



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:46 PM GMT

PDB ID : 3UNH
Title : Mouse 20S immunoproteasome
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on : 2011-11-15
Resolution : 3.20 Å(reported)

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

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

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

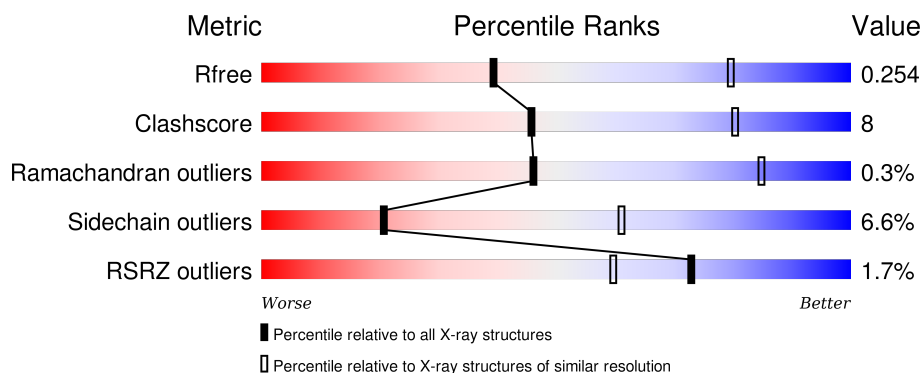
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	234	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	O	234	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	B	261	<div> <div>3%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div>
2	P	261	<div> <div>5%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
3	C	248	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	199	
14	b	199	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49084 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	6			
1	O	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	P	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	5			
3	Q	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	5			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	0	0
			1777	1116	294	356	11			
4	R	233	Total	C	N	O	S	0	0	0
			1777	1116	294	356	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			
5	S	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	T	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	U	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			

- Molecule 8 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			
8	V	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1591	1013	265	294	19			
9	W	204	Total	C	N	O	S	0	0	0
			1591	1013	265	294	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

- Molecule 11 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			
11	Y	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	0	0
			1653	1047	284	312	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1653	1047	284	312	10			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	a	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			
14	b	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			

- Molecule 15 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	I	0	0
			1	1		
15	E	1	Total	I	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total I 1 1	0	0
15	b	2	Total I 2 2	0	0
15	I	1	Total I 1 1	0	0
15	C	1	Total I 1 1	0	0
15	V	1	Total I 1 1	0	0
15	W	1	Total I 1 1	0	0
15	A	1	Total I 1 1	0	0
15	N	2	Total I 2 2	0	0
15	O	1	Total I 1 1	0	0
15	Y	1	Total I 1 1	0	0

- 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	G	1	Total Cl 1 1	0	0
16	Q	2	Total Cl 2 2	0	0
16	D	1	Total Cl 1 1	0	0
16	K	1	Total Cl 1 1	0	0
16	a	2	Total Cl 2 2	0	0
16	E	1	Total Cl 1 1	0	0
16	H	1	Total Cl 1 1	0	0
16	B	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	b	1	Total 1	Cl 1	0	0
16	V	2	Total 2	Cl 2	0	0
16	Z	1	Total 1	Cl 1	0	0
16	A	1	Total 1	Cl 1	0	0
16	N	2	Total 2	Cl 2	0	0
16	U	1	Total 1	Cl 1	0	0
16	R	1	Total 1	Cl 1	0	0
16	L	1	Total 1	Cl 1	0	0
16	S	1	Total 1	Cl 1	0	0
16	M	1	Total 1	Cl 1	0	0

- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	D	1	Total 1	K 1	0	0
17	K	1	Total 1	K 1	0	0
17	E	1	Total 1	K 1	0	0
17	H	1	Total 1	K 1	0	0
17	b	1	Total 1	K 1	0	0
17	C	1	Total 1	K 1	0	0
17	T	1	Total 1	K 1	0	0
17	Y	1	Total 1	K 1	0	0
17	S	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	F	1	Total K 1 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	20	Total O 20 20	0	0
18	B	18	Total O 18 18	0	0
18	C	24	Total O 24 24	0	0
18	D	16	Total O 16 16	0	0
18	E	22	Total O 22 22	0	0
18	F	17	Total O 17 17	0	0
18	G	23	Total O 23 23	0	0
18	H	18	Total O 18 18	0	0
18	I	18	Total O 18 18	0	0
18	J	14	Total O 14 14	0	0
18	K	14	Total O 14 14	0	0
18	L	22	Total O 22 22	0	0
18	M	24	Total O 24 24	0	0
18	N	18	Total O 18 18	0	0
18	O	10	Total O 10 10	0	0
18	P	20	Total O 20 20	0	0
18	Q	21	Total O 21 21	0	0
18	R	17	Total O 17 17	0	0

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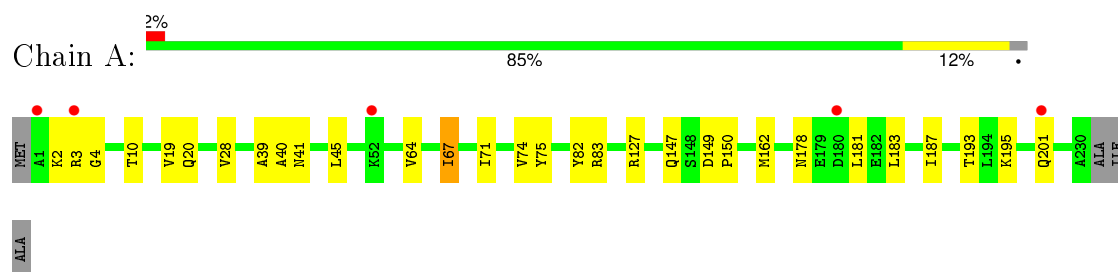
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	S	23	Total 23	O 23	0	0
18	T	24	Total 24	O 24	0	0
18	U	15	Total 15	O 15	0	0
18	V	14	Total 14	O 14	0	0
18	W	17	Total 17	O 17	0	0
18	X	15	Total 15	O 15	0	0
18	Y	26	Total 26	O 26	0	0
18	Z	25	Total 25	O 25	0	0
18	a	21	Total 21	O 21	0	0
18	b	19	Total 19	O 19	0	0

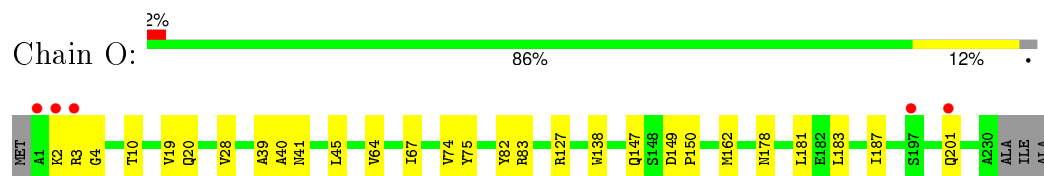
3 Residue-property plots [i](#)

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

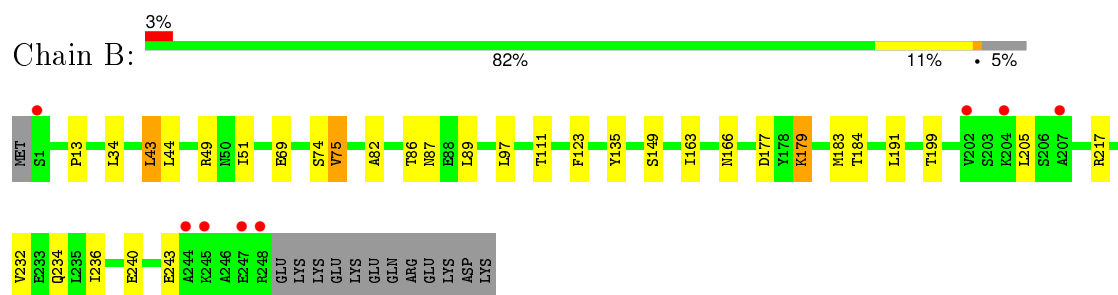
- Molecule 1: Proteasome subunit alpha type-2



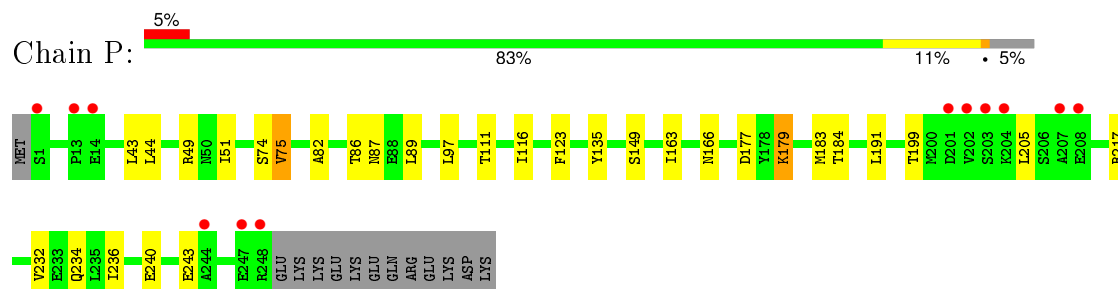
- Molecule 1: Proteasome subunit alpha type-2



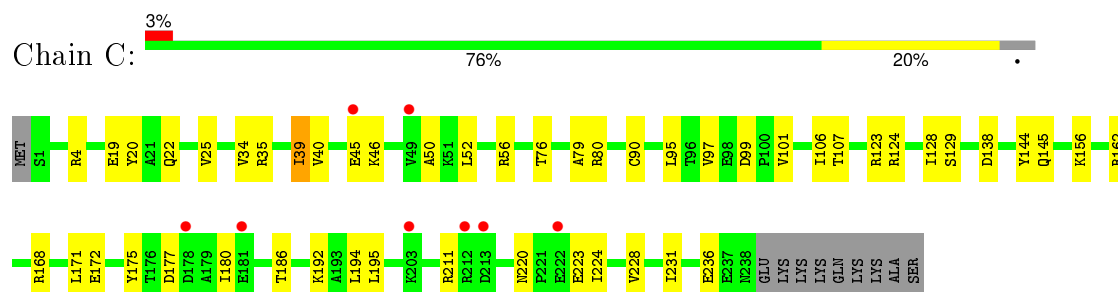
- Molecule 2: Proteasome subunit alpha type-4



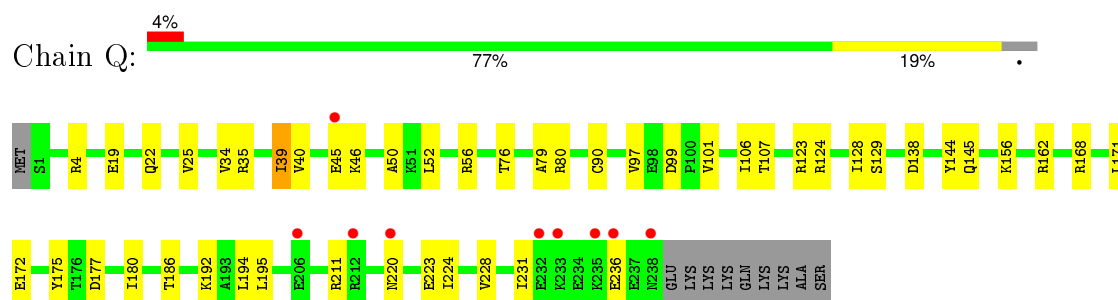
- Molecule 2: Proteasome subunit alpha type-4



