



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:18 am GMT

PDB ID : 1RYP
Title : CRYSTAL STRUCTURE OF THE 20S PROTEASOME FROM YEAST AT 2.4 ANGSTROMS RESOLUTION
Authors : Groll, M.; Ditzel, L.; Loewe, J.; Stock, D.; Bochtler, M.; Bartunik, H.D.; Huber, R.
Deposited on : 1997-02-26
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

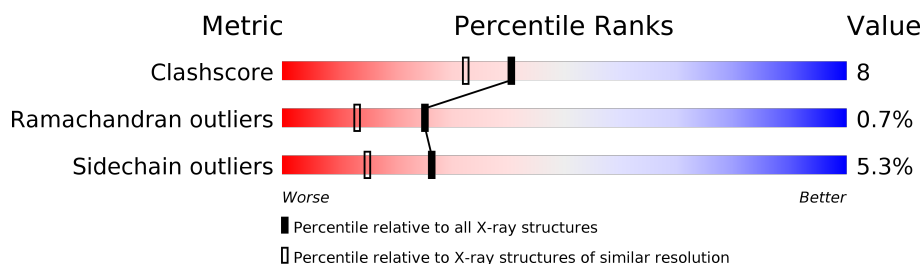
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)






















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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	
1	O	243	
2	B	250	
2	P	250	
3	C	244	
3	Q	244	
4	D	241	

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Mol	Chain	Length	Quality of chain
4	R	241	 68% 27% 5%
5	E	242	 79% 18% .
5	S	242	 75% 24% .
6	F	233	 70% 27% .
6	T	233	 70% 27% .
7	G	244	 80% 16% .
7	U	244	 75% 20% 5%
8	H	205	 76% 23% .
8	V	205	 78% 21%
9	I	222	 82% 16% .
9	W	222	 81% 18% .
10	J	204	 85% 14%
10	X	204	 83% 17%
11	K	198	 79% 21% .
11	Y	198	 77% 23% .
12	L	212	 85% 13% .
12	Z	212	 89% 9% .
13	1	222	 84% 15% .
13	M	222	 81% 18% .
14	2	233	 80% 19% .
14	N	233	 83% 16% .

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52604 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 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	O	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 2 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
2	P	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 3 is a protein called 20S PROTEASOME.

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

- Molecule 4 is a protein called 20S PROTEASOME.

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

- Molecule 5 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
5	S	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 6 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
6	T	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 7 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
7	U	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 8 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	205	Total	C	N	O	S	0	0	0
			1574	995	261	311	7			
8	V	205	Total	C	N	O	S	0	0	0
			1574	995	261	311	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	ALA	THR	CONFLICT	UNP P38624
V	1	ALA	THR	CONFLICT	UNP P38624

- Molecule 9 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	W	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 10 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
10	X	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 11 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	Y	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 12 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	CONFLICT	UNP P30656
Z	33	ARG	LYS	CONFLICT	UNP P30656

- Molecule 13 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	1	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called 20S PROTEASOME.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	J	2	Total	Mg	0	0
			2	2		
15	1	1	Total	Mg	0	0
			1	1		
15	E	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		
15	A	2	Total	Mg	0	0
			2	2		
15	U	1	Total	Mg	0	0
			1	1		
15	X	2	Total	Mg	0	0
			2	2		
15	O	2	Total	Mg	0	0
			2	2		
15	L	1	Total	Mg	0	0
			1	1		
15	S	1	Total	Mg	0	0
			1	1		
15	M	1	Total	Mg	0	0
			1	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	1	139	Total O 139 139	0	0
16	2	153	Total O 153 153	0	0
16	A	113	Total O 113 113	0	0
16	B	109	Total O 109 109	0	0
16	C	73	Total O 73 73	0	0
16	D	66	Total O 66 66	0	0
16	E	88	Total O 88 88	0	0
16	F	58	Total O 58 58	0	0
16	G	91	Total O 91 91	0	0
16	H	114	Total O 114 114	0	0
16	I	122	Total O 122 122	0	0
16	J	113	Total O 113 113	0	0
16	K	117	Total O 117 117	0	0
16	L	100	Total O 100 100	0	0
16	M	135	Total O 135 135	0	0
16	N	158	Total O 158 158	0	0
16	O	108	Total O 108 108	0	0
16	P	105	Total O 105 105	0	0
16	Q	78	Total O 78 78	0	0
16	R	63	Total O 63 63	0	0
16	S	88	Total O 88 88	0	0
16	T	55	Total O 55 55	0	0

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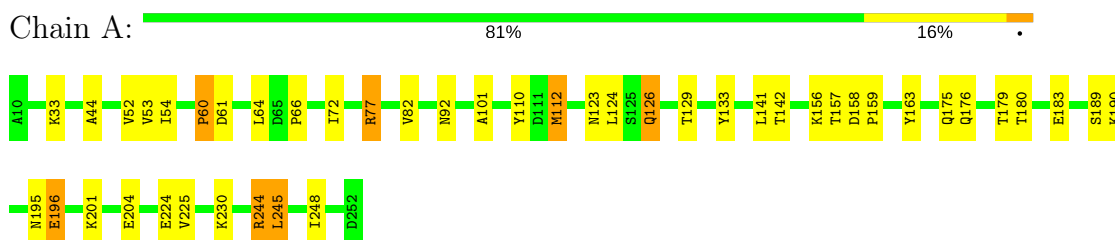
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	U	92	Total 92	O 92	0	0
16	V	121	Total 121	O 121	0	0
16	W	124	Total 124	O 124	0	0
16	X	110	Total 110	O 110	0	0
16	Y	115	Total 115	O 115	0	0
16	Z	100	Total 100	O 100	0	0

3 Residue-property plots [i](#)

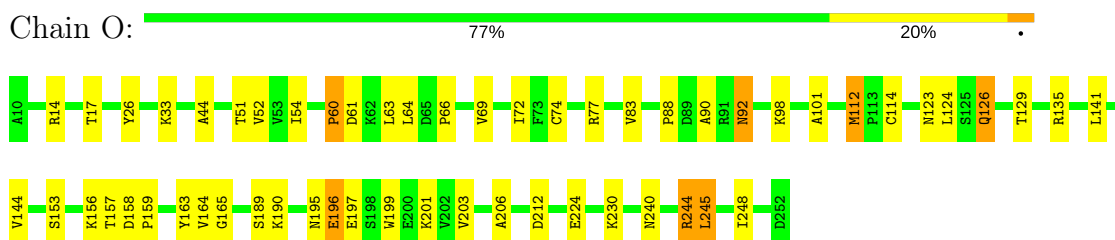
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

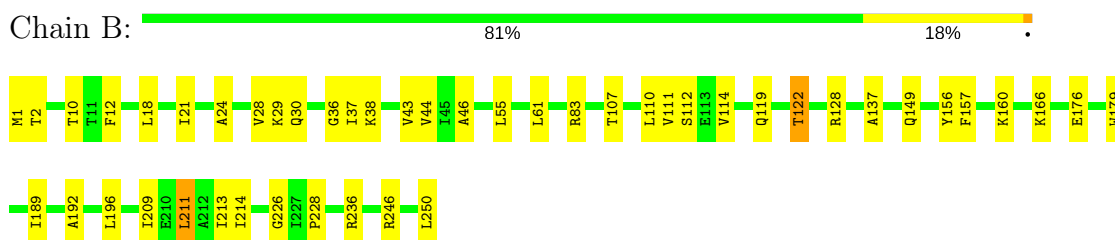
• Molecule 1: 20S PROTEASOME



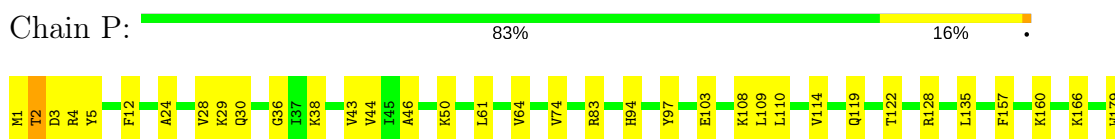
• Molecule 1: 20S PROTEASOME



• Molecule 2: 20S PROTEASOME

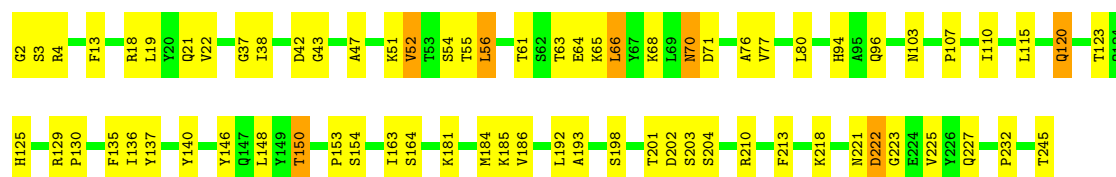


• Molecule 2: 20S PROTEASOME

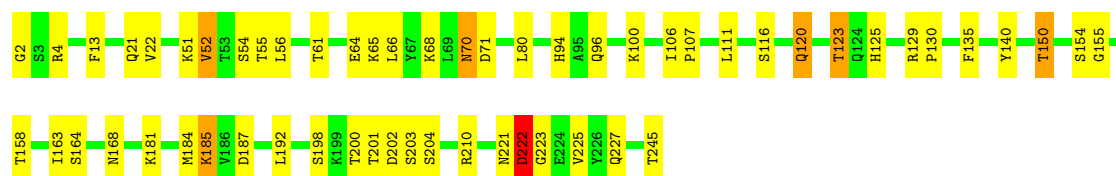
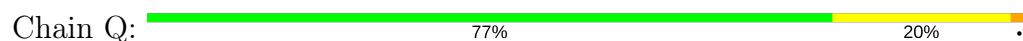




