Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:14 am BST

PDB ID	:	5NIF
Title	:	Yeast 20S proteasome in complex with Blm-pep activator
Authors	:	Witkowska, J.; Grudnik, P.; Golik, P.; Dubin, G.; Jankowska, E.
Deposited on	:	2017-03-23
Resolution	:	3.00 Å(reported)

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

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

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

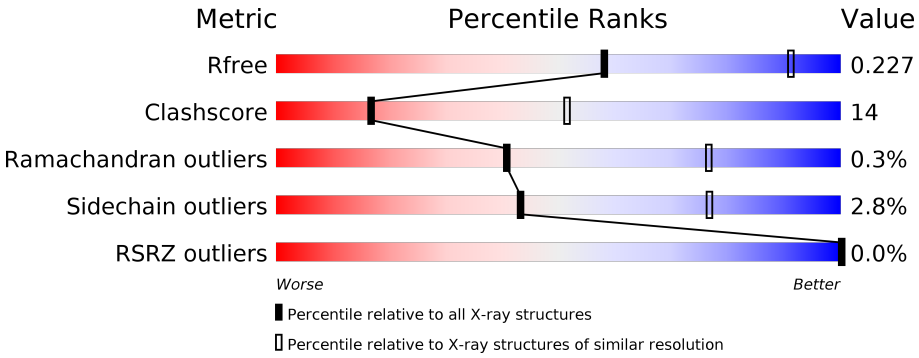
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	67% 27%
1	O	252	67% 27%
2	B	250	73% 26%
2	P	250	70% 29%
3	C	258	60% 32% 7%
3	Q	258	66% 28% 6%

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Mol	Chain	Length	Quality of chain
4	D	254	66% 28% • 5%
4	R	254	66% 28% 5%
5	E	260	64% 26% • 9%
5	S	260	63% 27% • 9%
6	F	234	75% 24% •
6	T	234	70% 27% • •
7	G	288	60% 23% • 15%
7	U	288	60% 23% • 15%
8	H	215	66% 24% • 9%
8	V	215	69% 21% 9%
9	I	261	61% 23% • 15%
9	W	261	61% 23% • 15%
10	J	205	72% 26% •
10	X	205	75% 24%
11	K	198	65% 32% • •
11	Y	198	69% 27% • •
12	L	287	55% 19% 26%
12	Z	287	55% 19% 26%
13	1	241	69% 22% • 8%
13	M	241	65% 27% 8%
14	2	266	64% 22% • 12%
14	N	266	65% 20% • 13%
15	3	14	14% 29% 57%
15	4	14	21% 21% 57%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49177 atoms, of which 104 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	2	0
			1910	1217	317	368	8			
1	O	241	Total	C	N	O	S	0	0	0
			1862	1183	312	359	8			

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1882	1200	306	372	4			
2	P	250	Total	C	N	O	S	0	0	0
			1904	1212	312	377	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1848	1167	305	373	3			
3	Q	242	Total	C	N	O	S	0	0	0
			1844	1163	307	371	3			

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1821	1135	316	366	4			
4	R	241	Total	C	N	O	S	0	0	0
			1837	1147	321	365	4			

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	236	Total	C	N	O	S	0	0	0
			1801	1133	295	366	7			
5	S	236	Total	C	N	O	S	0	0	0
			1800	1129	299	365	7			

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	232	Total	C	N	O	S	0	0	0
			1756	1104	300	348	4			
6	T	232	Total	C	N	O	S	0	0	0
			1769	1110	307	348	4			

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	0	0
			1865	1184	324	353	4			
7	U	244	Total	C	N	O	S	0	0	0
			1882	1196	327	355	4			

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1504	950	248	299	7			
8	V	196	Total	C	N	O	S	0	0	0
			1508	953	249	299	7			

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1678	1059	292	320	7			
9	W	222	Total	C	N	O	S	0	0	0
			1680	1058	292	323	7			

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1566	1000	253	305	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1563	997	253	305	8			

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	196	Total	C	N	O	S	0	0	0
			1549	986	263	294	6			
11	Y	196	Total	C	N	O	S	0	0	0
			1565	995	265	299	6			

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1634	1039	278	310	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1626	1033	274	312	7			

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1742	1104	299	335	4			
13	1	222	Total	C	N	O	S	0	0	0
			1740	1103	298	335	4			

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	232	Total	C	N	O	S	0	0	0
			1817	1150	311	349	7			
14	2	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is a protein called TRP-ARG-SER-TYR-TYR-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	6	Total	C	N	O	0	0	0
			52	33	9	10			
15	4	6	Total	C	N	O	0	0	0
			52	33	9	10			

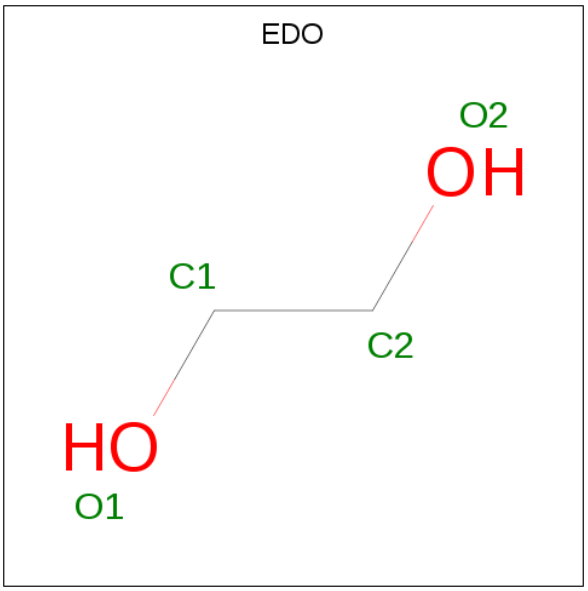
- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	P	1	Total Cl 1 1	0	0
16	2	3	Total Cl 3 3	0	0
16	K	2	Total Cl 2 2	0	0
16	V	1	Total Cl 1 1	0	0
16	A	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	O	1	Total Cl 1 1	0	0
16	R	1	Total Cl 1 1	0	0
16	S	1	Total Cl 1 1	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	J	1	Total Mg 1 1	0	0
17	Q	1	Total Mg 1 1	0	0
17	D	1	Total Mg 1 1	0	0
17	H	1	Total Mg 1 1	0	0
17	I	1	Total Mg 1 1	0	0
17	C	1	Total Mg 1 1	0	0
17	N	2	Total Mg 2 2	0	0

- Molecule 18 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	C	H	O	0	0
			10	2	6	2		
18	F	1	Total	C	H	O	0	0
			10	2	6	2		
18	G	1	Total	C	H	O	0	0
			10	2	6	2		
18	I	1	Total	C	H	O	0	0
			10	2	6	2		
18	L	1	Total	C	H	O	0	0
			10	2	6	2		
18	M	1	Total	C	H	O	0	0
			10	2	6	2		
18	O	1	Total	C	H	O	0	0
			10	2	6	2		
18	O	1	Total	C	H	O	0	0
			10	2	6	2		
18	U	1	Total	C	H	O	0	0
			10	2	6	2		
18	W	1	Total	C	H	O	0	0
			10	2	6	2		
18	W	1	Total	C	H	O	0	0
			10	2	6	2		
18	W	1	Total	C	H	O	0	0
			10	2	6	2		
18	Y	1	Total	C	H	O	0	0
			10	2	6	2		
18	Y	1	Total	C	H	O	0	0
			10	2	6	2		

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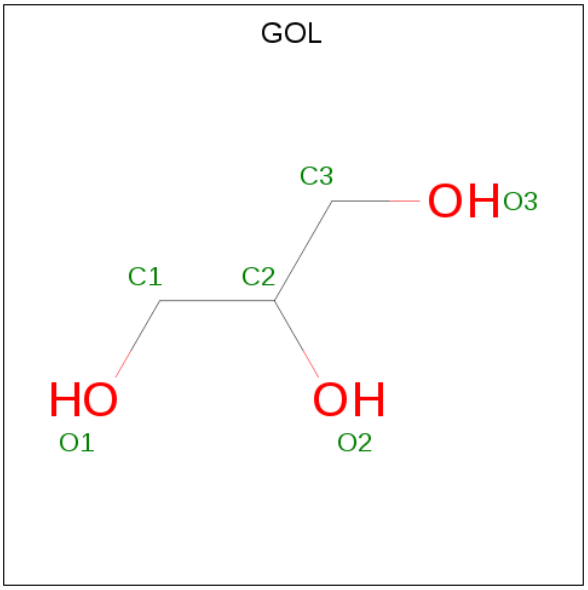
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	1	1	Total C H O 10 2 6 2	0	0
18	2	1	Total C H O 10 2 6 2	0	0

- Molecule 19 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	J	1	Total C O 6 3 3	0	0
19	L	1	Total C O 6 3 3	0	0
19	M	1	Total C H O 14 3 8 3	0	0
19	Q	1	Total C O 6 3 3	0	0
19	V	1	Total C O 6 3 3	0	0
19	Z	1	Total C O 6 3 3	0	0
19	1	1	Total C O 6 3 3	0	0

- Molecule 20 is water.

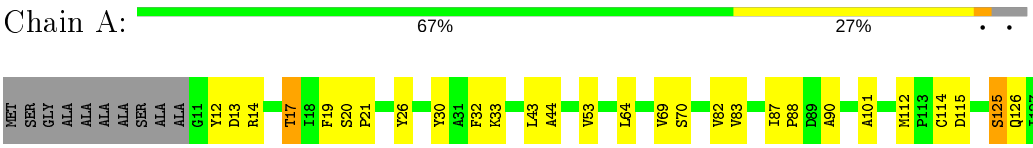
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	2	Total O 2 2	0	0
20	C	2	Total O 2 2	0	0
20	D	1	Total O 1 1	0	0
20	G	2	Total O 2 2	0	0
20	H	8	Total O 8 8	0	0
20	I	2	Total O 2 2	0	0
20	J	1	Total O 1 1	0	0
20	L	1	Total O 1 1	0	0
20	M	4	Total O 4 4	0	0
20	N	4	Total O 4 4	0	0
20	O	4	Total O 4 4	0	0
20	U	2	Total O 2 2	0	0
20	V	5	Total O 5 5	0	0
20	W	2	Total O 2 2	0	0
20	X	2	Total O 2 2	0	0
20	Z	6	Total O 6 6	0	0
20	1	9	Total O 9 9	0	0
20	2	9	Total O 9 9	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.

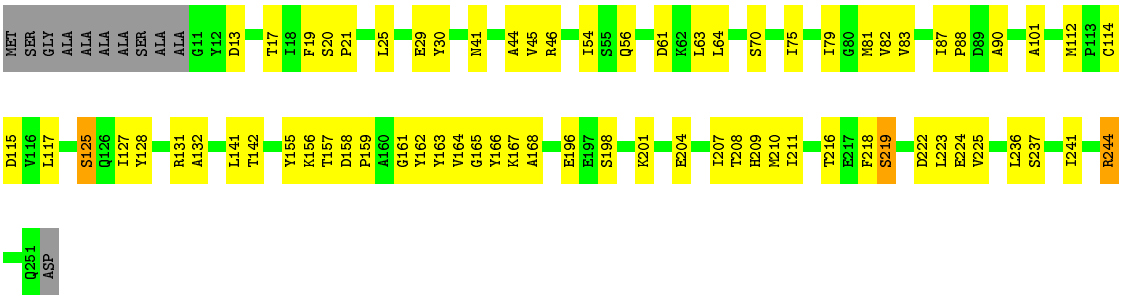
- Molecule 1: Proteasome subunit alpha type-1

Chain A:



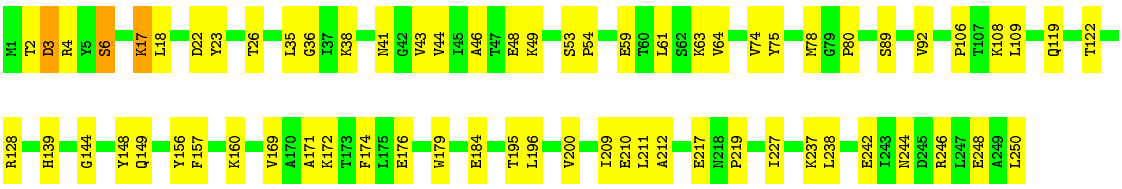
- Molecule 1: Proteasome subunit alpha type-1

Chain O:



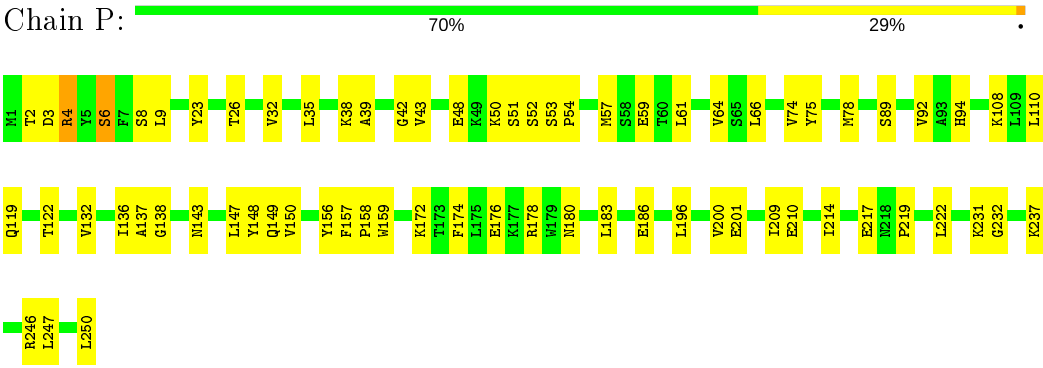
- Molecule 2: Proteasome subunit alpha type-2

Chain B:



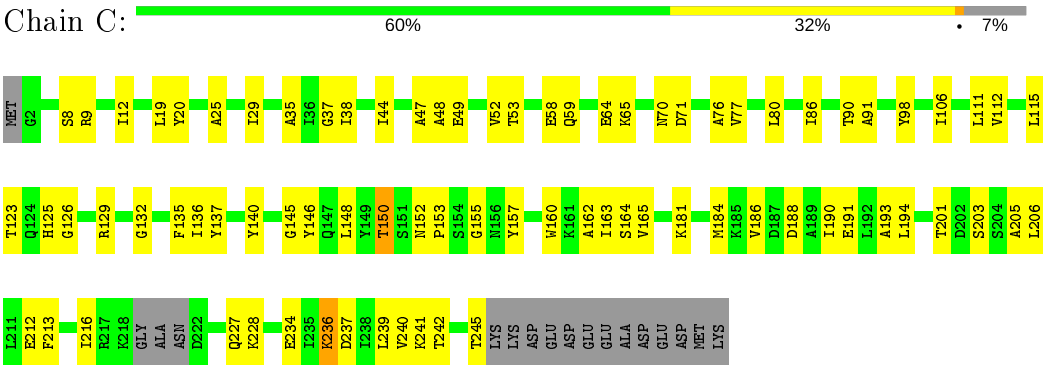
- Molecule 2: Proteasome subunit alpha type-2

Chain P:



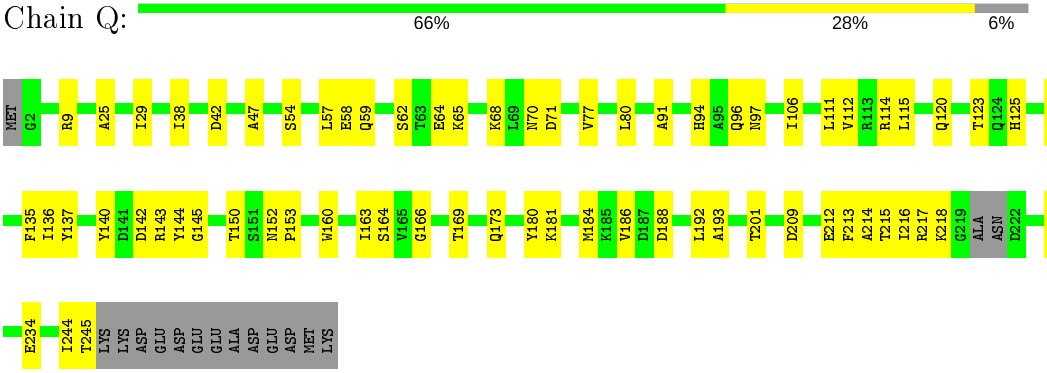
- Molecule 3: Proteasome subunit alpha type-3

Chain C:



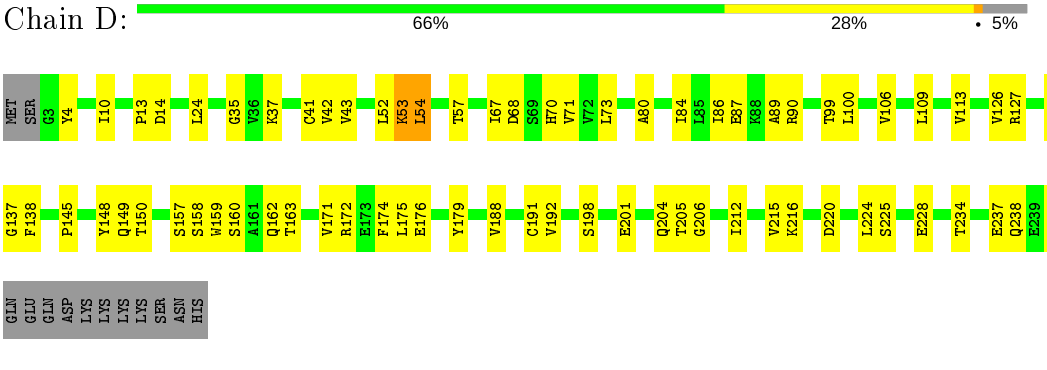
- Molecule 3: Proteasome subunit alpha type-3

Chain Q:



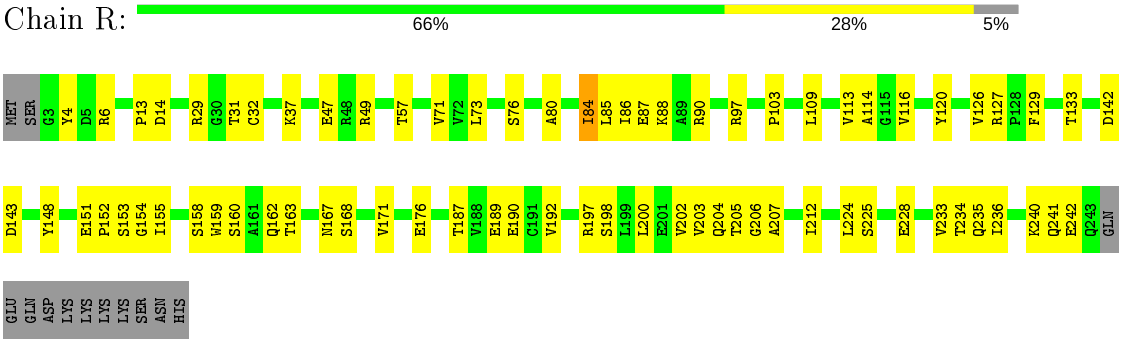
- Molecule 4: Proteasome subunit alpha type-4

Chain D:



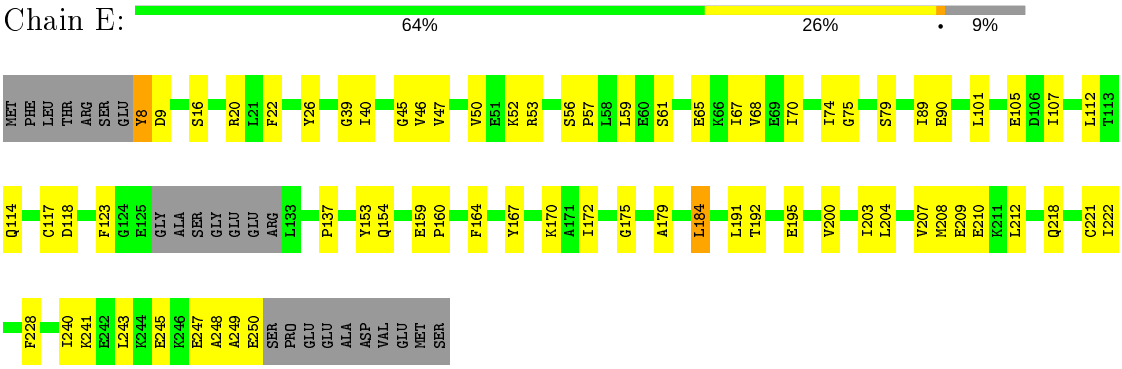
• Molecule 4: Proteasome subunit alpha type-4

Chain R:



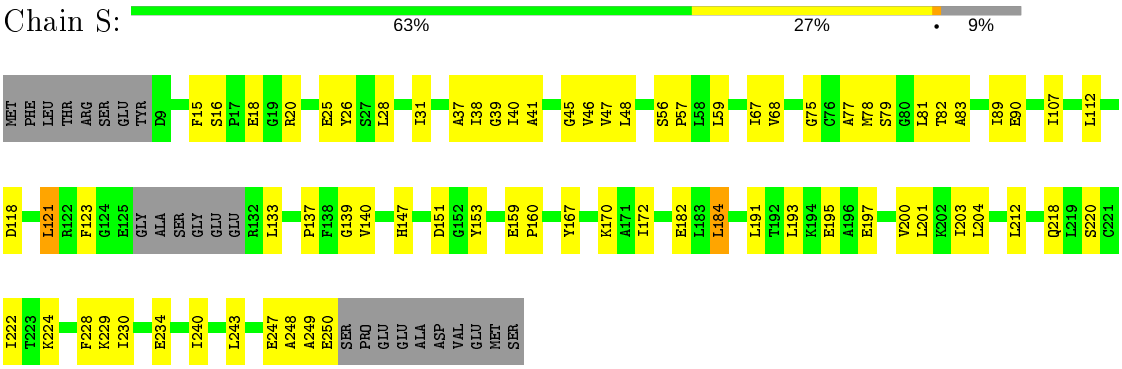
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



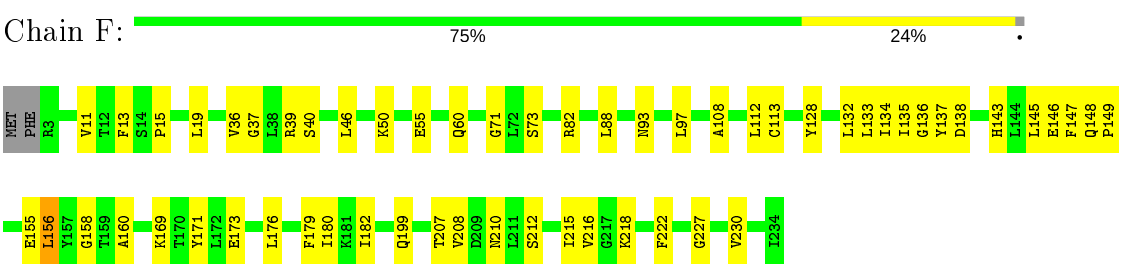
• Molecule 5: Proteasome subunit alpha type-5