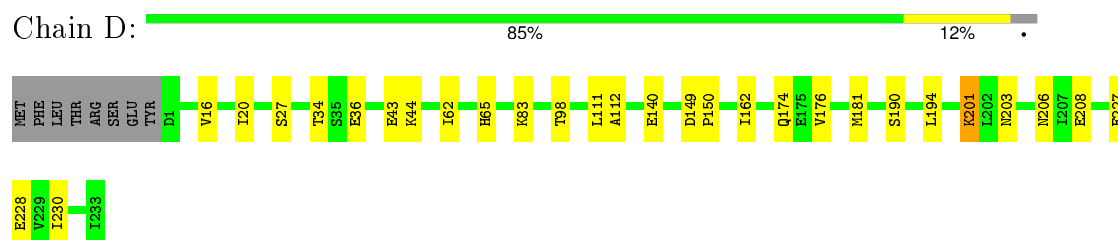
- Molecule 3: Proteasome subunit alpha type-7



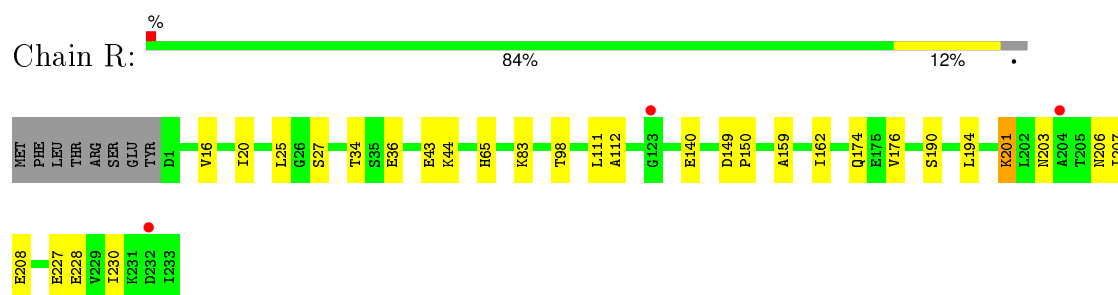
- Molecule 3: Proteasome subunit alpha type-7



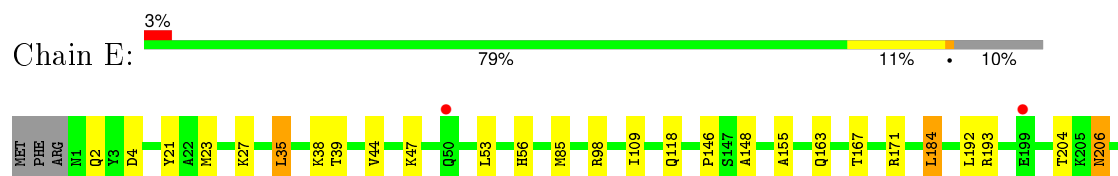
- Molecule 4: Proteasome subunit alpha type-5

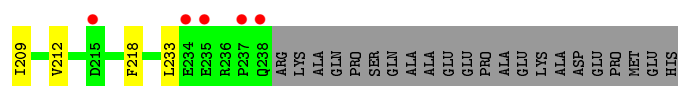


- Molecule 4: Proteasome subunit alpha type-5

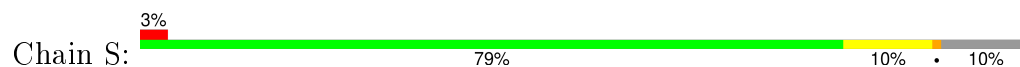


- Molecule 5: Proteasome subunit alpha type-1

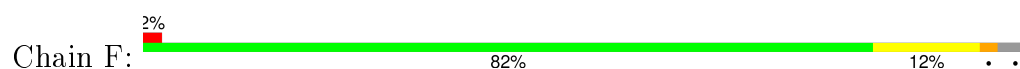




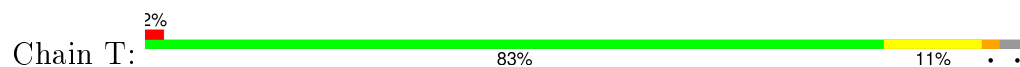
- Molecule 5: Proteasome subunit alpha type-1



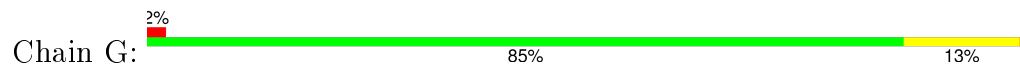
- Molecule 6: Proteasome subunit alpha type-3



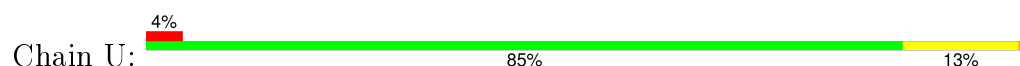
- Molecule 6: Proteasome subunit alpha type-3

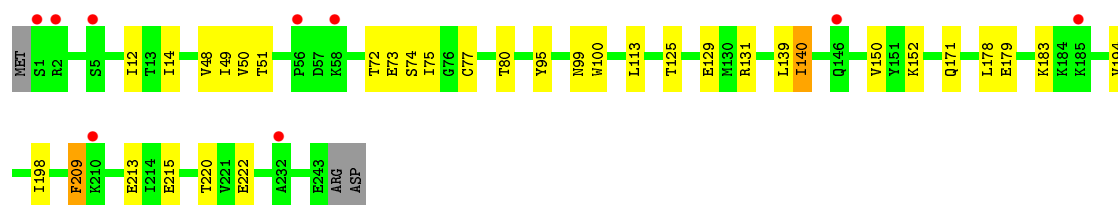


- Molecule 7: Proteasome subunit alpha type-6

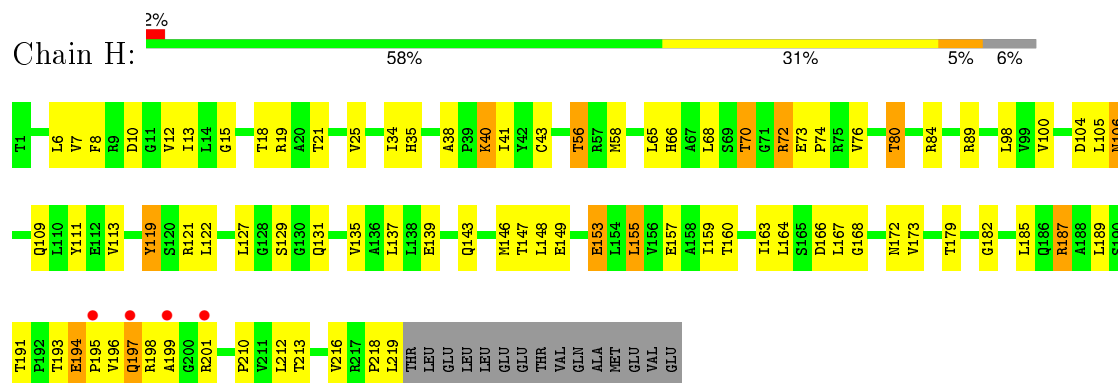


- Molecule 7: Proteasome subunit alpha type-6

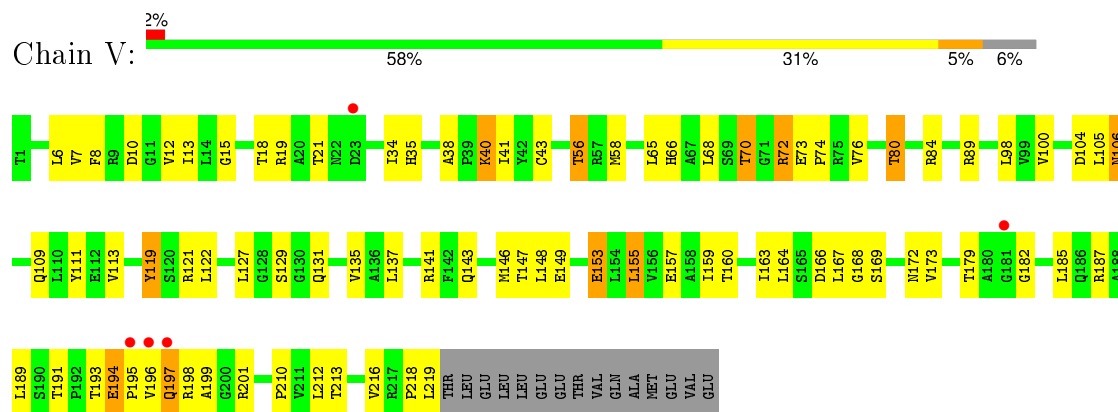




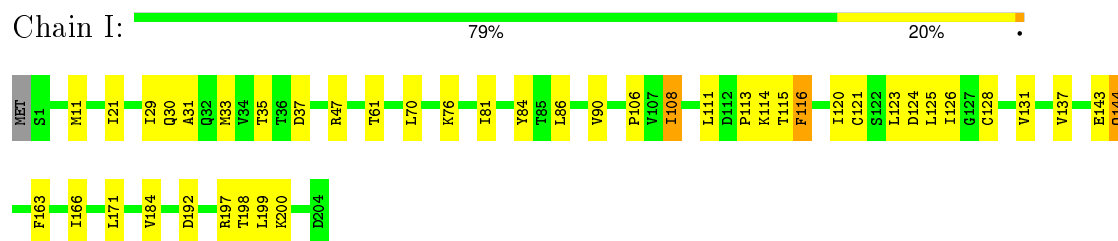
• Molecule 8: Proteasome subunit beta type-10



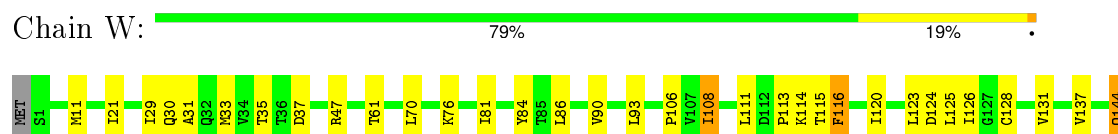
• Molecule 8: Proteasome subunit beta type-10

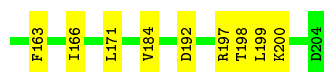


• Molecule 9: Proteasome subunit beta type-3



• Molecule 9: Proteasome subunit beta type-3





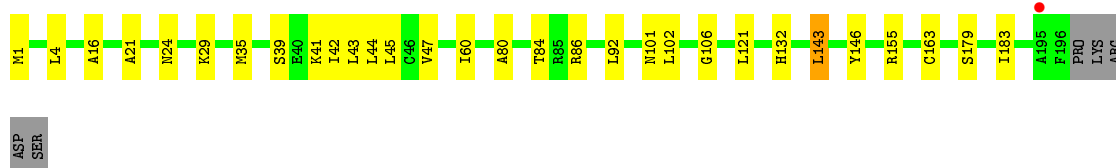
• Molecule 10: Proteasome subunit beta type-2

Chain J: 84% 13% .