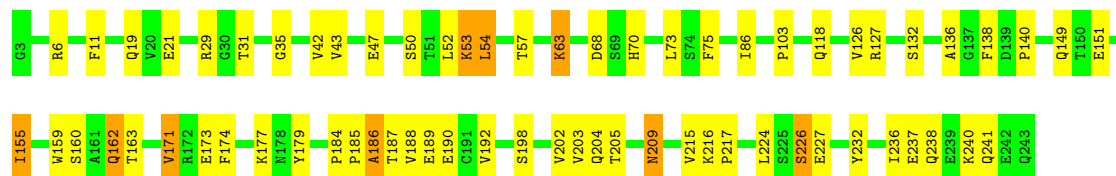
• Molecule 3: 20S PROTEASOME



• Molecule 3: 20S PROTEASOME



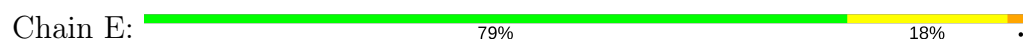
• Molecule 4: 20S PROTEASOME



• Molecule 4: 20S PROTEASOME



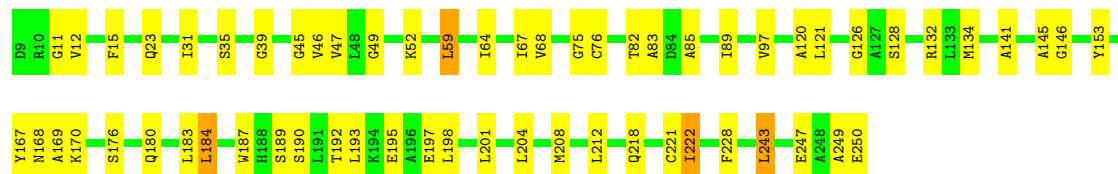
• Molecule 5: 20S PROTEASOME





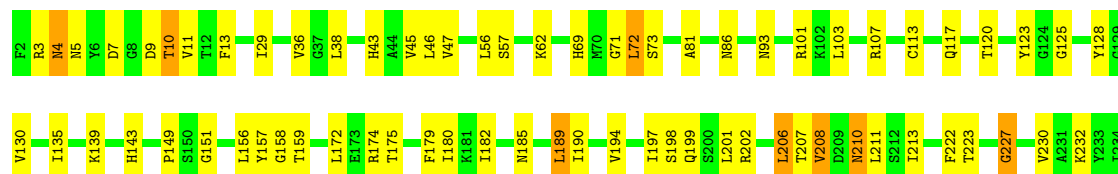
• Molecule 5: 20S PROTEASOME

Chain S: 75% 24%



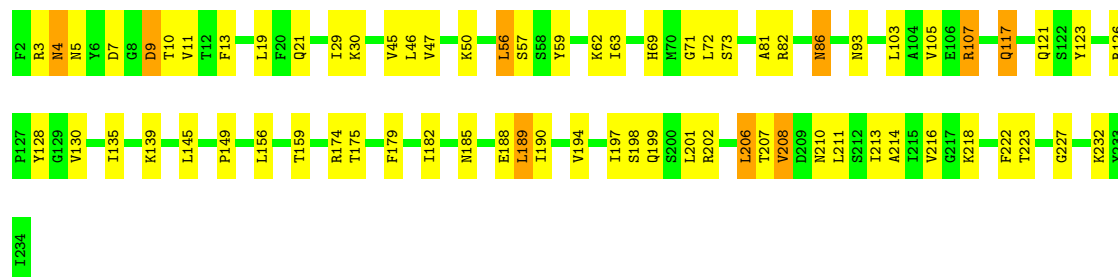
• Molecule 6: 20S PROTEASOME

Chain F: 70% 27%



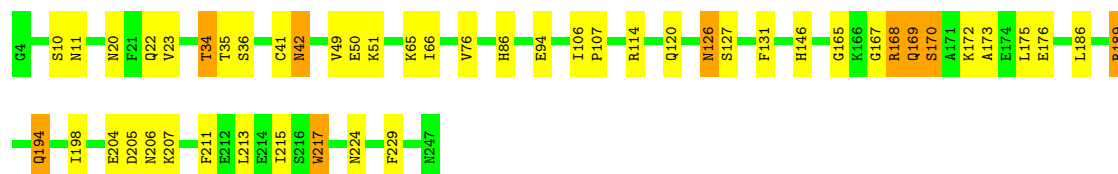
• Molecule 6: 20S PROTEASOME

Chain T: 70% 27%



• Molecule 7: 20S PROTEASOME

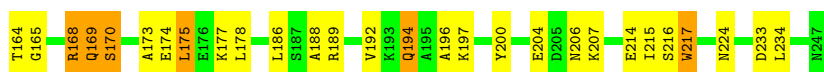
Chain G: 80% 16%



• Molecule 7: 20S PROTEASOME

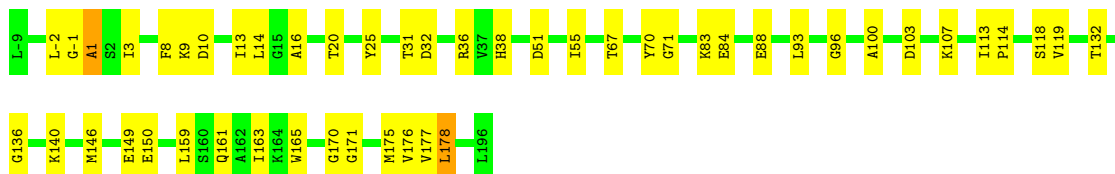
Chain U: 75% 20% 5%





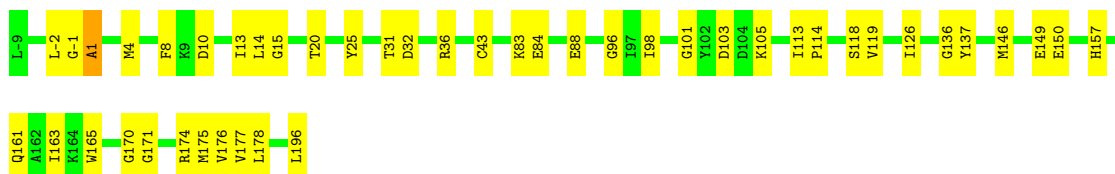
• Molecule 8: 20S PROTEASOME

Chain H: 76% 23%



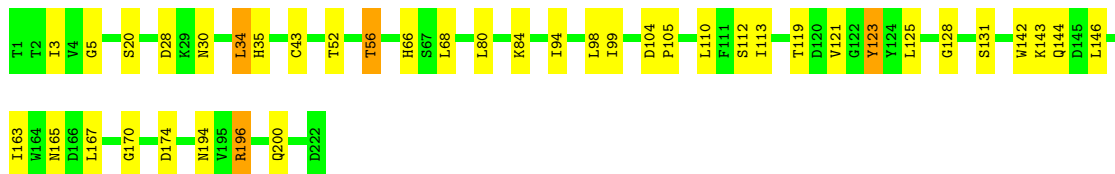
• Molecule 8: 20S PROTEASOME

Chain V: 78% 21%



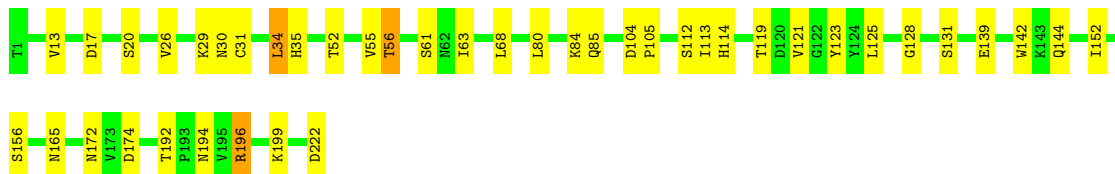
• Molecule 9: 20S PROTEASOME

Chain I: 82% 16%



• Molecule 9: 20S PROTEASOME

Chain W: 81% 18%

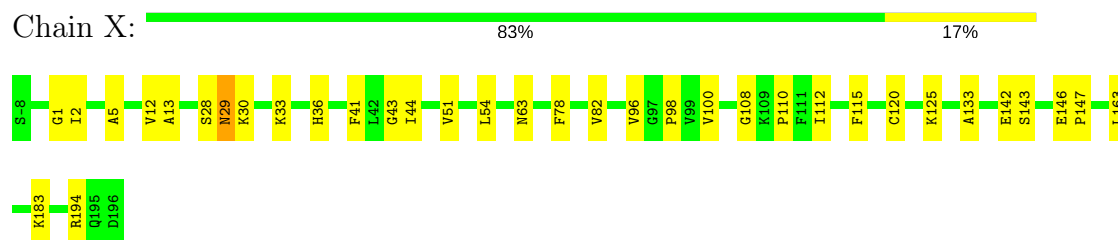


• Molecule 10: 20S PROTEASOME

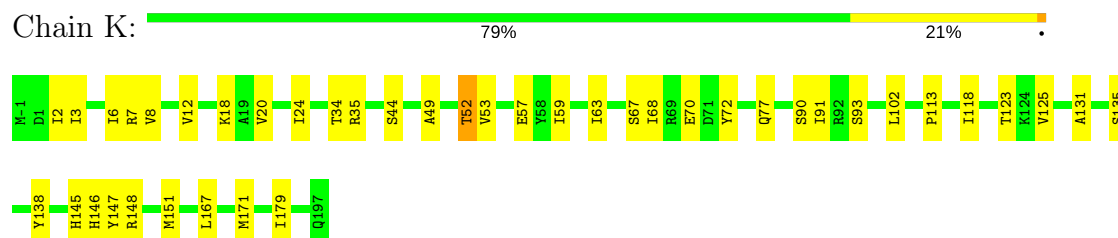
Chain J: 85% 14%



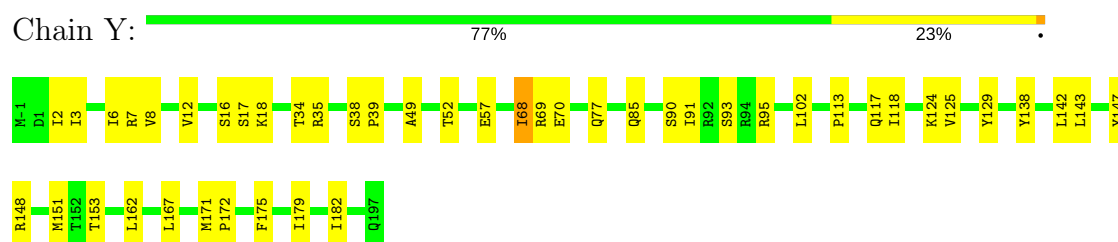
• Molecule 10: 20S PROTEASOME



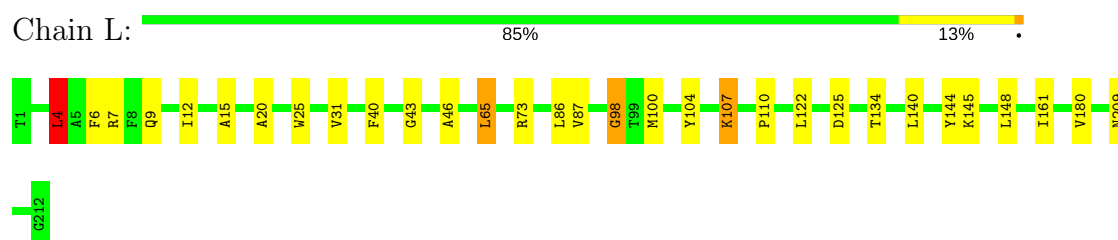
• Molecule 11: 20S PROTEASOME



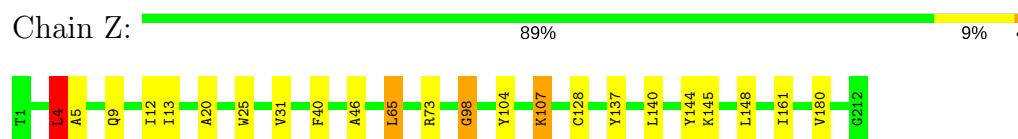
• Molecule 11: 20S PROTEASOME



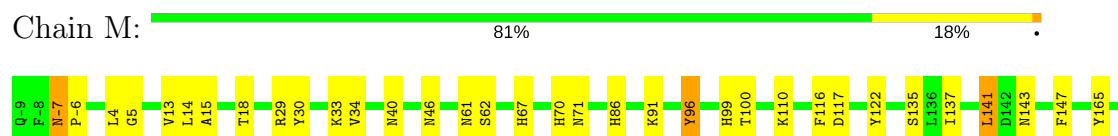
• Molecule 12: 20S PROTEASOME



• Molecule 12: 20S PROTEASOME



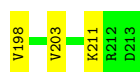
• Molecule 13: 20S PROTEASOME





• Molecule 13: 20S PROTEASOME

Chain 1: 84% 15%



• Molecule 14: 20S PROTEASOME

Chain N: 83% 16%



• Molecule 14: 20S PROTEASOME

Chain 2: 80% 19%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.49Å 300.70Å 144.42Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	90.5 (50.00-1.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.286 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	52604	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.56	1/1959 (0.1%)	0.72	0/2652
1	O	0.58	1/1959 (0.1%)	0.73	0/2652
2	B	0.54	0/1952	0.75	1/2642 (0.0%)
2	P	0.52	0/1952	0.74	1/2642 (0.0%)
3	C	0.52	0/1935	0.74	1/2618 (0.0%)
3	Q	0.52	0/1935	0.75	0/2618
4	D	0.53	0/1920	0.74	1/2598 (0.0%)
4	R	0.53	0/1920	0.74	1/2598 (0.0%)
5	E	0.52	0/1887	0.76	2/2541 (0.1%)
5	S	0.52	0/1887	0.73	2/2541 (0.1%)
6	F	0.50	0/1823	0.72	1/2463 (0.0%)
6	T	0.49	0/1823	0.70	0/2463
7	G	0.54	0/1937	0.73	0/2614
7	U	0.53	0/1937	0.76	0/2614
8	H	0.58	0/1603	0.77	2/2168 (0.1%)
8	V	0.58	0/1603	0.76	2/2168 (0.1%)
9	I	0.55	0/1716	0.76	0/2326
9	W	0.54	0/1716	0.77	1/2326 (0.0%)
10	J	0.56	0/1611	0.77	0/2174
10	X	0.55	0/1611	0.76	0/2174
11	K	0.56	0/1613	0.78	0/2173
11	Y	0.57	0/1613	0.79	0/2173
12	L	0.55	0/1683	0.76	2/2277 (0.1%)
12	Z	0.53	0/1683	0.76	2/2277 (0.1%)
13	1	0.56	0/1795	0.77	0/2420
13	M	0.55	0/1795	0.77	1/2420 (0.0%)
14	2	0.57	0/1855	0.81	2/2514 (0.1%)
14	N	0.55	0/1855	0.77	3/2514 (0.1%)
All	All	0.54	2/50578 (0.0%)	0.75	25/68360 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	MET	SD-CE	-5.62	1.46	1.77
1	O	112	MET	SD-CE	-5.05	1.49	1.77

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	52	LEU	CA-CB-CG	6.80	130.93	115.30
5	S	134	MET	N-CA-C	-6.60	93.17	111.00
5	E	134	MET	N-CA-C	-6.44	93.61	111.00
12	L	4	LEU	CA-CB-CG	6.42	130.07	115.30
4	R	52	LEU	CA-CB-CG	6.03	129.17	115.30
6	F	72	LEU	CA-CB-CG	5.98	129.04	115.30
14	2	102	LEU	N-CA-C	-5.87	95.14	111.00
12	Z	4	LEU	CA-CB-CG	5.84	128.74	115.30
2	B	214	ILE	N-CA-C	-5.68	95.66	111.00
14	N	102	LEU	N-CA-C	-5.66	95.72	111.00
5	E	59	LEU	CA-CB-CG	5.60	128.17	115.30
12	L	98	GLY	N-CA-C	-5.59	99.13	113.10
14	N	105	ALA	N-CA-C	-5.53	96.06	111.00
8	H	96	GLY	N-CA-C	-5.47	99.42	113.10
8	V	96	GLY	N-CA-C	-5.47	99.42	113.10
13	M	96	TYR	N-CA-C	-5.35	96.56	111.00
5	S	59	LEU	CA-CB-CG	5.25	127.38	115.30
14	N	27	ARG	N-CA-C	5.23	125.13	111.00
9	W	222	ASP	CB-CG-OD1	5.21	122.99	118.30
8	H	1	ALA	N-CA-C	5.20	125.03	111.00
8	V	1	ALA	N-CA-C	5.17	124.97	111.00
3	C	136	ILE	N-CA-C	-5.09	97.25	111.00
2	P	214	ILE	N-CA-C	-5.05	97.35	111.00
12	Z	98	GLY	N-CA-C	-5.04	100.50	113.10
14	2	105	ALA	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	123	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1921	0	1910	35	0
1	O	1921	0	1910	42	0
2	B	1915	0	1929	30	0
2	P	1915	0	1929	28	0
3	C	1905	0	1901	46	0
3	Q	1905	0	1901	38	0
4	D	1891	0	1900	47	0
4	R	1891	0	1900	57	0
5	E	1862	0	1836	33	0
5	S	1862	0	1836	34	0
6	F	1795	0	1797	47	0
6	T	1795	0	1797	46	0
7	G	1897	0	1886	30	0
7	U	1897	0	1886	40	0
8	H	1574	0	1553	31	0
8	V	1574	0	1553	31	0
9	I	1685	0	1688	27	0
9	W	1685	0	1688	30	0
10	J	1581	0	1574	18	0
10	X	1581	0	1574	24	0
11	K	1585	0	1590	29	0
11	Y	1585	0	1590	31	0
12	L	1646	0	1595	27	0
12	Z	1646	0	1595	16	0
13	1	1757	0	1711	26	0
13	M	1757	0	1711	31	0
14	2	1824	0	1832	29	0
14	N	1824	0	1832	22	0
15	1	1	0	0	0	0
15	A	2	0	0	0	0
15	E	1	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	I	1	0	0	0	0
15	J	2	0	0	0	0
15	L	1	0	0	0	0
15	M	1	0	0	0	0
15	O	2	0	0	0	0
15	S	1	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	2	0	0	0	0
15	Z	1	0	0	0	0
16	1	139	0	0	3	0
16	2	153	0	0	1	0
16	A	113	0	0	0	0
16	B	109	0	0	1	0
16	C	73	0	0	4	0
16	D	66	0	0	0	0
16	E	88	0	0	2	0
16	F	58	0	0	1	0
16	G	91	0	0	1	0
16	H	114	0	0	2	0
16	I	122	0	0	0	0
16	J	113	0	0	0	0
16	K	117	0	0	1	0
16	L	100	0	0	0	0
16	M	135	0	0	2	0
16	N	158	0	0	0	0
16	O	108	0	0	3	0
16	P	105	0	0	1	0
16	Q	78	0	0	3	0
16	R	63	0	0	0	0
16	S	88	0	0	1	0
16	T	55	0	0	0	0
16	U	92	0	0	1	0
16	V	121	0	0	1	0
16	W	124	0	0	1	0
16	X	110	0	0	0	0
16	Y	115	0	0	2	0
16	Z	100	0	0	0	0
All	All	52604	0	49404	812	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 8.