Chain S:



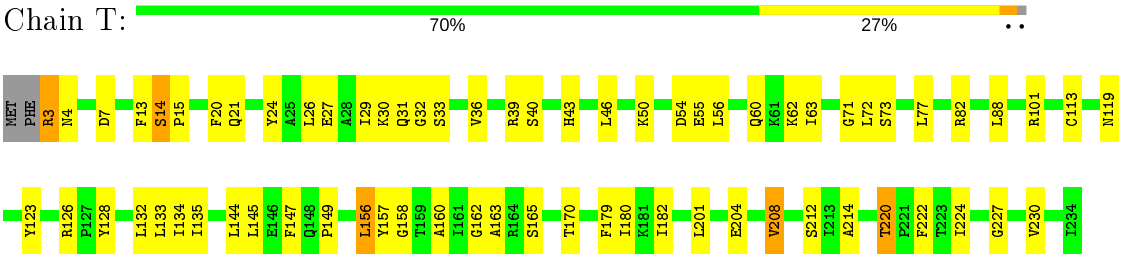
• Molecule 6: Proteasome subunit alpha type-6

Chain F:



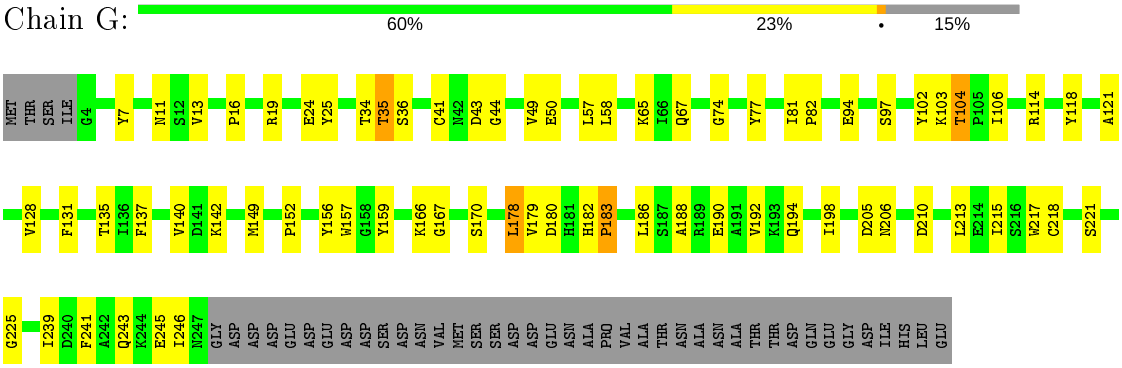
• Molecule 6: Proteasome subunit alpha type-6

Chain T:



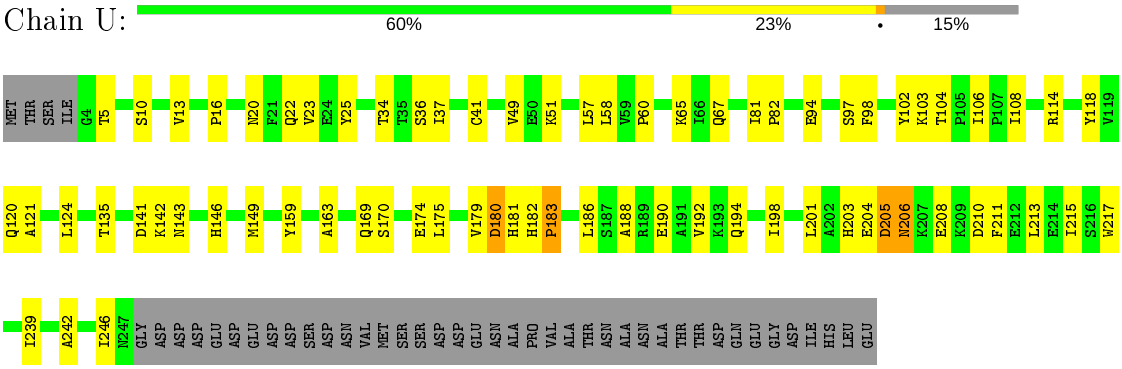
• Molecule 7: Probable proteasome subunit alpha type-7

Chain G:



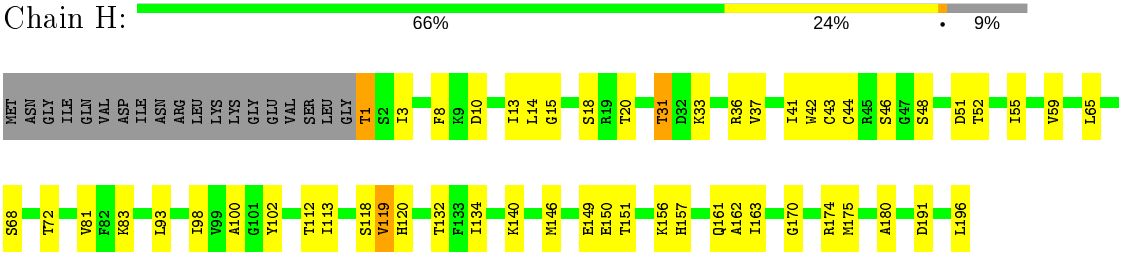
• Molecule 7: Probable proteasome subunit alpha type-7

Chain U:



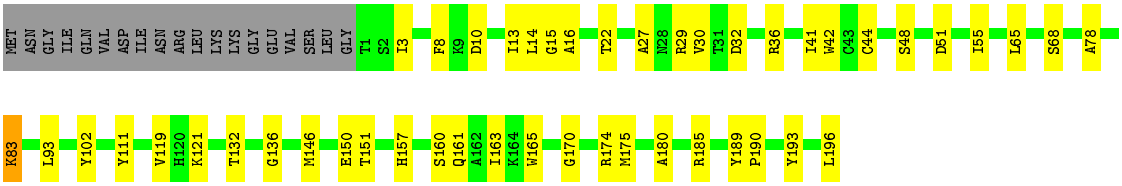
• Molecule 8: Proteasome subunit beta type-1

Chain H:



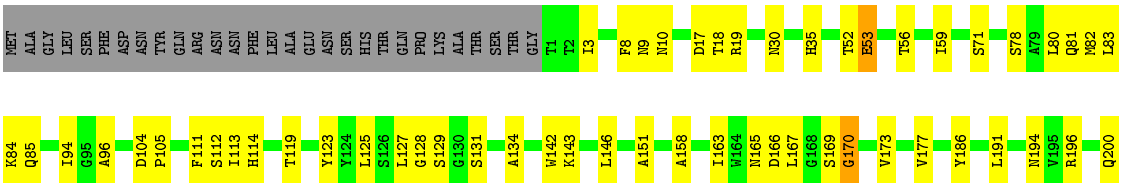
• Molecule 8: Proteasome subunit beta type-1

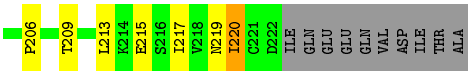
Chain V:



• Molecule 9: Proteasome subunit beta type-2

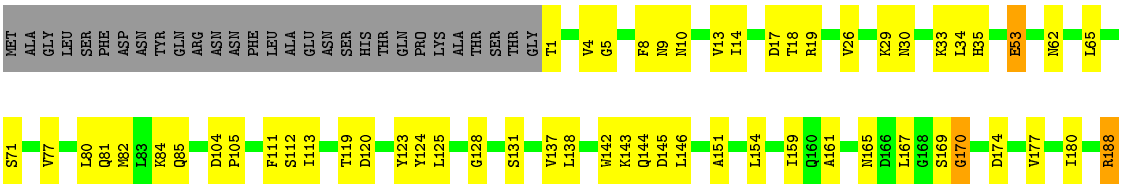
Chain I:





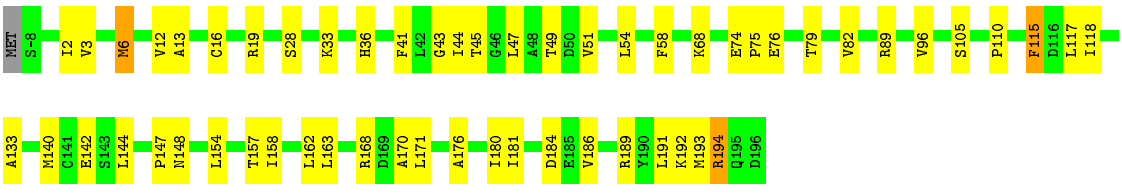
• Molecule 9: Proteasome subunit beta type-2

Chain W:



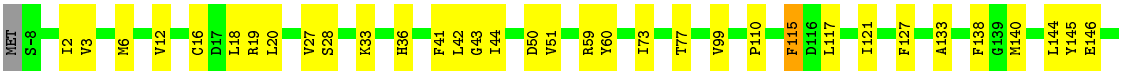
• Molecule 10: Proteasome subunit beta type-3

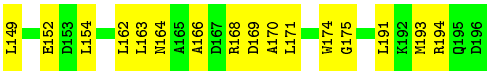
Chain J:



• Molecule 10: Proteasome subunit beta type-3

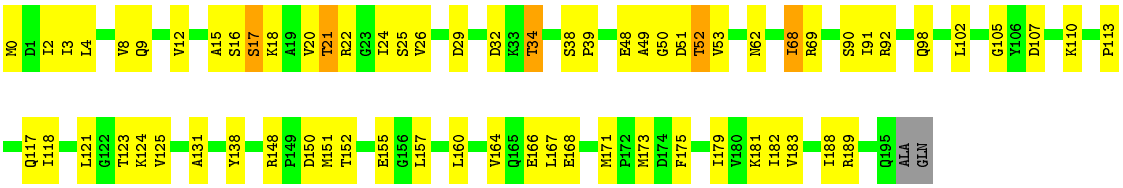
Chain X:





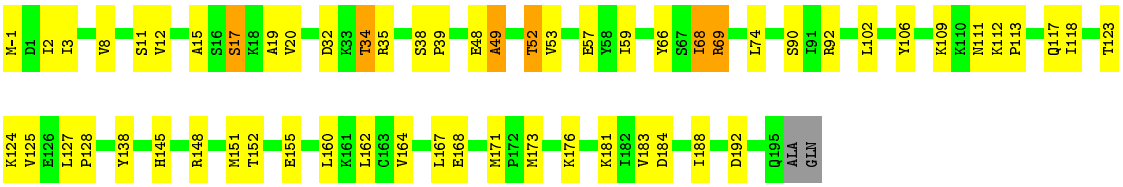
• Molecule 11: Proteasome subunit beta type-4

Chain K:



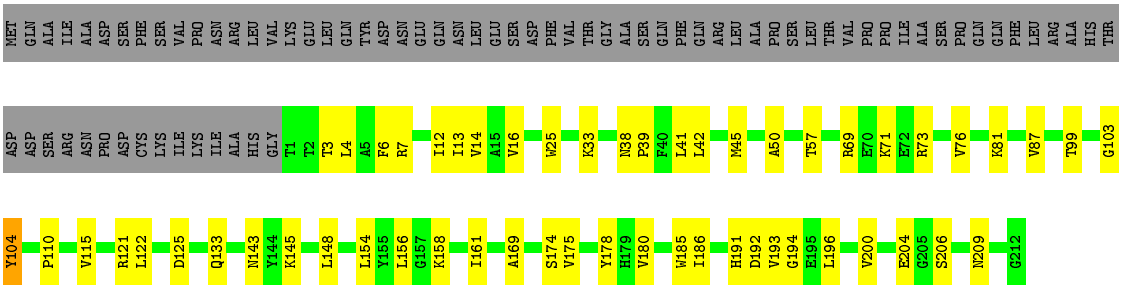
• Molecule 11: Proteasome subunit beta type-4

Chain Y:



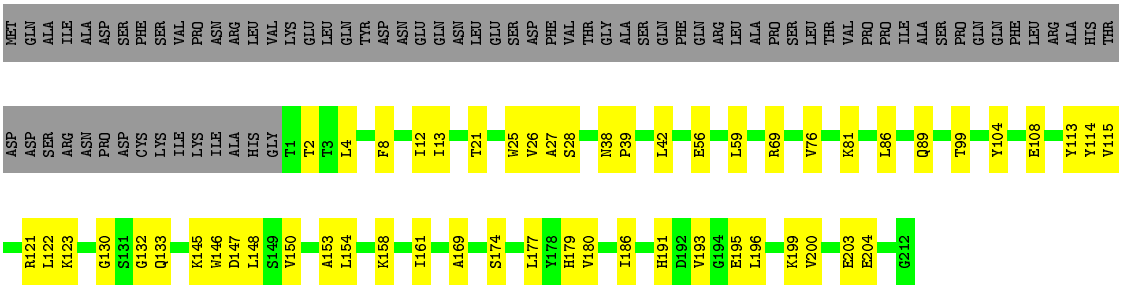
• Molecule 12: Proteasome subunit beta type-5

Chain L:



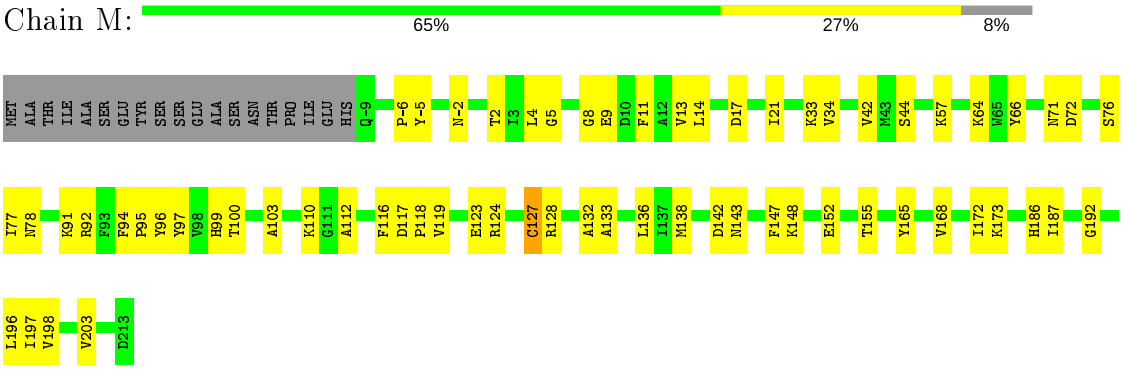
• Molecule 12: Proteasome subunit beta type-5

Chain Z:



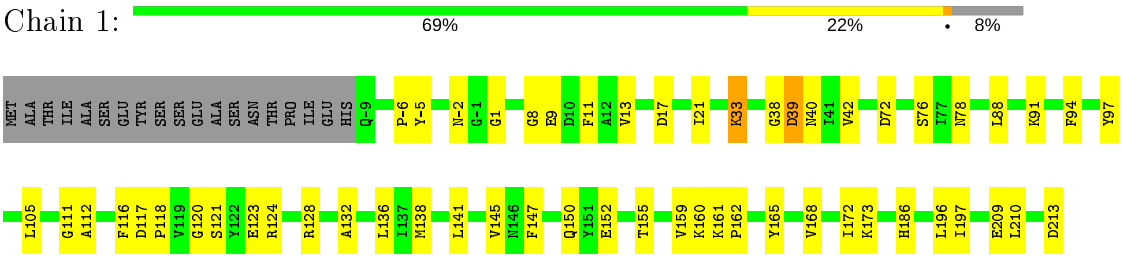
• Molecule 13: Proteasome subunit beta type-6

Chain M:



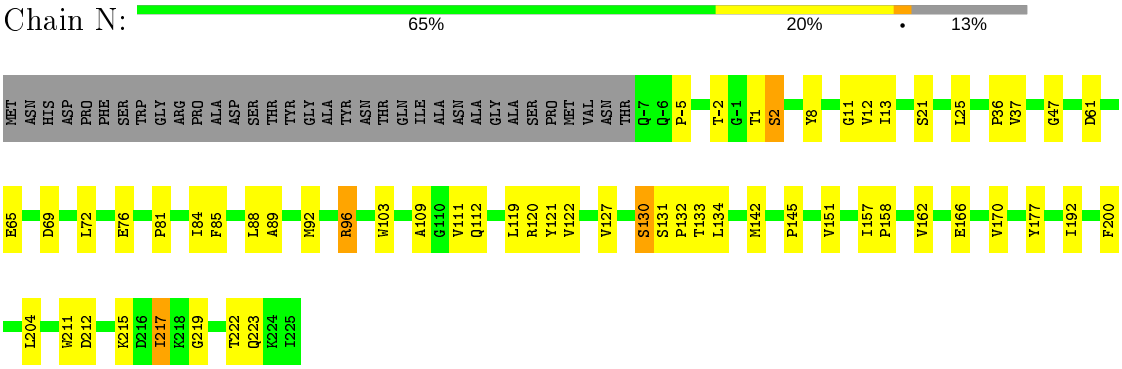
• Molecule 13: Proteasome subunit beta type-6

Chain 1:



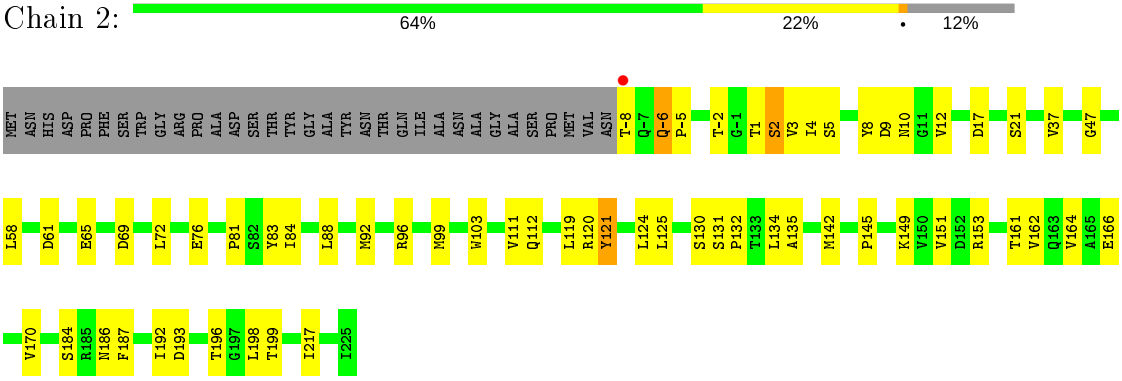
• Molecule 14: Proteasome subunit beta type-7

Chain N:



• Molecule 14: Proteasome subunit beta type-7

Chain 2:



• Molecule 15: TRP-ARG-SER-TYR-TYR-ALA

Chain 3:

- Molecule 15: TRP-ARG-SER-TYR-TYR-ALA

Chain 4:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.04Å 302.01Å 143.84Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	50.01 – 3.00 50.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.01-3.00) 100.0 (50.01-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.174 , 0.227 0.174 , 0.227	Depositor DCC
R_{free} test set	10362 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49177	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	0/1955	0.63	0/2652
1	O	0.47	0/1899	0.65	0/2581
2	B	0.46	0/1919	0.63	0/2605
2	P	0.47	0/1941	0.65	0/2631
3	C	0.44	0/1877	0.64	0/2550
3	Q	0.44	0/1873	0.65	0/2545
4	D	0.44	0/1850	0.61	0/2518
4	R	0.45	0/1866	0.63	0/2538
5	E	0.46	0/1826	0.63	0/2465
5	S	0.45	0/1824	0.63	1/2462 (0.0%)
6	F	0.44	0/1782	0.61	0/2412
6	T	0.45	0/1796	0.64	0/2431
7	G	0.52	0/1905	0.64	0/2581
7	U	0.46	0/1922	0.65	0/2599
8	H	0.47	0/1533	0.63	0/2078
8	V	0.47	0/1537	0.65	0/2082
9	I	0.53	2/1709 (0.1%)	0.67	2/2318 (0.1%)
9	W	0.51	2/1711 (0.1%)	0.68	2/2322 (0.1%)
10	J	0.46	0/1596	0.66	0/2159
10	X	0.46	0/1593	0.62	1/2156 (0.0%)
11	K	0.49	0/1577	0.66	0/2129
11	Y	0.48	0/1593	0.69	1/2148 (0.0%)
12	L	0.44	0/1671	0.61	0/2263
12	Z	0.45	0/1663	0.64	0/2255
13	1	0.46	0/1778	0.63	0/2403
13	M	0.48	1/1780 (0.1%)	0.62	0/2405
14	2	0.46	0/1855	0.65	0/2514
14	N	0.47	0/1848	0.71	0/2504
15	3	0.38	0/53	0.60	0/69
15	4	0.43	0/53	0.55	0/69
All	All	0.47	5/49785 (0.0%)	0.64	7/67444 (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
7	U	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	53	GLU	CB-CG	7.75	1.66	1.52
9	I	53	GLU	CG-CD	7.44	1.63	1.51
9	W	53	GLU	CG-CD	7.20	1.62	1.51
9	W	53	GLU	CB-CG	6.91	1.65	1.52
13	M	127	CYS	CB-SG	-6.15	1.71	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	69	ARG	NE-CZ-NH1	-6.25	117.17	120.30
9	W	53	GLU	OE1-CD-OE2	-5.84	116.29	123.30
9	I	170	GLY	N-CA-C	-5.65	98.98	113.10
5	S	121	LEU	CA-CB-CG	-5.47	102.71	115.30
9	W	170	GLY	N-CA-C	-5.41	99.58	113.10
9	I	53	GLU	OE1-CD-OE2	-5.22	117.03	123.30
10	X	59	ARG	NE-CZ-NH1	-5.17	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	U	180	ASP	Peptide

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	1910	0	1883	62	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1862	0	1804	64	0
2	B	1882	0	1863	59	0
2	P	1904	0	1897	64	1
3	C	1848	0	1796	69	0
3	Q	1844	0	1782	63	0
4	D	1821	0	1744	73	0
4	R	1837	0	1788	61	0
5	E	1801	0	1759	73	0
5	S	1800	0	1756	56	0
6	F	1756	0	1736	49	0
6	T	1769	0	1751	61	0
7	G	1865	0	1814	45	0
7	U	1882	0	1853	56	0
8	H	1504	0	1464	40	0
8	V	1508	0	1475	39	0
9	I	1678	0	1682	53	0
9	W	1680	0	1677	47	0
10	J	1566	0	1529	49	0
10	X	1563	0	1523	40	0
11	K	1549	0	1543	57	0
11	Y	1565	0	1571	55	0
12	L	1634	0	1573	46	0
12	Z	1626	0	1551	34	0
13	1	1740	0	1662	55	0
13	M	1742	0	1669	53	0
14	2	1824	0	1832	50	0
14	N	1817	0	1825	53	0
15	3	52	0	42	7	0
15	4	52	0	42	3	0
16	2	3	0	0	0	0
16	A	1	0	0	0	0
16	K	2	0	0	0	0
16	N	1	0	0	0	0
16	O	1	0	0	0	0
16	P	1	0	0	0	0
16	R	1	0	0	0	0
16	S	1	0	0	0	0
16	V	1	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
17	H	1	0	0	0	0
17	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	1	0	0	0	0
17	N	2	0	0	0	0
17	Q	1	0	0	0	0
18	1	4	6	6	0	0
18	2	4	6	6	0	0
18	C	4	6	6	2	0
18	F	4	6	6	1	0
18	G	4	6	6	1	0
18	I	4	6	6	0	0
18	L	4	6	6	0	0
18	M	4	6	6	0	0
18	O	8	12	12	2	0
18	U	4	6	6	1	0
18	W	12	18	18	0	0
18	Y	8	12	12	2	0
19	1	6	0	8	0	0
19	J	6	0	8	0	0
19	L	6	0	8	0	0
19	M	6	8	8	0	0
19	Q	6	0	8	1	0
19	V	6	0	8	2	0
19	Z	6	0	8	0	0
20	1	9	0	0	0	0
20	2	9	0	0	1	0
20	A	2	0	0	3	0
20	C	2	0	0	0	0
20	D	1	0	0	0	0
20	G	2	0	0	0	0
20	H	8	0	0	1	0
20	I	2	0	0	1	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	4	0	0	0	0
20	N	4	0	0	0	0
20	O	4	0	0	0	0
20	U	2	0	0	0	0
20	V	5	0	0	0	0
20	W	2	0	0	0	0
20	X	2	0	0	0	0
20	Z	6	0	0	0	0
All	All	49073	104	48038	1369	1

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 14.