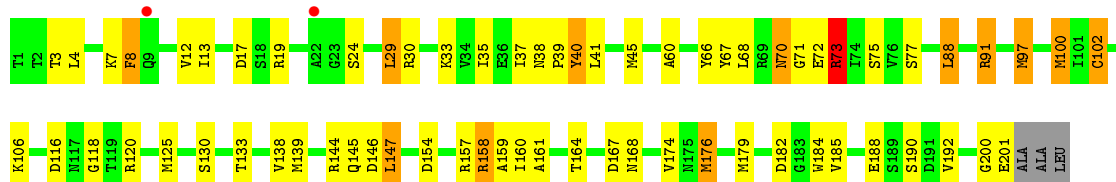
• Molecule 10: Proteasome subunit beta type-2

Chain X: 83% 14% .



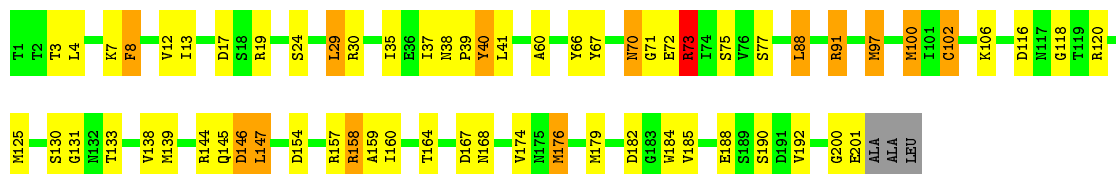
• Molecule 11: Proteasome subunit beta type-8

Chain K: 66% 26% 6% .



• Molecule 11: Proteasome subunit beta type-8

Chain Y: 67% 25% 6% .



• Molecule 12: Proteasome subunit beta type-1

Chain L: 88% 10% .



• Molecule 12: Proteasome subunit beta type-1

Chain Z: 88% 11% .



- Molecule 13: Proteasome subunit beta type-4

Chain M: 86% 11% ..



PHE
GLU

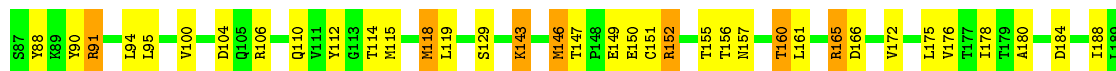
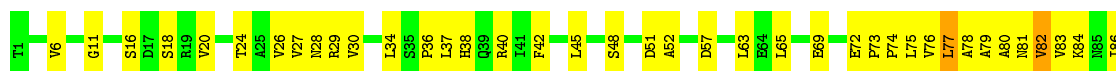
- Molecule 13: Proteasome subunit beta type-4

Chain a: 93% 5% •



- Molecule 14: Proteasome subunit beta type-9

Chain N: 59% 35% 6%



G190, D191, E192, L193, P194, E199

- Molecule 14: Proteasome subunit beta type-9

Chain b: 89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.28Å 205.22Å 161.94Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 29.83 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-3.20) 99.3 (29.83-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.239 , 0.254 0.239 , 0.254	Depositor DCC
R_{free} test set	6015 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 121329 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	49084	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, IOD, 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	0.38	0/1840	0.47	0/2491
1	O	0.38	1/1840 (0.1%)	0.47	0/2491
2	B	0.37	0/1980	0.48	0/2667
2	P	0.37	0/1980	0.48	0/2667
3	C	0.33	0/1903	0.48	0/2569
3	Q	0.33	0/1903	0.48	0/2569
4	D	0.36	0/1804	0.45	0/2437
4	R	0.35	0/1804	0.45	0/2437
5	E	0.37	0/1907	0.48	0/2578
5	S	0.37	0/1907	0.48	0/2578
6	F	0.38	0/1938	0.46	0/2608
6	T	0.38	0/1938	0.46	0/2608
7	G	0.37	1/1924 (0.1%)	0.46	0/2600
7	U	0.37	1/1924 (0.1%)	0.46	0/2600
8	H	0.32	0/1645	0.53	0/2235
8	V	0.32	0/1645	0.53	0/2235
9	I	0.34	0/1620	0.48	0/2185
9	W	0.34	0/1620	0.48	0/2185
10	J	0.33	0/1602	0.47	0/2167
10	X	0.32	0/1602	0.47	0/2167
11	K	0.40	0/1597	0.51	0/2151
11	Y	0.40	0/1597	0.50	0/2151
12	L	0.32	0/1684	0.46	0/2271
12	Z	0.32	0/1684	0.46	0/2271
13	M	0.40	0/1718	0.48	0/2325
13	a	0.40	1/1718 (0.1%)	0.48	0/2325
14	N	0.35	0/1526	0.50	0/2071
14	b	0.35	0/1526	0.50	0/2071
All	All	0.36	4/49376 (0.0%)	0.48	0/66710