All (812) 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)
1:O:101:ALA:HA	1:O:112:MET:HE2	1.37	1.06
1:A:101:ALA:HA	1:A:112:MET:HE2	1.46	0.96
3:C:125:HIS:HB3	4:D:126:VAL:HG12	1.50	0.94
13:1:18:THR:CG2	13:1:30:TYR:HA	1.98	0.93
12:Z:107:LYS:HD2	12:Z:107:LYS:H	1.34	0.92
13:M:33:LYS:HD2	13:M:46:ASN:HD22	1.37	0.89
8:H:136:GLY:HA2	8:V:161:GLN:HE21	1.37	0.88
13:1:33:LYS:HD2	13:1:46:ASN:HD22	1.40	0.87
13:M:18:THR:CG2	13:M:30:TYR:HA	2.05	0.87
12:L:107:LYS:HD2	12:L:107:LYS:H	1.40	0.86
14:2:171:ASN:HD22	14:2:174:ARG:HH21	1.15	0.86
3:C:201:THR:HG22	3:C:203:SER:H	1.41	0.86
2:P:122:THR:HG22	3:Q:129:ARG:HH21	1.41	0.84
9:W:35:HIS:HB3	9:W:56:THR:HG21	1.57	0.84
14:N:171:ASN:HD22	14:N:174:ARG:HH21	1.26	0.84
6:T:13:PHE:H	7:U:22:GLN:HE22	1.23	0.82
7:G:94:GLU:HG3	7:G:114:ARG:HH11	1.44	0.81
1:A:129:THR:HG22	2:B:128:ARG:HH21	1.44	0.80
3:Q:201:THR:HG22	3:Q:203:SER:H	1.46	0.80
4:D:11:PHE:H	5:E:23:GLN:HE22	1.27	0.80
2:B:12:PHE:H	3:C:21:GLN:HE22	1.28	0.80
6:F:13:PHE:H	7:G:22:GLN:HE22	1.30	0.79
7:U:94:GLU:HG2	7:U:114:ARG:HB3	1.62	0.79
13:1:198:VAL:HG22	13:1:203:VAL:HG22	1.65	0.78
2:P:12:PHE:H	3:Q:21:GLN:HE22	1.32	0.78
3:C:120:GLN:O	3:C:123:THR:HB	1.85	0.77
14:2:171:ASN:HD22	14:2:174:ARG:NH2	1.85	0.74
13:1:18:THR:HG22	13:1:29:ARG:O	1.88	0.73
13:M:18:THR:HG23	13:M:30:TYR:HA	1.70	0.73
3:Q:64:GLU:HG3	3:Q:65:LYS:HG3	1.68	0.73
4:D:171:VAL:HG12	4:D:202:VAL:HG21	1.71	0.73
5:E:97:VAL:HG21	12:L:65:LEU:HD13	1.71	0.73
3:Q:125:HIS:HB3	4:R:126:VAL:HG12	1.71	0.73
14:N:171:ASN:HD22	14:N:174:ARG:NH2	1.87	0.72
3:C:123:THR:HG22	4:D:127:ARG:HH21	1.54	0.72
14:2:171:ASN:ND2	14:2:174:ARG:HH21	1.87	0.71
9:I:35:HIS:HB3	9:I:56:THR:HG21	1.73	0.71
13:M:18:THR:HG22	13:M:29:ARG:O	1.91	0.71
14:N:148:ARG:HH11	9:W:165:ASN:HD22	1.39	0.71
1:A:196:GLU:HG2	1:A:201:LYS:CB	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:136:GLY:HA2	8:V:161:GLN:NE2	2.05	0.70
5:S:67:ILE:HG22	5:S:228:PHE:HZ	1.57	0.70
3:Q:96:GLN:HE22	10:X:63:ASN:HD22	1.40	0.70
4:R:151:GLU:HG2	4:R:155:ILE:HG22	1.74	0.70
6:F:45:VAL:HG23	6:F:189:LEU:HD13	1.74	0.69
4:D:53:LYS:HD2	4:D:54:LEU:N	2.06	0.69
14:N:119:LEU:HG	14:N:134:LEU:HD12	1.73	0.69
1:O:126:GLN:O	1:O:129:THR:HB	1.92	0.69
3:C:4:ARG:HG3	6:F:123:TYR:OH	1.92	0.69
6:T:69:HIS:HE1	6:T:103:LEU:O	1.75	0.68
4:D:68:ASP:HA	11:K:68:ILE:CD1	2.23	0.68
14:2:153:ARG:HH11	14:2:153:ARG:HG3	1.57	0.68
13:M:18:THR:HG21	13:M:30:TYR:HD1	1.59	0.68
14:N:171:ASN:ND2	14:N:174:ARG:HH21	1.90	0.68
1:A:157:THR:HG22	1:A:163:TYR:HB2	1.76	0.67
4:D:159:TRP:CZ2	5:E:59:LEU:HD23	2.29	0.67
7:U:34:THR:HG21	7:U:50:GLU:O	1.94	0.67
11:Y:138:TYR:CZ	11:Y:171:MET:HG3	2.29	0.67
1:A:129:THR:CG2	2:B:128:ARG:HH21	2.07	0.67
1:O:129:THR:HG22	2:P:128:ARG:HH21	1.60	0.67
5:E:146:GLY:HA2	5:E:222:ILE:HG12	1.76	0.67
7:G:34:THR:HG21	7:G:50:GLU:O	1.95	0.67
4:R:29:ARG:O	4:R:29:ARG:HG2	1.95	0.66
5:E:40:ILE:HD12	5:E:200:VAL:HG23	1.77	0.66
7:U:41:CYS:HB2	7:U:186:LEU:O	1.95	0.66
3:Q:140:TYR:CD1	3:Q:225:VAL:HG21	2.31	0.66
9:W:35:HIS:CB	9:W:56:THR:HG21	2.25	0.66
13:1:18:THR:HG23	13:1:30:TYR:HA	1.77	0.65
4:R:187:THR:HB	4:R:190:GLU:HG2	1.78	0.65
5:S:204:LEU:O	5:S:208:MET:HG3	1.94	0.65
11:K:2:ILE:HD13	11:K:167:LEU:HD13	1.78	0.65
2:P:122:THR:CG2	3:Q:129:ARG:HH21	2.08	0.65
6:T:190:ILE:HG23	6:T:213:ILE:HD13	1.76	0.65
1:O:123:ASN:HD21	2:P:83:ARG:HE	1.43	0.65
12:Z:12:ILE:HB	12:Z:180:VAL:HB	1.78	0.65
7:U:94:GLU:HG3	7:U:114:ARG:HH11	1.60	0.65
4:R:43:VAL:HG23	4:R:191:CYS:SG	2.37	0.64
4:R:189:GLU:HA	4:R:232:TYR:OH	1.97	0.64
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.80	0.64
4:D:151:GLU:HG2	4:D:155:ILE:HG22	1.78	0.64
7:G:168:ARG:HG3	7:G:172:LYS:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:120:GLN:O	3:Q:123:THR:HB	1.98	0.64
3:Q:13:PHE:H	4:R:19:GLN:HE22	1.46	0.64
12:L:144:TYR:O	12:L:145:LYS:HD2	1.98	0.64
4:D:162:GLN:HE21	4:D:163:THR:H	1.47	0.63
7:U:126:ASN:C	7:U:126:ASN:HD22	2.02	0.63
13:M:186:HIS:HD2	13:M:188:GLN:H	1.45	0.63
11:Y:2:ILE:HD13	11:Y:167:LEU:HD13	1.80	0.63
1:A:123:ASN:HD21	2:B:83:ARG:HE	1.47	0.63
4:D:155:ILE:HD12	5:E:83:ALA:HB2	1.79	0.63
7:G:126:ASN:C	7:G:126:ASN:HD22	2.01	0.63
10:J:2:ILE:HG21	10:J:133:ALA:HB3	1.81	0.63
1:O:199:TRP:O	1:O:203:VAL:HG23	1.99	0.62
2:P:1:MET:SD	2:P:2:THR:N	2.71	0.62
9:W:172:ASN:HD22	9:W:192:THR:HA	1.63	0.62
13:1:186:HIS:HD2	13:1:188:GLN:H	1.46	0.62
8:H:38:HIS:HD2	16:H:276:HOH:O	1.82	0.62
4:R:53:LYS:HD2	4:R:54:LEU:N	2.14	0.62
8:H:161:GLN:HE21	8:V:136:GLY:HA2	1.64	0.62
9:I:165:ASN:ND2	14:2:148:ARG:HH11	1.97	0.62
2:P:196:LEU:HD23	2:P:209:ILE:HD12	1.81	0.62
5:E:167:TYR:CE1	6:F:57:SER:HB3	2.35	0.62
10:X:2:ILE:HG21	10:X:133:ALA:HB3	1.82	0.62
1:A:179:THR:O	1:A:183:GLU:HG3	1.99	0.62
12:L:7:ARG:HD2	12:L:110:PRO:O	1.99	0.62
7:G:146:HIS:HD2	16:G:295:HOH:O	1.81	0.61
2:B:196:LEU:HD23	2:B:209:ILE:HD12	1.82	0.61
3:C:47:ALA:HB2	3:C:213:PHE:CE1	2.36	0.61
4:R:53:LYS:O	4:R:54:LEU:HB2	2.00	0.61
2:P:4:ARG:HH22	5:S:126:GLY:HA3	1.64	0.61
4:D:53:LYS:O	4:D:54:LEU:HB2	1.99	0.61
1:A:196:GLU:HG2	1:A:201:LYS:HB3	1.82	0.61
10:J:28:SER:HB2	11:K:125:VAL:HG21	1.81	0.60
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.82	0.60
8:H:8:PHE:CE2	8:H:10:ASP:HB2	2.36	0.60
6:F:93:ASN:HD21	13:M:61:ASN:HD21	1.48	0.60
6:F:139:LYS:HE3	14:N:83:TYR:OH	2.01	0.60
8:H:146:MET:HE3	8:H:150:GLU:HB3	1.83	0.60
5:S:146:GLY:HA2	5:S:222:ILE:HG12	1.82	0.60
13:1:18:THR:HG21	13:1:30:TYR:HD1	1.66	0.60
2:B:119:GLN:O	2:B:122:THR:HB	2.02	0.60
12:Z:107:LYS:CD	12:Z:107:LYS:H	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:18:THR:HG22	13:1:30:TYR:HA	1.83	0.60
11:Y:3:ILE:HG22	11:Y:102:LEU:HD12	1.84	0.60
13:1:186:HIS:HE1	16:1:309:HOH:O	1.85	0.60
11:K:3:ILE:HG22	11:K:102:LEU:HD12	1.84	0.60
6:T:190:ILE:CG2	6:T:213:ILE:HD13	2.31	0.60
5:S:97:VAL:HG21	12:Z:65:LEU:HD13	1.83	0.60
3:C:181:LYS:O	3:C:184:MET:HG3	2.02	0.60
3:C:123:THR:CG2	4:D:127:ARG:HH21	2.15	0.59
13:M:33:LYS:HD2	13:M:46:ASN:ND2	2.12	0.59
14:N:153:ARG:HG3	14:N:153:ARG:HH11	1.67	0.59
7:G:94:GLU:HG2	7:G:114:ARG:HB3	1.84	0.59
14:2:89:ALA:HA	14:2:122:VAL:HG21	1.83	0.59
11:K:3:ILE:HG21	16:K:311:HOH:O	2.02	0.59
5:E:39:GLY:HA2	5:E:47:VAL:O	2.03	0.59
8:H:140:LYS:HG3	8:V:137:TYR:CE1	2.37	0.59
7:G:169:GLN:CD	7:G:169:GLN:H	2.05	0.59
4:D:163:THR:HG21	4:D:171:VAL:HG22	1.83	0.59
3:C:18:ARG:HE	4:D:29:ARG:HH21	1.49	0.59
2:P:119:GLN:O	2:P:122:THR:HB	2.02	0.59
9:I:194:ASN:HB3	13:1:211:LYS:HE3	1.83	0.59
9:I:35:HIS:CB	9:I:56:THR:HG21	2.32	0.59
4:D:68:ASP:HA	11:K:68:ILE:HD13	1.84	0.58
7:G:41:CYS:HB2	7:G:186:LEU:O	2.03	0.58
3:Q:123:THR:CG2	4:R:127:ARG:HH21	2.15	0.58
1:A:245:LEU:O	1:A:248:ILE:HG13	2.02	0.58
3:C:96:GLN:HE22	10:J:63:ASN:HD22	1.51	0.58
2:P:64:VAL:HG11	2:P:212:ALA:HB2	1.84	0.58
5:S:184:LEU:HD22	6:T:56:LEU:HD22	1.85	0.58
1:O:64:LEU:O	1:O:66:PRO:HD3	2.03	0.58
3:Q:2:GLY:HA3	6:T:123:TYR:CE1	2.38	0.58
3:Q:4:ARG:HG3	6:T:123:TYR:OH	2.04	0.58
6:T:139:LYS:HE3	14:2:83:TYR:OH	2.04	0.58
2:B:122:THR:CG2	3:C:129:ARG:HH21	2.16	0.58
2:B:10:THR:HG22	2:B:18:LEU:HD22	1.86	0.58
11:K:18:LYS:HD3	11:K:179:ILE:HG13	1.86	0.58
9:W:112:SER:HB3	9:W:125:LEU:HD13	1.84	0.58
11:K:148:ARG:O	11:K:151:MET:HG3	2.04	0.58
12:L:43:GLY:HA2	12:L:100:MET:O	2.04	0.58
1:O:212:ASP:HB3	16:O:1011:HOH:O	2.03	0.57
1:O:245:LEU:O	1:O:248:ILE:HG13	2.04	0.57
7:G:213:LEU:HD21	7:G:215:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:4:LEU:HD11	13:M:141:LEU:HD21	1.84	0.57
10:X:28:SER:HB2	11:Y:125:VAL:HG21	1.84	0.57
4:R:103:PRO:HG2	4:R:140:PRO:HG3	1.85	0.57
6:F:190:ILE:HG23	6:F:213:ILE:HD13	1.85	0.57
6:T:9:ASP:HB2	6:T:11:VAL:HG12	1.86	0.57
6:T:208:VAL:O	6:T:227:GLY:HA2	2.05	0.57
3:C:140:TYR:CD1	3:C:225:VAL:HG21	2.40	0.57
12:L:107:LYS:CD	12:L:107:LYS:H	2.13	0.57
1:A:126:GLN:O	1:A:129:THR:HB	2.03	0.57
4:D:162:GLN:NE2	4:D:163:THR:H	2.02	0.57
8:H:25:TYR:HD1	14:2:138:PHE:HZ	1.53	0.57
9:W:84:LYS:HE2	9:W:119:THR:HG23	1.86	0.57
6:F:198:SER:HA	6:F:201:LEU:HG	1.87	0.56
1:O:72:ILE:CD1	1:O:224:GLU:HG2	2.35	0.56
4:R:103:PRO:HG2	4:R:140:PRO:CG	2.35	0.56
4:R:151:GLU:CG	4:R:155:ILE:HG22	2.35	0.56
3:C:19:LEU:HD13	3:C:123:THR:HG23	1.87	0.56
3:C:64:GLU:HG3	3:C:65:LYS:HG3	1.85	0.56
12:L:145:LYS:HB2	12:L:148:LEU:HD13	1.88	0.56
1:O:123:ASN:ND2	2:P:83:ARG:HE	2.03	0.56
9:W:128:GLY:O	9:W:131:SER:HB2	2.04	0.56
11:Y:118:ILE:HG12	11:Y:124:LYS:HG3	1.86	0.56
4:D:11:PHE:N	5:E:23:GLN:HE22	2.01	0.56
13:M:137:ILE:HG22	13:M:141:LEU:HD22	1.87	0.56
6:T:103:LEU:HD11	6:T:107:ARG:HG2	1.86	0.56
11:Y:138:TYR:CE2	11:Y:171:MET:HG3	2.40	0.56
4:D:187:THR:HB	4:D:190:GLU:HG2	1.88	0.56
4:D:203:VAL:HG11	4:D:209:ASN:HB3	1.88	0.56
1:O:196:GLU:HG2	1:O:201:LYS:CB	2.36	0.56
9:I:165:ASN:HD22	14:2:148:ARG:HH11	1.51	0.56
14:N:89:ALA:HA	14:N:122:VAL:HG21	1.88	0.56
11:K:3:ILE:HG22	11:K:102:LEU:CD1	2.36	0.56
3:C:13:PHE:H	4:D:19:GLN:HE22	1.54	0.55
7:U:37:ILE:HG22	7:U:163:ALA:CB	2.36	0.55
4:D:29:ARG:O	4:D:29:ARG:HG2	2.05	0.55
14:N:148:ARG:HH11	9:W:165:ASN:ND2	2.03	0.55
5:S:39:GLY:HA2	5:S:47:VAL:O	2.06	0.55
8:V:83:LYS:HD3	16:V:912:HOH:O	2.06	0.55
11:Y:3:ILE:HG21	16:Y:858:HOH:O	2.07	0.55
2:B:38:LYS:HG3	2:B:43:VAL:HG22	1.89	0.55
6:F:190:ILE:CG2	6:F:213:ILE:HD13	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:146:HIS:HD2	16:U:1060:HOH:O	1.89	0.55
4:D:188:VAL:HG21	4:D:216:LYS:HE2	1.89	0.55
5:E:24:VAL:O	5:E:27:SER:HB3	2.07	0.55
1:O:101:ALA:CA	1:O:112:MET:HE2	2.24	0.55