All (1369) 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)
3:C:201:THR:HG22	3:C:203:SER:H	1.09	1.10
3:C:123:THR:HG22	4:D:127:ARG:HH21	1.16	1.07
8:H:20:THR:HG23	8:H:31:THR:HG21	1.29	1.07
1:O:101:ALA:HA	1:O:112:MET:HE2	1.30	1.07
1:A:129:THR:HG22	2:B:128:ARG:HH21	1.21	1.05
5:E:248:ALA:HA	5:E:249:ALA:HB3	1.40	1.03
2:B:122:THR:HG22	3:C:129:ARG:HH21	1.24	1.00
9:W:19:ARG:HB3	9:W:170:GLY:HA2	1.43	0.99
1:A:101:ALA:HA	1:A:112:MET:HE2	1.41	0.98
4:D:54:LEU:H	4:D:54:LEU:HD12	1.28	0.98
2:P:122:THR:HG22	3:Q:129:ARG:HH21	1.27	0.98
14:N:111:VAL:HG23	14:N:192:ILE:HG22	1.49	0.94
6:T:36:VAL:HG22	6:T:160:ALA:HB2	1.47	0.94
7:G:94:GLU:HG2	7:G:114:ARG:HB3	1.51	0.93
4:D:205:THR:HG22	4:D:206:GLY:H	1.33	0.93
4:R:207:ALA:HB2	4:R:233:VAL:HG21	1.51	0.91
5:E:222:ILE:HD11	5:E:228:PHE:HD2	1.33	0.91
3:Q:123:THR:HG22	4:R:127:ARG:HH21	1.36	0.91
2:P:222:LEU:HD13	2:P:232:GLY:HA2	1.52	0.89
9:W:128:GLY:O	9:W:131:SER:HB2	1.72	0.89
13:1:152:GLU:HB2	13:1:159:VAL:HG13	1.55	0.89
12:L:33:LYS:HA	12:L:45:MET:HE2	1.55	0.89
5:S:40:ILE:HD12	5:S:200:VAL:HG23	1.53	0.88
4:R:197:ARG:HG3	4:R:236:ILE:HD12	1.55	0.88
3:C:201:THR:HG22	3:C:203:SER:N	1.89	0.87
7:U:182:HIS:NE2	7:U:190:GLU:OE1	2.09	0.86
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.57	0.85
5:E:40:ILE:HD12	5:E:200:VAL:HG23	1.58	0.85
1:O:82:VAL:HG12	1:O:142:THR:HB	1.58	0.85
10:J:6:MET:HE3	10:J:158:ILE:HA	1.59	0.84
11:K:48:GLU:HB3	11:K:98:GLN:HB2	1.60	0.84
10:X:140:MET:HE3	10:X:144:LEU:HD11	1.61	0.83
11:Y:34:THR:HG21	11:Y:181:LYS:HZ2	1.43	0.82
2:B:38:LYS:NZ	3:C:58:GLU:OE1	2.12	0.81
5:S:79:SER:HB3	5:S:172:ILE:HD12	1.62	0.81
7:G:34:THR:HG21	7:G:50:GLU:O	1.81	0.81
3:Q:123:THR:CG2	4:R:127:ARG:HH21	1.93	0.81
9:W:19:ARG:CB	9:W:170:GLY:HA2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:179:PHE:HA	6:T:182:ILE:HG13	1.64	0.80
14:N:12:VAL:HG21	14:N:109:ALA:HB1	1.64	0.80
9:I:209:THR:CG2	13:1:150:GLN:HG3	2.11	0.80
13:1:9:GLU:HB2	13:1:165:TYR:CD2	2.16	0.80
6:F:179:PHE:HA	6:F:182:ILE:HG13	1.64	0.80
1:A:126:GLN:O	1:A:129:THR:HB	1.81	0.79
10:J:2:ILE:HG21	10:J:133:ALA:HB3	1.63	0.79
5:S:90:GLU:OE2	12:Z:69:ARG:NH1	2.15	0.79
13:1:91:LYS:HE2	13:1:94:PHE:O	1.81	0.79
10:X:6:MET:HE3	10:X:145:TYR:HD1	1.46	0.79
11:Y:173:MET:HA	11:Y:173:MET:HE2	1.65	0.79
9:I:128:GLY:O	9:I:131:SER:HB2	1.81	0.78
4:D:204:GLN:HA	4:D:205:THR:OG1	1.84	0.78
6:T:13:PHE:N	7:U:22:GLN:OE1	2.14	0.78
13:1:13:VAL:HG12	13:1:197:ILE:HG12	1.64	0.77
3:C:53:THR:HG21	3:C:210:ARG:HD3	1.64	0.77
7:U:205:ASP:O	7:U:206:ASN:HB2	1.84	0.77
6:F:36:VAL:HG22	6:F:160:ALA:HB2	1.66	0.77
12:L:145:LYS:O	12:L:148:LEU:HD13	1.85	0.77
7:G:182:HIS:CE1	7:G:190:GLU:OE2	2.38	0.77
1:A:129:THR:CG2	2:B:128:ARG:HH21	1.96	0.77
2:P:6:SER:HB2	4:R:4:TYR:HB2	1.65	0.77
3:C:228:LYS:NZ	3:C:234:GLU:OE2	2.16	0.77
2:P:38:LYS:NZ	3:Q:58:GLU:OE1	2.12	0.77
4:D:133:THR:HG1	4:D:150:THR:HG1	1.33	0.77
2:P:217:GLU:O	2:P:219:PRO:HD3	1.84	0.76
10:J:140:MET:HE3	10:J:144:LEU:HD11	1.68	0.76
5:E:175:GLY:HA3	5:E:207:VAL:HG21	1.67	0.76
9:I:19:ARG:CB	9:I:170:GLY:HA2	2.16	0.76
14:2:8:TYR:CE2	14:2:162:VAL:HG22	2.21	0.76
4:R:187:THR:HG22	4:R:189:GLU:H	1.50	0.76
9:I:19:ARG:HB3	9:I:170:GLY:HA2	1.68	0.76
1:O:167:LYS:N	2:P:57:MET:HE2	2.00	0.76
5:E:222:ILE:HD11	5:E:228:PHE:CD2	2.21	0.76
7:U:94:GLU:HG2	7:U:114:ARG:HB3	1.65	0.76
1:A:101:ALA:HA	1:A:112:MET:CE	2.16	0.75
12:L:13:ILE:HD12	12:L:154:LEU:HD23	1.67	0.75
3:C:49:GLU:OE2	3:C:201:THR:HG23	1.87	0.75
9:I:209:THR:HG21	13:1:150:GLN:HG3	1.68	0.75
8:H:36:ARG:HG3	8:H:42:TRP:CE2	2.22	0.75
6:F:176:LEU:CD1	6:F:180:ILE:HD11	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:187:THR:HG22	4:R:189:GLU:N	2.01	0.74
4:R:205:THR:HG22	4:R:206:GLY:H	1.51	0.74
11:Y:171:MET:CE	11:Y:173:MET:HB2	2.16	0.74
3:C:181:LYS:O	3:C:184:MET:HG3	1.88	0.74
1:O:83:VAL:HG11	1:O:90:ALA:CB	2.18	0.74
11:K:21:THR:CG2	11:K:26:VAL:HG22	2.17	0.74
13:M:8:GLY:HA3	13:M:11:PHE:CE1	2.22	0.74
7:U:174:GLU:HG3	7:U:201:LEU:HD23	1.70	0.74
13:M:9:GLU:HB2	13:M:165:TYR:CD2	2.23	0.73
3:C:126:GLY:HA3	18:C:302:EDO:H12	1.70	0.73
8:H:20:THR:CG2	8:H:31:THR:HG21	2.15	0.73
4:R:234:THR:O	4:R:235:GLN:HB3	1.86	0.73
3:C:125:HIS:HB3	4:D:126:VAL:HG12	1.70	0.73
9:I:104:ASP:HB2	9:I:105:PRO:HD2	1.71	0.73
10:J:58:PHE:CZ	10:J:82:VAL:HG22	2.24	0.73
1:A:178:ILE:HD13	1:A:210:MET:HE1	1.70	0.73
6:T:43:HIS:CD2	6:T:220:THR:HG21	2.24	0.72
1:O:101:ALA:HA	1:O:112:MET:CE	2.15	0.72
2:P:180:ASN:H	2:P:183:LEU:HD11	1.53	0.72
4:R:159:TRP:CE2	5:S:59:LEU:HD23	2.24	0.72
9:I:194:ASN:HD21	13:1:213:ASP:HB3	1.54	0.72
6:T:156:LEU:HD23	7:U:58:LEU:HD23	1.70	0.72
8:V:102:TYR:OH	8:V:180:ALA:HB2	1.89	0.72
11:K:138:TYR:CE2	11:K:171:MET:HG3	2.25	0.72
2:B:17:LYS:HE3	2:B:18:LEU:N	2.05	0.72
6:F:176:LEU:HD13	6:F:180:ILE:HD11	1.72	0.72
13:1:-6:PRO:HB3	14:2:99:MET:CE	2.20	0.72
4:R:167:ASN:HB2	4:R:202:VAL:HG11	1.72	0.72
6:F:128:TYR:O	6:F:149:PRO:HB3	1.90	0.71
14:2:120:ARG:HH11	14:2:130:SER:HB2	1.55	0.71
11:K:12:VAL:HG23	11:K:113:PRO:HB2	1.71	0.71
3:Q:184:MET:HG2	3:Q:188:ASP:HB2	1.73	0.71
13:1:152:GLU:HB2	13:1:159:VAL:CG1	2.21	0.71
10:X:140:MET:HE3	10:X:144:LEU:CD1	2.20	0.71
1:O:82:VAL:CG1	1:O:142:THR:HB	2.21	0.71
7:G:94:GLU:CG	7:G:114:ARG:HD2	2.21	0.70
8:H:48:SER:HB3	8:H:51:ASP:HB2	1.73	0.70
2:B:122:THR:CG2	3:C:129:ARG:HH21	2.03	0.70
12:L:200:VAL:O	12:L:204:GLU:HB2	1.91	0.70
14:N:8:TYR:CE1	14:N:162:VAL:HG22	2.25	0.70
1:A:83:VAL:HG11	1:A:90:ALA:CB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:36:ARG:HG3	8:V:42:TRP:CE2	2.26	0.70
3:C:120:GLN:O	3:C:123:THR:HB	1.92	0.70
3:C:91:ALA:HB2	3:C:115:LEU:HD22	1.71	0.70
14:N:85:PHE:CE2	14:N:120:ARG:HD3	2.27	0.70
1:O:101:ALA:CA	1:O:112:MET:HE2	2.17	0.70
1:A:83:VAL:HG11	1:A:90:ALA:HB2	1.72	0.70
2:B:49:LYS:HD3	2:B:210:GLU:OE1	1.91	0.70
8:V:13:ILE:HD12	8:V:151:THR:HG22	1.74	0.70
5:E:247:GLU:HA	5:E:248:ALA:HB2	1.72	0.69
8:H:13:ILE:HD12	8:H:151:THR:HG22	1.73	0.69
8:V:48:SER:HB3	8:V:51:ASP:HB2	1.73	0.69
4:R:225:SER:OG	4:R:228:GLU:HG3	1.92	0.69
13:1:-6:PRO:HB3	14:2:99:MET:HE1	1.75	0.69
13:1:152:GLU:O	13:1:155:THR:HG23	1.92	0.69
12:L:33:LYS:HA	12:L:45:MET:CE	2.22	0.69
3:Q:9:ARG:HD3	4:R:6:ARG:NH1	2.08	0.69
14:N:211:TRP:CH2	8:V:29:ARG:HD2	2.27	0.69
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.75	0.69
9:I:219:ASN:C	9:I:220:ILE:HD13	2.12	0.69
11:Y:138:TYR:CE2	11:Y:171:MET:HG3	2.28	0.69
11:Y:2:ILE:HD13	11:Y:167:LEU:HD13	1.74	0.69
15:3:9:TRP:O	15:3:10:ARG:HD3	1.93	0.69
2:B:17:LYS:HE3	2:B:18:LEU:H	1.58	0.68
1:O:196:GLU:HG2	1:O:201:LYS:HB3	1.75	0.68
14:2:166:GLU:O	14:2:170:VAL:HG23	1.93	0.68
8:V:189:TYR:HB3	8:V:190:PRO:HD2	1.76	0.68
2:P:111:VAL:HG22	2:P:136:ILE:HD12	1.76	0.68
11:Y:15:ALA:HB2	11:Y:160:LEU:HD21	1.74	0.68
8:H:48:SER:O	8:H:52:THR:HG23	1.94	0.68
6:F:88:LEU:HD11	6:F:108:ALA:HB1	1.76	0.68
8:H:36:ARG:HG3	8:H:42:TRP:CZ2	2.29	0.68
10:J:79:THR:HG23	10:J:115:PHE:CZ	2.29	0.68
6:T:29:ILE:HD11	6:T:149:PRO:HD3	1.76	0.68
3:Q:152:ASN:HB2	3:Q:153:PRO:CD	2.23	0.68
5:S:184:LEU:HD21	6:T:55:GLU:HB2	1.76	0.68
1:A:44:ALA:HB2	1:A:53:VAL:HG12	1.76	0.67
5:E:221:CYS:C	5:E:222:ILE:HD12	2.14	0.67
4:D:225:SER:OG	4:D:228:GLU:HG3	1.94	0.67
12:Z:99:THR:HG22	12:Z:115:VAL:O	1.94	0.67
12:Z:200:VAL:O	12:Z:204:GLU:HB2	1.94	0.67
12:L:33:LYS:HG2	12:L:45:MET:HE3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:155:THR:OG1	13:1:159:VAL:HG12	1.94	0.67
2:P:48:GLU:OE1	2:P:200:VAL:HG22	1.93	0.67
6:T:156:LEU:CD2	7:U:58:LEU:HD23	2.24	0.67
14:2:-5:PRO:HG3	14:2:103:TRP:CD1	2.29	0.67
2:P:172:LYS:O	2:P:176:GLU:HG3	1.95	0.67
13:M:173:LYS:HG2	9:W:200:GLN:HG2	1.75	0.67
2:B:119:GLN:O	2:B:122:THR:HB	1.94	0.67
1:O:196:GLU:HG2	1:O:201:LYS:CB	2.25	0.66
3:C:237:ASP:O	3:C:240:VAL:HG22	1.96	0.66
12:L:174:SER:HA	12:L:193:VAL:HG23	1.76	0.66
3:Q:125:HIS:HB3	4:R:126:VAL:HG12	1.77	0.66
11:K:32:ASP:OD1	11:K:34:THR:HG22	1.95	0.66
4:D:10:ILE:HD11	5:E:8:TYR:HB2	1.77	0.66
7:U:94:GLU:HG3	7:U:114:ARG:HH11	1.59	0.66
4:R:187:THR:HB	4:R:190:GLU:HG2	1.78	0.66
6:F:156:LEU:HD23	7:G:58:LEU:HD23	1.78	0.66
14:N:111:VAL:CG2	14:N:192:ILE:HG22	2.23	0.66
11:Y:38:SER:HB2	11:Y:39:PRO:HD2	1.78	0.66
5:E:8:TYR:HD1	5:E:9:ASP:H	1.44	0.66
11:K:148:ARG:O	11:K:151:MET:HG3	1.96	0.66
6:T:227:GLY:O	6:T:230:VAL:HG22	1.95	0.66
3:C:123:THR:CG2	4:D:127:ARG:HH21	2.02	0.65
6:F:146:GLU:OE2	6:F:148:GLN:NE2	2.29	0.65
11:K:38:SER:HB2	11:K:39:PRO:HD2	1.77	0.65
10:J:6:MET:HE3	10:J:158:ILE:CA	2.26	0.65
4:D:67:ILE:O	11:K:68:ILE:HD13	1.96	0.65
3:C:123:THR:HG22	4:D:127:ARG:NH2	2.01	0.65
6:F:11:VAL:HG12	6:F:11:VAL:O	1.96	0.65
7:G:166:LYS:HD3	7:G:206:ASN:OD1	1.96	0.65
14:N:1:THR:OG1	14:N:2:SER:N	2.29	0.65
14:N:222:THR:HG22	9:W:77:VAL:CG1	2.26	0.65
7:G:182:HIS:NE2	7:G:190:GLU:OE2	2.30	0.65
8:H:18:SER:O	8:H:31:THR:HG23	1.96	0.65
9:W:9:ASN:OD1	9:W:10:ASN:N	2.30	0.65
10:X:6:MET:CE	10:X:145:TYR:HD1	2.10	0.65
11:Y:102:LEU:HD21	11:Y:117:GLN:HG3	1.77	0.65
14:N:217:ILE:HD13	8:V:30:VAL:CG2	2.26	0.65
14:N:-5:PRO:HG3	14:N:103:TRP:CD1	2.32	0.65
12:Z:12:ILE:HB	12:Z:180:VAL:HB	1.78	0.65
4:D:242:GLU:N	4:D:242:GLU:OE1	2.30	0.65
11:K:49:ALA:O	11:K:51:ASP:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:94:HIS:HB2	3:Q:114:ARG:HH11	1.62	0.65
7:U:37:ILE:HG22	7:U:163:ALA:HB2	1.78	0.65
7:U:41:CYS:HB2	7:U:186:LEU:O	1.97	0.65
14:N:12:VAL:CG2	14:N:109:ALA:HB1	2.26	0.64
1:A:14:ARG:HD3	1:A:26:TYR:CD2	2.32	0.64
5:E:248:ALA:CA	5:E:249:ALA:HB3	2.24	0.64
9:W:8:PHE:HB3	9:W:151:ALA:HB2	1.80	0.64
12:L:185:TRP:C	12:L:186:ILE:HD13	2.17	0.64
4:R:31:THR:HB	4:R:47:GLU:HG3	1.77	0.64
11:K:21:THR:HG23	11:K:26:VAL:HG22	1.78	0.64
4:D:237:GLU:O	4:D:240:LYS:HB3	1.98	0.64
5:E:203:ILE:O	5:E:207:VAL:HG13	1.97	0.64
7:U:182:HIS:CE1	7:U:190:GLU:OE1	2.50	0.64
5:E:20:ARG:CZ	15:4:10:ARG:HD3	2.28	0.64
2:B:17:LYS:HE2	2:B:22:ASP:OD1	1.98	0.64
6:T:208:VAL:HG13	6:T:227:GLY:HA2	1.78	0.64
13:1:147:PHE:CG	13:1:161:LYS:HE2	2.33	0.64
5:E:241:LYS:HE2	5:E:245:GLU:OE2	1.99	0.64
11:K:0:MET:O	11:K:0:MET:HG3	1.97	0.64
8:V:8:PHE:CE2	8:V:10:ASP:HB2	2.33	0.64
11:Y:12:VAL:HG23	11:Y:113:PRO:HB2	1.78	0.64
7:G:243:GLN:O	7:G:246:ILE:HG22	1.98	0.63
7:G:41:CYS:HB2	7:G:186:LEU:O	1.97	0.63
6:T:33:SER:O	6:T:62:LYS:NZ	2.30	0.63
8:V:157:HIS:NE2	8:V:196:LEU:HD22	2.13	0.63
11:K:160:LEU:O	11:K:164:VAL:HG23	1.99	0.63
3:C:19:LEU:HD13	3:C:123:THR:HG23	1.79	0.63
1:O:83:VAL:HG11	1:O:90:ALA:HB2	1.80	0.63
1:A:13:ASP:OD2	1:A:20:SER:HA	1.99	0.63
1:O:237:SER:O	1:O:241:ILE:HG13	1.99	0.63
5:S:67:ILE:HD12	5:S:218:GLN:HG2	1.81	0.63
11:K:118:ILE:HG12	11:K:124:LYS:HG3	1.79	0.63
3:Q:152:ASN:HB2	3:Q:153:PRO:HD2	1.81	0.63
3:C:80:LEU:HD23	3:C:132:GLY:HA3	1.80	0.63
9:I:112:SER:HB3	9:I:125:LEU:HD13	1.80	0.63
13:M:17:ASP:O	13:M:33:LYS:HE3	1.99	0.63
1:O:87:ILE:HG22	1:O:88:PRO:HD3	1.80	0.63
4:R:13:PRO:HA	5:S:26:TYR:CD1	2.33	0.63
3:C:191:GLU:HG2	3:C:242:THR:CG2	2.28	0.63
2:P:186:GLU:OE2	2:P:246:ARG:NH1	2.32	0.63
10:X:6:MET:HE1	10:X:154:LEU:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:241:GLN:HA	4:D:242:GLU:HB2	1.81	0.63
14:N:37:VAL:HG11	14:N:84:ILE:HD13	1.80	0.63
3:Q:120:GLN:O	3:Q:123:THR:HB	1.99	0.63
7:U:206:ASN:HA	7:U:208:GLU:OE2	1.99	0.63
3:C:140:TYR:CE1	3:C:145:GLY:HA2	2.33	0.62
9:I:9:ASN:OD1	9:I:10:ASN:N	2.32	0.62
11:K:183:VAL:HG22	11:K:188:ILE:HG12	1.81	0.62
13:M:198:VAL:HG22	13:M:203:VAL:HG22	1.79	0.62
4:R:84:ILE:N	4:R:84:ILE:HD13	2.13	0.62
4:R:90:ARG:HG2	11:Y:68:ILE:HG21	1.82	0.62
8:V:55:ILE:HD11	8:V:93:LEU:HD13	1.81	0.62
12:L:196:LEU:O	12:L:200:VAL:HG23	1.99	0.62
5:S:123:PHE:CZ	5:S:137:PRO:HG3	2.34	0.62
1:A:240:ASN:HB3	20:A:402:HOH:O	1.99	0.62
2:B:17:LYS:HE2	2:B:22:ASP:OD2	1.99	0.62
5:E:248:ALA:HB1	5:E:250:GLU:N	2.15	0.62
13:M:173:LYS:HG2	9:W:200:GLN:CG	2.29	0.62
6:T:158:GLY:O	7:U:57:LEU:HD13	1.98	0.62
11:Y:118:ILE:HA	11:Y:123:THR:O	1.99	0.62
10:J:6:MET:CE	10:J:158:ILE:HA	2.29	0.62
9:W:104:ASP:HB2	9:W:105:PRO:HD2	1.81	0.62
9:W:206:PRO:O	9:W:209:THR:OG1	2.11	0.62
3:C:201:THR:HG21	3:C:203:SER:OG	1.99	0.62
12:L:145:LYS:HB2	12:L:148:LEU:CD1	2.30	0.62
4:D:171:VAL:O	4:D:175:LEU:HG	1.99	0.62
5:E:90:GLU:OE2	12:L:69:ARG:NH1	2.32	0.62
7:U:242:ALA:O	7:U:246:ILE:HG23	1.99	0.62
3:C:205:ALA:O	3:C:210:ARG:NH2	2.33	0.62
12:L:76:VAL:CG2	12:L:103:GLY:HA3	2.30	0.62
2:B:48:GLU:OE1	2:B:200:VAL:HG22	1.99	0.61
3:Q:244:ILE:O	3:Q:245:THR:HG23	2.00	0.61
11:Y:34:THR:HG21	11:Y:181:LYS:NZ	2.15	0.61
11:K:34:THR:HG21	11:K:181:LYS:NZ	2.15	0.61
3:Q:181:LYS:H	3:Q:184:MET:HE2	1.65	0.61
4:D:68:ASP:HA	11:K:68:ILE:CD1	2.31	0.61
14:N:217:ILE:HD13	8:V:30:VAL:HG21	1.82	0.61
2:B:17:LYS:HE2	2:B:22:ASP:CG	2.20	0.61
3:C:216:ILE:HG12	3:C:227:GLN:HG3	1.82	0.61
6:T:71:GLY:HA3	6:T:222:PHE:CE2	2.35	0.61
1:A:87:ILE:HG22	1:A:88:PRO:HD3	1.82	0.61
6:F:46:LEU:HG	6:F:135:ILE:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:55:ILE:HD11	8:H:93:LEU:HD13	1.82	0.61
3:Q:94:HIS:HB2	3:Q:114:ARG:NH1	2.16	0.61
8:V:163:ILE:CG2	8:V:170:GLY:HA2	2.30	0.61
2:P:222:LEU:HD13	2:P:232:GLY:CA	2.29	0.61
13:1:11:PHE:CE2	13:1:168:VAL:HA	2.35	0.61
14:2:119:LEU:HG	14:2:134:LEU:HD12	1.82	0.61
1:A:185:HIS:ND1	1:A:209:HIS:CE1	2.69	0.61
7:U:188:ALA:O	7:U:192:VAL:HG23	2.00	0.61
2:B:196:LEU:HD23	2:B:209:ILE:HD12	1.82	0.61
8:H:20:THR:HG23	8:H:31:THR:CG2	2.18	0.61
13:M:152:GLU:O	13:M:155:THR:HG23	2.00	0.61
7:U:94:GLU:CG	7:U:114:ARG:HD2	2.30	0.61
1:A:17:THR:HG21	1:A:129:THR:HA	1.83	0.61
4:R:32:CYS:H	4:R:47:GLU:HG2	1.65	0.61
1:A:129:THR:HG22	2:B:128:ARG:NH2	2.05	0.61
2:B:108:LYS:HD2	2:B:148:TYR:OH	2.00	0.61
2:B:64:VAL:O	2:B:237:LYS:NZ	2.33	0.61
4:D:87:GLU:OE2	11:K:69:ARG:NH1	2.34	0.61
10:J:181:ILE:HG12	10:J:186:VAL:HG22	1.83	0.60
7:G:19:ARG:NH2	7:G:24:GLU:OE1	2.29	0.60
8:V:14:LEU:O	8:V:175:MET:HA	2.01	0.60
12:L:145:LYS:HB2	12:L:148:LEU:HD11	1.83	0.60
13:1:8:GLY:HA3	13:1:11:PHE:CE1	2.37	0.60
3:C:152:ASN:HB2	3:C:153:PRO:CD	2.31	0.60
4:D:10:ILE:CD1	5:E:8:TYR:HB2	2.32	0.60
11:K:164:VAL:O	11:K:168:GLU:HG3	2.02	0.60
11:K:24:ILE:HG12	11:K:24:ILE:O	2.01	0.60
6:F:71:GLY:HA3	6:F:222:PHE:CE2	2.36	0.60
4:D:109:LEU:O	4:D:113:VAL:HG23	2.02	0.60
5:E:40:ILE:HD12	5:E:200:VAL:CG2	2.30	0.60
11:K:2:ILE:H	11:K:17:SER:HB3	1.65	0.60
4:D:54:LEU:H	4:D:54:LEU:CD1	2.00	0.60
2:P:50:LYS:HG3	2:P:50:LYS:O	2.02	0.60
3:Q:80:LEU:HD23	3:Q:132:GLY:HA3	1.84	0.60
6:T:132:LEU:HB2	6:T:147:PHE:HB3	1.84	0.60
10:X:140:MET:CE	10:X:144:LEU:HD11	2.30	0.60
6:F:50:LYS:HE2	6:F:212:SER:HB2	1.83	0.60
1:A:19:PHE:HE1	2:B:78:MET:CE	2.15	0.60
6:F:227:GLY:O	6:F:230:VAL:HG22	2.02	0.60
5:S:81:LEU:HD12	5:S:139:GLY:HA3	1.83	0.60
6:T:50:LYS:HE2	6:T:212:SER:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:42:VAL:HG12	13:1:196:LEU:HD23	1.82	0.59
2:B:59:GLU:OE1	2:B:59:GLU:N	2.22	0.59
4:D:159:TRP:CE2	5:E:59:LEU:HD23	2.37	0.59
11:K:18:LYS:HE2	11:K:29:ASP:O	2.02	0.59
13:M:132:ALA:HB1	13:M:186:HIS:CE1	2.37	0.59
1:A:167:LYS:NZ	1:A:192:ASP:HB3	2.17	0.59
4:D:148:TYR:CE2	4:D:158:SER:HB3	2.38	0.59
11:K:34:THR:HG21	11:K:181:LYS:HZ2	1.67	0.59
9:I:219:ASN:O	9:I:220:ILE:HD13	2.03	0.59
14:N:111:VAL:HG23	14:N:192:ILE:CG2	2.30	0.59
11:Y:3:ILE:HG22	11:Y:102:LEU:CD1	2.33	0.59
5:E:175:GLY:HA3	5:E:207:VAL:CG2	2.32	0.59
5:S:118:ASP:OD2	6:T:82:ARG:NH1	2.36	0.59
3:C:120:GLN:HG3	4:D:80:ALA:HB1	1.85	0.59
1:A:64:LEU:HD23	7:G:159:TYR:CE1	2.37	0.59
11:K:2:ILE:O	11:K:3:ILE:HD13	2.03	0.59
4:R:192:VAL:HG13	4:R:212:ILE:HG21	1.85	0.59
2:P:94:HIS:CD2	9:W:65:LEU:HD21	2.38	0.59
9:I:81:GLN:O	9:I:85:GLN:HG3	2.03	0.59
8:V:51:ASP:O	8:V:55:ILE:HG13	2.03	0.59
14:2:151:VAL:O	14:2:151:VAL:HG23	2.03	0.58
1:O:132:ALA:HB2	2:P:9:LEU:HD11	1.85	0.58
7:U:204:GLU:HA	7:U:204:GLU:OE1	2.03	0.58
1:A:21:PRO:HA	2:B:23:TYR:CD1	2.38	0.58
9:I:113:ILE:HG12	9:I:119:THR:HG22	1.84	0.58
6:T:30:LYS:O	6:T:163:ALA:HB2	2.03	0.58
9:W:13:VAL:HG22	9:W:177:VAL:HG13	1.84	0.58
3:Q:65:LYS:HB2	3:Q:212:GLU:OE1	2.02	0.58
4:R:159:TRP:CZ2	5:S:59:LEU:HD23	2.38	0.58
11:Y:2:ILE:O	11:Y:3:ILE:HD13	2.01	0.58
12:Z:145:LYS:O	12:Z:148:LEU:HD13	2.02	0.58
2:B:64:VAL:HB	2:B:237:LYS:NZ	2.18	0.58
6:F:137:TYR:CZ	6:F:218:LYS:HB2	2.39	0.58
9:I:213:LEU:HD12	10:J:191:LEU:O	2.02	0.58
11:Y:2:ILE:H	11:Y:17:SER:HB3	1.69	0.58
13:1:88:LEU:HD12	13:1:120:GLY:HA2	1.86	0.58
3:Q:160:TRP:CD2	3:Q:163:ILE:HD13	2.38	0.58
1:A:178:ILE:HD13	1:A:210:MET:CE	2.34	0.58
7:G:213:LEU:HD21	7:G:215:ILE:HD11	1.85	0.58
7:G:94:GLU:HG2	7:G:114:ARG:CB	2.30	0.58
11:K:9:GLN:HB2	11:K:150:ASP:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:-5:TYR:CE1	13:M:97:TYR:HB2	2.39	0.58
7:U:142:LYS:HG2	7:U:142:LYS:O	2.02	0.58
1:O:13:ASP:OD2	1:O:20:SER:HA	2.03	0.58
5:S:220:SER:CB	5:S:230:ILE:HA	2.34	0.58
5:S:39:GLY:HA2	5:S:47:VAL:O	2.03	0.58
8:V:36:ARG:HG3	8:V:42:TRP:CZ2	2.39	0.58
9:W:80:LEU:HD13	9:W:111:PHE:CB	2.33	0.58
10:X:133:ALA:HB2	10:X:169:ASP:HB2	1.85	0.57
11:Y:152:THR:OG1	11:Y:155:GLU:HG3	2.04	0.57
11:Y:-1:MET:HA	18:Y:201:EDO:C1	2.33	0.57
1:A:44:ALA:CB	1:A:53:VAL:HG12	2.34	0.57
8:H:3:ILE:HB	8:H:44:CYS:HB3	1.87	0.57
14:N:11:GLY:HA3	14:N:192:ILE:O	2.05	0.57
3:Q:70:ASN:OD1	3:Q:71:ASP:N	2.38	0.57
8:V:111:TYR:CE1	8:V:121:LYS:HB2	2.39	0.57
1:A:162[B]:TYR:CE1	2:B:80:PRO:HD3	2.40	0.57
5:E:179:ALA:HB2	5:E:207:VAL:HG11	1.87	0.57
8:H:13:ILE:HD12	8:H:151:THR:CG2	2.34	0.57
2:P:122:THR:CG2	3:Q:129:ARG:HH21	2.08	0.57
3:Q:59:GLN:OE1	3:Q:209:ASP:HA	2.03	0.57
11:Y:148:ARG:O	11:Y:151:MET:HG3	2.04	0.57
11:Y:32:ASP:OD1	11:Y:34:THR:HB	2.04	0.57
1:A:43:LEU:HD23	1:A:210:MET:CE	2.34	0.57
4:D:241:GLN:HA	4:D:242:GLU:CB	2.35	0.57
5:E:112:LEU:O	5:E:112:LEU:HG	2.03	0.57
14:2:120:ARG:NH1	14:2:130:SER:HB2	2.19	0.57
2:B:172:LYS:O	2:B:176:GLU:HG3	2.05	0.57
8:H:83:LYS:HG3	8:H:119:VAL:HG22	1.86	0.57
14:N:177:TYR:CE2	19:V:202:GOL:H12	2.40	0.57
1:O:211:ILE:HG23	1:O:216:THR:O	2.05	0.57
7:U:182:HIS:CD2	7:U:190:GLU:OE1	2.57	0.57
11:Y:34:THR:CG2	11:Y:181:LYS:HZ2	2.16	0.57
13:1:105:LEU:HD23	13:1:111:GLY:HA2	1.87	0.57
5:S:212:LEU:HD23	5:S:240:ILE:HD13	1.87	0.57
14:N:151:VAL:HG23	14:N:151:VAL:O	2.04	0.56
10:X:36:HIS:HB3	10:X:41:PHE:CD2	2.39	0.56
10:J:13:ALA:HB2	10:J:180:ILE:HD13	1.85	0.56
8:V:13:ILE:HD12	8:V:151:THR:CG2	2.35	0.56
3:C:59:GLN:OE1	3:C:209:ASP:HA	2.06	0.56
10:J:54:LEU:CD1	10:J:96:VAL:HG21	2.35	0.56
14:N:145:PRO:HA	9:W:165:ASN:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:173:MET:HA	11:Y:173:MET:CE	2.34	0.56
4:D:67:ILE:HG21	4:D:109:LEU:HD21	1.87	0.56
9:I:19:ARG:HB2	9:I:170:GLY:HA2	1.86	0.56
6:T:29:ILE:CD1	6:T:149:PRO:HD3	2.35	0.56
9:W:113:ILE:HG12	9:W:119:THR:HG22	1.87	0.56
7:G:94:GLU:HG3	7:G:114:ARG:HD2	1.86	0.56
3:Q:215:THR:HG23	3:Q:230:PHE:CE1	2.40	0.56
10:X:20:LEU:HD23	10:X:27:VAL:HB	1.86	0.56
8:H:113:ILE:HG23	8:H:118:SER:O	2.06	0.56
8:H:191:ASP:OD2	20:H:301:HOH:O	2.18	0.56
5:S:248:ALA:C	5:S:250:GLU:H	2.09	0.56
8:H:8:PHE:CE2	8:H:10:ASP:HB2	2.41	0.56
12:L:42:LEU:HD12	12:L:180:VAL:CG2	2.36	0.56
1:O:81:MET:SD	1:O:141:LEU:HD22	2.46	0.56
2:P:217:GLU:OE2	2:P:231:LYS:HD3	2.06	0.56
14:2:3:VAL:O	14:2:135:ALA:HA	2.06	0.56
3:C:216:ILE:CG1	3:C:227:GLN:HG3	2.36	0.56
4:D:73:LEU:HD12	4:D:135:ILE:HG12	1.88	0.56
1:O:21:PRO:HA	2:P:23:TYR:CD1	2.41	0.56
4:R:167:ASN:CB	4:R:202:VAL:HG11	2.36	0.56
3:C:186:VAL:O	3:C:190:ILE:HG13	2.05	0.56
11:K:15:ALA:HB2	11:K:160:LEU:HD21	1.88	0.55
14:N:37:VAL:HG11	14:N:84:ILE:CD1	2.36	0.55
14:N:61:ASP:O	14:N:65:GLU:HG3	2.06	0.55
5:S:40:ILE:CD1	5:S:200:VAL:HG23	2.31	0.55
12:Z:150:VAL:HG11	12:Z:179:HIS:CE1	2.41	0.55
1:A:125:SER:HB3	1:A:161:GLY:HA2	1.88	0.55
13:M:-6:PRO:O	14:N:96:ARG:NH1	2.34	0.55
7:U:175:LEU:O	7:U:179:VAL:HG23	2.06	0.55
8:V:14:LEU:N	8:V:14:LEU:HD12	2.21	0.55
3:C:191:GLU:HG2	3:C:242:THR:HG21	1.88	0.55
6:F:176:LEU:O	6:F:180:ILE:HG13	2.07	0.55
9:W:18:THR:HB	9:W:30:ASN:HA	1.88	0.55
3:C:65:LYS:HB2	3:C:212:GLU:OE1	2.07	0.55
14:N:120:ARG:NH1	14:N:130:SER:HB2	2.21	0.55
4:D:24:LEU:HD23	4:D:24:LEU:O	2.06	0.55
7:G:140:VAL:HG21	7:G:225:GLY:HA2	1.87	0.55
4:R:148:TYR:CE2	4:R:158:SER:HB3	2.41	0.55
9:W:213:LEU:HD12	10:X:191:LEU:O	2.06	0.55
1:A:199:TRP:O	1:A:203:VAL:HG23	2.07	0.55
2:B:44:VAL:HG23	2:B:211:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:84:LYS:HE2	9:I:119:THR:CG2	2.37	0.55
9:I:84:LYS:HG3	9:I:85:GLN:N	2.21	0.55
11:K:138:TYR:CZ	11:K:171:MET:HG3	2.41	0.55
9:W:84:LYS:HE2	9:W:119:THR:CG2	2.37	0.55
6:F:176:LEU:HD11	6:F:180:ILE:HD11	1.89	0.55