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	138	TRP	CD2-CE2	5.08	1.47	1.41
13	a	209	TRP	CD2-CE2	5.06	1.47	1.41
7	G	188	TRP	CD2-CE2	5.05	1.47	1.41
7	U	100	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1801	0	1800	15	0
1	O	1801	0	1800	14	0
2	B	1950	0	1973	18	0
2	P	1950	0	1973	12	0
3	C	1876	0	1902	22	0
3	Q	1876	0	1902	20	0
4	D	1777	0	1767	15	0
4	R	1777	0	1767	15	0
5	E	1872	0	1859	18	0
5	S	1872	0	1858	18	0
6	F	1903	0	1894	20	0
6	T	1903	0	1894	17	0
7	G	1890	0	1900	18	0
7	U	1890	0	1900	19	0
8	H	1619	0	1643	69	0
8	V	1619	0	1643	65	0
9	I	1591	0	1612	23	0
9	W	1591	0	1612	23	0
10	J	1570	0	1573	16	0
10	X	1570	0	1573	17	0
11	K	1566	0	1518	71	0
11	Y	1566	0	1518	69	0
12	L	1653	0	1652	24	0
12	Z	1653	0	1652	26	0
13	M	1685	0	1664	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	1685	0	1664	0	0
14	N	1498	0	1478	59	0
14	b	1498	0	1478	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	E	1	0	0	1	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	2	0	0	0	0
15	O	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	b	2	0	0	0	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	D	1	0	0	0	0
16	E	1	0	0	0	0
16	G	1	0	0	1	0
16	H	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	N	2	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	0	0
16	R	1	0	0	0	0
16	S	1	0	0	1	0
16	U	1	0	0	1	0
16	V	2	0	0	0	0
16	Z	1	0	0	0	0
16	a	2	0	0	0	0
16	b	1	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
17	E	1	0	0	0	0
17	F	1	0	0	0	0
17	H	1	0	0	0	0
17	K	1	0	0	0	0
17	S	1	0	0	0	0
17	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Y	1	0	0	0	0
17	b	1	0	0	0	0
18	A	20	0	0	0	0
18	B	18	0	0	2	0
18	C	24	0	0	0	0
18	D	16	0	0	0	0
18	E	22	0	0	0	0
18	F	17	0	0	0	0
18	G	23	0	0	1	0
18	H	18	0	0	1	0
18	I	18	0	0	0	0
18	J	14	0	0	0	0
18	K	14	0	0	0	0
18	L	22	0	0	0	0
18	M	24	0	0	1	0
18	N	18	0	0	0	0
18	O	10	0	0	0	0
18	P	20	0	0	0	0
18	Q	21	0	0	1	0
18	R	17	0	0	0	0
18	S	23	0	0	2	0
18	T	24	0	0	0	0
18	U	15	0	0	4	0
18	V	14	0	0	0	0
18	W	17	0	0	1	0
18	X	15	0	0	1	0
18	Y	26	0	0	1	0
18	Z	25	0	0	1	0
18	a	21	0	0	0	0
18	b	19	0	0	0	0
All	All	49084	0	48469	650	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (650) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:125:MET:HE2	11:Y:139:MET:HE3	1.21	1.18
11:K:125:MET:HE2	11:K:139:MET:HE3	1.23	1.16
11:K:144:ARG:O	11:K:147:LEU:HD12	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:144:ARG:O	11:Y:147:LEU:HD12	1.57	1.04
14:N:152:ARG:HH21	14:N:152:ARG:HG3	1.26	1.00
14:N:160:THR:HG23	14:N:193:LEU:HD23	1.46	0.98
11:K:138:VAL:HG21	11:K:159:ALA:HA	1.43	0.98
11:Y:138:VAL:HG21	11:Y:159:ALA:HA	1.43	0.97
8:H:199:ALA:HB3	12:Z:173:ARG:CZ	1.96	0.96
11:Y:125:MET:HE2	11:Y:139:MET:CE	1.95	0.95
11:K:125:MET:HE2	11:K:139:MET:CE	1.97	0.95
8:H:131:GLN:O	8:H:135:VAL:HG23	1.68	0.94
12:L:173:ARG:CZ	8:V:199:ALA:HB3	1.98	0.93
8:V:131:GLN:O	8:V:135:VAL:HG23	1.68	0.91
8:H:199:ALA:CB	12:Z:173:ARG:CZ	2.50	0.90
11:K:125:MET:CE	11:K:139:MET:HE3	2.02	0.89
11:Y:125:MET:CE	11:Y:139:MET:HE3	2.01	0.88
12:L:173:ARG:CZ	8:V:199:ALA:CB	2.52	0.88
10:J:60:ILE:HG21	10:J:84:THR:HG22	1.56	0.88
10:X:60:ILE:HG21	10:X:84:THR:HG22	1.55	0.88
8:H:199:ALA:HB3	12:Z:173:ARG:HD2	1.56	0.85
11:K:66:TYR:O	11:K:70:ASN:ND2	2.10	0.84
11:K:37:ILE:C	11:K:38:ASN:HD22	1.81	0.83
11:Y:66:TYR:O	11:Y:70:ASN:ND2	2.11	0.83
11:Y:144:ARG:O	11:Y:147:LEU:CD1	2.26	0.83
14:N:20:VAL:HG23	14:N:27:VAL:HG23	1.61	0.83
8:H:199:ALA:HB3	12:Z:173:ARG:CD	2.09	0.83
8:H:199:ALA:HB3	12:Z:173:ARG:NH1	1.93	0.83
12:L:173:ARG:HD2	8:V:199:ALA:HB3	1.59	0.82
11:K:144:ARG:O	11:K:147:LEU:CD1	2.26	0.82
12:L:173:ARG:NH1	8:V:199:ALA:HB3	1.93	0.82
11:Y:37:ILE:C	11:Y:38:ASN:HD22	1.83	0.82
14:N:72:GLU:HG3	14:N:73:PRO:HD2	1.62	0.81
7:G:152:LYS:NZ	16:G:246:CL:CL	2.51	0.81
13:M:152:GLU:OE1	8:V:141:ARG:NH1	2.14	0.81
14:N:152:ARG:HG3	14:N:152:ARG:NH2	1.91	0.80
8:V:129:SER:OG	8:V:166:ASP:OD2	1.99	0.80
14:N:157:ASN:O	14:N:161:LEU:HD12	1.81	0.79
8:H:84:ARG:NH1	14:N:57:ASP:OD2	2.14	0.79
8:V:212:LEU:HD11	9:W:200:LYS:HA	1.64	0.79
12:L:173:ARG:CD	8:V:199:ALA:HB3	2.13	0.78
8:H:212:LEU:HD11	9:I:200:LYS:HA	1.63	0.78
8:V:40:LYS:HE2	8:V:74:PRO:HD2	1.66	0.77
8:H:199:ALA:HB3	12:Z:173:ARG:NE	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LYS:HE2	8:H:74:PRO:HD2	1.66	0.76
8:H:129:SER:OG	8:H:166:ASP:OD2	2.01	0.76
4:R:201:LYS:H	4:R:201:LYS:HE2	1.51	0.76
14:N:18:SER:OG	14:N:29:ARG:O	2.03	0.76
13:M:35:ARG:NH2	18:M:461:HOH:O	2.18	0.76
4:D:201:LYS:H	4:D:201:LYS:HE2	1.51	0.76
11:K:125:MET:CE	11:K:139:MET:CE	2.61	0.76
14:N:18:SER:OG	14:N:30:VAL:HA	1.86	0.75
7:U:152:LYS:NZ	16:U:246:CL:CL	2.57	0.74
14:N:77:LEU:HD22	14:N:81:ASN:ND2	2.03	0.74
14:N:6:VAL:HG21	14:N:155:THR:HG22	1.69	0.74
8:H:84:ARG:HD3	8:H:119:TYR:HB3	1.71	0.73
11:Y:125:MET:CE	11:Y:139:MET:CE	2.62	0.73
11:Y:138:VAL:HG21	11:Y:159:ALA:CA	2.18	0.73
8:H:199:ALA:CB	12:Z:173:ARG:NE	2.52	0.73
8:V:84:ARG:HD3	8:V:119:TYR:HB3	1.71	0.73
8:V:166:ASP:OD1	8:V:168:GLY:N	2.21	0.73
8:H:166:ASP:OD1	8:H:168:GLY:N	2.22	0.72
12:L:173:ARG:NE	8:V:199:ALA:HB3	2.03	0.72
14:N:6:VAL:CG2	14:N:155:THR:HG22	2.19	0.72
11:K:138:VAL:HG21	11:K:159:ALA:CA	2.19	0.72
14:N:20:VAL:CG2	14:N:27:VAL:HG23	2.20	0.71
7:U:51:THR:HB	18:U:507:HOH:O	1.90	0.71
11:Y:3:THR:HG22	11:Y:100:MET:CE	2.20	0.71
5:S:23:MET:HE3	18:S:506:HOH:O	1.89	0.71
11:K:125:MET:CE	11:K:139:MET:HB3	2.21	0.70
5:E:47:LYS:HB3	5:E:56:HIS:HB3	1.73	0.70
11:K:3:THR:HG22	11:K:100:MET:CE	2.21	0.70
14:N:152:ARG:CG	14:N:152:ARG:HH21	2.03	0.69
5:S:47:LYS:HB3	5:S:56:HIS:HB3	1.73	0.69
11:K:37:ILE:HG22	11:K:38:ASN:ND2	2.08	0.69
8:H:199:ALA:CB	12:Z:173:ARG:HD2	2.22	0.69
12:L:173:ARG:NE	8:V:199:ALA:CB	2.56	0.69
14:N:160:THR:CG2	14:N:193:LEU:HD23	2.22	0.68
11:Y:125:MET:CE	11:Y:139:MET:HB3	2.22	0.68
12:L:173:ARG:HD2	8:V:199:ALA:CB	2.24	0.68
11:Y:37:ILE:HG22	11:Y:38:ASN:ND2	2.09	0.68
8:H:139:GLU:OE2	14:N:29:ARG:NH2	2.27	0.68
1:O:4:GLY:HA2	7:U:129:GLU:HG2	1.74	0.68
1:A:4:GLY:HA2	7:G:129:GLU:HG2	1.74	0.67
14:N:160:THR:HG23	14:N:193:LEU:CD2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:97:MET:H	11:K:116:ASP:HB3	1.59	0.67
13:M:46:ASN:HD22	13:M:48:SER:H	1.42	0.67
11:K:138:VAL:CG2	11:K:159:ALA:HA	2.23	0.67
11:Y:157:ARG:NH1	11:Y:188:GLU:OE2	2.28	0.66
11:K:157:ARG:NH1	11:K:188:GLU:OE2	2.29	0.66
12:L:8:ASN:HD22	12:L:58:HIS:H	1.44	0.65
11:Y:97:MET:H	11:Y:116:ASP:HB3	1.60	0.65
3:Q:35:ARG:HH21	3:Q:156:LYS:HG3	1.61	0.65
11:Y:138:VAL:CG2	11:Y:159:ALA:HA	2.23	0.65
12:Z:8:ASN:HD22	12:Z:58:HIS:H	1.44	0.65
9:W:93:LEU:HG	18:W:473:HOH:O	1.96	0.65
3:C:35:ARG:HH21	3:C:156:LYS:HG3	1.60	0.65
11:K:3:THR:HG22	11:K:100:MET:HE2	1.79	0.65
18:Q:476:HOH:O	4:R:25:LEU:HD11	1.96	0.64
14:N:147:THR:OG1	14:N:150:GLU:HG3	1.96	0.64
11:Y:3:THR:HG22	11:Y:100:MET:HE2	1.80	0.64
11:Y:40:TYR:CZ	11:Y:73:ARG:HD3	2.32	0.64
8:H:66:HIS:O	8:H:70:THR:OG1	2.15	0.64
11:K:40:TYR:CZ	11:K:73:ARG:HD3	2.33	0.64
11:K:40:TYR:CE1	11:K:73:ARG:HD3	2.33	0.64
8:V:66:HIS:O	8:V:70:THR:OG1	2.16	0.64
1:O:149:ASP:HB2	1:O:150:PRO:HD2	1.81	0.63
7:U:49:ILE:HG13	7:U:140:ILE:HD12	1.81	0.63
1:A:149:ASP:HB2	1:A:150:PRO:HD2	1.81	0.63
2:P:87:ASN:HD21	9:W:76:LYS:HE2	1.64	0.63
8:H:160:THR:O	8:H:164:LEU:HD12	1.99	0.63
7:G:49:ILE:HG13	7:G:140:ILE:HD12	1.81	0.63
14:N:20:VAL:HG23	14:N:27:VAL:CG2	2.29	0.63
11:Y:40:TYR:CE1	11:Y:73:ARG:HD3	2.34	0.63
7:U:179:GLU:O	7:U:183:LYS:HG2	1.99	0.63
12:L:13:LEU:HD11	12:L:149:LEU:HD11	1.79	0.62
14:N:188:ILE:HG22	14:N:193:LEU:HD12	1.80	0.62
14:N:151:CYS:O	14:N:155:THR:HG23	1.99	0.62
8:V:160:THR:O	8:V:164:LEU:HD12	1.99	0.62
12:Z:13:LEU:HD11	12:Z:149:LEU:HD11	1.80	0.62
5:S:145:CYS:HB3	18:S:506:HOH:O	1.98	0.62
6:T:39:ILE:HD13	6:T:39:ILE:H	1.63	0.62
2:B:87:ASN:HD21	9:I:76:LYS:HE2	1.64	0.62
8:V:149:GLU:HA	8:V:149:GLU:OE2	2.00	0.61
14:N:77:LEU:HD22	14:N:81:ASN:HD21	1.64	0.61
3:C:192:LYS:HD3	3:C:231:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:130:SER:OG	11:Y:167:ASP:OD2	2.14	0.61
6:F:39:ILE:H	6:F:39:ILE:HD13	1.63	0.61
7:G:179:GLU:O	7:G:183:LYS:HG2	2.01	0.61
11:Y:30:ARG:O	11:Y:30:ARG:HG3	2.00	0.61
8:V:212:LEU:CD1	9:W:200:LYS:HA	2.30	0.61
2:P:135:TYR:HE1	2:P:149:SER:HB2	1.66	0.61