2:P:24:ALA:O	2:P:28:VAL:HG23	2.06	0.55
4:R:42:VAL:HG11	4:R:136:ALA:HB1	1.87	0.55
1:A:101:ALA:HA	1:A:112:MET:CE	2.30	0.55
6:F:201:LEU:HD11	6:F:206:LEU:HD22	1.88	0.55
4:R:11:PHE:H	5:S:23:GLN:HE22	1.54	0.55
13:1:33:LYS:HD2	13:1:46:ASN:ND2	2.17	0.55
6:F:227:GLY:O	6:F:230:VAL:HG22	2.07	0.55
4:R:184:PRO:O	4:R:186:ALA:N	2.41	0.54
7:U:165:GLY:O	7:U:168:ARG:HB3	2.07	0.54
9:I:43:CYS:SG	9:I:98:LEU:HB3	2.48	0.54
4:R:163:THR:HG21	4:R:171:VAL:HG22	1.89	0.54
4:R:188:VAL:O	4:R:192:VAL:HG23	2.06	0.54
2:P:36:GLY:HA2	2:P:44:VAL:O	2.07	0.54
11:Y:148:ARG:O	11:Y:151:MET:HG3	2.07	0.54
10:J:100:VAL:O	10:J:112:ILE:HA	2.07	0.54
14:N:138:PHE:HZ	8:V:25:TYR:HD1	1.56	0.54
12:L:46:ALA:HB3	12:L:98:GLY:O	2.07	0.54
9:W:172:ASN:ND2	9:W:192:THR:HA	2.23	0.54
13:1:18:THR:HG21	13:1:30:TYR:CD1	2.42	0.54
1:O:129:THR:CG2	2:P:128:ARG:HH21	2.20	0.54
4:R:192:VAL:O	4:R:196:VAL:HG23	2.07	0.54
14:2:81:PRO:HD2	14:2:112:GLN:OE1	2.07	0.54
9:I:34:LEU:HD22	9:I:174:ASP:HB3	1.90	0.54
2:B:1:MET:SD	2:B:2:THR:N	2.79	0.54
5:E:249:ALA:O	5:E:250:GLU:HG2	2.08	0.54
9:I:128:GLY:O	9:I:131:SER:HB2	2.07	0.54
1:O:60:PRO:HG2	1:O:61:ASP:H	1.73	0.53
7:U:178:LEU:CD2	7:U:194:GLN:HG2	2.38	0.53
3:C:68:LYS:HG3	3:C:227:GLN:OE1	2.08	0.53
7:G:194:GLN:O	7:G:198:ILE:HG13	2.08	0.53
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.88	0.53
9:W:34:LEU:HD22	9:W:174:ASP:HB3	1.89	0.53
9:W:196:ARG:NH2	10:X:142:GLU:HG3	2.23	0.53
8:H:67:THR:HA	8:H:71:GLY:O	2.09	0.53
9:I:196:ARG:NH2	10:J:142:GLU:HG3	2.23	0.53
14:2:19:LEU:HB2	14:2:184:SER:HB2	1.90	0.53
8:V:14:LEU:O	8:V:175:MET:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:CG1	1:A:142:THR:HB	2.38	0.53
8:V:31:THR:HG22	8:V:32:ASP:H	1.74	0.53
11:Y:7:ARG:O	11:Y:7:ARG:HG2	2.09	0.53
13:1:137:ILE:HG22	13:1:141:LEU:HD22	1.91	0.53
4:D:31:THR:HB	4:D:47:GLU:HG3	1.90	0.53
5:E:75:GLY:HA3	5:E:228:PHE:CD1	2.44	0.53
8:H:114:PRO:HD2	8:H:118:SER:O	2.07	0.53
9:I:112:SER:HB3	9:I:125:LEU:HD13	1.90	0.53
3:C:210:ARG:HH11	3:C:210:ARG:HG2	1.72	0.53
8:H:9:LYS:O	8:H:107:LYS:HD3	2.08	0.53
13:M:198:VAL:HG22	13:M:203:VAL:HG22	1.90	0.53
8:V:31:THR:HG22	8:V:32:ASP:N	2.23	0.53
1:A:123:ASN:ND2	2:B:83:ARG:HE	2.07	0.53
4:R:160:SER:HB3	4:R:179:TYR:CE1	2.44	0.53
4:R:162:GLN:HA	4:R:162:GLN:HE21	1.74	0.53
4:R:180:ASP:OD2	4:R:182:LYS:HB2	2.07	0.53
2:B:122:THR:HG22	3:C:129:ARG:HH21	1.73	0.52
8:H:-2:LEU:O	8:H:1:ALA:N	2.42	0.52
16:S:1049:HOH:O	13:1:70:HIS:HE1	1.91	0.52
2:B:37:ILE:HD12	2:B:192:ALA:HB2	1.90	0.52
7:U:196:ALA:O	7:U:200:TYR:HD1	1.92	0.52
4:R:159:TRP:CZ2	5:S:59:LEU:HD23	2.45	0.52
6:F:10:THR:HG21	6:F:120:THR:HA	1.91	0.52
1:O:83:VAL:HG11	1:O:90:ALA:CB	2.39	0.52
4:R:68:ASP:HA	11:Y:68:ILE:HD13	1.90	0.52
8:H:161:GLN:NE2	8:V:136:GLY:HA2	2.24	0.52
7:U:178:LEU:HD21	7:U:194:GLN:HG2	1.91	0.52
1:A:44:ALA:HB2	1:A:53:VAL:HG12	1.91	0.52
5:S:45:GLY:HA2	5:S:153:TYR:CE1	2.44	0.52
8:H:171:GLY:HA2	14:2:211:TRP:CH2	2.44	0.52
5:E:67:ILE:HG22	5:E:228:PHE:HZ	1.75	0.52
8:V:161:GLN:HE22	8:V:165:TRP:HE1	1.56	0.52
8:V:176:VAL:HG12	8:V:178:LEU:HD13	1.91	0.52
4:R:155:ILE:HD11	5:S:82:THR:OG1	2.10	0.52
5:E:167:TYR:CD1	6:F:57:SER:HB3	2.46	0.51
4:R:155:ILE:HD12	5:S:83:ALA:HB2	1.92	0.51
5:S:249:ALA:O	5:S:250:GLU:HG2	2.09	0.51
4:R:171:VAL:HG12	4:R:202:VAL:HG21	1.92	0.51
5:E:46:VAL:HG11	5:E:145:ALA:HB1	1.93	0.51
10:J:33:LYS:O	10:J:43:GLY:HA2	2.09	0.51
11:K:138:TYR:CE1	11:K:171:MET:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:8:TYR:CE2	14:N:162:VAL:HG22	2.45	0.51
1:O:83:VAL:HG11	1:O:90:ALA:HB2	1.93	0.51
1:A:157:THR:HG22	1:A:163:TYR:CB	2.39	0.51
6:F:208:VAL:O	6:F:227:GLY:HA2	2.10	0.51
11:K:138:TYR:CZ	11:K:171:MET:HG3	2.46	0.51
10:X:1:GLY:HA3	10:X:33:LYS:HE2	1.92	0.51
7:U:178:LEU:HD21	7:U:194:GLN:CG	2.40	0.51
14:2:166:GLU:O	14:2:170:VAL:HG23	2.11	0.51
1:A:82:VAL:HG12	1:A:142:THR:HB	1.92	0.51
12:L:4:LEU:HD12	12:L:161:ILE:HD11	1.93	0.51
9:W:104:ASP:HB2	9:W:105:PRO:CD	2.40	0.51
1:A:60:PRO:HG2	1:A:61:ASP:H	1.74	0.51
7:U:34:THR:CG2	7:U:50:GLU:O	2.58	0.51
11:Y:3:ILE:HG22	11:Y:102:LEU:CD1	2.41	0.51
5:S:52:LYS:HG3	5:S:64:ILE:HG21	1.92	0.50
8:H:84:GLU:O	8:H:88:GLU:HB2	2.11	0.50
7:U:17:ASP:OD2	7:U:19:ARG:HD3	2.11	0.50
7:U:94:GLU:HG2	7:U:114:ARG:CB	2.37	0.50
14:2:111:VAL:HG23	14:2:192:ILE:HG22	1.93	0.50
4:R:162:GLN:HE21	4:R:163:THR:H	1.59	0.50
7:U:37:ILE:HG22	7:U:163:ALA:HB2	1.93	0.50
6:T:62:LYS:O	6:T:73:SER:HA	2.10	0.50
4:R:68:ASP:HA	11:Y:68:ILE:CD1	2.41	0.50
1:A:141:LEU:O	1:A:156:LYS:HA	2.11	0.50
6:F:69:HIS:HE1	6:F:103:LEU:O	1.93	0.50
2:P:64:VAL:HG11	2:P:212:ALA:CB	2.41	0.50
3:Q:123:THR:HG22	4:R:127:ARG:HH21	1.76	0.50
14:2:40:ASN:H	14:2:40:ASN:HD22	1.59	0.50
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.93	0.50
9:W:52:THR:O	9:W:56:THR:HB	2.12	0.50
10:X:33:LYS:O	10:X:43:GLY:HA2	2.11	0.50
4:D:70:HIS:CE1	4:D:103:PRO:HB2	2.47	0.50
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.41	0.50
3:Q:163:ILE:HG13	3:Q:164:SER:N	2.27	0.50
4:R:162:GLN:NE2	4:R:163:THR:H	2.08	0.50
14:2:151:VAL:O	14:2:151:VAL:HG23	2.11	0.50
3:C:51:LYS:HG2	3:C:52:VAL:HG23	1.94	0.50
11:Y:18:LYS:HD3	11:Y:179:ILE:HG13	1.92	0.49
11:K:20:VAL:HG11	12:L:122:LEU:HD11	1.94	0.49
7:U:66:ILE:HG13	7:U:214:GLU:OE1	2.13	0.49
5:E:75:GLY:HA3	5:E:228:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:175:VAL:O	14:N:178:TYR:HB2	2.13	0.49
5:S:121:LEU:HD13	6:T:126:ARG:HH21	1.77	0.49
8:H:83:LYS:HD3	16:H:337:HOH:O	2.11	0.49
11:K:59:ILE:O	11:K:63:ILE:HG12	2.12	0.49
13:M:186:HIS:CD2	13:M:188:GLN:H	2.29	0.49
5:E:243:LEU:HD22	5:E:247:GLU:HG3	1.95	0.49
14:N:179:ARG:HD3	9:W:139:GLU:OE2	2.12	0.49
4:R:29:ARG:HH11	4:R:29:ARG:CB	2.26	0.49
10:X:5:ALA:HA	10:X:13:ALA:O	2.12	0.49
1:A:72:ILE:CD1	1:A:224:GLU:HG2	2.42	0.49
6:T:45:VAL:HG23	6:T:189:LEU:HD13	1.95	0.49
12:Z:145:LYS:HB2	12:Z:148:LEU:HD13	1.94	0.49
5:E:202:LYS:O	5:E:205:LYS:HB3	2.13	0.49
5:S:46:VAL:HG11	5:S:145:ALA:HB1	1.94	0.49
5:S:75:GLY:HA3	5:S:228:PHE:CD1	2.48	0.49
14:N:211:TRP:CH2	8:V:171:GLY:HA2	2.48	0.49
1:O:157:THR:HG22	1:O:163:TYR:HB2	1.95	0.49
3:Q:210:ARG:HG2	3:Q:210:ARG:HH11	1.78	0.49
3:C:163:ILE:HG13	3:C:164:SER:N	2.27	0.49
12:L:4:LEU:HD13	12:L:15:ALA:O	2.12	0.48
7:U:169:GLN:H	7:U:169:GLN:CD	2.15	0.48
5:S:193:LEU:O	5:S:197:GLU:HG3	2.13	0.48
3:C:94:HIS:HE1	16:C:253:HOH:O	1.97	0.48
7:G:167:GLY:HA2	7:G:205:ASP:OD2	2.14	0.48
8:H:31:THR:HG22	8:H:32:ASP:N	2.28	0.48
9:I:200:GLN:HG2	13:I:173:LYS:HG2	1.95	0.48
13:M:18:THR:HG21	13:M:30:TYR:CD1	2.43	0.48
1:O:123:ASN:HD22	2:P:83:ARG:HH21	1.60	0.48
13:I:86:HIS:HD2	16:I:343:HOH:O	1.96	0.48
4:D:184:PRO:O	4:D:186:ALA:N	2.46	0.48
8:H:176:VAL:HG12	8:H:178:LEU:HD13	1.95	0.48
13:M:211:LYS:HE3	9:W:194:ASN:HB3	1.96	0.48
14:2:153:ARG:HH11	14:2:153:ARG:CG	2.25	0.48
1:A:156:LYS:O	1:A:163:TYR:HA	2.14	0.48
5:E:127:ALA:HA	6:F:125:GLY:HA2	1.96	0.48
5:E:204:LEU:O	5:E:208:MET:HG3	2.13	0.48
11:K:118:ILE:HA	11:K:123:THR:O	2.14	0.48
14:N:27:ARG:HD3	14:N:28:PHE:CE2	2.49	0.48
6:T:194:VAL:O	6:T:197:ILE:HG22	2.14	0.48
6:T:50:LYS:HB3	6:T:59:TYR:HB3	1.96	0.48
12:L:4:LEU:CD1	12:L:161:ILE:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:42:VAL:CG2	4:R:145:PRO:HB2	2.43	0.48
10:X:108:GLY:HA2	10:X:183:LYS:HD3	1.96	0.48
10:X:115:PHE:HA	10:X:120:CYS:O	2.13	0.48
2:P:94:HIS:HD2	9:W:61:SER:OG	1.96	0.48
5:S:167:TYR:CE1	6:T:57:SER:HB3	2.49	0.48
3:C:96:GLN:NE2	10:J:63:ASN:HD22	2.12	0.47
7:G:165:GLY:O	7:G:168:ARG:HB3	2.14	0.47
10:J:36:HIS:HB3	10:J:41:PHE:CD2	2.49	0.47
13:M:34:VAL:HG12	13:M:196:LEU:HD22	1.96	0.47
7:U:170:SER:O	7:U:173:ALA:HB3	2.14	0.47
12:Z:4:LEU:CD1	12:Z:161:ILE:HD11	2.43	0.47
1:A:204:GLU:HG3	1:A:244:ARG:HG3	1.96	0.47
4:D:232:TYR:O	4:D:236:ILE:HG13	2.14	0.47
6:F:3:ARG:O	6:F:5:ASN:N	2.47	0.47
10:J:1:GLY:HA3	10:J:33:LYS:HE2	1.96	0.47
14:N:122:VAL:HA	14:N:127:VAL:O	2.14	0.47
6:T:128:TYR:O	6:T:149:PRO:HB3	2.14	0.47
3:Q:96:GLN:NE2	10:X:63:ASN:HD22	2.10	0.47
3:C:70:ASN:ND2	3:C:71:ASP:H	2.13	0.47
7:G:51:LYS:HG2	7:G:65:LYS:HD2	1.96	0.47
8:H:14:LEU:O	8:H:175:MET:HA	2.14	0.47
10:J:29:ASN:HD22	10:J:30:LYS:HG3	1.78	0.47
11:Y:95:ARG:HD2	16:Y:861:HOH:O	2.14	0.47
4:D:162:GLN:HE21	4:D:162:GLN:HA	1.79	0.47
11:K:91:ILE:HA	11:K:91:ILE:HD12	1.78	0.47
8:V:161:GLN:NE2	8:V:165:TRP:HE1	2.12	0.47
6:T:93:ASN:HD21	13:1:61:ASN:HD21	1.61	0.47
13:1:67:HIS:HD2	16:1:366:HOH:O	1.97	0.47
14:2:120:ARG:HH11	14:2:130:SER:HB2	1.79	0.47
2:B:107:THR:O	2:B:111:VAL:HG23	2.14	0.47
6:F:103:LEU:HD11	6:F:107:ARG:HG2	1.97	0.47
3:Q:70:ASN:HD22	3:Q:71:ASP:H	1.61	0.47
4:D:159:TRP:CE2	5:E:59:LEU:HD23	2.50	0.47
4:D:160:SER:HB3	4:D:179:TYR:CE1	2.50	0.47
3:Q:22:VAL:HG11	3:Q:154:SER:HB3	1.95	0.47
6:T:156:LEU:HD13	6:T:159:THR:HB	1.97	0.47
8:V:146:MET:HE2	8:V:150:GLU:HB3	1.96	0.47
11:Y:91:ILE:HD12	11:Y:91:ILE:HA	1.77	0.47
4:D:188:VAL:O	4:D:192:VAL:HG23	2.14	0.47
6:F:3:ARG:C	6:F:5:ASN:H	2.17	0.47
2:P:38:LYS:HG3	2:P:43:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:40:ASN:HD22	14:2:40:ASN:N	2.12	0.47
1:A:189:SER:O	1:A:190:LYS:HB2	2.15	0.47
8:V:15:GLY:HA2	8:V:174:ARG:O	2.14	0.47
9:W:152:ILE:O	9:W:156:SER:HB2	2.14	0.47
10:X:100:VAL:O	10:X:112:ILE:HA	2.15	0.47
1:A:52:VAL:HG12	1:A:54:ILE:HD12	1.97	0.47
3:C:70:ASN:HD22	3:C:71:ASP:H	1.61	0.47
6:F:206:LEU:HD23	6:F:206:LEU:H	1.80	0.47
7:G:126:ASN:HD22	7:G:127:SER:N	2.12	0.47
1:O:135:ARG:HB3	7:U:12:SER:HB2	1.97	0.47
6:T:46:LEU:HG	6:T:135:ILE:HD13	1.96	0.47
7:U:81:ILE:HB	7:U:82:PRO:HD3	1.97	0.47