3:Q:217:ARG:HG2	3:Q:218:LYS:N	2.21	0.55
10:X:19:ARG:HD3	10:X:171:LEU:O	2.06	0.55
4:D:137:GLY:HA2	4:D:215:VAL:HG21	1.88	0.55
11:K:4:LEU:HD23	11:K:131:ALA:HB2	1.88	0.55
14:N:142:MET:O	14:N:145:PRO:HD2	2.07	0.55
14:N:204:LEU:HD23	14:N:204:LEU:N	2.21	0.55
3:C:152:ASN:HB2	3:C:153:PRO:HD2	1.88	0.54
4:R:97:ARG:HH11	4:R:103:PRO:HG3	1.70	0.54
12:Z:76:VAL:N	12:Z:108:GLU:OE1	2.39	0.54
1:A:164:VAL:HG22	1:A:165:GLY:N	2.21	0.54
4:D:84:ILE:N	4:D:84:ILE:HD13	2.22	0.54
5:S:45:GLY:HA2	5:S:153:TYR:CE1	2.43	0.54
10:X:12:VAL:CG1	10:X:110:PRO:HB3	2.36	0.54
5:E:79:SER:HB3	5:E:172:ILE:HD12	1.89	0.54
7:U:20:ASN:ND2	7:U:23:VAL:HG23	2.22	0.54
11:Y:102:LEU:CD2	11:Y:117:GLN:HG3	2.37	0.54
14:2:-6:GLN:HG3	14:2:-6:GLN:O	2.06	0.54
9:I:52:THR:O	9:I:56:THR:HG23	2.07	0.54
2:P:89:SER:O	2:P:92:VAL:HG12	2.06	0.54
13:1:42:VAL:CG1	13:1:196:LEU:HD23	2.38	0.54
4:R:197:ARG:CG	4:R:236:ILE:HD12	2.34	0.54
6:T:62:LYS:HD3	15:3:14:ALA:O	2.07	0.54
4:D:42:VAL:HB	4:D:215:VAL:CG1	2.38	0.54
5:E:167:TYR:CZ	5:E:170:LYS:HD3	2.42	0.54
10:X:6:MET:HE3	10:X:145:TYR:CD1	2.36	0.54
2:B:89:SER:O	2:B:92:VAL:HG12	2.08	0.54
4:D:205:THR:HG22	4:D:206:GLY:N	2.14	0.54
10:X:28:SER:HB2	11:Y:125:VAL:HG21	1.89	0.54
14:2:217:ILE:HG22	14:2:217:ILE:O	2.06	0.54
1:A:207:ILE:O	1:A:211:ILE:HG13	2.07	0.54
5:S:68:VAL:HG21	5:S:89:ILE:HD12	1.90	0.54
9:W:84:LYS:HG3	9:W:85:GLN:N	2.22	0.54
3:C:52:VAL:HG12	3:C:64:GLU:OE1	2.08	0.54
9:I:200:GLN:CG	13:1:173:LYS:HG2	2.38	0.54
7:U:37:ILE:HG22	7:U:163:ALA:CB	2.37	0.54
13:1:161:LYS:HG2	13:1:162:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:VAL:HG22	4:D:106:VAL:HG22	1.89	0.53
9:I:173:VAL:HB	9:I:191:LEU:HB3	1.90	0.53
9:I:196:ARG:HH12	10:J:142:GLU:HG3	1.73	0.53
5:S:193:LEU:O	5:S:197:GLU:HG3	2.07	0.53
7:U:194:GLN:O	7:U:198:ILE:HG13	2.07	0.53
8:V:83:LYS:HB2	8:V:119:VAL:HG22	1.90	0.53
2:P:180:ASN:H	2:P:183:LEU:CD1	2.19	0.53
11:Y:183:VAL:HG22	11:Y:188:ILE:HG12	1.89	0.53
2:B:160:LYS:HD3	2:B:179:TRP:CZ3	2.44	0.53
11:K:105:GLY:HA2	11:K:183:VAL:HG11	1.91	0.53
11:K:182:ILE:HD12	11:K:189:ARG:NH2	2.23	0.53
3:C:65:LYS:O	3:C:76:ALA:HA	2.07	0.53
4:D:192:VAL:HG13	4:D:212:ILE:HG21	1.90	0.53
6:T:72:LEU:HD12	6:T:72:LEU:O	2.08	0.53
11:Y:3:ILE:HG22	11:Y:102:LEU:HD12	1.89	0.53
13:1:-6:PRO:HB3	14:2:99:MET:HE3	1.91	0.53
3:C:70:ASN:OD1	3:C:71:ASP:N	2.42	0.53
7:U:67:GLN:HG2	14:2:69:ASP:OD1	2.08	0.53
3:C:136:ILE:HD11	3:C:165:VAL:HG22	1.90	0.53
4:D:159:TRP:CZ2	5:E:59:LEU:HD23	2.42	0.53
9:I:129:SER:OG	9:I:166:ASP:OD2	2.18	0.53
3:Q:192:LEU:O	3:Q:192:LEU:HD12	2.09	0.53
9:W:123:TYR:HB3	9:W:142:TRP:CZ2	2.43	0.53
14:2:161:THR:OG1	14:2:164:VAL:HG23	2.09	0.53
10:J:74:GLU:OE2	10:J:105:SER:OG	2.23	0.53
7:U:36:SER:HB3	7:U:49:VAL:HG23	1.90	0.53
5:E:105:GLU:OE2	13:M:66:TYR:OH	2.25	0.53
8:H:14:LEU:O	8:H:175:MET:HA	2.08	0.53
1:A:194:ILE:HD11	1:A:205:PHE:CE1	2.44	0.53
5:E:118:ASP:OD2	6:F:82:ARG:NH1	2.42	0.53
6:T:63:ILE:HG21	6:T:214:ALA:HB2	1.91	0.53
9:W:143:LYS:HG3	9:W:146:LEU:HD23	1.91	0.53
10:X:33:LYS:O	10:X:43:GLY:HA2	2.08	0.53
2:P:180:ASN:O	2:P:183:LEU:HD13	2.09	0.53
11:Y:52:THR:CG2	11:Y:53:VAL:N	2.72	0.53
5:E:123:PHE:CZ	5:E:137:PRO:HG3	2.45	0.52
3:C:194:LEU:HD21	3:C:213:PHE:CE2	2.45	0.52
14:N:89:ALA:HA	14:N:122:VAL:HG21	1.92	0.52
1:O:167:LYS:NZ	2:P:54:PRO:O	2.41	0.52
2:P:180:ASN:OD1	2:P:183:LEU:HD12	2.09	0.52
3:Q:68:LYS:HG3	3:Q:227:GLN:OE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:216:LYS:HE3	4:D:220:ASP:OD2	2.10	0.52
5:E:74:ILE:HD13	5:E:112:LEU:HD22	1.92	0.52
12:L:12:ILE:HB	12:L:180:VAL:HB	1.91	0.52
2:P:64:VAL:O	2:P:237:LYS:NZ	2.42	0.52
4:R:203:VAL:HG12	4:R:204:GLN:O	2.09	0.52
5:S:38:ILE:HD12	5:S:204:LEU:HG	1.90	0.52
6:T:162:GLY:O	6:T:165:SER:HB3	2.08	0.52
3:C:112:VAL:HG22	3:C:137:TYR:CG	2.44	0.52
7:G:118:TYR:O	7:G:121:ALA:HB3	2.10	0.52
7:G:35:THR:HB	7:G:167:GLY:H	1.73	0.52
9:I:196:ARG:NH1	10:J:142:GLU:HG3	2.24	0.52
11:K:118:ILE:HA	11:K:123:THR:O	2.09	0.52
14:N:-5:PRO:HG3	14:N:103:TRP:CG	2.45	0.52
1:O:79:ILE:HD13	1:O:114:CYS:HA	1.90	0.52
1:O:166:TYR:C	2:P:57:MET:HE2	2.30	0.52
3:Q:135:PHE:O	3:Q:150:THR:HA	2.09	0.52
8:V:15:GLY:HA2	8:V:174:ARG:O	2.08	0.52
12:Z:113:TYR:CE1	12:Z:123:LYS:HB2	2.45	0.52
13:1:9:GLU:HB2	13:1:165:TYR:CE2	2.45	0.52
5:E:67:ILE:HD12	5:E:218:GLN:HG2	1.91	0.52
14:N:133:THR:O	14:N:134:LEU:HD23	2.09	0.52
3:Q:163:ILE:HG13	3:Q:164:SER:H	1.74	0.52
7:U:108:ILE:HG21	7:U:146:HIS:HB2	1.92	0.52
9:W:188:ARG:HG3	9:W:189:ASN:N	2.24	0.52
12:L:50:ALA:CB	13:M:119:VAL:HG23	2.39	0.52
14:N:72:LEU:HD13	14:N:76:GLU:HB2	1.90	0.52
2:P:119:GLN:O	2:P:122:THR:HB	2.09	0.52
11:Y:192:ASP:N	11:Y:192:ASP:OD1	2.42	0.52
2:B:41:ASN:ND2	2:B:184:GLU:OE2	2.34	0.52
5:E:191:LEU:HD22	5:E:195:GLU:CB	2.39	0.52
4:D:176:GLU:OE2	5:E:57:PRO:HD2	2.09	0.52
11:K:152:THR:OG1	11:K:155:GLU:HG3	2.09	0.52
13:M:77:ILE:HG23	13:M:78:ASN:N	2.25	0.52
6:F:176:LEU:HA	6:F:179:PHE:CE2	2.45	0.52
10:J:3:VAL:HG22	10:J:16:CYS:HB3	1.92	0.52
5:S:31:ILE:HD11	5:S:140:VAL:N	2.24	0.52
5:S:147:HIS:CD2	5:S:224:LYS:HG3	2.45	0.52
8:H:37:VAL:CG2	8:H:41:ILE:HG22	2.40	0.52
9:W:81:GLN:O	9:W:85:GLN:HG3	2.10	0.52
2:B:17:LYS:CE	2:B:18:LEU:H	2.22	0.52
13:M:91:LYS:HE3	13:M:94:PHE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:81:PRO:HD2	14:2:112:GLN:OE1	2.10	0.51
14:2:37:VAL:HG11	14:2:84:ILE:CD1	2.40	0.51
10:X:3:VAL:HG22	10:X:16:CYS:HB3	1.92	0.51
11:Y:11:SER:HB3	11:Y:184:ASP:HB3	1.92	0.51
13:1:209:GLU:O	13:1:210:LEU:HD23	2.10	0.51
4:D:68:ASP:HB3	4:D:70:HIS:CE1	2.46	0.51
8:H:163:ILE:CG2	8:H:170:GLY:HA2	2.40	0.51
10:J:6:MET:HG3	10:J:154:LEU:HD11	1.91	0.51
13:M:42:VAL:HG12	13:M:196:LEU:HD23	1.91	0.51
3:Q:163:ILE:HG13	3:Q:164:SER:N	2.25	0.51
1:A:53:VAL:CG1	1:A:144:VAL:HG11	2.41	0.51
3:C:191:GLU:HG2	3:C:242:THR:HG22	1.93	0.51
1:O:44:ALA:O	1:O:168:ALA:HB1	2.09	0.51
8:H:161:GLN:OE1	8:V:136:GLY:HA2	2.10	0.51
6:T:46:LEU:HG	6:T:135:ILE:HD13	1.91	0.51
11:Y:15:ALA:CB	11:Y:160:LEU:HD21	2.41	0.51
11:Y:164:VAL:O	11:Y:168:GLU:HG3	2.10	0.51
1:A:167:LYS:HZ1	1:A:192:ASP:HB3	1.74	0.51
7:G:241:PHE:CZ	7:G:245:GLU:HG3	2.45	0.51
3:Q:184:MET:HG2	3:Q:188:ASP:CB	2.40	0.51
3:Q:58:GLU:O	3:Q:62:SER:HB2	2.11	0.51
1:A:156:LYS:O	1:A:163:TYR:HA	2.11	0.51
2:B:171:ALA:HB1	2:B:195:THR:CG2	2.40	0.51
4:D:13:PRO:HA	5:E:26:TYR:CD1	2.46	0.51
11:K:3:ILE:HG22	11:K:102:LEU:CD1	2.40	0.51
13:M:187:ILE:O	9:W:167:LEU:HD22	2.10	0.51
13:M:4:LEU:HD12	13:M:5:GLY:N	2.25	0.51
3:Q:166:GLY:O	3:Q:169:THR:HG23	2.10	0.51
3:Q:42:ASP:CG	3:Q:186:VAL:HG23	2.31	0.51
11:K:20:VAL:HG11	12:L:122:LEU:HD11	1.92	0.51
14:N:217:ILE:HG22	14:N:217:ILE:O	2.11	0.51
1:O:156:LYS:O	1:O:163:TYR:HA	2.09	0.51
4:R:87:GLU:OE1	11:Y:69:ARG:NH1	2.43	0.51
10:X:12:VAL:HG13	10:X:110:PRO:HB3	1.93	0.51
13:1:1:GLY:HA3	13:1:33:LYS:HZ2	1.76	0.51
2:B:2:THR:HG22	2:B:3:ASP:N	2.26	0.51
13:M:152:GLU:HB3	13:M:155:THR:HG21	1.92	0.51
2:P:148:TYR:CE1	2:P:158:PRO:HB3	2.45	0.51
6:T:72:LEU:HD12	6:T:72:LEU:C	2.31	0.51
9:W:80:LEU:HD13	9:W:111:PHE:CG	2.46	0.51
4:D:205:THR:CG2	4:D:206:GLY:H	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:42:VAL:HG22	4:D:145:PRO:HB2	1.92	0.51
4:R:109:LEU:O	4:R:113:VAL:HG23	2.11	0.51
5:S:107:ILE:HD13	5:S:112:LEU:HB2	1.92	0.51
9:W:62:ASN:HB3	9:W:82:MET:HE1	1.93	0.51
10:X:163:LEU:HD23	10:X:193:MET:HE1	1.92	0.51
5:E:45:GLY:HA2	5:E:153:TYR:CE1	2.45	0.51
9:I:84:LYS:HE2	9:I:119:THR:HG23	1.93	0.51
1:O:41:ASN:HB2	1:O:56:GLN:OE1	2.10	0.51
6:T:36:VAL:HG22	6:T:160:ALA:CB	2.31	0.51
3:C:163:ILE:HG13	3:C:164:SER:N	2.25	0.50
5:E:50:VAL:HG22	5:E:67:ILE:HD11	1.92	0.50
10:X:50:ASP:OD2	11:Y:92:ARG:NH2	2.44	0.50
12:Z:27:ALA:O	13:1:128:ARG:NH1	2.35	0.50
3:C:240:VAL:HG12	3:C:245:THR:HB	1.93	0.50
5:E:191:LEU:HD22	5:E:195:GLU:HB3	1.93	0.50
9:I:143:LYS:HG3	9:I:146:LEU:HD23	1.93	0.50
2:B:227:ILE:HG13	9:I:186:TYR:HD2	1.76	0.50
4:D:157:SER:OG	5:E:59:LEU:HD21	2.11	0.50
5:E:222:ILE:CD1	5:E:228:PHE:HD2	2.13	0.50
11:K:102:LEU:HD21	11:K:117:GLN:HG3	1.93	0.50
1:O:208:THR:HG22	1:O:209:HIS:N	2.26	0.50
3:Q:120:GLN:HG3	4:R:80:ALA:HB1	1.94	0.50
13:M:168:VAL:O	13:M:172:ILE:HG13	2.12	0.50
2:P:239:THR:OG1	2:P:242:GLU:HG3	2.11	0.50
3:Q:216:ILE:HG12	3:Q:227:GLN:HG3	1.92	0.50
2:B:242:GLU:O	2:B:246:ARG:HG3	2.12	0.50
5:E:107:ILE:HD13	5:E:112:LEU:HB2	1.93	0.50
9:I:8:PHE:HB3	9:I:151:ALA:HB2	1.93	0.50
12:L:4:LEU:C	12:L:4:LEU:HD12	2.31	0.50
3:Q:80:LEU:HD22	3:Q:80:LEU:N	2.27	0.50
4:R:176:GLU:OE2	5:S:57:PRO:HD2	2.12	0.50
9:W:137:VAL:HG21	9:W:161:ALA:HB2	1.94	0.50
10:X:6:MET:CE	10:X:145:TYR:CD1	2.92	0.50
1:A:17:THR:OG1	20:A:401:HOH:O	2.04	0.50
4:D:54:LEU:HD12	4:D:54:LEU:N	2.11	0.50
7:G:102:TYR:O	7:G:104:THR:HG22	2.12	0.50
4:R:87:GLU:CD	11:Y:69:ARG:HH12	2.15	0.50
8:V:111:TYR:CD1	8:V:121:LYS:HB2	2.47	0.50
14:2:5:SER:OG	14:2:119:LEU:HD11	2.11	0.50
1:A:82:VAL:HG12	1:A:142:THR:HB	1.93	0.50
4:R:88:LYS:HD2	4:R:116:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:72:LEU:HA	6:T:133:LEU:O	2.11	0.50
6:T:39:ARG:NH1	6:T:40:SER:O	2.44	0.50
10:X:162:LEU:C	10:X:162:LEU:HD23	2.32	0.50
4:D:54:LEU:CD1	4:D:54:LEU:N	2.74	0.50
6:F:148:GLN:HA	6:F:148:GLN:OE1	2.11	0.50
12:L:174:SER:CA	12:L:193:VAL:HG23	2.41	0.50
1:O:225:VAL:HG11	1:O:236:LEU:HD12	1.94	0.50
6:T:26:LEU:CD2	6:T:149:PRO:HD2	2.42	0.50
4:D:241:GLN:HA	4:D:242:GLU:O	2.12	0.49
5:E:248:ALA:HA	5:E:249:ALA:CB	2.25	0.49
8:H:15:GLY:HA2	8:H:174:ARG:O	2.12	0.49
10:J:13:ALA:CB	10:J:180:ILE:HD13	2.42	0.49
1:O:225:VAL:HB	1:O:236:LEU:HD12	1.94	0.49
2:P:74:VAL:HG22	2:P:75:TYR:H	1.77	0.49
4:R:205:THR:HG22	4:R:206:GLY:N	2.25	0.49
5:S:159:GLU:HB3	5:S:160:PRO:HD2	1.93	0.49
5:S:41:ALA:HA	5:S:46:VAL:HG22	1.94	0.49
6:F:132:LEU:HB2	6:F:147:PHE:HB3	1.94	0.49
10:J:44:ILE:HG22	10:J:51:VAL:HG22	1.93	0.49
8:V:8:PHE:HE2	8:V:10:ASP:HB2	1.76	0.49
10:X:115:PHE:CD1	10:X:115:PHE:N	2.80	0.49
12:Z:195:GLU:OE2	13:1:160:LYS:HD2	2.13	0.49
13:1:13:VAL:CG1	13:1:197:ILE:HG12	2.38	0.49
3:C:120:GLN:CG	4:D:80:ALA:HB1	2.41	0.49
4:D:52:LEU:O	4:D:53:LYS:CB	2.59	0.49
11:K:166:GLU:HA	11:K:166:GLU:OE1	2.12	0.49
10:X:163:LEU:HD23	10:X:193:MET:CE	2.42	0.49
11:Y:52:THR:HG23	11:Y:53:VAL:N	2.27	0.49
1:A:158:ASP:HB2	1:A:159:PRO:CD	2.42	0.49
5:E:53:ARG:O	5:E:53:ARG:HG2	2.12	0.49
8:H:102:TYR:OH	8:H:180:ALA:HB2	2.12	0.49
1:O:79:ILE:CD1	1:O:114:CYS:HA	2.42	0.49
2:P:32:VAL:HG21	2:P:50:LYS:HG2	1.94	0.49
6:T:54:ASP:HB3	6:T:56:LEU:H	1.76	0.49
6:T:60:GLN:HG2	15:3:14:ALA:HB2	1.93	0.49
8:V:22:THR:HG23	8:V:27:ALA:HB2	1.94	0.49
9:W:112:SER:HB3	9:W:125:LEU:HD13	1.93	0.49
13:M:9:GLU:HG3	13:M:165:TYR:CE2	2.46	0.49
1:A:128:TYR:N	1:A:128:TYR:CD1	2.80	0.49
1:A:82:VAL:CG1	1:A:142:THR:HB	2.43	0.49
7:G:94:GLU:HG3	7:G:114:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:228:LYS:NZ	3:Q:234:GLU:OE2	2.37	0.49
6:T:63:ILE:HG22	6:T:224:ILE:HD11	1.93	0.49
5:E:20:ARG:HG2	15:4:13:TYR:OH	2.12	0.49
10:J:33:LYS:O	10:J:43:GLY:HA2	2.12	0.49
4:R:162:GLN:OE1	4:R:163:THR:N	2.41	0.49
10:X:36:HIS:HB3	10:X:41:PHE:CE2	2.48	0.49
11:Y:118:ILE:HG12	11:Y:124:LYS:HG3	1.94	0.49
1:A:237:SER:O	1:A:241:ILE:HG13	2.12	0.49
3:C:52:VAL:HG13	3:C:52:VAL:O	2.13	0.49
1:O:164:VAL:HG22	1:O:165:GLY:H	1.78	0.49
2:P:147:LEU:HD23	2:P:159:TRP:HB2	1.95	0.49
3:Q:57:LEU:HG	3:Q:58:GLU:N	2.26	0.49
7:U:182:HIS:N	7:U:183:PRO:HD3	2.28	0.49
1:A:183:GLU:CD	2:B:54:PRO:HG2	2.33	0.49
10:J:6:MET:HE3	10:J:158:ILE:CB	2.43	0.49
14:N:81:PRO:HD2	14:N:112:GLN:OE1	2.13	0.49
7:G:149:MET:O	7:G:156:TYR:HA	2.12	0.49
10:J:184:ASP:N	10:J:184:ASP:OD1	2.40	0.49
6:T:119:ASN:HB3	6:T:126:ARG:O	2.13	0.49
12:L:186:ILE:HD13	12:L:186:ILE:N	2.28	0.48
14:N:142:MET:C	14:N:145:PRO:HD2	2.33	0.48
1:O:241:ILE:O	1:O:244:ARG:HB2	2.13	0.48
12:Z:114:TYR:O	12:Z:121:ARG:HA	2.13	0.48
13:1:159:VAL:HG13	13:1:159:VAL:O	2.12	0.48
14:2:88:LEU:O	14:2:92:MET:HG2	2.13	0.48
11:K:2:ILE:HD13	11:K:167:LEU:HD13	1.95	0.48
14:N:119:LEU:HG	14:N:134:LEU:HD12	1.95	0.48
4:R:31:THR:O	4:R:76:SER:OG	2.20	0.48
6:T:7:ASP:OD2	6:T:24:TYR:OH	2.15	0.48
8:V:8:PHE:HB2	8:V:146:MET:O	2.14	0.48
10:X:2:ILE:HD11	10:X:166:ALA:HB2	1.95	0.48
11:Y:48:GLU:HG3	11:Y:49:ALA:N	2.27	0.48
3:C:77:VAL:HG22	3:C:135:PHE:CE1	2.48	0.48
3:C:25:ALA:O	3:C:29:ILE:HG13	2.13	0.48
3:C:35:ALA:CB	3:C:48:ALA:HB2	2.43	0.48
4:D:99:THR:OG1	4:D:100:LEU:HD22	2.13	0.48
5:E:75:GLY:HA3	5:E:228:PHE:CD2	2.48	0.48
2:P:108:LYS:NZ	2:P:143:ASN:OD1	2.47	0.48
3:Q:180:TYR:CD1	3:Q:184:MET:HE1	2.48	0.48
3:Q:215:THR:HG23	3:Q:230:PHE:HE1	1.79	0.48
1:A:141:LEU:O	1:A:156:LYS:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:ARG:NH1	6:F:40:SER:O	2.46	0.48
9:I:217:ILE:N	9:I:217:ILE:HD12	2.29	0.48
5:S:182:GLU:HG2	5:S:203:ILE:CD1	2.44	0.48
12:Z:174:SER:HA	12:Z:193:VAL:HG23	1.95	0.48
6:F:11:VAL:CG1	6:F:11:VAL:O	2.60	0.48
9:I:163:ILE:HG23	9:I:170:GLY:O	2.14	0.48
5:S:184:LEU:HD21	6:T:55:GLU:CB	2.44	0.48
14:2:8:TYR:HD2	14:2:9:ASP:OD1	1.97	0.48
7:G:194:GLN:O	7:G:198:ILE:HG13	2.12	0.48
13:M:136:LEU:N	13:M:136:LEU:HD12	2.28	0.48
13:M:152:GLU:CB	13:M:155:THR:HG21	2.43	0.48
2:P:66:LEU:HD23	2:P:66:LEU:C	2.34	0.48
6:T:201:LEU:HB3	6:T:204:GLU:HG3	1.95	0.48
6:T:62:LYS:CD	15:3:14:ALA:O	2.61	0.48
3:C:126:GLY:HA3	18:C:302:EDO:C1	2.42	0.48
9:I:78:SER:O	9:I:82:MET:HG3	2.13	0.48
10:J:140:MET:CE	10:J:144:LEU:HD11	2.38	0.48
11:K:152:THR:HG23	11:K:155:GLU:OE1	2.14	0.48
1:O:225:VAL:CG1	1:O:236:LEU:HD12	2.43	0.48
11:Y:-1:MET:HA	18:Y:201:EDO:H11	1.95	0.48
12:Z:81:LYS:HD2	12:Z:121:ARG:NH1	2.28	0.48
2:B:210:GLU:HG2	2:B:237:LYS:HE3	1.95	0.48
11:K:2:ILE:O	11:K:16:SER:HA	2.14	0.48
2:P:8:SER:OG	3:Q:128:LEU:HA	2.14	0.48
8:V:157:HIS:O	8:V:160:SER:OG	2.28	0.48
8:H:140:LYS:HD3	8:V:161:GLN:HE21	1.78	0.48
10:X:42:LEU:HD12	10:X:99:VAL:O	2.14	0.48
5:E:70:ILE:HB	5:E:74:ILE:HG22	1.95	0.48
9:I:3:ILE:HD11	9:I:127:LEU:HB2	1.96	0.48
10:J:163:LEU:HD23	10:J:193:MET:CE	2.44	0.48
13:M:13:VAL:HG12	13:M:197:ILE:HG23	1.96	0.48
3:Q:97:ASN:OD1	10:X:60:TYR:HE2	1.97	0.48
1:A:32:PHE:CZ	1:A:158:ASP:HB2	2.49	0.48
4:R:171:VAL:HG23	4:R:202:VAL:HG21	1.95	0.48
12:Z:42:LEU:HD12	12:Z:180:VAL:CG2	2.44	0.48
1:A:129:THR:CG2	2:B:128:ARG:NH2	2.73	0.47
1:A:43:LEU:HD21	1:A:210:MET:HB2	1.94	0.47
1:A:69:VAL:HG22	7:G:157:TRP:CE3	2.49	0.47
12:L:13:ILE:HD12	12:L:154:LEU:CD2	2.40	0.47
14:N:119:LEU:O	14:N:130:SER:OG	2.29	0.47
1:O:164:VAL:HG22	1:O:165:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:212:LEU:CD2	5:E:240:ILE:HD13	2.44	0.47
7:G:179:VAL:O	7:G:179:VAL:HG12	2.14	0.47
6:T:43:HIS:NE2	6:T:220:THR:HG21	2.28	0.47
13:1:21:ILE:C	13:1:21:ILE:HD12	2.35	0.47
7:G:188:ALA:O	7:G:192:VAL:HG23	2.14	0.47
12:L:158:LYS:HD3	12:L:196:LEU:HD11	1.96	0.47
1:O:210:MET:CG	1:O:218:PHE:HE2	2.28	0.47
13:1:17:ASP:O	13:1:33:LYS:HE3	2.15	0.47
8:H:156:LYS:HG2	8:H:196:LEU:HD11	1.96	0.47
10:J:117:LEU:HG	10:J:118:ILE:HG23	1.96	0.47
11:K:2:ILE:HD12	11:K:175:PHE:CD1	2.49	0.47
13:M:14:LEU:HD23	13:M:34:VAL:HG13	1.96	0.47
13:M:9:GLU:HB2	13:M:165:TYR:HD2	1.75	0.47
14:N:-2:THR:HA	14:N:47:GLY:O	2.15	0.47
2:P:4:ARG:NH1	6:T:123:TYR:HE2	2.13	0.47
5:S:79:SER:HB3	5:S:172:ILE:CD1	2.40	0.47
5:S:18:GLU:O	6:T:31:GLN:NE2	2.47	0.47
8:V:146:MET:HE3	8:V:150:GLU:HB3	1.96	0.47
9:W:124:TYR:HB2	9:W:138:LEU:HD13	1.96	0.47
9:I:200:GLN:HG3	13:1:173:LYS:HG2	1.97	0.47
4:D:157:SER:CB	5:E:59:LEU:HD21	2.44	0.47
7:G:44:GLY:HA3	7:G:218:CYS:O	2.14	0.47
8:H:3:ILE:CD1	8:H:46:SER:HB3	2.43	0.47
8:H:59:VAL:HG22	8:H:81:VAL:HG12	1.97	0.47
9:I:59:ILE:HG12	9:I:83:LEU:HD23	1.96	0.47
11:K:2:ILE:HD12	11:K:175:PHE:CG	2.49	0.47
2:P:149:GLN:O	2:P:156:TYR:HA	2.14	0.47
4:R:200:LEU:HD12	4:R:236:ILE:HG21	1.97	0.47
12:Z:21:THR:HG22	12:Z:26:VAL:HA	1.95	0.47
13:1:155:THR:HG21	13:1:159:VAL:CG1	2.45	0.47
12:L:192:ASP:OD1	12:L:194:GLY:N	2.46	0.47
1:O:30:TYR:CG	7:U:16:PRO:HA	2.49	0.47
4:R:171:VAL:HG13	4:R:198:SER:HB2	1.96	0.47
6:T:26:LEU:HD23	6:T:149:PRO:HD2	1.96	0.47
7:U:181:HIS:C	7:U:183:PRO:HD3	2.34	0.47
2:B:46:ALA:HB2	2:B:211:LEU:HG	1.97	0.47
13:1:136:LEU:N	13:1:136:LEU:HD12	2.30	0.47
4:D:241:GLN:CA	4:D:242:GLU:HB2	2.45	0.47
14:N:217:ILE:HD13	8:V:30:VAL:HG23	1.96	0.47
14:2:142:MET:O	14:2:145:PRO:HD2	2.15	0.47
2:B:149:GLN:O	2:B:156:TYR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:146:MET:HE3	8:H:150:GLU:HB3	1.97	0.47
10:J:193:MET:HG3	10:J:194:ARG:O	2.15	0.47
11:K:102:LEU:CD2	11:K:117:GLN:HG3	2.44	0.47
3:Q:163:ILE:HD12	3:Q:173:GLN:NE2	2.30	0.47
6:T:27:GLU:OE2	6:T:30:LYS:HD2	2.14	0.47
8:V:32:ASP:OD2	8:V:185:ARG:NH2	2.48	0.47
14:2:153:ARG:HH11	14:2:153:ARG:HG3	1.80	0.47
2:B:61:LEU:HD12	2:B:61:LEU:HA	1.56	0.47
1:O:196:GLU:HG2	1:O:201:LYS:HB2	1.97	0.47
4:R:84:ILE:CD1	4:R:84:ILE:N	2.78	0.47
5:S:15:PHE:HB2	6:T:21:GLN:OE1	2.15	0.47
2:B:108:LYS:HD2	2:B:148:TYR:CZ	2.50	0.47
2:B:74:VAL:HG22	2:B:75:TYR:H	1.79	0.47
6:F:143:HIS:ND1	6:F:155:GLU:OE2	2.44	0.47
9:I:200:GLN:HG2	13:1:173:LYS:HG2	1.96	0.47
10:J:44:ILE:CG2	10:J:51:VAL:HG22	2.45	0.47
2:P:122:THR:HG22	3:Q:129:ARG:NH2	2.12	0.47
3:Q:91:ALA:HB2	3:Q:115:LEU:HD22	1.97	0.47
5:S:81:LEU:N	5:S:139:GLY:O	2.42	0.47
9:W:26:VAL:HG11	9:W:29:LYS:HG2	1.95	0.47
1:A:164:VAL:HG22	1:A:165:GLY:H	1.80	0.46
5:E:159:GLU:HB3	5:E:160:PRO:HD2	1.97	0.46
8:H:157:HIS:NE2	8:H:196:LEU:HD22	2.31	0.46
9:I:165:ASN:ND2	14:2:145:PRO:HB3	2.30	0.46
10:J:54:LEU:HD12	10:J:96:VAL:HG21	1.97	0.46
6:T:72:LEU:HD22	6:T:132:LEU:HD22	1.97	0.46
8:V:190:PRO:HA	8:V:193:TYR:CE2	2.50	0.46
9:W:1:THR:OG1	9:W:33:LYS:NZ	2.34	0.46
9:W:5:GLY:O	9:W:124:TYR:HA	2.15	0.46
11:Y:138:TYR:CZ	11:Y:171:MET:HG3	2.50	0.46
9:I:194:ASN:ND2	13:1:213:ASP:HB3	2.27	0.46
1:A:196:GLU:HG2	1:A:201:LYS:CB	2.46	0.46
3:C:112:VAL:HG22	3:C:137:TYR:CD2	2.50	0.46
6:F:176:LEU:HD13	6:F:180:ILE:CD1	2.45	0.46
8:H:112:THR:HG22	8:H:120:HIS:HB2	1.97	0.46
8:H:1:THR:HB	8:H:33:LYS:NZ	2.30	0.46
12:L:158:LYS:HD3	12:L:196:LEU:CD1	2.46	0.46
5:E:101:LEU:CD1	12:L:57:THR:HG22	2.46	0.46
1:O:204:GLU:OE2	1:O:244:ARG:NH1	2.47	0.46
11:Y:111:ASN:O	11:Y:112:LYS:HD3	2.16	0.46
10:J:170:ALA:O	12:Z:169:ALA:HB1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:9:ASP:OD1	14:2:10:ASN:N	2.48	0.46
3:C:86:ILE:O	3:C:90:THR:HG23	2.15	0.46
18:O:302:EDO:H11	2:P:57:MET:CE	2.45	0.46
5:S:220:SER:HB3	5:S:230:ILE:HA	1.96	0.46
9:W:84:LYS:HE2	9:W:119:THR:HG23	1.96	0.46
14:2:17:ASP:HA	14:2:187:PHE:CB	2.45	0.46
14:2:37:VAL:HG11	14:2:84:ILE:HD11	1.98	0.46
1:A:166:TYR:HB3	1:A:168:ALA:O	2.15	0.46
4:D:174:PHE:CD2	4:D:201:GLU:HG3	2.51	0.46
5:E:248:ALA:HB1	5:E:250:GLU:O	2.15	0.46
6:F:11:VAL:HG13	7:G:128:VAL:C	2.36	0.46
12:L:38:ASN:HB2	12:L:39:PRO:CD	2.46	0.46
12:L:7:ARG:HG2	12:L:110:PRO:HB2	1.98	0.46
2:P:111:VAL:HG22	2:P:136:ILE:CD1	2.45	0.46
4:R:142:ASP:OD1	4:R:143:ASP:N	2.49	0.46
13:1:1:GLY:HA3	13:1:33:LYS:NZ	2.31	0.46
4:D:42:VAL:HG11	4:D:136:ALA:HB1	1.98	0.46
10:J:28:SER:HB2	11:K:125:VAL:HG21	1.98	0.46
3:Q:142:ASP:O	11:Y:109:LYS:NZ	2.33	0.46
6:T:128:TYR:O	6:T:149:PRO:HB3	2.15	0.46
9:I:213:LEU:HG	10:J:192:LYS:HB2	1.97	0.46
13:M:42:VAL:CG1	13:M:196:LEU:HD23	2.45	0.46
2:P:43:VAL:HG11	2:P:137:ALA:HB1	1.97	0.46
3:Q:25:ALA:O	3:Q:29:ILE:HG13	2.16	0.46
1:A:115:ASP:HB3	1:A:155:TYR:CZ	2.50	0.46
1:A:87:ILE:CG2	1:A:88:PRO:HD3	2.44	0.46
11:K:91:ILE:HG12	11:K:121:LEU:HD23	1.97	0.46
2:P:247:LEU:HA	2:P:247:LEU:HD23	1.66	0.46
3:Q:228:LYS:HZ1	3:Q:234:GLU:CD	2.19	0.46
11:Y:125:VAL:HG13	11:Y:127:LEU:HG	1.97	0.46
11:Y:19:ALA:HB2	11:Y:176:LYS:HG2	1.98	0.46
11:Y:-1:MET:HG3	11:Y:-1:MET:O	2.14	0.46
1:A:131:ARG:HD2	1:A:133:TYR:HE1	1.81	0.46
5:E:207:VAL:HG23	5:E:207:VAL:O	2.15	0.46
5:E:248:ALA:HB1	5:E:249:ALA:C	2.36	0.46
7:G:67:GLN:HG2	14:N:69:ASP:OD1	2.16	0.46
2:P:210:GLU:HG2	2:P:237:LYS:HE3	1.98	0.46
8:V:65:LEU:O	8:V:68:SER:HB2	2.15	0.46
2:B:6:SER:HB2	4:D:4:TYR:HB2	1.97	0.46
6:F:39:ARG:HH11	6:F:39:ARG:HG3	1.81	0.46
10:J:47:LEU:HG	10:J:49:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:LEU:HD22	13:M:57:LYS:HE2	1.98	0.46
4:R:32:CYS:N	4:R:47:GLU:HG2	2.30	0.46
13:M:187:ILE:HD12	9:W:167:LEU:HB3	1.97	0.46
7:G:103:LYS:HD2	18:G:301:EDO:H21	1.97	0.46
6:F:15:PRO:HA	7:G:25:TYR:CD2	2.51	0.46
13:M:34:VAL:HG12	13:M:196:LEU:HD22	1.98	0.46
14:N:36:PRO:HG3	14:N:200:PHE:CE2	2.51	0.46
12:Z:86:LEU:O	12:Z:89:GLN:HB2	2.16	0.46
1:A:101:ALA:CA	1:A:112:MET:HE2	2.29	0.45
1:A:211:ILE:HG23	1:A:216:THR:O	2.17	0.45
5:E:192:THR:OG1	5:E:195:GLU:HG3	2.16	0.45
7:G:36:SER:HB3	7:G:49:VAL:HG23	1.98	0.45