3:Q:39:ILE:HG22	3:Q:211:ARG:HA	1.82	0.61
3:Q:192:LYS:HD3	3:Q:231:ILE:HD11	1.82	0.60
8:H:149:GLU:OE2	8:H:149:GLU:HA	2.00	0.60
4:D:227:GLU:HA	4:D:230:ILE:HG22	1.82	0.60
11:K:174:VAL:HG23	11:K:192:VAL:HG23	1.84	0.60
8:H:187:ARG:NH1	18:H:245:HOH:O	2.34	0.60
4:R:227:GLU:HA	4:R:230:ILE:HG22	1.83	0.60
11:Y:174:VAL:HG23	11:Y:192:VAL:HG23	1.84	0.60
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.84	0.60
2:B:135:TYR:HE1	2:B:149:SER:HB2	1.66	0.59
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.84	0.59
1:A:183:LEU:O	1:A:187:ILE:HD12	2.02	0.59
3:C:39:ILE:HG22	3:C:211:ARG:HA	1.84	0.59
11:K:30:ARG:HG3	11:K:30:ARG:O	2.00	0.59
1:O:183:LEU:O	1:O:187:ILE:HD12	2.02	0.59
11:K:200:GLY:O	11:K:201:GLU:HB2	2.03	0.59
8:V:197:GLN:HA	8:V:197:GLN:OE1	2.03	0.59
8:H:179:THR:HG23	8:H:182:GLY:H	1.68	0.58
12:L:14:ALA:HA	12:L:22:ILE:O	2.04	0.58
4:R:27:SER:HB2	4:R:43:GLU:HG3	1.85	0.58
8:H:212:LEU:CD1	9:I:200:LYS:HA	2.31	0.58
8:H:70:THR:HB	8:H:72:ARG:HG3	1.84	0.58
11:K:88:LEU:O	11:K:91:ARG:HG3	2.03	0.58
8:V:70:THR:HB	8:V:72:ARG:HG3	1.85	0.58
6:T:168:ALA:HB3	6:T:200:VAL:HG13	1.84	0.58
6:F:168:ALA:HB3	6:F:200:VAL:HG13	1.85	0.58
8:V:179:THR:HG23	8:V:182:GLY:H	1.68	0.58
4:D:27:SER:HB2	4:D:43:GLU:HG3	1.85	0.58
11:K:125:MET:HE1	11:K:139:MET:HB3	1.85	0.58
11:Y:200:GLY:O	11:Y:201:GLU:HB2	2.03	0.58
5:E:27:LYS:HG2	15:E:261:IOD:I	2.74	0.58
11:Y:125:MET:HE1	11:Y:139:MET:HB3	1.85	0.57
2:P:166:ASN:HB2	2:P:199:THR:HG23	1.85	0.57
12:L:173:ARG:CD	8:V:199:ALA:CB	2.82	0.57
11:Y:88:LEU:O	11:Y:91:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:84:ARG:CD	8:V:119:TYR:HB3	2.34	0.57
8:H:84:ARG:CD	8:H:119:TYR:HB3	2.34	0.57
14:N:65:LEU:O	14:N:69:GLU:HG3	2.05	0.57
8:H:197:GLN:HA	8:H:197:GLN:OE1	2.03	0.57
8:H:100:VAL:HG13	8:H:111:TYR:HB2	1.86	0.57
8:H:199:ALA:HB2	12:Z:173:ARG:CZ	2.33	0.57
2:B:166:ASN:HB2	2:B:199:THR:HG23	1.85	0.57
10:J:80:ALA:O	10:J:84:THR:HG23	2.05	0.57
8:V:15:GLY:HA3	8:V:159:ILE:CD1	2.35	0.57
11:K:88:LEU:HD13	11:K:118:GLY:HA3	1.87	0.57
6:T:66:LEU:HD22	6:T:212:GLU:HB3	1.85	0.57
8:V:100:VAL:HG13	8:V:111:TYR:HB2	1.87	0.57
12:L:137:ALA:H	12:L:146:GLN:HE21	1.53	0.57
10:J:43:LEU:HD12	10:J:183:ILE:HD11	1.86	0.57
11:Y:88:LEU:HD13	11:Y:118:GLY:HA3	1.87	0.57
8:H:15:GLY:HA3	8:H:159:ILE:CD1	2.35	0.57
12:Z:14:ALA:HA	12:Z:22:ILE:O	2.04	0.57
14:N:40:ARG:NH2	14:N:180:ALA:O	2.34	0.57
10:X:43:LEU:HD12	10:X:183:ILE:HD11	1.86	0.56
6:F:66:LEU:HD22	6:F:212:GLU:HB3	1.86	0.56
12:L:173:ARG:CZ	8:V:199:ALA:HB2	2.36	0.56
12:Z:137:ALA:H	12:Z:146:GLN:HE21	1.54	0.56
10:X:80:ALA:O	10:X:84:THR:HG23	2.06	0.56
12:L:12:VAL:HG21	12:L:53:GLY:HA3	1.86	0.56
13:M:46:ASN:ND2	13:M:48:SER:H	2.04	0.56
12:Z:12:VAL:HG21	12:Z:53:GLY:HA3	1.87	0.56
1:A:45:LEU:HB3	1:A:74:VAL:HG21	1.87	0.56
11:K:8:PHE:N	11:K:8:PHE:CD1	2.74	0.55
9:I:11:MET:HG3	9:I:137:VAL:HG12	1.88	0.55
8:H:199:ALA:CB	12:Z:173:ARG:NH1	2.67	0.55
11:Y:37:ILE:HG22	11:Y:38:ASN:HD22	1.71	0.55
9:W:11:MET:HG3	9:W:137:VAL:HG12	1.87	0.55
14:N:11:GLY:HA3	14:N:178:ILE:O	2.07	0.55
14:N:34:LEU:HD13	14:N:176:VAL:HG13	1.89	0.55
11:K:37:ILE:HG22	11:K:38:ASN:HD22	1.71	0.55
11:Y:8:PHE:N	11:Y:8:PHE:CD1	2.74	0.55
1:O:45:LEU:HB3	1:O:74:VAL:HG21	1.87	0.55
8:H:13:ILE:HG12	8:H:155:LEU:HD22	1.89	0.55
8:V:104:ASP:HB3	8:V:106:ASN:H	1.72	0.55
11:K:30:ARG:O	11:K:30:ARG:CG	2.54	0.55
14:N:175:LEU:HD12	14:N:188:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:13:ILE:HG12	8:V:155:LEU:HD22	1.89	0.54
8:V:80:THR:O	8:V:84:ARG:HG3	2.07	0.54
8:H:80:THR:O	8:H:84:ARG:HG3	2.07	0.54
8:H:104:ASP:HB3	8:H:106:ASN:H	1.72	0.54
4:D:149:ASP:HB2	4:D:150:PRO:HD2	1.88	0.54
3:C:79:ALA:HA	3:C:128:ILE:HD13	1.88	0.54
5:S:35:LEU:HD13	5:S:184:LEU:HD22	1.90	0.54
3:Q:79:ALA:HA	3:Q:128:ILE:HD13	1.88	0.54
7:G:45:ASP:HB3	18:G:253:HOH:O	2.06	0.54
11:K:144:ARG:H	11:K:147:LEU:CD1	2.20	0.54
11:Y:30:ARG:CG	11:Y:30:ARG:O	2.56	0.54
11:K:160:ILE:O	11:K:164:THR:HG23	2.08	0.54
4:R:149:ASP:HB2	4:R:150:PRO:HD2	1.88	0.54
11:K:88:LEU:O	11:K:91:ARG:CG	2.56	0.54
10:X:47:VAL:HG11	18:X:202:HOH:O	2.07	0.54
11:Y:144:ARG:H	11:Y:147:LEU:CD1	2.21	0.54
10:J:86:ARG:HA	10:J:86:ARG:HE	1.72	0.54
4:R:65:HIS:CE1	4:R:98:THR:HB	2.43	0.54
1:A:127:ARG:HH21	7:G:125:THR:HG22	1.72	0.54
4:D:65:HIS:CE1	4:D:98:THR:HB	2.43	0.53
5:E:35:LEU:HD13	5:E:184:LEU:HD22	1.90	0.53
6:F:152:ASP:HB2	6:F:153:PRO:HD2	1.90	0.53
10:X:86:ARG:HE	10:X:86:ARG:HA	1.72	0.53
8:H:84:ARG:HD3	8:H:119:TYR:CB	2.38	0.53
6:T:152:ASP:HB2	6:T:153:PRO:HD2	1.91	0.53
9:W:124:ASP:HB2	9:W:128:CYS:H	1.72	0.53
8:H:76:VAL:CG1	8:H:109:GLN:NE2	2.71	0.53
8:H:199:ALA:CB	12:Z:173:ARG:CD	2.79	0.53
12:L:173:ARG:NH1	8:V:199:ALA:CB	2.67	0.53
13:M:92:LEU:O	13:M:96:MET:HG2	2.09	0.53
11:Y:88:LEU:O	11:Y:91:ARG:CG	2.57	0.53
8:V:76:VAL:CG1	8:V:109:GLN:NE2	2.71	0.53
8:H:15:GLY:HA3	8:H:159:ILE:HD11	1.91	0.53
9:I:124:ASP:HB2	9:I:128:CYS:H	1.73	0.53
6:F:37:ILE:HD11	6:F:176:ILE:HD11	1.91	0.53
3:Q:101:VAL:HG11	3:Q:106:ILE:HG13	1.91	0.53
9:I:47:ARG:HG2	9:I:111:LEU:HB2	1.91	0.53
6:T:37:ILE:HD11	6:T:176:ILE:HD11	1.91	0.53
11:Y:160:ILE:O	11:Y:164:THR:HG23	2.08	0.52
8:V:15:GLY:HA3	8:V:159:ILE:HD11	1.91	0.52
11:K:130:SER:OG	11:K:167:ASP:OD2	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:39:ILE:N	6:T:39:ILE:HD13	2.24	0.52
9:W:47:ARG:HG2	9:W:111:LEU:HB2	1.91	0.52
3:C:101:VAL:HG11	3:C:106:ILE:HG13	1.91	0.52
6:F:39:ILE:N	6:F:39:ILE:HD13	2.24	0.52
11:K:8:PHE:N	11:K:8:PHE:HD1	2.07	0.52
4:R:174:GLN:HA	5:S:53:LEU:HD21	1.92	0.52
5:E:85:MET:HG2	5:E:109:ILE:HD11	1.90	0.52
11:Y:8:PHE:N	11:Y:8:PHE:HD1	2.07	0.52
8:H:76:VAL:HG13	8:H:109:GLN:NE2	2.25	0.52
14:N:45:LEU:HG	14:N:52:ALA:HB1	1.92	0.52
8:V:76:VAL:HG13	8:V:109:GLN:NE2	2.25	0.52
5:S:85:MET:HG2	5:S:109:ILE:HD11	1.91	0.52
2:B:111:THR:HG23	3:C:80:ARG:HD3	1.92	0.51
11:Y:125:MET:CE	11:Y:139:MET:HE2	2.40	0.51
8:V:212:LEU:HD11	9:W:200:LYS:CA	2.38	0.51
13:M:15:LYS:HE2	13:M:135:PRO:HA	1.93	0.51
10:J:39:SER:HB2	10:J:42:ILE:HG12	1.91	0.51
10:X:39:SER:HB2	10:X:42:ILE:HG12	1.91	0.51
11:K:157:ARG:HG3	11:K:176:MET:HE1	1.93	0.51
2:B:69:GLU:HG2	18:U:250:HOH:O	106.15	0.51
11:K:125:MET:CE	11:K:139:MET:HE2	2.40	0.51
11:K:37:ILE:O	11:K:38:ASN:ND2	2.44	0.51
8:V:43:CYS:SG	8:V:98:LEU:HB3	2.51	0.51
9:W:86:LEU:O	9:W:90:VAL:HG23	2.11	0.51
8:H:43:CYS:SG	8:H:98:LEU:HB3	2.51	0.51
8:V:213:THR:HB	9:W:198:THR:OG1	2.11	0.51
8:H:212:LEU:HD11	9:I:200:LYS:CA	2.37	0.50
8:V:194:GLU:OE1	8:V:196:VAL:HG12	2.11	0.50
2:B:34:LEU:HD12	18:B:477:HOH:O	2.10	0.50
9:I:144:GLN:H	9:I:144:GLN:HE21	1.58	0.50
11:K:8:PHE:C	11:K:145:GLN:HE21	2.14	0.50
9:W:144:GLN:H	9:W:144:GLN:HE21	1.58	0.50
8:V:84:ARG:HD3	8:V:119:TYR:CB	2.38	0.50
8:V:35:HIS:CG	8:V:56:THR:HG21	2.47	0.50
8:V:8:PHE:HE1	8:V:10:ASP:HB2	1.76	0.50
14:N:72:GLU:HG3	14:N:73:PRO:CD	2.37	0.50
7:U:215:GLU:HB2	18:U:507:HOH:O	2.11	0.50
11:Y:8:PHE:C	11:Y:145:GLN:HE21	2.14	0.50
13:M:96:MET:HE3	13:M:127:MET:HA	1.94	0.50
10:J:101:ASN:HB3	10:J:132:HIS:CE1	2.47	0.50
8:H:18:THR:HG23	8:H:172:ASN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:193:THR:HG23	13:M:195:LYS:H	1.77	0.50
11:K:29:LEU:HD23	11:K:29:LEU:H	1.77	0.50
11:K:70:ASN:H	11:K:70:ASN:ND2	2.10	0.50
14:N:6:VAL:HG23	14:N:155:THR:HG22	1.94	0.50
9:I:61:THR:HG23	10:J:86:ARG:HH22	1.76	0.50
9:W:61:THR:HG23	10:X:86:ARG:HH22	1.75	0.50
9:I:86:LEU:O	9:I:90:VAL:HG23	2.11	0.50
11:K:154:ASP:O	11:K:158:ARG:HB2	2.12	0.50
11:K:4:LEU:C	11:K:4:LEU:HD12	2.32	0.49
14:N:82:VAL:O	14:N:86:ILE:HG13	2.11	0.49
14:N:90:TYR:HB2	14:N:94:LEU:HD12	1.94	0.49
8:H:194:GLU:OE1	8:H:196:VAL:HG12	2.12	0.49
5:S:44:VAL:HG12	5:S:192:LEU:HD22	1.93	0.49
8:V:18:THR:HG23	8:V:172:ASN:O	2.12	0.49
8:V:40:LYS:H	8:V:40:LYS:HD3	1.77	0.49
8:H:35:HIS:CG	8:H:56:THR:HG21	2.47	0.49
8:H:212:LEU:CD1	9:I:200:LYS:CA	2.90	0.49
5:S:47:LYS:HB2	5:S:206:ASN:HA	1.94	0.49
14:N:190:GLY:HA2	14:N:193:LEU:HD13	1.94	0.49
11:Y:70:ASN:H	11:Y:70:ASN:ND2	2.10	0.49
8:H:40:LYS:H	8:H:40:LYS:HD3	1.77	0.49
5:E:47:LYS:HB2	5:E:206:ASN:HA	1.95	0.49
8:H:8:PHE:HE1	8:H:10:ASP:HB2	1.76	0.49
11:Y:37:ILE:O	11:Y:38:ASN:ND2	2.45	0.49
11:Y:3:THR:HG22	11:Y:100:MET:HE3	1.93	0.49
11:K:144:ARG:H	11:K:147:LEU:HD11	1.76	0.49
11:Y:4:LEU:C	11:Y:4:LEU:HD12	2.32	0.49
2:P:232:VAL:O	2:P:236:ILE:HG12	2.13	0.49