2:B:160:LYS:HD3	2:B:179:TRP:CZ3	2.50	0.47
4:D:11:PHE:H	5:E:23:GLN:NE2	2.06	0.47
2:P:196:LEU:HA	2:P:196:LEU:HD12	1.80	0.47
4:R:43:VAL:CG2	4:R:191:CYS:SG	3.02	0.47
10:X:36:HIS:HB3	10:X:41:PHE:CD2	2.50	0.47
7:G:94:GLU:HG3	7:G:114:ARG:NH1	2.22	0.47
11:K:44:SER:OG	11:K:102:LEU:HB2	2.14	0.47
13:M:67:HIS:HD2	16:M:288:HOH:O	1.97	0.47
3:Q:135:PHE:O	3:Q:150:THR:HA	2.15	0.47
13:1:7:ALA:HB2	13:1:113:VAL:HG23	1.97	0.46
4:D:103:PRO:HG2	4:D:140:PRO:HG3	1.97	0.46
11:K:131:ALA:HB1	11:K:135:SER:HB2	1.98	0.46
9:W:17:ASP:HA	9:W:172:ASN:O	2.15	0.46
14:2:119:LEU:HG	14:2:134:LEU:HD12	1.97	0.46
5:E:49:GLY:HA2	5:E:218:GLN:O	2.15	0.46
12:Z:25:TRP:HH2	13:1:138:MET:HB2	1.80	0.46
1:A:196:GLU:HG2	1:A:201:LYS:HB2	1.93	0.46
6:F:113:CYS:SG	6:F:151:GLY:O	2.74	0.46
1:O:141:LEU:O	1:O:156:LYS:HA	2.15	0.46
6:T:82:ARG:O	6:T:86:ASN:HB2	2.16	0.46
1:A:244:ARG:O	1:A:248:ILE:HG23	2.16	0.46
6:F:46:LEU:HG	6:F:135:ILE:HD13	1.96	0.46
12:L:86:LEU:C	12:L:86:LEU:HD13	2.35	0.46
12:Z:145:LYS:HB2	12:Z:148:LEU:CD1	2.45	0.46
5:S:192:THR:OG1	5:S:195:GLU:HG3	2.15	0.46
10:J:108:GLY:HA2	10:J:183:LYS:HD3	1.97	0.46
6:F:47:VAL:CG1	6:F:211:LEU:HD11	2.45	0.46
9:I:123:TYR:HB3	9:I:142:TRP:CZ2	2.51	0.46
3:Q:4:ARG:CZ	5:S:11:GLY:HA2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:157:HIS:CD2	8:V:196:LEU:HD13	2.51	0.46
7:G:42:ASN:N	7:G:42:ASN:HD22	2.14	0.46
14:N:121:TYR:O	14:N:128:THR:HA	2.16	0.46
4:R:35:GLY:HA2	4:R:43:VAL:O	2.16	0.46
1:A:158:ASP:HB2	1:A:159:PRO:CD	2.46	0.46
7:G:34:THR:CG2	7:G:50:GLU:O	2.62	0.46
8:H:83:LYS:HD2	8:H:119:VAL:CG2	2.46	0.46
10:J:11:CYS:HA	10:J:103:ILE:HD11	1.97	0.46
11:K:12:VAL:HG23	11:K:113:PRO:HB2	1.96	0.46
6:T:47:VAL:CG1	6:T:211:LEU:HD11	2.46	0.46
11:K:24:ILE:HG12	11:K:24:ILE:O	2.16	0.46
5:S:31:ILE:HD13	5:S:141:ALA:HB2	1.98	0.46
7:U:135:THR:O	7:U:149:MET:HA	2.15	0.46
9:W:84:LYS:HG3	9:W:85:GLN:N	2.31	0.46
12:L:4:LEU:HD11	12:L:15:ALA:HB3	1.98	0.45
13:M:186:HIS:HE1	16:M:234:HOH:O	1.99	0.45
14:N:7:LYS:HD2	14:N:157:ILE:HD13	1.97	0.45
4:R:70:HIS:CE1	4:R:103:PRO:HB2	2.52	0.45
5:S:243:LEU:HD22	5:S:247:GLU:HG3	1.98	0.45
6:T:3:ARG:O	6:T:5:ASN:N	2.49	0.45
8:V:84:GLU:O	8:V:88:GLU:HB2	2.16	0.45
12:Z:128:CYS:HB2	12:Z:137:TYR:CE2	2.51	0.45
8:V:4:MET:HB3	8:V:126:ILE:HG22	1.98	0.45
13:1:4:LEU:HD11	13:1:141:LEU:HD21	1.97	0.45
2:B:43:VAL:HG11	2:B:137:ALA:HB1	1.99	0.45
3:C:146:TYR:OH	3:C:218:LYS:HB2	2.16	0.45
7:G:170:SER:O	7:G:173:ALA:HB3	2.16	0.45
9:I:20:SER:HB3	9:I:28:ASP:HB3	1.98	0.45
1:O:240:ASN:HB3	16:O:1085:HOH:O	2.16	0.45
9:W:196:ARG:NH2	10:X:142:GLU:O	2.50	0.45
10:X:78:PHE:O	10:X:82:VAL:HG23	2.16	0.45
12:Z:5:ALA:HA	12:Z:13:ILE:O	2.17	0.45
7:G:106:ILE:HA	7:G:107:PRO:HD3	1.88	0.45
8:H:159:LEU:O	8:H:163:ILE:HG13	2.16	0.45
4:R:199:LEU:O	4:R:203:VAL:HG23	2.16	0.45
8:V:83:LYS:HD2	8:V:119:VAL:CG2	2.47	0.45
10:X:12:VAL:HG13	10:X:110:PRO:HB3	1.98	0.45
12:L:25:TRP:CH2	13:M:135:SER:HA	2.51	0.45
1:O:74:CYS:O	1:O:98:LYS:HE2	2.16	0.45
6:T:182:ILE:HD13	6:T:188:GLU:HB3	1.98	0.45
8:V:8:PHE:CE2	8:V:10:ASP:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:189:GLU:HA	4:D:232:TYR:OH	2.16	0.45
10:J:181:ILE:HG23	10:J:186:VAL:HG22	1.97	0.45
1:O:164:VAL:HG22	1:O:165:GLY:N	2.32	0.45
4:R:29:ARG:NH1	4:R:29:ARG:HB2	2.32	0.45
1:A:72:ILE:HD12	1:A:224:GLU:HG2	1.98	0.45
9:I:113:ILE:HG12	9:I:119:THR:HG22	1.99	0.45
14:N:111:VAL:HG23	14:N:192:ILE:HG22	1.99	0.45
4:R:51:THR:HG22	4:R:52:LEU:HD22	1.99	0.45
6:T:117:GLN:OE1	6:T:121:GLN:NE2	2.50	0.45
3:Q:100:LYS:NZ	11:Y:85:GLN:NE2	2.64	0.45
11:Y:90:SER:O	11:Y:93:SER:HB3	2.16	0.45
4:D:42:VAL:HG11	4:D:136:ALA:HB1	1.98	0.45
7:G:36:SER:HB3	7:G:49:VAL:HG23	1.99	0.45
6:T:175:THR:O	6:T:175:THR:HG22	2.17	0.45
6:T:19:LEU:HD21	7:U:129:ARG:HD2	1.99	0.45
9:I:52:THR:O	9:I:56:THR:HB	2.17	0.45
4:R:203:VAL:HG11	4:R:209:ASN:HB3	1.98	0.45
9:W:123:TYR:HB3	9:W:142:TRP:CZ2	2.52	0.45
11:Y:17:SER:HB2	11:Y:175:PHE:HB2	1.99	0.45
3:C:130:PRO:HG3	16:C:263:HOH:O	2.16	0.44
2:B:12:PHE:N	3:C:21:GLN:HE22	2.07	0.44
4:D:174:PHE:CD2	4:D:198:SER:HB3	2.53	0.44
6:F:93:ASN:HD21	13:M:61:ASN:ND2	2.14	0.44
11:K:6:ILE:HD11	11:K:147:TYR:CE1	2.52	0.44
3:Q:111:LEU:HD23	3:Q:111:LEU:C	2.37	0.44
3:Q:70:ASN:ND2	3:Q:71:ASP:H	2.15	0.44
5:S:176:SER:O	5:S:180:GLN:HB2	2.17	0.44
9:W:114:HIS:HE1	16:W:340:HOH:O	2.00	0.44
14:2:175:VAL:O	14:2:178:TYR:HB2	2.17	0.44
9:I:143:LYS:O	9:I:146:LEU:HG	2.17	0.44
10:J:5:ALA:HA	10:J:13:ALA:O	2.17	0.44
11:K:35:ARG:NH1	11:K:57:GLU:OE2	2.51	0.44
5:S:169:ALA:HB1	5:S:183:LEU:HD22	1.99	0.44
5:S:46:VAL:O	5:S:221:CYS:HA	2.18	0.44
9:W:84:LYS:HE2	9:W:119:THR:CG2	2.46	0.44
5:E:46:VAL:O	5:E:221:CYS:HA	2.18	0.44
6:F:135:ILE:HA	6:F:143:HIS:O	2.17	0.44
3:Q:181:LYS:HG3	3:Q:184:MET:HG3	2.00	0.44
8:V:-2:LEU:O	8:V:1:ALA:N	2.51	0.44
2:B:110:LEU:O	2:B:114:VAL:HG23	2.17	0.44
3:C:66:LEU:HD12	3:C:76:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:168:ASN:HB3	5:S:187:TRP:CE2	2.53	0.44
6:F:43:HIS:HB2	6:F:189:LEU:HD12	2.00	0.44
8:H:113:ILE:HG12	8:H:119:VAL:HG22	2.00	0.44
13:M:143:ASN:O	13:M:147:PHE:HA	2.17	0.44
4:R:226:SER:HB2	4:R:227:GLU:OE2	2.18	0.44
4:R:63:LYS:HE2	4:R:75:PHE:CZ	2.52	0.44
6:T:4:ASN:HA	6:T:7:ASP:OD1	2.18	0.44
10:X:44:ILE:HB	10:X:51:VAL:HG13	1.98	0.44
1:A:54:ILE:HG13	1:A:225:VAL:HG22	1.99	0.44
1:A:77:ARG:HB2	1:A:77:ARG:HH11	1.82	0.44
3:C:221:ASN:O	3:C:222:ASP:HB2	2.18	0.44
4:D:237:GLU:O	4:D:241:GLN:HB2	2.18	0.44
5:E:192:THR:OG1	5:E:195:GLU:HG3	2.17	0.44
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.98	0.44
11:K:52:THR:CG2	11:K:53:VAL:N	2.81	0.44
2:P:3:ASP:OD1	2:P:5:TYR:HB2	2.16	0.44
3:Q:51:LYS:HG2	3:Q:52:VAL:HG23	1.99	0.44
3:C:77:VAL:HG22	3:C:135:PHE:CE1	2.52	0.44
12:L:4:LEU:CD1	12:L:15:ALA:HB3	2.47	0.44
13:M:196:LEU:CD1	13:M:205:LYS:HG2	2.47	0.44
1:O:69:VAL:HA	7:U:157:TRP:CZ3	2.53	0.44
3:Q:125:HIS:CB	4:R:126:VAL:HG12	2.46	0.44
8:H:20:THR:HG23	8:H:31:THR:OG1	2.17	0.44
2:P:110:LEU:O	2:P:114:VAL:HG23	2.18	0.44
6:T:207:THR:H	6:T:210:ASN:HB2	1.82	0.44
6:T:3:ARG:C	6:T:5:ASN:H	2.20	0.44
11:Y:12:VAL:HG23	11:Y:113:PRO:HB2	2.00	0.44
3:C:107:PRO:HD2	3:C:110:ILE:HD12	1.99	0.44
10:J:9:LYS:HD3	10:J:148:ASN:HB3	1.99	0.44
7:U:11:ASN:O	7:U:13:VAL:N	2.51	0.44
4:R:90:ARG:NH1	11:Y:69:ARG:HA	2.33	0.44
6:F:179:PHE:HA	6:F:182:ILE:HG13	2.00	0.43
7:G:217:TRP:N	7:G:217:TRP:CD1	2.86	0.43
8:V:105:LYS:O	8:V:105:LYS:HD3	2.18	0.43
3:C:2:GLY:HA3	6:F:123:TYR:CE1	2.53	0.43
11:K:90:SER:HA	11:K:93:SER:HB2	2.00	0.43
3:Q:100:LYS:HZ2	11:Y:85:GLN:HE21	1.66	0.43
11:Y:129:TYR:CD1	11:Y:143:LEU:HD13	2.53	0.43
12:Z:144:TYR:O	12:Z:145:LYS:HD2	2.18	0.43
3:C:22:VAL:HG11	3:C:154:SER:HB3	2.01	0.43
9:I:200:GLN:CG	13:1:173:LYS:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:7:ARG:HG2	11:K:7:ARG:O	2.18	0.43
13:M:116:PHE:CD1	13:M:116:PHE:N	2.86	0.43
1:O:17:THR:HB	1:O:129:THR:O	2.19	0.43
14:2:144:ASN:O	14:2:148:ARG:HG3	2.19	0.43
4:D:35:GLY:HA2	4:D:43:VAL:O	2.18	0.43
7:G:126:ASN:C	7:G:126:ASN:ND2	2.71	0.43
1:O:101:ALA:HA	1:O:112:MET:CE	2.28	0.43
1:O:52:VAL:HG12	1:O:54:ILE:CD1	2.49	0.43
2:P:160:LYS:HD3	2:P:179:TRP:CZ3	2.52	0.43
3:Q:94:HIS:CE1	16:Q:1058:HOH:O	2.71	0.43
4:R:66:LYS:HA	4:R:72:VAL:HG12	1.99	0.43
7:U:42:ASN:HD22	7:U:43:ASP:N	2.16	0.43
9:W:26:VAL:HG11	9:W:29:LYS:HG2	1.99	0.43
4:D:103:PRO:HG2	4:D:140:PRO:CG	2.48	0.43
11:K:145:HIS:HD2	11:K:146:HIS:CE1	2.37	0.43
11:K:24:ILE:HD13	12:L:134:THR:HG21	2.01	0.43
1:O:14:ARG:HG2	1:O:26:TYR:CD2	2.53	0.43
4:R:237:GLU:O	4:R:241:GLN:HB2	2.18	0.43
6:T:105:VAL:HG12	6:T:145:LEU:HD22	2.00	0.43
6:T:206:LEU:HD12	6:T:211:LEU:HD13	2.01	0.43
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.99	0.43
9:W:80:LEU:HD12	9:W:113:ILE:HD11	2.00	0.43
9:W:196:ARG:HH21	10:X:142:GLU:HG3	1.82	0.43
4:D:238:GLN:C	4:D:240:LYS:H	2.21	0.43
6:F:29:ILE:HD11	6:F:149:PRO:CD	2.48	0.43
7:G:189:ARG:HH11	7:G:189:ARG:HG3	1.84	0.43
11:K:6:ILE:HD11	11:K:147:TYR:CD1	2.53	0.43
3:Q:116:SER:HB3	3:Q:155:GLY:O	2.19	0.43
3:Q:68:LYS:HG3	3:Q:227:GLN:OE1	2.19	0.43
5:S:68:VAL:HG21	5:S:89:ILE:HD12	2.01	0.43
2:B:18:LEU:HD13	2:B:21:ILE:HD12	2.01	0.43
6:F:71:GLY:HA3	6:F:222:PHE:CZ	2.53	0.43
8:H:14:LEU:HD11	8:H:100:ALA:HB3	2.00	0.43
9:I:196:ARG:HH21	10:J:142:GLU:HG3	1.82	0.43
12:L:145:LYS:HB2	12:L:148:LEU:CD1	2.49	0.43
4:R:31:THR:HB	4:R:47:GLU:HG3	2.00	0.43
6:T:71:GLY:HA3	6:T:222:PHE:CE2	2.53	0.43
14:2:131:SER:HB3	14:2:133:THR:O	2.19	0.43
1:A:176:GLN:HE21	1:A:180:THR:HG23	1.84	0.43
4:D:138:PHE:CE2	4:D:217:PRO:HG3	2.53	0.43
6:F:62:LYS:O	6:F:73:SER:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:80:LEU:HD12	9:I:113:ILE:HD11	2.00	0.43
3:Q:54:SER:OG	3:Q:55:THR:N	2.50	0.43
1:A:64:LEU:O	1:A:66:PRO:HD3	2.19	0.43
7:G:86:HIS:HD2	7:G:131:PHE:CE2	2.37	0.43
2:P:97:TYR:HD1	2:P:103:GLU:O	2.02	0.43
3:Q:221:ASN:O	3:Q:222:ASP:HB2	2.19	0.43
6:T:13:PHE:HB2	7:U:22:GLN:HE22	1.83	0.43
4:D:63:LYS:HE2	4:D:75:PHE:CZ	2.54	0.43
5:E:168:ASN:HB3	5:E:187:TRP:CE2	2.53	0.43
9:I:84:LYS:HE2	9:I:119:THR:HG23	2.00	0.43
1:O:88:PRO:HB2	7:U:120:GLN:HG3	1.99	0.43
4:R:151:GLU:HB2	4:R:152:PRO:CD	2.49	0.43
5:S:75:GLY:HA3	5:S:228:PHE:CE1	2.53	0.43
7:U:194:GLN:HE21	7:U:197:LYS:HD3	1.83	0.43
13:1:116:PHE:CD2	13:1:122:TYR:HB3	2.54	0.42
13:1:14:LEU:HA	13:1:14:LEU:HD23	1.87	0.42
14:2:7:LYS:HD2	14:2:157:ILE:HD13	2.01	0.42
2:B:36:GLY:HA2	2:B:44:VAL:O	2.19	0.42
6:F:101:ARG:NH1	16:F:252:HOH:O	2.51	0.42
6:F:45:VAL:HG12	6:F:46:LEU:N	2.34	0.42