1:O:158:ASP:HB2	1:O:159:PRO:CD	2.46	0.45
5:S:167:TYR:CZ	5:S:170:LYS:HD3	2.51	0.45
5:S:201:LEU:HD22	5:S:240:ILE:HG12	1.98	0.45
5:S:40:ILE:HD12	5:S:200:VAL:CG2	2.34	0.45
10:X:193:MET:HE3	10:X:193:MET:HB2	1.84	0.45
2:B:23:TYR:O	2:B:26:THR:HB	2.16	0.45
9:I:80:LEU:HD13	9:I:111:PHE:CG	2.52	0.45
4:R:163:THR:HG23	4:R:168:SER:HB2	1.97	0.45
5:S:121:LEU:HD23	5:S:121:LEU:HA	1.76	0.45
4:D:234:THR:O	4:D:238:GLN:HG2	2.16	0.45
5:E:247:GLU:HA	5:E:248:ALA:CB	2.39	0.45
9:I:220:ILE:N	9:I:220:ILE:HD13	2.30	0.45
10:J:162:LEU:CD2	10:J:176:ALA:HB1	2.47	0.45
1:O:125:SER:HB3	1:O:161:GLY:HA2	1.98	0.45
5:S:75:GLY:HA3	5:S:228:PHE:CD2	2.52	0.45
13:1:132:ALA:HB1	13:1:186:HIS:CE1	2.51	0.45
1:A:131:ARG:O	20:A:401:HOH:O	2.21	0.45
3:C:9:ARG:HB2	3:C:12:ILE:HD13	1.99	0.45
3:C:240:VAL:HG23	3:C:241:LYS:N	2.32	0.45
13:M:128:ARG:HA	13:M:128:ARG:HD3	1.84	0.45
14:N:120:ARG:HH11	14:N:130:SER:HB2	1.82	0.45
5:S:220:SER:HB2	5:S:229:LYS:O	2.16	0.45
7:U:94:GLU:HG2	7:U:114:ARG:HD2	1.98	0.45
9:W:174:ASP:OD2	9:W:188:ARG:NH1	2.47	0.45
11:Y:66:TYR:CE1	11:Y:74:LEU:HG	2.51	0.45
14:2:-2:THR:HA	14:2:47:GLY:O	2.17	0.45
5:E:46:VAL:O	5:E:221:CYS:HA	2.17	0.45
7:G:11:ASN:O	7:G:13:VAL:N	2.50	0.45
7:G:81:ILE:HB	7:G:82:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:174:ARG:HG2	8:H:174:ARG:HH11	1.80	0.45
11:K:25:SER:HB2	12:L:133:GLN:NE2	2.31	0.45
2:P:150:VAL:HG22	2:P:156:TYR:HB3	1.96	0.45
3:Q:140:TYR:CE1	3:Q:145:GLY:HA2	2.52	0.45
10:X:146:GLU:HG3	10:X:149:LEU:HD21	1.97	0.45
12:L:169:ALA:HB1	10:X:170:ALA:O	2.16	0.45
12:L:143:ASN:HB2	12:L:156:LEU:CD1	2.47	0.45
3:Q:96:GLN:OE1	19:Q:301:GOL:H11	2.17	0.45
5:S:243:LEU:O	5:S:247:GLU:HG3	2.16	0.45
7:U:10:SER:HB2	7:U:13:VAL:HG21	1.98	0.45
7:U:135:THR:O	7:U:149:MET:HA	2.17	0.45
2:B:44:VAL:CG2	2:B:211:LEU:HD21	2.46	0.45
8:H:43:CYS:HA	8:H:98:ILE:O	2.16	0.45
9:I:35:HIS:ND1	9:I:53:GLU:OE1	2.50	0.45
4:R:151:GLU:HB2	4:R:152:PRO:CD	2.47	0.45
13:1:76:SER:HB2	13:1:78:ASN:OD1	2.16	0.45
4:D:89:ALA:HB1	4:D:109:LEU:HD11	1.99	0.45
7:G:180:ASP:O	7:G:183:PRO:HD3	2.16	0.45
1:O:207:ILE:HG23	1:O:223:LEU:HD11	1.99	0.45
5:S:16:SER:O	6:T:24:TYR:HB3	2.17	0.45
6:T:88:LEU:HD12	6:T:88:LEU:HA	1.64	0.45
11:Y:171:MET:HE2	11:Y:173:MET:HB2	1.95	0.45
4:D:42:VAL:O	4:D:215:VAL:HG12	2.17	0.45
6:F:158:GLY:O	7:G:57:LEU:HD13	2.17	0.45
6:F:39:ARG:NH1	6:F:39:ARG:HG3	2.31	0.45
9:I:35:HIS:CE1	9:I:53:GLU:OE2	2.70	0.45
10:J:54:LEU:HD23	10:J:54:LEU:HA	1.60	0.45
2:P:48:GLU:OE2	2:P:50:LYS:HB3	2.17	0.45
3:Q:65:LYS:HE3	3:Q:77:VAL:O	2.16	0.45
3:Q:80:LEU:H	3:Q:80:LEU:HD22	1.82	0.45
12:Z:38:ASN:HB2	12:Z:39:PRO:CD	2.47	0.45
4:D:162:GLN:OE1	4:D:163:THR:N	2.37	0.45
11:K:91:ILE:HA	11:K:91:ILE:HD12	1.86	0.45
2:P:2:THR:CG2	2:P:4:ARG:HD3	2.47	0.45
3:Q:115:LEU:HA	3:Q:115:LEU:HD12	1.69	0.45
10:X:18:LEU:HD12	10:X:175:GLY:HA3	1.99	0.45
15:3:9:TRP:C	15:3:10:ARG:HD3	2.37	0.44
2:B:238:LEU:HD22	2:B:242:GLU:OE1	2.17	0.44
3:C:163:ILE:HG13	3:C:164:SER:H	1.82	0.44
6:F:215:ILE:HG12	6:F:216:VAL:N	2.32	0.44
6:F:36:VAL:HG22	6:F:160:ALA:CB	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:151:GLU:HB2	4:R:152:PRO:HD2	1.98	0.44
7:U:179:VAL:O	7:U:183:PRO:HB3	2.17	0.44
3:C:206:LEU:HA	3:C:206:LEU:HD12	1.73	0.44
5:E:114:GLN:NE2	6:F:82:ARG:HD2	2.32	0.44
10:J:163:LEU:HD23	10:J:193:MET:HE1	2.00	0.44
12:L:185:TRP:O	12:L:186:ILE:HD13	2.17	0.44
14:2:121:TYR:C	14:2:121:TYR:CD1	2.90	0.44
3:C:208:TYR:CD1	3:C:236:LYS:HG3	2.53	0.44
4:D:37:LYS:HD2	4:D:159:TRP:O	2.17	0.44
5:E:39:GLY:HA2	5:E:47:VAL:O	2.17	0.44
7:G:65:LYS:HE2	7:G:81:ILE:HD11	1.99	0.44
13:M:117:ASP:HB2	13:M:118:PRO:CD	2.48	0.44
14:N:177:TYR:OH	19:V:202:GOL:H32	2.17	0.44
1:O:46:ARG:HG3	1:O:167:LYS:O	2.17	0.44
2:P:42:GLY:HA2	2:P:214:ILE:O	2.17	0.44
7:U:102:TYR:O	7:U:103:LYS:HB3	2.18	0.44
10:X:44:ILE:HG22	10:X:51:VAL:HG22	1.99	0.44
11:Y:35:ARG:NH1	11:Y:57:GLU:OE2	2.48	0.44
12:Z:199:LYS:O	12:Z:203:GLU:HG3	2.17	0.44
13:1:168:VAL:O	13:1:172:ILE:HG13	2.17	0.44
1:A:64:LEU:CD2	7:G:159:TYR:CE1	3.00	0.44
4:D:133:THR:O	4:D:149:GLN:HA	2.18	0.44
11:K:52:THR:CG2	11:K:53:VAL:N	2.81	0.44
12:L:76:VAL:HG21	12:L:103:GLY:HA3	1.99	0.44
12:L:25:TRP:HH2	13:M:138:MET:HB2	1.82	0.44
12:L:6:PHE:HA	12:L:125:ASP:O	2.17	0.44
13:M:13:VAL:HG12	13:M:197:ILE:HG12	1.98	0.44
3:Q:112:VAL:HG22	3:Q:137:TYR:CG	2.53	0.44
7:U:36:SER:CB	7:U:49:VAL:HG23	2.48	0.44
5:E:16:SER:HB2	5:E:22:PHE:CE1	2.53	0.44
9:I:123:TYR:HB3	9:I:142:TRP:CZ2	2.53	0.44
10:J:68:LYS:HB3	10:J:68:LYS:HZ2	1.83	0.44
14:N:212:ASP:OD2	14:N:215:LYS:HE3	2.17	0.44
5:E:184:LEU:HD21	6:F:55:GLU:HB2	1.99	0.44
10:J:19:ARG:HD3	10:J:171:LEU:O	2.17	0.44
11:K:157:LEU:HA	11:K:157:LEU:HD23	1.80	0.44
12:L:81:LYS:HD2	12:L:121:ARG:NH1	2.33	0.44
2:P:6:SER:CB	4:R:4:TYR:HB2	2.41	0.44
5:S:75:GLY:HA3	5:S:228:PHE:CE2	2.52	0.44
6:T:32:GLY:HA2	15:3:13:TYR:HB3	1.99	0.44
7:U:201:LEU:CD1	7:U:246:ILE:HG22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:117:ASP:HB2	13:1:118:PRO:CD	2.47	0.44
4:D:14:ASP:OD1	4:D:14:ASP:N	2.45	0.44
8:H:1:THR:HB	8:H:33:LYS:HZ3	1.83	0.44
9:I:143:LYS:HG3	9:I:146:LEU:CD2	2.48	0.44
10:J:117:LEU:H	10:J:117:LEU:HD23	1.83	0.44
10:J:193:MET:HE3	10:J:193:MET:HB2	1.64	0.44
12:L:99:THR:HG22	12:L:115:VAL:O	2.17	0.44
1:O:210:MET:HG2	1:O:218:PHE:CE2	2.53	0.44
3:Q:181:LYS:H	3:Q:184:MET:CE	2.30	0.44
9:W:17:ASP:OD2	9:W:170:GLY:HA3	2.18	0.44
9:W:35:HIS:ND1	9:W:53:GLU:OE2	2.50	0.44
14:2:72:LEU:HD13	14:2:76:GLU:HB2	2.00	0.44
1:A:14:ARG:CD	1:A:26:TYR:CD2	3.00	0.44
4:D:35:GLY:HA2	4:D:43:VAL:O	2.18	0.44
13:M:-5:TYR:CD1	13:M:97:TYR:HB2	2.53	0.44
14:N:157:ILE:N	14:N:158:PRO:HD2	2.33	0.44
1:O:30:TYR:CD2	7:U:16:PRO:HA	2.53	0.44
4:R:224:LEU:HD12	4:R:224:LEU:N	2.33	0.44
9:W:35:HIS:ND1	9:W:53:GLU:CD	2.70	0.44
14:2:198:LEU:HD12	14:2:198:LEU:C	2.38	0.44
2:B:64:VAL:HB	2:B:237:LYS:HZ2	1.83	0.44
3:C:47:ALA:HB2	3:C:213:PHE:CE2	2.53	0.44
4:D:41:CYS:HA	4:D:138:PHE:HZ	1.83	0.44
8:H:113:ILE:HG12	8:H:119:VAL:HG13	2.00	0.44
6:T:134:ILE:O	6:T:144:LEU:HD12	2.18	0.44
6:F:71:GLY:HA3	6:F:222:PHE:CZ	2.52	0.43
7:G:131:PHE:O	7:G:152:PRO:HB3	2.18	0.43
10:J:147:PRO:O	10:J:148:ASN:HB2	2.18	0.43
13:M:-2:ASN:HA	13:M:21:ILE:O	2.18	0.43
1:O:115:ASP:HB3	1:O:155:TYR:CZ	2.52	0.43
1:O:128:TYR:N	1:O:128:TYR:CD1	2.85	0.43
1:O:167:LYS:CA	2:P:57:MET:HE2	2.47	0.43
2:B:248:GLU:C	2:B:250:LEU:H	2.21	0.43
5:E:204:LEU:O	5:E:208:MET:HG3	2.17	0.43
5:E:52:LYS:HE3	5:E:218:GLN:HB2	2.00	0.43
5:E:65:GLU:CD	12:L:71:LYS:HZ1	2.21	0.43
1:O:115:ASP:HB3	1:O:155:TYR:CE1	2.53	0.43
1:O:219:SER:HB3	1:O:222:ASP:OD2	2.18	0.43
3:Q:38:ILE:HD12	3:Q:193:ALA:HB2	2.01	0.43
12:Z:56:GLU:O	12:Z:59:LEU:HB3	2.18	0.43
13:1:116:PHE:HA	13:1:121:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:GLU:C	2:B:219:PRO:HD3	2.39	0.43
5:E:167:TYR:CE2	5:E:170:LYS:HD3	2.53	0.43
6:F:15:PRO:HA	7:G:25:TYR:CG	2.53	0.43
1:O:127:ILE:HG23	1:O:131:ARG:HH21	1.84	0.43
1:O:70:SER:CB	1:O:224:GLU:OE2	2.66	0.43
11:Y:19:ALA:HB2	11:Y:176:LYS:CG	2.48	0.43
12:Z:13:ILE:HD12	12:Z:154:LEU:HD23	2.01	0.43
6:F:13:PHE:CE1	6:F:19:LEU:HD21	2.53	0.43
6:F:207:THR:HG23	6:F:210:ASN:ND2	2.34	0.43
14:N:72:LEU:HD23	14:N:72:LEU:HA	1.78	0.43
5:S:220:SER:HB2	5:S:230:ILE:HA	1.99	0.43
7:U:203:HIS:CD2	7:U:211:PHE:CD1	3.06	0.43
2:P:110:LEU:O	2:P:114:VAL:HG23	2.18	0.43
7:U:106:ILE:O	7:U:106:ILE:HG23	2.18	0.43
7:U:22:GLN:NE2	7:U:22:GLN:HA	2.33	0.43
10:X:117:LEU:HD23	10:X:117:LEU:H	1.82	0.43
3:C:44:ILE:HD11	3:C:146:TYR:HB3	2.01	0.43
4:D:171:VAL:HG13	4:D:198:SER:HB2	2.00	0.43
9:I:17:ASP:OD2	9:I:170:GLY:HA3	2.18	0.43
4:R:71:VAL:HG11	4:R:109:LEU:CD2	2.48	0.43
1:A:101:ALA:CA	1:A:112:MET:CE	2.93	0.43
4:D:43:VAL:HG23	4:D:191:CYS:SG	2.58	0.43
4:D:67:ILE:HG21	4:D:109:LEU:CD2	2.48	0.43
4:D:68:ASP:HB3	4:D:70:HIS:ND1	2.34	0.43
10:J:115:PHE:N	10:J:115:PHE:CD1	2.87	0.43
11:K:107:ASP:OD2	11:K:110:LYS:HD3	2.19	0.43
13:M:92:ARG:HD2	13:M:92:ARG:O	2.18	0.43
14:N:88:LEU:O	14:N:92:MET:HG2	2.18	0.43
3:Q:64:GLU:O	3:Q:64:GLU:HG2	2.19	0.43
7:U:94:GLU:HG2	7:U:114:ARG:CB	2.43	0.43
10:X:73:ILE:HD11	10:X:77:THR:HG22	2.00	0.43
9:I:114:HIS:HB3	20:I:402:HOH:O	2.19	0.43
11:K:52:THR:HG23	11:K:53:VAL:N	2.33	0.43
12:L:143:ASN:HB2	12:L:156:LEU:HD13	2.01	0.43
14:N:166:GLU:O	14:N:170:VAL:HG23	2.19	0.43
18:O:302:EDO:H11	2:P:57:MET:HE1	2.00	0.43
1:O:75:ILE:HG21	1:O:117:LEU:HD21	1.99	0.43
2:P:39:ALA:HB1	2:P:183:LEU:O	2.18	0.43
5:S:37:ALA:C	5:S:38:ILE:HG13	2.39	0.43
6:T:157:TYR:OH	7:U:60:PRO:HD2	2.18	0.43
7:U:81:ILE:HB	7:U:82:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:60:GLN:HG2	15:4:14:ALA:HB2	2.01	0.43
6:F:37:GLY:O	6:F:158:GLY:HA2	2.19	0.43
13:M:2:THR:HG21	13:M:133:ALA:HB3	2.01	0.43
4:R:90:ARG:HG2	11:Y:68:ILE:CG2	2.48	0.43
7:U:118:TYR:O	7:U:121:ALA:HB3	2.19	0.43
13:1:141:LEU:O	13:1:145:VAL:HB	2.19	0.43
13:1:-2:ASN:HA	13:1:21:ILE:O	2.19	0.43
3:C:37:GLY:O	3:C:162:ALA:HA	2.18	0.43
11:K:34:THR:CG2	11:K:181:LYS:NZ	2.82	0.43
13:M:112:ALA:HB2	13:M:124:ARG:NH2	2.34	0.43
1:O:64:LEU:HD23	7:U:159:TYR:CE1	2.53	0.43
1:O:87:ILE:CG2	1:O:88:PRO:HD3	2.47	0.43
3:Q:214:ALA:HB2	3:Q:229:ILE:HG12	2.01	0.43
4:R:32:CYS:H	4:R:47:GLU:CG	2.32	0.43
13:M:138:MET:CE	10:X:168:ARG:NH2	2.82	0.43
2:B:43:VAL:HG12	2:B:44:VAL:N	2.34	0.42
4:D:224:LEU:HB3	4:D:228:GLU:HB2	2.00	0.42
6:F:134:ILE:HB	6:F:145:LEU:HB2	1.99	0.42
7:G:77:TYR:HB3	7:G:135:THR:HG23	2.00	0.42
7:G:74:GLY:O	7:G:137:PHE:HA	2.18	0.42
8:H:65:LEU:O	8:H:68:SER:HB2	2.18	0.42
9:I:206:PRO:HG2	9:I:209:THR:OG1	2.18	0.42
11:K:2:ILE:HB	11:K:17:SER:HB3	1.99	0.42
12:L:73:ARG:NH2	12:L:104:TYR:O	2.43	0.42
14:N:222:THR:HG22	9:W:77:VAL:HG12	2.01	0.42
5:S:191:LEU:CD2	5:S:195:GLU:HB3	2.48	0.42
5:S:78:MET:HG3	5:S:82:THR:HG22	2.01	0.42
7:U:213:LEU:HD21	7:U:215:ILE:HD11	2.01	0.42
12:Z:4:LEU:HD23	12:Z:161:ILE:CD1	2.49	0.42
14:2:198:LEU:HD12	14:2:199:THR:N	2.34	0.42
1:A:114:CYS:HB2	1:A:145:SER:OG	2.19	0.42
2:B:2:THR:O	2:B:4:ARG:N	2.52	0.42
3:C:190:ILE:HG23	3:C:213:PHE:CZ	2.54	0.42
5:E:117:CYS:HG	5:E:164:PHE:HD2	1.66	0.42
8:H:134:ILE:HD13	8:H:162:ALA:HB2	2.01	0.42
11:K:0:MET:CG	11:K:0:MET:O	2.65	0.42
14:N:219:GLY:HA3	14:N:223:GLN:HB3	2.00	0.42
1:O:166:TYR:HB3	1:O:168:ALA:O	2.19	0.42
12:Z:130:GLY:O	12:Z:133:GLN:HB3	2.18	0.42
4:D:225:SER:H	4:D:228:GLU:HG3	1.85	0.42
13:M:142:ASP:O	13:M:148:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:239:THR:HG23	2:P:242:GLU:CD	2.40	0.42
6:T:101:ARG:HG3	14:2:83:TYR:CZ	2.55	0.42
14:2:193:ASP:HB3	14:2:196:THR:OG1	2.18	0.42
6:T:101:ARG:HB2	14:2:83:TYR:CD1	2.54	0.42
14:2:99:MET:CE	14:2:99:MET:HA	2.49	0.42
5:S:20:ARG:HD3	15:3:10:ARG:NH1	2.34	0.42
3:C:98:TYR:CD1	3:C:106:ILE:HA	2.54	0.42
9:I:94:ILE:O	9:I:96:ALA:N	2.50	0.42
13:M:143:ASN:O	13:M:147:PHE:HA	2.19	0.42
6:T:15:PRO:HA	7:U:25:TYR:CD2	2.54	0.42
14:2:131:SER:OG	14:2:132:PRO:HD2	2.20	0.42
14:2:99:MET:HE2	14:2:99:MET:HA	2.01	0.42
2:B:35:LEU:HD12	2:B:35:LEU:C	2.40	0.42
3:C:38:ILE:HD12	3:C:193:ALA:HB2	2.02	0.42
5:E:74:ILE:CD1	5:E:112:LEU:HD22	2.49	0.42
4:D:157:SER:HB2	5:E:59:LEU:HD21	2.01	0.42
7:G:7:TYR:CD2	7:G:16:PRO:HD3	2.54	0.42
10:J:79:THR:HG23	10:J:115:PHE:CE2	2.54	0.42
13:M:117:ASP:OD1	13:M:117:ASP:C	2.58	0.42
13:M:91:LYS:HD3	13:M:96:TYR:CE2	2.54	0.42
13:M:9:GLU:O	13:M:110:LYS:HA	2.18	0.42
1:O:127:ILE:CG2	1:O:131:ARG:HH21	2.31	0.42
4:R:153:SER:OG	4:R:155:ILE:HG13	2.19	0.42
7:U:205:ASP:OD1	7:U:205:ASP:N	2.53	0.42
12:L:206:SER:HB2	11:Y:145:HIS:HA	2.02	0.42
11:Y:59:ILE:HD13	11:Y:59:ILE:HA	1.91	0.42
12:Z:154:LEU:HD23	12:Z:154:LEU:HA	1.79	0.42
12:Z:177:LEU:HA	12:Z:177:LEU:HD23	1.82	0.42
14:2:111:VAL:HG23	14:2:192:ILE:HG22	2.02	0.42
3:C:239:LEU:HD23	3:C:239:LEU:HA	1.91	0.42
10:J:12:VAL:CG1	10:J:110:PRO:HB3	2.50	0.42
10:J:89:ARG:HH12	11:K:92:ARG:HD3	1.84	0.42
11:K:32:ASP:OD1	11:K:34:THR:CG2	2.64	0.42
1:O:63:LEU:HA	1:O:63:LEU:HD23	1.65	0.42
5:S:191:LEU:HD22	5:S:195:GLU:CB	2.50	0.42
6:T:62:LYS:O	6:T:73:SER:HA	2.19	0.42
10:X:121:ILE:H	10:X:121:ILE:HD12	1.84	0.42
12:L:209:ASN:ND2	11:Y:128:PRO:HG3	2.34	0.42
2:B:211:LEU:HD23	2:B:212:ALA:N	2.34	0.42
6:F:136:GLY:HA2	6:F:216:VAL:HG11	2.02	0.42
6:F:169:LYS:O	6:F:173:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:4:LEU:HD12	13:M:5:GLY:H	1.84	0.42
1:O:225:VAL:CB	1:O:236:LEU:HD12	2.49	0.42
3:Q:143:ARG:NE	3:Q:144:TYR:CE2	2.88	0.42
4:R:29:ARG:O	4:R:49:ARG:NH2	2.53	0.42
11:Y:11:SER:HB2	11:Y:183:VAL:O	2.19	0.42
13:1:155:THR:CB	13:1:159:VAL:HG12	2.50	0.42
13:1:38:GLY:O	13:1:40:ASN:N	2.53	0.42
9:I:165:ASN:HD22	14:2:145:PRO:HB3	1.85	0.42
14:2:162:VAL:HG23	20:2:402:HOH:O	2.20	0.42
14:2:17:ASP:HA	14:2:187:PHE:HA	2.02	0.42
2:B:122:THR:HG22	3:C:129:ARG:NH2	2.09	0.42
3:C:111:LEU:HD23	3:C:111:LEU:C	2.40	0.42
3:C:116:SER:HB3	3:C:155:GLY:O	2.20	0.42
5:E:212:LEU:HD21	5:E:240:ILE:CD1	2.50	0.42
10:J:36:HIS:HB3	10:J:41:PHE:CD2	2.55	0.42
14:N:122:VAL:HA	14:N:127:VAL:O	2.20	0.42
2:P:174:PHE:HE1	2:P:178:ARG:NE	2.18	0.42
2:P:250:LEU:HA	2:P:250:LEU:HD12	1.89	0.42
5:S:247:GLU:O	5:S:250:GLU:N	2.53	0.42
9:W:14:ILE:HD12	9:W:34:LEU:HD22	2.02	0.42
9:W:62:ASN:HB3	9:W:82:MET:CE	2.49	0.42
13:1:38:GLY:O	13:1:39:ASP:C	2.57	0.42
3:C:184:MET:HE3	3:C:188:ASP:HB3	2.02	0.42
5:E:184:LEU:HD23	5:E:184:LEU:O	2.19	0.42
12:Z:158:LYS:HD3	12:Z:196:LEU:HD11	2.01	0.42
13:1:116:PHE:N	13:1:116:PHE:CD1	2.87	0.42
4:D:86:ILE:HG22	4:D:90:ARG:HD2	2.02	0.42
2:P:138:GLY:HA2	2:P:214:ILE:HG13	2.01	0.42
5:S:212:LEU:HD23	5:S:240:ILE:CD1	2.48	0.42
7:U:120:GLN:HE22	7:U:124:LEU:HD21	1.85	0.42
7:U:98:PHE:CE2	7:U:106:ILE:HA	2.54	0.42
10:X:140:MET:HE2	10:X:164:ASN:HB2	2.02	0.42
12:Z:25:TRP:HH2	13:1:138:MET:HB2	1.84	0.42
14:2:1:THR:OG1	14:2:2:SER:N	2.53	0.41
14:2:-5:PRO:HG3	14:2:103:TRP:CG	2.55	0.41
5:E:191:LEU:HD22	5:E:195:GLU:HB2	2.02	0.41
6:F:138:ASP:HB2	18:F:301:EDO:O2	2.20	0.41
11:K:22:ARG:HA	11:K:22:ARG:HD3	1.79	0.41
13:M:17:ASP:HA	13:M:192:GLY:O	2.20	0.41
14:N:13:ILE:HG21	14:N:13:ILE:HD13	1.82	0.41
9:W:144:GLN:O	9:W:145:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:4:VAL:HG22	9:W:159:ILE:HD11	2.02	0.41
11:Y:106:TYR:CE1	11:Y:111:ASN:HA	2.55	0.41
12:Z:2:THR:OG1	12:Z:132:GLY:HA3	2.19	0.41
2:B:160:LYS:HD3	2:B:179:TRP:CH2	2.54	0.41
2:B:244:ASN:O	2:B:248:GLU:OE1	2.37	0.41
2:B:36:GLY:HA2	2:B:44:VAL:O	2.20	0.41
3:C:65:LYS:HE3	3:C:77:VAL:O	2.20	0.41
4:D:241:GLN:HG3	4:D:242:GLU:O	2.21	0.41
6:F:133:LEU:CD2	6:F:146:GLU:HG3	2.50	0.41
14:N:37:VAL:CG1	14:N:84:ILE:CD1	2.98	0.41
2:P:78:MET:N	2:P:132:VAL:HG12	2.35	0.41
3:Q:47:ALA:HB2	3:Q:213:PHE:CE2	2.55	0.41
4:R:155:ILE:HG12	5:S:83:ALA:HB2	2.02	0.41
4:D:138:PHE:CZ	4:D:145:PRO:HB3	2.55	0.41
6:F:171:TYR:HB2	6:F:199:GLN:HG3	2.01	0.41
13:M:173:LYS:HG2	9:W:200:GLN:HG3	2.01	0.41
2:P:59:GLU:OE1	2:P:59:GLU:N	2.31	0.41
7:U:103:LYS:HD3	18:U:301:EDO:H21	2.03	0.41
12:Z:191:HIS:CD2	12:Z:191:HIS:N	2.88	0.41
14:2:124:LEU:N	14:2:124:LEU:HD23	2.36	0.41
2:B:139:HIS:HA	2:B:144:GLY:O	2.21	0.41
1:O:19:PHE:HE1	2:P:78:MET:CE	2.33	0.41
5:S:48:LEU:HD13	5:S:77:ALA:HB2	2.01	0.41
7:U:57:LEU:HA	7:U:57:LEU:HD23	1.87	0.41
11:K:173:MET:SD	11:Y:173:MET:CE	3.09	0.41
13:1:112:ALA:HB2	13:1:124:ARG:NH2	2.35	0.41
12:Z:28:SER:HB2	13:1:128:ARG:HH22	1.86	0.41
14:2:96:ARG:HD2	14:2:125:LEU:O	2.20	0.41
4:D:71:VAL:HG11	4:D:109:LEU:HD23	2.02	0.41
9:I:215:GLU:CD	10:J:189:ARG:HE	2.24	0.41
10:J:45:THR:O	10:J:96:VAL:HA	2.20	0.41
7:U:141:ASP:O	7:U:143:ASN:N	2.54	0.41
8:V:8:PHE:CE1	8:V:13:ILE:HG13	2.56	0.41
14:2:58:LEU:HA	14:2:58:LEU:HD23	1.79	0.41
1:A:30:TYR:N	1:A:30:TYR:CD1	2.87	0.41
5:E:56:SER:OG	5:E:57:PRO:HD2	2.21	0.41
6:F:73:SER:OG	6:F:133:LEU:HB2	2.21	0.41
13:M:8:GLY:HA3	13:M:11:PHE:CD1	2.56	0.41
7:U:180:ASP:C	7:U:181:HIS:O	2.57	0.41
1:A:12:TYR:C	1:A:14:ARG:H	2.23	0.41
4:D:160:SER:HB3	4:D:179:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:88:LEU:HD12	6:F:88:LEU:HA	1.90	0.41
9:I:18:THR:HB	9:I:30:ASN:HA	2.02	0.41
10:J:168:ARG:NH2	13:1:138:MET:CE	2.84	0.41
10:J:3:VAL:HG22	10:J:16:CYS:CB	2.51	0.41
14:N:131:SER:OG	14:N:132:PRO:HD2	2.21	0.41
1:O:70:SER:OG	1:O:224:GLU:OE2	2.32	0.41
1:O:61:ASP:OD1	1:O:63:LEU:HB2	2.21	0.41
2:P:23:TYR:O	2:P:26:THR:HB	2.21	0.41
10:X:121:ILE:HD12	10:X:121:ILE:N	2.36	0.41
11:Y:20:VAL:HG11	12:Z:122:LEU:HD11	2.03	0.41
12:Z:42:LEU:HD23	12:Z:42:LEU:HA	1.88	0.41
14:2:61:ASP:O	14:2:65:GLU:HG3	2.20	0.41
6:F:112:LEU:HD23	6:F:112:LEU:HA	1.85	0.41
12:L:191:HIS:CD2	12:L:191:HIS:N	2.89	0.41
13:M:94:PHE:N	13:M:95:PRO:HD3	2.35	0.41
2:P:210:GLU:OE2	2:P:237:LYS:NZ	2.41	0.41
3:Q:106:ILE:O	3:Q:106:ILE:HG23	2.21	0.41
3:Q:91:ALA:HB1	3:Q:111:LEU:HD21	2.03	0.41
4:R:114:ALA:HB1	4:R:154:GLY:O	2.20	0.41
4:R:85:LEU:HD23	4:R:85:LEU:HA	1.82	0.41
6:T:14:SER:HB2	6:T:20:PHE:CE2	2.56	0.41
7:U:51:LYS:HG2	7:U:65:LYS:HD2	2.03	0.41
13:1:11:PHE:CZ	13:1:168:VAL:HA	2.55	0.41
7:G:106:ILE:O	7:G:106:ILE:HG23	2.20	0.41
14:N:25:LEU:HD12	8:V:165:TRP:O	2.21	0.41
9:W:112:SER:OG	9:W:120:ASP:HB2	2.20	0.41
1:A:70:SER:HA	1:A:224:GLU:OE2	2.20	0.41
2:B:63:LYS:N	2:B:210:GLU:OE2	2.53	0.41
11:K:18:LYS:CG	11:K:179:ILE:HG13	2.51	0.41
1:O:141:LEU:O	1:O:156:LYS:HG3	2.20	0.41
2:P:35:LEU:C	2:P:35:LEU:HD12	2.41	0.41
3:Q:143:ARG:HG2	3:Q:144:TYR:CD2	2.56	0.41
3:Q:136:ILE:HG12	3:Q:150:THR:HG22	2.02	0.41
14:2:142:MET:C	14:2:145:PRO:HD2	2.42	0.41
1:A:158:ASP:HB2	1:A:159:PRO:HD2	2.01	0.41
3:C:148:LEU:HB3	3:C:160:TRP:O	2.21	0.41
3:C:19:LEU:O	3:C:20:TYR:C	2.59	0.41
5:E:212:LEU:C	5:E:212:LEU:HD23	2.41	0.41
5:E:68:VAL:HG21	5:E:89:ILE:HD12	2.03	0.41
7:G:43:ASP:OD2	7:G:221:SER:HB3	2.21	0.41
9:I:84:LYS:HE2	9:I:119:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:33:LYS:O	13:M:44:SER:OG	2.27	0.41
2:P:61:LEU:HA	2:P:61:LEU:HD12	1.85	0.41
5:S:191:LEU:HD22	5:S:195:GLU:HB3	2.03	0.41
5:S:28:LEU:HA	5:S:28:LEU:HD23	1.84	0.41
2:P:4:ARG:NH1	6:T:123:TYR:CE2	2.89	0.41
12:Z:148:LEU:HD23	12:Z:153:ALA:HA	2.03	0.41
5:E:153:TYR:C	5:E:154:GLN:HG3	2.40	0.40
5:E:240:ILE:O	5:E:243:LEU:HB3	2.21	0.40
8:H:51:ASP:OD2	8:H:93:LEU:HA	2.21	0.40
12:L:14:VAL:HB	12:L:178:TYR:HB2	2.02	0.40
5:S:133:LEU:H	5:S:133:LEU:HD12	1.85	0.40
6:T:180:ILE:HD13	6:T:180:ILE:HG21	1.90	0.40
6:T:3:ARG:HG3	6:T:4:ASN:N	2.36	0.40
6:T:63:ILE:HG22	6:T:224:ILE:CD1	2.51	0.40
8:V:41:ILE:HD13	8:V:78:ALA:HB2	2.03	0.40
9:W:154:LEU:HD12	9:W:154:LEU:O	2.20	0.40
9:W:207:ARG:CZ	10:X:152:GLU:HB2	2.51	0.40
10:X:6:MET:HG2	10:X:127:PHE:HB3	2.02	0.40
5:E:192:THR:HG23	5:E:195:GLU:OE1	2.21	0.40
8:H:14:LEU:HD11	8:H:100:ALA:HB3	2.04	0.40
12:L:3:THR:HG22	12:L:16:VAL:HG12	2.03	0.40
13:M:91:LYS:HB3	13:M:94:PHE:O	2.22	0.40
1:O:101:ALA:CA	1:O:112:MET:CE	2.89	0.40
4:R:120:TYR:CD1	4:R:129:PHE:HE1	2.40	0.40
13:1:-5:TYR:CE1	13:1:97:TYR:HB2	2.57	0.40
14:2:-8:THR:O	14:2:-8:THR:HG22	2.20	0.40
13:1:-6:PRO:CB	14:2:99:MET:HE3	2.51	0.40
7:G:178:LEU:HA	7:G:178:LEU:HD23	1.89	0.40
10:J:75:PRO:HD2	10:J:76:GLU:OE1	2.22	0.40
14:N:36:PRO:HG3	14:N:200:PHE:CD2	2.57	0.40
1:O:210:MET:HG3	1:O:218:PHE:HE2	1.86	0.40
1:O:25:LEU:O	1:O:29:GLU:HG3	2.21	0.40
3:Q:201:THR:O	3:Q:201:THR:HG23	2.21	0.40
4:R:73:LEU:HD22	4:R:86:ILE:HG12	2.04	0.40
6:T:15:PRO:HA	7:U:25:TYR:CG	2.56	0.40
8:V:3:ILE:HD12	8:V:44:CYS:HB3	2.02	0.40
1:A:156:LYS:HB3	1:A:166:TYR:HE1	1.86	0.40
2:B:106:PRO:CG	2:B:109:LEU:HD12	2.50	0.40
9:I:134:ALA:HB1	9:I:158:ALA:HB1	2.04	0.40
12:L:41:LEU:HA	12:L:41:LEU:HD23	1.85	0.40
13:M:42:VAL:CG2	13:M:103:ALA:HB3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:157:THR:HA	1:O:162:TYR:O	2.22	0.40
1:O:45:VAL:HG12	1:O:168:ALA:CB	2.52	0.40
4:R:73:LEU:HD11	4:R:133:THR:HG21	2.03	0.40
4:R:37:LYS:HD3	4:R:160:SER:HA	2.03	0.40
5:S:56:SER:OG	5:S:57:PRO:HD2	2.21	0.40
6:T:134:ILE:HB	6:T:145:LEU:HB2	2.03	0.40
6:T:77:LEU:HD23	6:T:77:LEU:HA	1.83	0.40
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.52	0.40
2:B:18:LEU:HD23	2:B:18:LEU:HA	2.01	0.40
3:C:150:THR:O	3:C:157:TYR:HA	2.21	0.40
8:H:3:ILE:HD13	8:H:46:SER:HB3	2.02	0.40
9:I:166:ASP:OD1	9:I:167:LEU:N	2.54	0.40
12:L:161:ILE:CG2	12:L:175:VAL:HG22	2.52	0.40
13:M:100:THR:HB	13:M:116:PHE:HB2	2.04	0.40
2:P:196:LEU:HD23	2:P:209:ILE:HD12	2.02	0.40
4:R:14:ASP:OD1	4:R:14:ASP:N	2.48	0.40
4:R:224:LEU:CD1	4:R:224:LEU:N	2.84	0.40
14:N:211:TRP:CZ3	8:V:29:ARG:HD2	2.57	0.40
12:Z:8:PHE:HA	12:Z:146:TRP:CE3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:HIS:ND1	2:P:201:GLU:OE2[2_546]	1.89	0.31