1:A:193:THR:HG23	1:A:195:LYS:H	6.38	0.49
14:N:36:PRO:HB3	14:N:42:PHE:CE1	2.47	0.49
11:K:37:ILE:HG23	11:K:60:ALA:HA	1.95	0.49
5:E:44:VAL:HG12	5:E:192:LEU:HD22	1.93	0.49
10:X:35:MET:HG2	10:X:45:LEU:HD22	1.93	0.49
11:Y:37:ILE:HG23	11:Y:60:ALA:HA	1.95	0.49
10:J:35:MET:HG2	10:J:45:LEU:HD22	1.93	0.49
11:Y:154:ASP:O	11:Y:158:ARG:HB2	2.13	0.49
10:X:101:ASN:HB3	10:X:132:HIS:CE1	2.47	0.49
11:K:19:ARG:NH1	11:K:168:ASN:O	2.46	0.49
14:N:165:ARG:HA	14:N:165:ARG:HD3	1.59	0.48
8:V:212:LEU:CD1	9:W:200:LYS:CA	2.91	0.48
8:H:15:GLY:C	8:H:159:ILE:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:VAL:HG12	3:C:99:ASP:H	1.78	0.48
13:M:192:VAL:HG12	13:M:197:VAL:HG22	1.95	0.48
8:V:15:GLY:C	8:V:159:ILE:CD1	2.82	0.48
3:Q:90:CYS:SG	3:Q:106:ILE:HD11	2.54	0.48
11:K:3:THR:HG22	11:K:100:MET:HE3	1.94	0.48
2:B:135:TYR:HB3	14:N:165:ARG:HG3	83.57	0.48
11:Y:19:ARG:NH1	11:Y:168:ASN:O	2.46	0.48
14:N:79:ALA:O	14:N:83:VAL:HG23	2.14	0.48
5:E:2:GLN:HE22	6:F:5:THR:HA	1.79	0.48
3:Q:97:VAL:HG12	3:Q:99:ASP:H	1.79	0.48
3:Q:34:VAL:HG23	3:Q:175:TYR:HE1	1.79	0.48
11:Y:144:ARG:H	11:Y:147:LEU:HD11	1.77	0.48
3:Q:35:ARG:HA	3:Q:40:VAL:HG13	1.96	0.48
1:O:127:ARG:HH21	7:U:125:THR:HG22	1.77	0.48
6:T:151:ILE:HG12	6:T:157:SER:HB3	1.95	0.48
14:N:156:THR:O	14:N:160:THR:OG1	2.27	0.48
4:D:174:GLN:HA	5:E:53:LEU:HD21	1.96	0.48
14:N:191:ASP:OD1	14:N:191:ASP:N	2.47	0.48
6:F:151:ILE:HG12	6:F:157:SER:HB3	1.96	0.48
2:B:232:VAL:O	2:B:236:ILE:HG12	2.13	0.48
8:H:213:THR:HB	9:I:198:THR:OG1	2.13	0.48
11:K:125:MET:HE1	11:K:139:MET:HE2	1.95	0.47
11:K:67:TYR:O	11:K:71:GLY:HA2	2.14	0.47
3:C:34:VAL:HG23	3:C:175:TYR:HE1	1.79	0.47
3:C:35:ARG:HA	3:C:40:VAL:HG13	1.96	0.47
8:H:153:GLU:O	8:H:157:GLU:HG3	2.14	0.47
4:D:44:LYS:HE2	4:D:208:GLU:HG3	1.97	0.47
4:R:44:LYS:HE2	4:R:208:GLU:HG3	1.97	0.47
11:Y:29:LEU:HD23	11:Y:29:LEU:H	1.78	0.47
11:K:37:ILE:C	11:K:38:ASN:ND2	2.61	0.47
1:A:67:ILE:HG13	1:A:71:ILE:HG22	1.97	0.47
3:C:25:VAL:HG21	3:C:129:SER:HB2	1.96	0.47
10:J:143:LEU:HD13	10:J:163:CYS:SG	2.55	0.47
10:X:21:ALA:HB3	10:X:29:LYS:HB2	1.97	0.47
10:J:21:ALA:HB3	10:J:29:LYS:HB2	1.97	0.47
12:L:8:ASN:HA	12:L:30:SER:O	2.15	0.47
12:Z:8:ASN:HA	12:Z:30:SER:O	2.15	0.47
3:C:90:CYS:SG	3:C:106:ILE:HD11	2.54	0.47
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.96	0.47
2:P:111:THR:HG23	3:Q:80:ARG:HD3	1.96	0.47
11:Y:67:TYR:O	11:Y:71:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ALA:O	1:A:41:ASN:N	2.42	0.47
3:Q:25:VAL:HG21	3:Q:129:SER:HB2	1.95	0.47
11:Y:157:ARG:HG3	11:Y:176:MET:HE1	1.97	0.47
7:U:74:SER:HB2	7:U:75:ILE:HD12	1.97	0.47
11:Y:72:GLU:O	11:Y:73:ARG:CB	2.62	0.47
14:N:75:LEU:HD11	14:N:106:ARG:HH21	1.80	0.47
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.96	0.46
5:S:193:ARG:HH22	5:S:233:LEU:HD12	1.80	0.46
3:Q:180:ILE:HA	3:Q:186:THR:HG23	1.98	0.46
8:V:153:GLU:O	8:V:157:GLU:HG3	2.15	0.46
7:G:74:SER:HB2	7:G:75:ILE:HD12	1.96	0.46
11:K:125:MET:HE1	11:K:139:MET:CE	2.45	0.46
11:K:179:MET:SD	11:K:184:TRP:HB3	2.55	0.46
11:K:72:GLU:O	11:K:73:ARG:CB	2.63	0.46
11:K:29:LEU:N	11:K:29:LEU:CD2	2.79	0.46
4:R:34:THR:HG22	4:R:36:GLU:H	1.80	0.46
6:F:47:PHE:HB2	6:F:214:SER:HB2	1.98	0.46
14:N:76:VAL:HG12	14:N:112:TYR:CE1	2.51	0.46
12:L:99:ARG:HD2	12:L:102:PHE:O	2.16	0.46
6:T:47:PHE:HB2	6:T:214:SER:HB2	1.98	0.46
11:K:125:MET:HE3	11:K:139:MET:HB3	1.97	0.46
7:U:171:GLN:NE2	18:U:247:HOH:O	2.48	0.46
3:C:180:ILE:HA	3:C:186:THR:HG23	1.98	0.46
12:L:173:ARG:NH2	12:L:176:LYS:HD3	2.31	0.46
6:F:113:ASP:O	6:F:117:MET:HG2	2.16	0.46
1:O:39:ALA:O	1:O:41:ASN:N	2.43	0.46
12:Z:173:ARG:NH2	12:Z:176:LYS:HD3	2.31	0.46
7:G:49:ILE:CG1	7:G:140:ILE:HD12	2.46	0.46
11:Y:29:LEU:CD2	11:Y:29:LEU:N	2.79	0.46
14:N:76:VAL:HB	14:N:110:GLN:NE2	2.31	0.46
5:E:148:ALA:HB3	6:F:82:ALA:HB1	1.97	0.46
3:Q:168:ARG:O	3:Q:172:GLU:HG3	2.16	0.46
11:Y:179:MET:SD	11:Y:184:TRP:HB3	2.56	0.46
12:Z:99:ARG:HD2	12:Z:102:PHE:O	2.16	0.46
11:Y:37:ILE:C	11:Y:38:ASN:ND2	2.63	0.45
8:V:210:PRO:HB2	9:W:200:LYS:HB3	1.97	0.45
11:Y:39:PRO:O	11:Y:184:TRP:CD1	2.68	0.45
11:K:39:PRO:O	11:K:184:TRP:CD1	2.69	0.45
8:V:143:GLN:O	8:V:146:MET:CG	2.64	0.45
8:H:148:LEU:HD23	8:H:148:LEU:C	2.36	0.45
10:J:4:LEU:HB2	10:J:132:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:148:LEU:C	8:V:148:LEU:HD23	2.36	0.45
7:G:140:ILE:HG22	7:G:150:VAL:HG22	1.98	0.45
3:C:107:THR:HG21	3:C:144:TYR:HB3	1.98	0.45
4:D:34:THR:HG22	4:D:36:GLU:H	1.80	0.45
6:T:123:THR:O	7:U:131:ARG:NH1	2.50	0.45
10:X:143:LEU:HD13	10:X:163:CYS:SG	2.56	0.45
11:Y:72:GLU:O	11:Y:73:ARG:HB2	2.17	0.45
6:T:168:ALA:HB1	6:T:171:ALA:HB3	1.99	0.45
11:K:77:SER:O	11:K:120:ARG:NH2	2.49	0.45
9:W:108:ILE:N	9:W:108:ILE:HD13	2.31	0.45
1:A:178:ASN:O	1:A:181:LEU:HG	2.17	0.45
3:C:168:ARG:O	3:C:172:GLU:HG3	2.16	0.45
5:E:193:ARG:HH22	5:E:233:LEU:HD12	1.80	0.45
7:G:50:VAL:HG21	7:G:198:ILE:HD13	1.99	0.45
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.52	0.45
9:W:35:THR:HG22	9:W:37:ASP:H	1.81	0.45
7:U:140:ILE:HG22	7:U:150:VAL:HG22	1.99	0.45
6:F:168:ALA:HB1	6:F:171:ALA:HB3	1.99	0.45
13:M:57:TYR:CD2	14:N:118:MET:HE1	2.52	0.45
4:D:176:VAL:O	4:D:176:VAL:HG12	2.17	0.45
5:S:38:LYS:HG3	5:S:39:THR:HG23	1.98	0.45
8:H:84:ARG:HD3	8:H:119:TYR:CG	2.52	0.45
9:I:35:THR:HG22	9:I:37:ASP:H	1.81	0.45
11:Y:125:MET:HE3	11:Y:139:MET:HB3	1.99	0.45
2:B:43:LEU:HD22	18:B:477:HOH:O	2.17	0.45
8:H:143:GLN:O	8:H:146:MET:CG	2.64	0.45
10:X:4:LEU:HB2	10:X:132:HIS:HB2	1.98	0.45
3:Q:224:ILE:O	3:Q:228:VAL:HG23	2.17	0.45
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.52	0.45
11:Y:157:ARG:HH11	11:Y:188:GLU:CD	2.21	0.44
5:E:38:LYS:HG3	5:E:39:THR:HG23	1.99	0.44
5:S:4:ASP:HB2	5:S:21:TYR:CE1	2.52	0.44
5:E:4:ASP:HB2	5:E:21:TYR:CE1	2.52	0.44
8:V:84:ARG:HD3	8:V:119:TYR:CG	2.52	0.44
12:L:8:ASN:ND2	12:L:58:HIS:H	2.11	0.44
4:D:203:ASN:HB3	4:D:206:ASN:HB2	2.00	0.44
6:T:113:ASP:O	6:T:117:MET:HG2	2.16	0.44
4:R:203:ASN:HB3	4:R:206:ASN:HB2	2.00	0.44
3:Q:107:THR:HG21	3:Q:144:TYR:HB3	1.98	0.44
4:R:83:LYS:HD2	4:R:111:LEU:HD11	1.97	0.44
8:H:35:HIS:CB	8:H:56:THR:HG21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:83:LYS:HD2	4:D:111:LEU:HD11	1.98	0.44
7:U:50:VAL:HG21	7:U:198:ILE:HD13	1.99	0.44
7:G:72:THR:HG22	7:G:73:GLU:N	2.32	0.44
11:K:72:GLU:O	11:K:73:ARG:HB2	2.17	0.44
1:A:64:VAL:HG22	1:A:74:VAL:HG22	1.99	0.44
7:U:72:THR:HG22	7:U:73:GLU:N	2.33	0.44
7:G:95:TYR:O	7:G:99:ASN:HB2	2.18	0.44
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.00	0.44
8:V:166:ASP:OD1	8:V:167:LEU:N	2.51	0.44
13:M:46:ASN:HD21	13:M:49:THR:HG22	1.83	0.44
6:F:39:ILE:HD11	6:F:193:VAL:CG2	2.47	0.44
8:V:35:HIS:CB	8:V:56:THR:HG21	2.46	0.44
14:N:114:THR:HA	14:N:118:MET:O	2.16	0.44
8:H:166:ASP:OD1	8:H:167:LEU:N	2.51	0.44
11:K:157:ARG:HH11	11:K:188:GLU:CD	2.21	0.44
11:Y:164:THR:HG21	11:Y:192:VAL:HG21	2.00	0.44
9:W:184:VAL:HB	9:W:199:LEU:HD12	1.98	0.44
1:O:178:ASN:O	1:O:181:LEU:HG	2.17	0.44
9:I:106:PRO:HG2	9:I:123:LEU:HB2	1.98	0.44
9:W:163:PHE:CE1	9:W:197:ARG:HD3	2.53	0.44
6:T:39:ILE:HD11	6:T:193:VAL:CG2	2.47	0.44
11:K:164:THR:HG21	11:K:192:VAL:HG21	2.00	0.44
14:N:176:VAL:HA	14:N:184:ASP:O	2.17	0.44
5:S:167:THR:O	5:S:171:ARG:HG3	2.17	0.44
4:D:16:VAL:O	4:D:20:ILE:HG12	2.17	0.44
14:N:18:SER:HB3	14:N:172:VAL:H	1.83	0.44
9:I:113:PRO:O	9:I:114:LYS:HB2	2.18	0.44
9:I:70:LEU:HD11	9:I:81:ILE:HG21	2.00	0.44
7:U:95:TYR:O	7:U:99:ASN:HB2	2.18	0.44
3:C:224:ILE:O	3:C:228:VAL:HG23	2.18	0.44
3:C:95:LEU:HG	10:J:62:LYS:HG2	2.00	0.44
6:T:83:ASP:OD2	6:T:129:ARG:NH2	2.51	0.44
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.00	0.43
14:N:129:SER:OG	14:N:166:ASP:OD2	2.33	0.43
9:W:106:PRO:HG2	9:W:123:LEU:HB2	1.99	0.43
14:N:80:ALA:HB1	14:N:119:LEU:HD11	2.01	0.43
11:Y:40:TYR:OH	11:Y:73:ARG:HD3	2.18	0.43
8:V:35:HIS:HB3	8:V:56:THR:CG2	2.48	0.43
6:F:83:ASP:OD2	6:F:129:ARG:NH2	2.51	0.43
3:C:50:ALA:C	3:C:52:LEU:H	2.22	0.43
2:P:44:LEU:HD13	2:P:74:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:HD13	2:B:74:SER:HB2	2.00	0.43
12:Z:8:ASN:ND2	12:Z:58:HIS:H	2.11	0.43
7:G:143:ASP:CG	8:H:72:ARG:HH12	2.21	0.43
5:E:44:VAL:HG22	5:E:209:ILE:HG23	1.99	0.43
2:P:86:THR:HA	2:P:89:LEU:HD12	2.00	0.43
11:Y:7:LYS:HB3	11:Y:12:VAL:HG22	2.00	0.43