12:L:12:ILE:HB	12:L:180:VAL:HB	2.02	0.42
12:L:40:PHE:CD2	12:L:73:ARG:CZ	3.02	0.42
1:O:92:ASN:C	1:O:92:ASN:HD22	2.22	0.42
2:P:46:ALA:HB2	2:P:211:LEU:HG	2.01	0.42
3:Q:185:LYS:HD2	3:Q:187:ASP:H	1.83	0.42
12:Z:4:LEU:HD12	12:Z:161:ILE:HD11	2.00	0.42
2:B:46:ALA:HB2	2:B:211:LEU:HG	2.02	0.42
7:G:49:VAL:HG22	7:G:50:GLU:N	2.34	0.42
9:W:113:ILE:HG12	9:W:119:THR:HG22	2.00	0.42
4:D:171:VAL:HG12	4:D:202:VAL:CG2	2.46	0.42
5:E:201:LEU:HA	5:E:201:LEU:HD12	1.89	0.42
8:H:146:MET:CE	8:H:150:GLU:HB3	2.47	0.42
8:H:55:ILE:HD11	8:H:93:LEU:HD13	2.00	0.42
12:L:6:PHE:HA	12:L:125:ASP:O	2.20	0.42
14:N:88:LEU:O	14:N:92:MET:HG2	2.20	0.42
2:P:226:GLY:O	2:P:228:PRO:HD3	2.19	0.42
7:U:69:VAL:HB	7:U:73:ILE:HB	2.01	0.42
6:F:206:LEU:CD2	6:F:206:LEU:H	2.32	0.42
7:G:172:LYS:O	7:G:176:GLU:HG3	2.20	0.42
10:J:92:GLY:N	10:J:93:PRO:CD	2.83	0.42
7:U:217:TRP:CZ2	7:U:234:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:171:MET:HA	11:Y:172:PRO:HD3	1.86	0.42
11:Y:35:ARG:NH1	11:Y:57:GLU:OE2	2.53	0.42
2:B:189:ILE:HG21	2:B:246:ARG:HD3	2.01	0.42
8:H:51:ASP:OD2	8:H:93:LEU:HA	2.19	0.42
12:L:4:LEU:HD12	12:L:161:ILE:CD1	2.50	0.42
4:R:42:VAL:HG11	4:R:136:ALA:CB	2.49	0.42
8:V:114:PRO:HD2	8:V:118:SER:O	2.20	0.42
9:I:167:LEU:HD22	13:1:187:ILE:O	2.19	0.42
6:F:194:VAL:HA	6:F:197:ILE:HG22	2.00	0.42
4:R:48:ARG:HD2	4:R:208:LYS:O	2.18	0.42
6:T:29:ILE:HD11	6:T:149:PRO:CD	2.50	0.42
7:U:215:ILE:HG22	7:U:216:SER:N	2.34	0.42
3:C:137:TYR:O	3:C:148:LEU:HA	2.19	0.42
3:C:38:ILE:HD12	3:C:193:ALA:HB2	2.02	0.42
4:D:68:ASP:HA	11:K:68:ILE:HD11	2.01	0.42
6:F:201:LEU:CD1	6:F:206:LEU:HD22	2.49	0.42
13:M:186:HIS:CD2	13:M:188:GLN:HB2	2.54	0.42
1:O:54:ILE:HD13	1:O:206:ALA:HB1	2.02	0.42
6:T:135:ILE:HD12	6:T:216:VAL:HG12	2.01	0.42
8:V:-2:LEU:HD23	8:V:20:THR:HG22	2.02	0.42
3:C:42:ASP:OD1	3:C:42:ASP:N	2.53	0.42
4:D:203:VAL:O	4:D:204:GLN:HB2	2.19	0.42
9:I:3:ILE:HG13	9:I:99:ILE:HD12	2.02	0.42
10:J:12:VAL:HG13	10:J:110:PRO:HB3	2.01	0.42
1:O:51:THR:HG21	1:O:144:VAL:HB	2.02	0.42
4:R:29:ARG:CG	4:R:29:ARG:O	2.65	0.42
6:T:63:ILE:HG21	6:T:214:ALA:HB2	2.01	0.42
8:V:113:ILE:HG12	8:V:119:VAL:HG22	2.01	0.42
9:W:199:LYS:HE3	10:X:143:SER:O	2.20	0.42
14:2:121:TYR:O	14:2:128:THR:HA	2.20	0.42
6:F:175:THR:HG22	6:F:175:THR:O	2.19	0.42
16:E:274:HOH:O	13:M:86:HIS:HD2	2.03	0.42
4:R:215:VAL:HB	4:R:221:ILE:HG12	2.01	0.42
1:A:110:TYR:OH	9:I:66:HIS:HE1	2.02	0.42
2:B:149:GLN:O	2:B:156:TYR:HA	2.20	0.42
7:G:20:ASN:ND2	7:G:23:VAL:HG23	2.35	0.42
7:G:49:VAL:HB	7:G:76:VAL:HG21	2.02	0.42
9:I:5:GLY:HA3	9:I:110:LEU:HD11	2.02	0.42
12:L:140:LEU:HD12	12:L:140:LEU:HA	1.88	0.42
1:O:63:LEU:HA	1:O:63:LEU:HD23	1.82	0.42
6:T:198:SER:HA	6:T:201:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:35:THR:HA	7:U:164:THR:O	2.20	0.42
2:B:226:GLY:O	2:B:228:PRO:HD3	2.20	0.41
4:D:203:VAL:HG13	4:D:209:ASN:OD1	2.20	0.41
6:F:4:ASN:HA	6:F:7:ASP:OD1	2.20	0.41
12:L:209:ASN:O	10:X:30:LYS:NZ	2.50	0.41
1:O:197:GLU:H	1:O:197:GLU:CD	2.24	0.41
2:P:109:LEU:HA	2:P:109:LEU:HD23	1.89	0.41
4:R:200:LEU:HA	4:R:200:LEU:HD23	1.73	0.41
5:S:85:ALA:O	5:S:89:ILE:HG12	2.19	0.41
7:U:106:ILE:HA	7:U:107:PRO:HD3	1.86	0.41
11:Y:2:ILE:O	11:Y:16:SER:HA	2.20	0.41
11:Y:38:SER:HB2	11:Y:39:PRO:HD2	2.02	0.41
2:B:24:ALA:O	2:B:28:VAL:HG23	2.20	0.41
3:C:115:LEU:HA	3:C:115:LEU:HD23	1.80	0.41
3:C:135:PHE:O	3:C:150:THR:HA	2.20	0.41
13:M:91:LYS:HD3	13:M:96:TYR:CE2	2.55	0.41
5:S:52:LYS:HG3	5:S:64:ILE:CG2	2.50	0.41
9:W:20:SER:HB2	9:W:31:CYS:SG	2.60	0.41
10:X:29:ASN:HD22	10:X:30:LYS:HG3	1.85	0.41
12:Z:40:PHE:CD2	12:Z:73:ARG:CZ	3.04	0.41
13:1:63:VAL:HG22	13:1:75:LEU:HD23	2.01	0.41
14:2:219:GLY:HA3	14:2:223:GLN:HB3	2.03	0.41
9:I:104:ASP:HB2	9:I:105:PRO:CD	2.50	0.41
11:K:67:SER:HA	11:K:72:TYR:O	2.20	0.41
8:V:83:LYS:HD2	8:V:119:VAL:HG21	2.01	0.41
9:W:104:ASP:HB2	9:W:105:PRO:HD2	2.02	0.41
2:B:196:LEU:CD2	2:B:209:ILE:HD12	2.49	0.41
5:E:170:LYS:HE3	5:E:171:ALA:O	2.21	0.41
12:L:40:PHE:CD2	12:L:73:ARG:NH1	2.89	0.41
13:M:15:ALA:HB1	13:M:193:LEU:HD11	2.01	0.41
5:E:68:VAL:HG21	5:E:89:ILE:HD12	2.02	0.41
16:E:276:HOH:O	13:M:70:HIS:HE1	2.03	0.41
14:N:138:PHE:HE2	14:N:142:MET:SD	2.43	0.41
1:O:158:ASP:HB2	1:O:159:PRO:CD	2.51	0.41
2:P:74:VAL:HG12	2:P:135:LEU:HB2	2.01	0.41
5:S:15:PHE:HB2	6:T:21:GLN:OE1	2.20	0.41
11:Y:102:LEU:HD23	11:Y:117:GLN:HA	2.02	0.41
11:Y:6:ILE:HD11	11:Y:147:TYR:CD1	2.56	0.41
4:D:226:SER:HB2	4:D:227:GLU:OE2	2.21	0.41
6:F:194:VAL:HG13	6:F:206:LEU:HD11	2.03	0.41
7:G:66:ILE:HB	7:G:229:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:244:ARG:O	1:O:248:ILE:HG23	2.21	0.41
1:O:44:ALA:HA	1:O:52:VAL:O	2.21	0.41
6:T:179:PHE:HA	6:T:182:ILE:HG13	2.03	0.41
6:T:63:ILE:HD13	6:T:214:ALA:HB2	2.02	0.41
6:F:157:TYR:CD1	6:F:180:ILE:HD13	2.56	0.41
1:O:245:LEU:HA	1:O:245:LEU:HD12	1.88	0.41
4:R:232:TYR:O	4:R:236:ILE:HG13	2.20	0.41
6:T:194:VAL:HG13	6:T:206:LEU:HD11	2.02	0.41
2:B:55:LEU:HA	2:B:55:LEU:HD23	1.82	0.41
5:E:243:LEU:HD23	5:E:243:LEU:HA	1.88	0.41
8:H:161:GLN:HE22	8:H:165:TRP:HE1	1.67	0.41
13:M:110:LYS:HA	13:M:110:LYS:HD3	1.89	0.41
1:O:88:PRO:HG2	16:O:1037:HOH:O	2.21	0.41
4:R:74:SER:OG	4:R:134:LEU:HB2	2.21	0.41
4:R:59:ILE:HG13	4:R:60:THR:N	2.36	0.41
10:X:28:SER:CB	11:Y:125:VAL:HG21	2.50	0.41
11:Y:142:LEU:HD13	11:Y:162:LEU:HG	2.03	0.41
5:E:198:LEU:HA	5:E:198:LEU:HD12	1.81	0.41
12:L:65:LEU:HD12	12:L:65:LEU:HA	1.89	0.41
1:O:189:SER:O	1:O:190:LYS:HB2	2.20	0.41
1:O:52:VAL:HG12	1:O:54:ILE:HD12	2.03	0.41
8:V:101:GLY:HA2	8:V:178:LEU:HD23	2.02	0.41
12:Z:140:LEU:HD12	12:Z:140:LEU:HA	1.94	0.41
1:A:133:TYR:HD1	16:B:283:HOH:O	2.04	0.41
2:B:43:VAL:O	2:B:213:ILE:HA	2.21	0.41
1:A:123:ASN:HD22	2:B:83:ARG:HH21	1.68	0.41
5:E:76:CYS:HB2	5:E:143:LEU:O	2.20	0.41
6:F:156:LEU:HD13	6:F:159:THR:HB	2.02	0.41
9:I:163:ILE:HG23	9:I:170:GLY:HA2	2.03	0.41
9:I:94:ILE:HG21	9:I:94:ILE:HD13	1.84	0.41
13:M:5:GLY:HA2	13:M:13:VAL:O	2.21	0.41
5:S:167:TYR:CZ	5:S:170:LYS:HD3	2.56	0.41
6:T:107:ARG:HH11	6:T:107:ARG:HG2	1.86	0.41
7:U:39:ILE:HG12	7:U:175:LEU:HD11	2.02	0.41
7:U:174:GLU:O	7:U:177:LYS:HB2	2.21	0.41
14:2:138:PHE:HE1	14:2:142:MET:SD	2.44	0.41
3:C:63:THR:HG23	3:C:66:LEU:O	2.21	0.41
3:C:71:ASP:HB2	16:C:294:HOH:O	2.21	0.41
6:F:207:THR:H	6:F:210:ASN:HB2	1.86	0.41
8:H:13:ILE:HG12	8:H:177:VAL:HG13	2.02	0.41
13:M:-7:ASN:HD22	13:M:-6:PRO:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:168:ASN:ND2	3:Q:200:THR:O	2.54	0.41
4:R:185:PRO:HB3	4:R:191:CYS:HA	2.03	0.41
5:S:49:GLY:HA2	5:S:218:GLN:O	2.21	0.41
7:U:138:GLY:HA3	7:U:146:HIS:O	2.21	0.41
7:U:188:ALA:O	7:U:192:VAL:HG23	2.21	0.41
12:Z:46:ALA:HB3	12:Z:98:GLY:O	2.21	0.41
14:2:35:ILE:HA	14:2:36:PRO:HD3	1.85	0.40
3:C:54:SER:OG	3:C:55:THR:N	2.55	0.40
6:F:38:LEU:HA	6:F:158:GLY:HA2	2.03	0.40
6:F:3:ARG:C	6:F:5:ASN:N	2.74	0.40
6:T:13:PHE:H	7:U:22:GLN:NE2	2.03	0.40
3:C:37:GLY:C	3:C:148:LEU:HD21	2.42	0.40
3:C:94:HIS:CE1	16:C:253:HOH:O	2.72	0.40
5:E:167:TYR:CZ	5:E:170:LYS:HD3	2.57	0.40
6:F:36:VAL:HG13	6:F:172:LEU:HD11	2.04	0.40
3:Q:94:HIS:HE1	16:Q:1058:HOH:O	2.03	0.40
2:B:176:GLU:HG3	3:C:56:LEU:HD22	2.03	0.40
13:M:116:PHE:CD2	13:M:122:TYR:HB3	2.57	0.40
1:O:144:VAL:HA	1:O:153:SER:O	2.21	0.40
3:Q:130:PRO:HG3	16:Q:1068:HOH:O	2.21	0.40
6:F:128:TYR:O	6:F:149:PRO:HB3	2.20	0.40
14:N:18:ASN:HA	14:N:31:VAL:O	2.21	0.40
2:P:108:LYS:HG2	16:P:1045:HOH:O	2.21	0.40
8:V:43:CYS:HA	8:V:98:ILE:O	2.20	0.40
10:X:146:GLU:HA	10:X:147:PRO:HD3	1.89	0.40
10:X:54:LEU:CD1	10:X:96:VAL:HG21	2.52	0.40
10:X:98:PRO:HB2	10:X:115:PHE:CD1	2.56	0.40
11:Y:153:THR:HG21	11:Y:182:ILE:HD13	2.03	0.40
14:2:167:GLU:HG3	16:2:348:HOH:O	2.22	0.40
1:A:52:VAL:HG12	1:A:54:ILE:CD1	2.52	0.40
3:C:43:GLY:HA3	3:C:186:VAL:HG21	2.04	0.40
4:D:73:LEU:HD22	4:D:86:ILE:HG12	2.04	0.40
3:Q:106:ILE:HA	3:Q:107:PRO:HD3	1.97	0.40
8:V:13:ILE:HG12	8:V:177:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	38	26
1	O	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	38	26
2	B	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	38	26
2	P	248/250 (99%)	235 (95%)	10 (4%)	3 (1%)	15	5
3	C	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	11	2
3	Q	242/244 (99%)	224 (93%)	14 (6%)	4 (2%)	11	2
4	D	239/241 (99%)	223 (93%)	12 (5%)	4 (2%)	11	2
4	R	239/241 (99%)	222 (93%)	13 (5%)	4 (2%)	11	2
5	E	240/242 (99%)	231 (96%)	7 (3%)	2 (1%)	22	11
5	S	240/242 (99%)	228 (95%)	9 (4%)	3 (1%)	14	4
6	F	231/233 (99%)	214 (93%)	14 (6%)	3 (1%)	14	4
6	T	231/233 (99%)	209 (90%)	19 (8%)	3 (1%)	14	4
7	G	242/244 (99%)	230 (95%)	10 (4%)	2 (1%)	22	11
7	U	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	15	5
8	H	203/205 (99%)	193 (95%)	9 (4%)	1 (0%)	32	20
8	V	203/205 (99%)	192 (95%)	10 (5%)	1 (0%)	32	20
9	I	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
9	W	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
10	J	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
10	X	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
11	K	196/198 (99%)	191 (97%)	3 (2%)	2 (1%)	18	7
11	Y	196/198 (99%)	188 (96%)	6 (3%)	2 (1%)	18	7
12	L	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	Z	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
13	1	220/222 (99%)	212 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
14	2	231/233 (99%)	219 (95%)	12 (5%)	0	100	100
14	N	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
All	All	6330/6386 (99%)	6017 (95%)	269 (4%)	44 (1%)	25	13