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	241/252 (96%)	232 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
2	B	248/250 (99%)	231 (93%)	15 (6%)	2 (1%)	19	57
2	P	248/250 (99%)	233 (94%)	13 (5%)	2 (1%)	19	57
3	C	237/258 (92%)	222 (94%)	15 (6%)	0	100	100
3	Q	238/258 (92%)	225 (94%)	13 (6%)	0	100	100
4	D	239/254 (94%)	226 (95%)	11 (5%)	2 (1%)	19	57
4	R	239/254 (94%)	227 (95%)	10 (4%)	2 (1%)	19	57
5	E	232/260 (89%)	220 (95%)	12 (5%)	0	100	100
5	S	232/260 (89%)	218 (94%)	13 (6%)	1 (0%)	34	72
6	F	230/234 (98%)	213 (93%)	17 (7%)	0	100	100
6	T	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
7	G	242/288 (84%)	226 (93%)	15 (6%)	1 (0%)	34	72
7	U	242/288 (84%)	228 (94%)	12 (5%)	2 (1%)	19	57
8	H	194/215 (90%)	183 (94%)	11 (6%)	0	100	100
8	V	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
9	I	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
9	W	220/261 (84%)	212 (96%)	8 (4%)	0	100	100
10	J	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	X	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
11	K	194/198 (98%)	182 (94%)	10 (5%)	2 (1%)	15	53
11	Y	194/198 (98%)	184 (95%)	8 (4%)	2 (1%)	15	53
12	L	210/287 (73%)	201 (96%)	9 (4%)	0	100	100
12	Z	210/287 (73%)	204 (97%)	6 (3%)	0	100	100
13	1	220/241 (91%)	209 (95%)	9 (4%)	2 (1%)	17	55
13	M	220/241 (91%)	209 (95%)	10 (4%)	1 (0%)	29	68
14	2	231/266 (87%)	222 (96%)	9 (4%)	0	100	100
14	N	230/266 (86%)	222 (96%)	8 (4%)	0	100	100
15	3	4/14 (29%)	4 (100%)	0	0	100	100
15	4	4/14 (29%)	3 (75%)	1 (25%)	0	100	100
All	All	6286/6966 (90%)	5973 (95%)	294 (5%)	19 (0%)	41	76