14:N:78:ALA:O	14:N:82:VAL:HG13	2.18	0.43
8:H:143:GLN:O	8:H:146:MET:HG2	2.18	0.43
9:I:125:LEU:HD12	9:I:126:ILE:HG23	2.00	0.43
3:Q:50:ALA:C	3:Q:52:LEU:H	2.22	0.43
9:W:113:PRO:O	9:W:114:LYS:HB2	2.18	0.43
6:F:34:SER:HB2	6:F:50:GLU:HG3	2.01	0.43
11:K:4:LEU:CD2	11:K:159:ALA:HB3	2.49	0.43
1:A:149:ASP:HB2	1:A:150:PRO:CD	2.49	0.43
1:O:64:VAL:HG22	1:O:74:VAL:HG22	2.00	0.43
8:V:143:GLN:O	8:V:146:MET:HG2	2.19	0.43
3:Q:19:GLU:HA	3:Q:22:GLN:HE21	1.83	0.43
13:M:72:ILE:O	13:M:76:LEU:HG	2.19	0.43
9:W:29:ILE:O	9:W:31:ALA:N	2.52	0.43
4:R:16:VAL:O	4:R:20:ILE:HG12	2.18	0.43
11:Y:125:MET:HE1	11:Y:139:MET:HE2	2.00	0.43
7:U:49:ILE:CG1	7:U:140:ILE:HD12	2.46	0.43
12:L:136:LYS:HA	12:L:146:GLN:HE22	1.84	0.43
14:N:63:LEU:HD21	14:N:79:ALA:HA	1.99	0.43
10:J:44:LEU:HD11	10:J:102:LEU:HD13	2.01	0.43
10:X:44:LEU:HD11	10:X:102:LEU:HD13	2.01	0.43
9:I:184:VAL:HB	9:I:199:LEU:HD12	1.99	0.43
1:O:149:ASP:HB2	1:O:150:PRO:CD	2.48	0.43
2:P:135:TYR:CE1	2:P:149:SER:HB2	2.51	0.43
2:B:86:THR:HA	2:B:89:LEU:HD12	2.01	0.43
9:W:125:LEU:HD12	9:W:126:ILE:HG23	2.00	0.43
9:W:70:LEU:HD11	9:W:81:ILE:HG21	2.00	0.43
6:T:34:SER:HB2	6:T:50:GLU:HG3	2.01	0.43
10:X:146:TYR:HB3	10:X:155:ARG:HH22	1.83	0.43
11:Y:4:LEU:CD2	11:Y:159:ALA:HB3	2.49	0.43
8:V:15:GLY:HA3	8:V:159:ILE:HD12	2.01	0.43
12:Z:136:LYS:HA	12:Z:146:GLN:HE22	1.84	0.43
1:O:45:LEU:HD13	1:O:74:VAL:HG23	2.00	0.43
9:I:163:PHE:CE1	9:I:197:ARG:HD3	2.53	0.43
12:Z:56:GLY:HA2	18:Z:218:HOH:O	2.19	0.43
8:H:35:HIS:HB3	8:H:56:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:2:GLN:HE22	6:T:5:THR:HA	1.83	0.43
11:Y:77:SER:O	11:Y:120:ARG:NH2	2.50	0.43
5:E:212:VAL:HB	5:E:218:PHE:HD1	1.84	0.43
10:J:146:TYR:HB3	10:J:155:ARG:HH22	1.83	0.43
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.54	0.43
5:E:167:THR:O	5:E:171:ARG:HG3	2.17	0.43
5:S:212:VAL:HB	5:S:218:PHE:HD1	1.84	0.42
8:V:189:LEU:HD13	8:V:189:LEU:C	2.38	0.42
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.54	0.42
5:S:44:VAL:HG22	5:S:209:ILE:HG23	1.99	0.42
5:E:118:GLN:HG3	6:F:129:ARG:HG3	1.99	0.42
7:U:77:CYS:HB3	7:U:139:LEU:HD23	2.01	0.42
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.00	0.42
11:K:7:LYS:HB3	11:K:12:VAL:HG22	2.00	0.42
9:I:29:ILE:O	9:I:31:ALA:N	2.52	0.42
4:R:176:VAL:HG12	4:R:176:VAL:O	2.18	0.42
8:H:189:LEU:C	8:H:189:LEU:HD13	2.38	0.42
7:G:77:CYS:HB3	7:G:139:LEU:HD23	2.01	0.42
14:N:149:GLU:HA	14:N:152:ARG:NH2	2.34	0.42
2:P:205:LEU:HD23	2:P:236:ILE:HG23	2.01	0.42
2:B:75:VAL:HG21	2:B:82:ALA:HB1	2.02	0.42
11:Y:144:ARG:NH2	11:Y:146:ASP:O	2.53	0.42
2:B:205:LEU:HD23	2:B:236:ILE:HG23	2.01	0.42
3:C:171:LEU:O	3:C:175:TYR:HB2	2.20	0.42
2:B:123:PHE:HB3	3:C:123:ARG:HB3	2.00	0.42
11:K:40:TYR:CZ	11:K:73:ARG:CD	3.02	0.42
1:A:45:LEU:HD13	1:A:74:VAL:HG23	2.01	0.42
3:Q:171:LEU:O	3:Q:175:TYR:HB2	2.20	0.42
3:C:19:GLU:HA	3:C:22:GLN:HE21	1.83	0.42
10:X:16:ALA:HA	10:X:179:SER:O	2.19	0.42
8:V:218:PRO:C	8:V:219:LEU:HD12	2.39	0.42
14:N:38:HIS:CD2	14:N:74:PRO:HD2	2.54	0.42
6:F:123:THR:O	7:G:131:ARG:NH1	2.52	0.42
8:H:218:PRO:C	8:H:219:LEU:HD12	2.39	0.42
8:H:15:GLY:HA3	8:H:159:ILE:HD12	2.01	0.42
4:R:190:SER:O	4:R:194:LEU:HB2	2.20	0.42
2:P:179:LYS:O	2:P:183:MET:HG2	2.20	0.42
13:M:122:LEU:HG	13:M:137:LEU:HD12	2.01	0.42
2:B:135:TYR:CE1	2:B:149:SER:HB2	2.50	0.42
11:Y:39:PRO:HG2	11:Y:73:ARG:HH21	1.85	0.42
11:K:40:TYR:OH	11:K:73:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:SER:O	4:D:194:LEU:HB2	2.20	0.42
2:B:179:LYS:O	2:B:183:MET:HG2	2.20	0.42
2:P:75:VAL:HG21	2:P:82:ALA:HB1	2.02	0.41
2:B:135:TYR:CD2	14:N:165:ARG:NH1	84.92	0.41
14:N:193:LEU:HA	14:N:194:PRO:HD3	1.96	0.41
11:K:41:LEU:HD23	11:K:102:CYS:O	2.20	0.41
8:H:210:PRO:HB2	9:I:200:LYS:HB3	2.02	0.41
11:Y:8:PHE:C	11:Y:145:GLN:NE2	2.73	0.41
8:V:105:LEU:HD23	8:V:106:ASN:H	1.85	0.41
11:K:33:LYS:HA	11:K:45:MET:HE2	2.02	0.41
10:J:92:LEU:HD11	10:J:121:LEU:HD23	2.02	0.41
11:Y:70:ASN:ND2	11:Y:70:ASN:N	2.67	0.41
8:V:19:ARG:NH1	8:V:167:LEU:O	2.54	0.41
11:K:8:PHE:C	11:K:145:GLN:NE2	2.74	0.41
3:C:45:GLU:OE2	3:C:194:LEU:HB3	2.20	0.41
1:O:10:THR:HG23	1:O:20:GLN:HB2	2.01	0.41
8:V:38:ALA:HB3	8:V:41:ILE:HB	2.03	0.41
11:K:70:ASN:N	11:K:70:ASN:ND2	2.67	0.41
11:K:39:PRO:HG2	11:K:73:ARG:HH21	1.85	0.41
2:B:13:PRO:HA	3:C:20:TYR:CE2	2.55	0.41
12:Z:191:ASP:HA	12:Z:212:LYS:HG2	2.01	0.41
11:K:106:LYS:HE2	11:K:106:LYS:HB3	1.77	0.41
8:H:15:GLY:CA	8:H:159:ILE:HD11	2.50	0.41
8:H:105:LEU:HD23	8:H:106:ASN:H	1.85	0.41
14:N:88:TYR:O	14:N:91:ARG:HG2	2.19	0.41
12:L:191:ASP:HA	12:L:212:LYS:HG2	2.01	0.41
11:Y:41:LEU:HD23	11:Y:102:CYS:O	2.20	0.41
5:S:27:LYS:HG2	16:S:262:CL:CL	2.58	0.41
11:Y:131:GLY:HA3	18:Y:487:HOH:O	2.21	0.41
7:U:12:ILE:HG13	7:U:14:ILE:HG12	2.02	0.41
5:E:23:MET:HA	5:E:146:PRO:HG2	2.02	0.41
14:N:188:ILE:HG23	14:N:192:GLU:HB2	2.03	0.41
12:Z:68:ILE:HD11	12:Z:92:LEU:HD13	2.02	0.41
11:Y:106:LYS:HE2	11:Y:106:LYS:HB3	1.77	0.41
11:Y:167:ASP:OD1	11:Y:168:ASN:N	2.54	0.41
3:Q:45:GLU:OE2	3:Q:194:LEU:HB3	2.20	0.41
8:V:15:GLY:CA	8:V:159:ILE:HD11	2.50	0.41
5:E:155:ALA:O	6:F:57:LEU:HB3	2.20	0.41
8:H:38:ALA:HB3	8:H:41:ILE:HB	2.03	0.41
4:D:62:ILE:O	11:K:68:LEU:HD13	2.21	0.41
10:X:41:LYS:O	10:X:106:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ALA:HA	10:J:179:SER:O	2.19	0.41
8:H:15:GLY:C	8:H:159:ILE:HD11	2.42	0.41
4:R:159:ALA:HB3	5:S:53:LEU:HD12	2.03	0.41
7:U:209:PHE:HB2	7:U:213:GLU:HB2	2.03	0.41
7:G:12:ILE:HG13	7:G:14:ILE:HG12	2.02	0.41
1:A:10:THR:HG23	1:A:20:GLN:HB2	2.02	0.41
12:Z:31:GLU:HB2	12:Z:36:HIS:CD2	2.56	0.41
7:U:48:VAL:HG11	7:U:194:VAL:HA	2.03	0.41
5:S:23:MET:HA	5:S:146:PRO:HG2	2.03	0.40
8:H:194:GLU:CD	8:H:194:GLU:C	2.80	0.40
13:M:149:LEU:HD11	13:M:175:VAL:HG21	2.03	0.40
8:V:8:PHE:HB2	8:V:146:MET:O	2.22	0.40
4:D:34:THR:HG23	4:D:181:MET:O	2.21	0.40
8:H:25:VAL:HG21	9:I:143:GLU:HG2	2.03	0.40
10:X:92:LEU:HD11	10:X:121:LEU:HD23	2.03	0.40
12:L:68:ILE:HD11	12:L:92:LEU:HD13	2.03	0.40
1:O:74:VAL:HG12	1:O:75:TYR:N	2.37	0.40
8:V:194:GLU:CD	8:V:194:GLU:C	2.80	0.40
14:N:143:LYS:O	14:N:146:MET:HG2	2.22	0.40
2:P:123:PHE:HB3	3:Q:123:ARG:HB3	2.02	0.40
12:Z:136:LYS:HA	12:Z:146:GLN:NE2	2.37	0.40
8:H:8:PHE:HB2	8:H:146:MET:O	2.22	0.40
14:N:84:LYS:HD2	14:N:119:LEU:HB2	2.02	0.40
6:F:86:SER:O	6:F:90:ILE:HG12	2.22	0.40
12:L:31:GLU:HB2	12:L:36:HIS:CD2	2.56	0.40
7:G:48:VAL:HG11	7:G:194:VAL:HA	2.04	0.40
7:G:209:PHE:HB2	7:G:213:GLU:HB2	2.03	0.40
9:I:108:ILE:HB	9:I:121:CYS:SG	2.61	0.40
8:V:166:ASP:HB3	8:V:169:SER:HB2	2.03	0.40
8:H:19:ARG:NH1	8:H:167:LEU:O	2.54	0.40
11:K:161:ALA:HA	11:K:192:VAL:HG22	2.03	0.40
6:T:86:SER:O	6:T:90:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/234 (97%)	219 (96%)	8 (4%)	1 (0%)	39	80
1	O	228/234 (97%)	220 (96%)	7 (3%)	1 (0%)	39	80
2	B	246/261 (94%)	241 (98%)	5 (2%)	0	100	100
2	P	246/261 (94%)	241 (98%)	5 (2%)	0	100	100
3	C	236/248 (95%)	227 (96%)	9 (4%)	0	100	100
3	Q	236/248 (95%)	227 (96%)	9 (4%)	0	100	100
4	D	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	39	80
4	R	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	39	80
5	E	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
5	S	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
6	F	242/255 (95%)	236 (98%)	5 (2%)	1 (0%)	39	80
6	T	242/255 (95%)	236 (98%)	5 (2%)	1 (0%)	39	80
7	G	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	U	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
8	H	217/234 (93%)	213 (98%)	3 (1%)	1 (0%)	34	78
8	V	217/234 (93%)	213 (98%)	3 (1%)	1 (0%)	34	78
9	I	202/205 (98%)	192 (95%)	8 (4%)	2 (1%)	19	65
9	W	202/205 (98%)	192 (95%)	8 (4%)	2 (1%)	19	65
10	J	194/201 (96%)	188 (97%)	5 (3%)	1 (0%)	34	78
10	X	194/201 (96%)	188 (97%)	5 (3%)	1 (0%)	34	78
11	K	199/204 (98%)	194 (98%)	4 (2%)	1 (0%)	34	78
11	Y	199/204 (98%)	194 (98%)	4 (2%)	1 (0%)	34	78
12	L	211/213 (99%)	206 (98%)	4 (2%)	1 (0%)	34	78
12	Z	211/213 (99%)	206 (98%)	4 (2%)	1 (0%)	34	78
13	M	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
13	a	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
14	N	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
14	b	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
All	All	6188/6446 (96%)	5999 (97%)	171 (3%)	18 (0%)	46	85