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	222	ASP
4	D	54	LEU
4	D	185	PRO
1	O	60	PRO
3	Q	222	ASP
4	R	54	LEU
4	R	185	PRO
7	U	11	ASN
3	C	204	SER
4	D	205	THR
7	G	11	ASN
11	K	49	ALA
2	P	50	LYS
3	Q	204	SER
4	R	205	THR
5	S	189	SER
6	T	202	ARG
6	T	218	LYS
7	U	12	SER
1	A	60	PRO
4	D	186	ALA
5	E	127	ALA
5	E	189	SER
6	F	4	ASN
6	F	202	ARG
3	Q	52	VAL
4	R	186	ALA
7	U	207	LYS
11	Y	49	ALA
3	C	52	VAL
8	H	-1	GLY
2	P	2	THR
5	S	120	ALA

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Mol	Chain	Res	Type
5	S	128	SER
6	T	4	ASN
2	B	166	LYS
7	G	207	LYS
2	P	166	LYS
8	V	-1	GLY
11	Y	8	VAL
3	C	223	GLY
11	K	8	VAL
6	F	227	GLY
3	Q	223	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/207 (100%)	196 (95%)	11 (5%)	26	15
1	O	207/207 (100%)	196 (95%)	11 (5%)	26	15
2	B	209/209 (100%)	200 (96%)	9 (4%)	33	22
2	P	209/209 (100%)	203 (97%)	6 (3%)	48	39
3	C	203/203 (100%)	187 (92%)	16 (8%)	14	6
3	Q	203/203 (100%)	188 (93%)	15 (7%)	16	7
4	D	213/213 (100%)	195 (92%)	18 (8%)	12	5
4	R	213/213 (100%)	196 (92%)	17 (8%)	14	5
5	E	198/198 (100%)	186 (94%)	12 (6%)	22	11
5	S	198/198 (100%)	187 (94%)	11 (6%)	25	13
6	F	192/192 (100%)	176 (92%)	16 (8%)	13	5
6	T	192/192 (100%)	176 (92%)	16 (8%)	13	5
7	G	201/201 (100%)	184 (92%)	17 (8%)	12	5
7	U	201/201 (100%)	183 (91%)	18 (9%)	11	4
8	H	168/168 (100%)	162 (96%)	6 (4%)	40	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	168/168 (100%)	165 (98%)	3 (2%)	64	60
9	I	181/181 (100%)	174 (96%)	7 (4%)	37	26
9	W	181/181 (100%)	171 (94%)	10 (6%)	25	14
10	J	172/172 (100%)	169 (98%)	3 (2%)	66	62
10	X	172/172 (100%)	168 (98%)	4 (2%)	56	49
11	K	175/175 (100%)	171 (98%)	4 (2%)	56	49
11	Y	175/175 (100%)	170 (97%)	5 (3%)	48	39
12	L	169/169 (100%)	163 (96%)	6 (4%)	40	29
12	Z	169/169 (100%)	164 (97%)	5 (3%)	46	37
13	1	185/185 (100%)	174 (94%)	11 (6%)	23	12
13	M	185/185 (100%)	175 (95%)	10 (5%)	26	14
14	2	199/199 (100%)	190 (96%)	9 (4%)	32	21
14	N	199/199 (100%)	191 (96%)	8 (4%)	36	25
All	All	5344/5344 (100%)	5060 (95%)	284 (5%)	26	15