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	53	SER
4	D	53	LYS
11	K	50	GLY
2	P	53	SER
4	R	240	LYS
4	R	241	GLN
11	Y	49	ALA
2	B	3	ASP
2	P	3	ASP
13	1	72	ASP
13	M	72	ASP
7	U	206	ASN
4	D	242	GLU
7	U	183	PRO
7	G	183	PRO
5	S	249	ALA
13	1	39	ASP
11	Y	8	VAL
11	K	8	VAL

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	205/210 (98%)	196 (96%)	9 (4%)	28	65
1	O	194/210 (92%)	188 (97%)	6 (3%)	40	75
2	B	201/209 (96%)	196 (98%)	5 (2%)	47	79
2	P	205/209 (98%)	200 (98%)	5 (2%)	49	79
3	C	193/216 (89%)	190 (98%)	3 (2%)	62	86
3	Q	190/216 (88%)	189 (100%)	1 (0%)	88	96
4	D	194/226 (86%)	189 (97%)	5 (3%)	46	78
4	R	199/226 (88%)	196 (98%)	3 (2%)	65	87
5	E	190/215 (88%)	185 (97%)	5 (3%)	46	78
5	S	189/215 (88%)	184 (97%)	5 (3%)	46	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	185/193 (96%)	181 (98%)	4 (2%)	52	81
6	T	187/193 (97%)	180 (96%)	7 (4%)	34	70
7	G	193/239 (81%)	183 (95%)	10 (5%)	23	59
7	U	197/239 (82%)	187 (95%)	10 (5%)	24	60
8	H	160/178 (90%)	154 (96%)	6 (4%)	33	69
8	V	161/178 (90%)	159 (99%)	2 (1%)	71	90
9	I	179/214 (84%)	175 (98%)	4 (2%)	52	81
9	W	180/214 (84%)	176 (98%)	4 (2%)	52	81
10	J	167/173 (96%)	163 (98%)	4 (2%)	49	79
10	X	167/173 (96%)	163 (98%)	4 (2%)	49	79
11	K	168/175 (96%)	161 (96%)	7 (4%)	30	66
11	Y	173/175 (99%)	167 (96%)	6 (4%)	36	71
12	L	166/235 (71%)	164 (99%)	2 (1%)	71	90
12	Z	165/235 (70%)	162 (98%)	3 (2%)	59	85
13	1	180/201 (90%)	178 (99%)	2 (1%)	73	90
13	M	181/201 (90%)	175 (97%)	6 (3%)	38	73
14	2	199/224 (89%)	190 (96%)	9 (4%)	27	64
14	N	198/224 (88%)	192 (97%)	6 (3%)	41	75
15	3	4/12 (33%)	4 (100%)	0	100	100
15	4	4/12 (33%)	4 (100%)	0	100	100
All	All	5174/5840 (89%)	5031 (97%)	143 (3%)	43	77

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	33	LYS
1	A	125	SER
1	A	128	TYR
1	A	174	LYS
1	A	210	MET
1	A	219	SER
1	A	244	ARG
1	A	251	GLN
2	B	6	SER

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Mol	Chain	Res	Type
2	B	17	LYS
2	B	157	PHE
2	B	169	VAL
2	B	174	PHE
3	C	8	SER
3	C	150	THR
3	C	236	LYS
4	D	54	LEU
4	D	57	THR
4	D	172	ARG
4	D	188	VAL
4	D	242	GLU
5	E	8	TYR
5	E	61	SER
5	E	184	LEU
5	E	209	GLU
5	E	210	GLU
6	F	93	ASN
6	F	113	CYS
6	F	156	LEU
6	F	208	VAL
7	G	35	THR
7	G	97	SER
7	G	104	THR
7	G	142	LYS
7	G	170	SER
7	G	178	LEU
7	G	205	ASP
7	G	210	ASP
7	G	217	TRP
7	G	239	ILE
8	H	1	THR
8	H	31	THR
8	H	72	THR
8	H	119	VAL
8	H	132	THR
8	H	149	GLU
9	I	71	SER
9	I	169	SER
9	I	177	VAL
9	I	220	ILE
10	J	6	MET

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Mol	Chain	Res	Type
10	J	115	PHE
10	J	157	THR
10	J	194	ARG
11	K	17	SER
11	K	21	THR
11	K	34	THR
11	K	52	THR
11	K	62	ASN
11	K	68	ILE
11	K	90	SER
12	L	87	VAL
12	L	104	TYR
13	M	64	LYS
13	M	71	ASN
13	M	76	SER
13	M	99	HIS
13	M	123	GLU
13	M	127	CYS
14	N	2	SER
14	N	21	SER
14	N	96	ARG
14	N	121	TYR
14	N	130	SER
14	N	217	ILE
1	O	17	THR
1	O	54	ILE
1	O	125	SER
1	O	198	SER
1	O	219	SER
1	O	244	ARG
2	P	4	ARG
2	P	6	SER
2	P	51	SER
2	P	52	SER
2	P	157	PHE
3	Q	54	SER
4	R	57	THR
4	R	84	ILE
4	R	242	GLU
5	S	25	GLU
5	S	151	ASP
5	S	184	LEU

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Mol	Chain	Res	Type
5	S	222	ILE
5	S	234	GLU
6	T	3	ARG
6	T	14	SER
6	T	113	CYS
6	T	156	LEU
6	T	170	THR
6	T	208	VAL
6	T	220	THR
7	U	5	THR
7	U	34	THR
7	U	97	SER
7	U	104	THR
7	U	169	GLN
7	U	170	SER
7	U	205	ASP
7	U	210	ASP
7	U	217	TRP
7	U	239	ILE
8	V	83	LYS
8	V	132	THR
9	W	71	SER
9	W	169	SER
9	W	180	ILE
9	W	188	ARG
10	X	115	PHE
10	X	138	PHE
10	X	174	TRP
10	X	194	ARG
11	Y	17	SER
11	Y	34	THR
11	Y	52	THR
11	Y	68	ILE
11	Y	90	SER
11	Y	162	LEU
12	Z	104	TYR
12	Z	147	ASP
12	Z	186	ILE
13	1	33	LYS
13	1	123	GLU
14	2	-6	GLN
14	2	2	SER

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Mol	Chain	Res	Type
14	2	4	ILE
14	2	12	VAL
14	2	21	SER
14	2	121	TYR
14	2	149	LYS
14	2	184	SER
14	2	186	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	30	ASN
9	I	189	ASN
9	I	194	ASN

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 43 ligands modelled in this entry, 20 are monoatomic - leaving 23 for Mogul analysis.

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	$\#\|Z\|>2$
18	EDO	U	301	-	3,3,3	0.32	0	2,2,2	0.72	0
18	EDO	C	302	-	3,3,3	0.56	0	2,2,2	0.50	0
19	GOL	Q	301	-	5,5,5	0.42	0	5,5,5	0.48	0
18	EDO	2	304	-	3,3,3	0.60	0	2,2,2	0.34	0
18	EDO	M	302	-	3,3,3	0.65	0	2,2,2	0.07	0
18	EDO	Y	202	-	3,3,3	0.42	0	2,2,2	0.76	0
19	GOL	L	301	-	5,5,5	0.38	0	5,5,5	0.28	0
18	EDO	G	301	-	3,3,3	0.45	0	2,2,2	0.36	0
19	GOL	V	202	-	5,5,5	0.56	0	5,5,5	0.91	0
18	EDO	W	301	-	3,3,3	0.95	0	2,2,2	0.44	0
18	EDO	I	302	-	3,3,3	0.53	0	2,2,2	0.22	0
18	EDO	W	303	-	3,3,3	0.69	0	2,2,2	0.13	0
18	EDO	W	302	-	3,3,3	0.62	0	2,2,2	0.19	0
18	EDO	F	301	-	3,3,3	0.28	0	2,2,2	0.57	0
19	GOL	J	201	-	5,5,5	0.36	0	5,5,5	0.35	0
19	GOL	Z	301	-	5,5,5	0.37	0	5,5,5	0.25	0
19	GOL	1	301	-	5,5,5	0.36	0	5,5,5	0.97	0
18	EDO	1	302	-	3,3,3	0.66	0	2,2,2	0.13	0
18	EDO	L	302	-	3,3,3	0.66	0	2,2,2	0.14	0
18	EDO	O	302	-	3,3,3	0.63	0	2,2,2	0.39	0
18	EDO	Y	201	-	3,3,3	0.65	0	2,2,2	0.15	0
18	EDO	O	303	-	3,3,3	0.78	0	2,2,2	0.06	0
19	GOL	M	301	-	5,5,5	0.52	0	5,5,5	0.45	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
18	EDO	U	301	-	-	0/1/1/1	-
18	EDO	C	302	-	-	0/1/1/1	-
19	GOL	Q	301	-	-	2/4/4/4	-
18	EDO	2	304	-	-	0/1/1/1	-
18	EDO	M	302	-	-	0/1/1/1	-
18	EDO	Y	202	-	-	0/1/1/1	-
19	GOL	L	301	-	-	2/4/4/4	-
18	EDO	G	301	-	-	0/1/1/1	-
19	GOL	V	202	-	-	3/4/4/4	-
18	EDO	W	301	-	-	1/1/1/1	-
18	EDO	I	302	-	-	0/1/1/1	-
18	EDO	W	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	EDO	W	302	-	-	0/1/1/1	-
18	EDO	F	301	-	-	0/1/1/1	-
19	GOL	J	201	-	-	1/4/4/4	-
19	GOL	Z	301	-	-	2/4/4/4	-
19	GOL	1	301	-	-	2/4/4/4	-
18	EDO	1	302	-	-	0/1/1/1	-
18	EDO	L	302	-	-	0/1/1/1	-
18	EDO	O	302	-	-	0/1/1/1	-
18	EDO	Y	201	-	-	0/1/1/1	-
18	EDO	O	303	-	-	1/1/1/1	-
19	GOL	M	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	Q	301	GOL	C1-C2-C3-O3
19	M	301	GOL	O1-C1-C2-O2
19	M	301	GOL	O1-C1-C2-C3
19	Q	301	GOL	O2-C2-C3-O3
19	Z	301	GOL	O1-C1-C2-O2
19	L	301	GOL	O1-C1-C2-C3
19	Z	301	GOL	O1-C1-C2-C3
19	V	202	GOL	O1-C1-C2-O2
18	W	303	EDO	O1-C1-C2-O2
19	V	202	GOL	O2-C2-C3-O3
18	W	301	EDO	O1-C1-C2-O2
19	L	301	GOL	O1-C1-C2-O2
19	1	301	GOL	O2-C2-C3-O3
18	O	303	EDO	O1-C1-C2-O2
19	1	301	GOL	C1-C2-C3-O3
19	V	202	GOL	O1-C1-C2-C3
19	J	201	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	U	301	EDO	1	0
18	C	302	EDO	2	0
19	Q	301	GOL	1	0
18	G	301	EDO	1	0
19	V	202	GOL	2	0
18	F	301	EDO	1	0
18	O	302	EDO	2	0
18	Y	201	EDO	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	241/252 (95%)	-0.78	0	100	100	22, 36, 56, 72	0
1	O	241/252 (95%)	-0.80	0	100	100	22, 34, 56, 74	0
2	B	250/250 (100%)	-0.65	0	100	100	25, 42, 71, 81	0
2	P	250/250 (100%)	-0.74	0	100	100	23, 36, 61, 82	0
3	C	241/258 (93%)	-0.65	0	100	100	26, 40, 70, 96	0
3	Q	242/258 (93%)	-0.73	0	100	100	24, 40, 67, 83	0
4	D	241/254 (94%)	-0.41	0	100	100	27, 49, 86, 100	1 (0%)
4	R	241/254 (94%)	-0.49	0	100	100	23, 44, 82, 95	1 (0%)
5	E	236/260 (90%)	-0.68	0	100	100	27, 44, 66, 83	0
5	S	236/260 (90%)	-0.75	0	100	100	26, 40, 61, 81	0
6	F	232/234 (99%)	-0.62	0	100	100	26, 42, 63, 73	0
6	T	232/234 (99%)	-0.64	0	100	100	27, 43, 64, 77	0
7	G	244/288 (84%)	-0.70	0	100	100	20, 36, 64, 81	0
7	U	244/288 (84%)	-0.70	0	100	100	24, 37, 65, 85	2 (0%)
8	H	196/215 (91%)	-0.85	0	100	100	22, 30, 46, 55	0
8	V	196/215 (91%)	-0.83	0	100	100	19, 29, 46, 54	0
9	I	222/261 (85%)	-0.80	0	100	100	22, 34, 52, 88	0
9	W	222/261 (85%)	-0.79	0	100	100	22, 33, 50, 91	0
10	J	204/205 (99%)	-0.85	0	100	100	22, 34, 50, 79	0
10	X	204/205 (99%)	-0.79	0	100	100	22, 35, 50, 73	0
11	K	196/198 (98%)	-0.77	0	100	100	22, 35, 50, 77	0
11	Y	196/198 (98%)	-0.82	0	100	100	24, 35, 51, 87	0
12	L	212/287 (73%)	-0.77	0	100	100	25, 36, 53, 68	0
12	Z	212/287 (73%)	-0.77	0	100	100	23, 35, 51, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	222/241 (92%)	-0.76	0 100 100	24, 34, 53, 70	0
13	M	222/241 (92%)	-0.71	0 100 100	21, 35, 57, 74	0
14	2	233/266 (87%)	-0.82	1 (0%) 92 79	19, 32, 46, 59	0
14	N	232/266 (87%)	-0.86	0 100 100	19, 30, 44, 57	0
15	3	6/14 (42%)	-0.21	0 100 100	45, 57, 69, 80	0
15	4	6/14 (42%)	-0.14	0 100 100	49, 69, 70, 73	0
All	All	6352/6966 (91%)	-0.73	1 (0%) 100 100	19, 37, 63, 100	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	2	-8	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	EDO	W	301	4/4	0.53	0.34	36,45,47,54	0
18	EDO	W	303	4/4	0.75	0.27	44,58,70,70	0
16	CL	2	301	1/1	0.83	0.20	60,60,60,60	0
18	EDO	Y	202	4/4	0.87	0.24	47,57,64,75	0
17	MG	I	301	1/1	0.87	0.23	38,38,38,38	0
19	GOL	Q	301	6/6	0.88	0.30	38,49,50,55	0
16	CL	A	301	1/1	0.89	0.17	53,53,53,53	0
18	EDO	1	302	4/4	0.91	0.22	33,47,50,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	EDO	L	302	4/4	0.91	0.29	38,45,49,49	0
16	CL	O	301	1/1	0.91	0.10	47,47,47,47	0
19	GOL	V	202	6/6	0.92	0.26	31,40,48,50	0
18	EDO	Y	201	4/4	0.92	0.19	32,54,69,69	0
19	GOL	J	201	6/6	0.92	0.21	40,46,53,54	0
18	EDO	C	302	4/4	0.93	0.31	41,48,57,66	0
17	MG	Q	302	1/1	0.93	0.12	29,29,29,29	0
16	CL	V	201	1/1	0.93	0.08	44,44,44,44	0
16	CL	K	201	1/1	0.93	0.10	46,46,46,46	0
19	GOL	Z	301	6/6	0.93	0.18	40,58,61,61	0
18	EDO	O	303	4/4	0.93	0.18	38,46,58,58	0
18	EDO	2	304	4/4	0.93	0.33	48,56,63,63	0
17	MG	C	301	1/1	0.94	0.11	30,30,30,30	0
17	MG	N	302	1/1	0.94	0.18	33,33,33,33	0
19	GOL	L	301	6/6	0.94	0.14	41,46,48,53	0
18	EDO	I	302	4/4	0.95	0.20	34,49,67,67	0
18	EDO	G	301	4/4	0.95	0.22	41,49,55,65	0
16	CL	2	303	1/1	0.95	0.10	54,54,54,54	0
17	MG	H	201	1/1	0.95	0.10	20,20,20,20	0
16	CL	P	301	1/1	0.96	0.08	41,41,41,41	0
16	CL	K	202	1/1	0.96	0.07	40,40,40,40	0
19	GOL	1	301	6/6	0.96	0.17	34,44,48,49	0
16	CL	R	301	1/1	0.96	0.10	60,60,60,60	0
18	EDO	U	301	4/4	0.96	0.20	38,45,53,63	0
18	EDO	M	302	4/4	0.97	0.33	31,37,42,44	0
18	EDO	W	302	4/4	0.97	0.13	38,45,49,49	0
17	MG	N	303	1/1	0.97	0.09	33,33,33,33	0
17	MG	D	301	1/1	0.97	0.07	31,31,31,31	0
18	EDO	O	302	4/4	0.97	0.24	33,43,51,51	0
19	GOL	M	301	6/6	0.97	0.17	42,52,56,67	0
16	CL	S	301	1/1	0.98	0.06	45,45,45,45	0
17	MG	J	202	1/1	0.98	0.09	32,32,32,32	0
18	EDO	F	301	4/4	0.98	0.17	34,39,42,44	0
16	CL	2	302	1/1	0.99	0.10	47,47,47,47	0
16	CL	N	301	1/1	0.99	0.06	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.