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

Mol	Chain	Res	Type
1	A	33	LYS
1	A	77	ARG
1	A	92	ASN
1	A	124	LEU
1	A	126	GLN
1	A	175	GLN
1	A	195	ASN
1	A	196	GLU
1	A	230	LYS
1	A	244	ARG
1	A	245	LEU
2	B	29	LYS
2	B	30	GLN
2	B	61	LEU
2	B	112	SER
2	B	122	THR
2	B	157	PHE
2	B	211	LEU
2	B	236	ARG

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Mol	Chain	Res	Type
2	B	250	LEU
3	C	3	SER
3	C	56	LEU
3	C	61	THR
3	C	66	LEU
3	C	70	ASN
3	C	80	LEU
3	C	103	ASN
3	C	120	GLN
3	C	150	THR
3	C	153	PRO
3	C	185	LYS
3	C	192	LEU
3	C	198	SER
3	C	202	ASP
3	C	232	PRO
3	C	245	THR
4	D	6	ARG
4	D	21	GLU
4	D	50	SER
4	D	53	LYS
4	D	57	THR
4	D	63	LYS
4	D	118	GLN
4	D	132	SER
4	D	149	GLN
4	D	155	ILE
4	D	162	GLN
4	D	171	VAL
4	D	173	GLU
4	D	177	LYS
4	D	209	ASN
4	D	215	VAL
4	D	224	LEU
4	D	226	SER
5	E	13	SER
5	E	28	LEU
5	E	48	LEU
5	E	76	CYS
5	E	132	ARG
5	E	177	GLU
5	E	184	LEU

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Mol	Chain	Res	Type
5	E	190	SER
5	E	198	LEU
5	E	201	LEU
5	E	222	ILE
5	E	243	LEU
6	F	9	ASP
6	F	10	THR
6	F	11	VAL
6	F	56	LEU
6	F	72	LEU
6	F	86	ASN
6	F	117	GLN
6	F	174	ARG
6	F	185	ASN
6	F	189	LEU
6	F	199	GLN
6	F	206	LEU
6	F	208	VAL
6	F	210	ASN
6	F	223	THR
6	F	232	LYS
7	G	10	SER
7	G	34	THR
7	G	35	THR
7	G	42	ASN
7	G	120	GLN
7	G	126	ASN
7	G	168	ARG
7	G	169	GLN
7	G	170	SER
7	G	175	LEU
7	G	189	ARG
7	G	194	GLN
7	G	204	GLU
7	G	206	ASN
7	G	211	PHE
7	G	217	TRP
7	G	224	ASN
8	H	36	ARG
8	H	70	TYR
8	H	103	ASP
8	H	132	THR

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Mol	Chain	Res	Type
8	H	149	GLU
8	H	178	LEU
9	I	30	ASN
9	I	34	LEU
9	I	56	THR
9	I	68	LEU
9	I	121	VAL
9	I	144	GLN
9	I	196	ARG
10	J	29	ASN
10	J	125	LYS
10	J	163	LEU
11	K	34	THR
11	K	52	THR
11	K	70	GLU
11	K	77	GLN
12	L	4	LEU
12	L	9	GLN
12	L	65	LEU
12	L	87	VAL
12	L	104	TYR
12	L	107	LYS
13	M	-7	ASN
13	M	14	LEU
13	M	40	ASN
13	M	62	SER
13	M	71	ASN
13	M	99	HIS
13	M	100	THR
13	M	117	ASP
13	M	141	LEU
13	M	165	TYR
14	N	40	ASN
14	N	61	ASP
14	N	74	ASP
14	N	96	ARG
14	N	153	ARG
14	N	204	LEU
14	N	205	GLN
14	N	218	LYS
1	O	33	LYS
1	O	77	ARG

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Mol	Chain	Res	Type
1	O	92	ASN
1	O	114	CYS
1	O	124	LEU
1	O	126	GLN
1	O	195	ASN
1	O	196	GLU
1	O	230	LYS
1	O	244	ARG
1	O	245	LEU
2	P	29	LYS
2	P	30	GLN
2	P	61	LEU
2	P	157	PHE
2	P	211	LEU
2	P	250	LEU
3	Q	56	LEU
3	Q	61	THR
3	Q	66	LEU
3	Q	70	ASN
3	Q	80	LEU
3	Q	120	GLN
3	Q	123	THR
3	Q	150	THR
3	Q	158	THR
3	Q	185	LYS
3	Q	192	LEU
3	Q	198	SER
3	Q	202	ASP
3	Q	222	ASP
3	Q	245	THR
4	R	6	ARG
4	R	21	GLU
4	R	50	SER
4	R	53	LYS
4	R	57	THR
4	R	63	LYS
4	R	118	GLN
4	R	132	SER
4	R	149	GLN
4	R	162	GLN
4	R	171	VAL
4	R	173	GLU

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Mol	Chain	Res	Type
4	R	177	LYS
4	R	209	ASN
4	R	215	VAL
4	R	224	LEU
4	R	241	GLN
5	S	12	VAL
5	S	35	SER
5	S	76	CYS
5	S	132	ARG
5	S	184	LEU
5	S	190	SER
5	S	198	LEU
5	S	201	LEU
5	S	212	LEU
5	S	222	ILE
5	S	243	LEU
6	T	9	ASP
6	T	10	THR
6	T	30	LYS
6	T	56	LEU
6	T	72	LEU
6	T	86	ASN
6	T	107	ARG
6	T	117	GLN
6	T	174	ARG
6	T	185	ASN
6	T	189	LEU
6	T	199	GLN
6	T	206	LEU
6	T	208	VAL
6	T	223	THR
6	T	232	LYS
7	U	10	SER
7	U	34	THR
7	U	35	THR
7	U	42	ASN
7	U	72	HIS
7	U	120	GLN
7	U	126	ASN
7	U	168	ARG
7	U	169	GLN
7	U	170	SER

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Mol	Chain	Res	Type
7	U	175	LEU
7	U	189	ARG
7	U	194	GLN
7	U	204	GLU
7	U	206	ASN
7	U	217	TRP
7	U	224	ASN
7	U	233	ASP
8	V	36	ARG
8	V	103	ASP
8	V	149	GLU
9	W	13	VAL
9	W	30	ASN
9	W	34	LEU
9	W	55	VAL
9	W	56	THR
9	W	63	ILE
9	W	68	LEU
9	W	121	VAL
9	W	144	GLN
9	W	196	ARG
10	X	29	ASN
10	X	125	LYS
10	X	163	LEU
10	X	194	ARG
11	Y	34	THR
11	Y	52	THR
11	Y	68	ILE
11	Y	70	GLU
11	Y	77	GLN
12	Z	4	LEU
12	Z	9	GLN
12	Z	65	LEU
12	Z	104	TYR
12	Z	107	LYS
13	1	-7	ASN
13	1	14	LEU
13	1	40	ASN
13	1	62	SER
13	1	94	PHE
13	1	99	HIS
13	1	100	THR

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Mol	Chain	Res	Type
13	1	117	ASP
13	1	141	LEU
13	1	156	ASN
13	1	165	TYR
14	2	40	ASN
14	2	61	ASP
14	2	62	LEU
14	2	74	ASP
14	2	96	ARG
14	2	153	ARG
14	2	162	VAL
14	2	205	GLN
14	2	218	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (172) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	39	ASN
1	A	92	ASN
1	A	123	ASN
1	A	126	GLN
1	A	130	GLN
1	A	175	GLN
1	A	176	GLN
1	A	184	ASN
1	A	193	HIS
1	A	195	ASN
1	A	251	GLN
2	B	94	HIS
2	B	218	ASN
3	C	21	GLN
3	C	70	ASN
3	C	94	HIS
3	C	96	GLN
3	C	120	GLN
3	C	124	GLN
3	C	156	ASN
3	C	177	GLN
4	D	19	GLN
4	D	79	ASN
4	D	149	GLN

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Mol	Chain	Res	Type
4	D	162	GLN
5	E	23	GLN
5	E	108	ASN
5	E	154	GLN
5	E	206	GLN
5	E	218	GLN
5	E	233	ASN
6	F	69	HIS
6	F	100	ASN
6	F	117	GLN
6	F	121	GLN
6	F	185	ASN
7	G	22	GLN
7	G	42	ASN
7	G	89	ASN
7	G	120	GLN
7	G	126	ASN
7	G	146	HIS
7	G	194	GLN
7	G	247	ASN
8	H	38	HIS
8	H	157	HIS
8	H	161	GLN
9	I	30	ASN
9	I	66	HIS
9	I	114	HIS
9	I	116	HIS
9	I	144	GLN
9	I	165	ASN
9	I	172	ASN
9	I	189	ASN
10	J	29	ASN
11	K	54	GLN
11	K	85	GLN
11	K	117	GLN
11	K	145	HIS
11	K	190	GLN
12	L	85	ASN
12	L	176	ASN
12	L	208	ASN
13	M	-7	ASN
13	M	40	ASN

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Mol	Chain	Res	Type
13	M	46	ASN
13	M	61	ASN
13	M	67	HIS
13	M	70	HIS
13	M	71	ASN
13	M	86	HIS
13	M	126	GLN
13	M	149	ASN
13	M	156	ASN
13	M	186	HIS
14	N	10	ASN
14	N	40	ASN
14	N	94	GLN
14	N	100	ASN
14	N	163	GLN
14	N	171	ASN
14	N	186	ASN
14	N	205	GLN
1	O	39	ASN
1	O	92	ASN
1	O	123	ASN
1	O	126	GLN
1	O	130	GLN
1	O	184	ASN
1	O	195	ASN
1	O	251	GLN
2	P	94	HIS
3	Q	21	GLN
3	Q	70	ASN
3	Q	94	HIS
3	Q	96	GLN
3	Q	120	GLN
3	Q	124	GLN
3	Q	156	ASN
3	Q	177	GLN
4	R	19	GLN
4	R	79	ASN
4	R	118	GLN
4	R	122	GLN
4	R	149	GLN
4	R	162	GLN
5	S	23	GLN

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Mol	Chain	Res	Type
5	S	108	ASN
5	S	154	GLN
5	S	206	GLN
5	S	218	GLN
5	S	233	ASN
6	T	31	GLN
6	T	69	HIS
6	T	100	ASN
6	T	117	GLN
6	T	121	GLN
6	T	185	ASN
6	T	199	GLN
7	U	22	GLN
7	U	42	ASN
7	U	89	ASN
7	U	120	GLN
7	U	126	ASN
7	U	146	HIS
7	U	194	GLN
8	V	38	HIS
8	V	69	GLN
8	V	157	HIS
8	V	161	GLN
9	W	30	ASN
9	W	66	HIS
9	W	114	HIS
9	W	116	HIS
9	W	144	GLN
9	W	165	ASN
9	W	172	ASN
9	W	189	ASN
10	X	29	ASN
10	X	148	ASN
11	Y	54	GLN
11	Y	77	GLN
11	Y	85	GLN
11	Y	117	GLN
11	Y	190	GLN
11	Y	197	GLN
12	Z	9	GLN
12	Z	85	ASN
12	Z	176	ASN

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Mol	Chain	Res	Type
12	Z	208	ASN
13	1	-7	ASN
13	1	40	ASN
13	1	46	ASN
13	1	61	ASN
13	1	71	ASN
13	1	86	HIS
13	1	99	HIS
13	1	126	GLN
13	1	149	ASN
13	1	156	ASN
13	1	186	HIS
14	2	-7	GLN
14	2	10	ASN
14	2	40	ASN
14	2	94	GLN
14	2	100	ASN
14	2	163	GLN
14	2	171	ASN
14	2	186	ASN
14	2	205	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

Of 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.