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	216	VAL
8	H	195	PRO
9	I	30	GLN
10	J	24	ASN
6	T	216	VAL
8	V	195	PRO
9	W	30	GLN
10	X	24	ASN
1	A	40	ALA
9	I	116	PHE
1	O	40	ALA
9	W	116	PHE
4	D	112	ALA
11	K	73	ARG
11	Y	73	ARG
12	L	191	ASP
4	R	112	ALA
12	Z	191	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/191 (99%)	182 (96%)	7 (4%)	41	79
1	O	189/191 (99%)	182 (96%)	7 (4%)	41	79
2	B	208/221 (94%)	194 (93%)	14 (7%)	20	60
2	P	208/221 (94%)	193 (93%)	15 (7%)	18	57
3	C	202/211 (96%)	188 (93%)	14 (7%)	19	59
3	Q	202/211 (96%)	188 (93%)	14 (7%)	19	59
4	D	195/203 (96%)	191 (98%)	4 (2%)	61	88
4	R	195/203 (96%)	190 (97%)	5 (3%)	54	85
5	E	204/224 (91%)	198 (97%)	6 (3%)	50	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	204/224 (91%)	198 (97%)	6 (3%)	50	83
6	F	200/211 (95%)	192 (96%)	8 (4%)	38	77
6	T	200/211 (95%)	192 (96%)	8 (4%)	38	77
7	G	207/210 (99%)	200 (97%)	7 (3%)	44	80
7	U	207/210 (99%)	200 (97%)	7 (3%)	44	80
8	H	169/183 (92%)	133 (79%)	36 (21%)	1	7
8	V	169/183 (92%)	133 (79%)	36 (21%)	1	7
9	I	174/175 (99%)	162 (93%)	12 (7%)	19	59
9	W	174/175 (99%)	162 (93%)	12 (7%)	19	59
10	J	166/171 (97%)	164 (99%)	2 (1%)	78	93
10	X	166/171 (97%)	164 (99%)	2 (1%)	78	93
11	K	165/166 (99%)	142 (86%)	23 (14%)	4	20
11	Y	165/166 (99%)	142 (86%)	23 (14%)	4	20
12	L	178/178 (100%)	173 (97%)	5 (3%)	51	84
12	Z	178/178 (100%)	173 (97%)	5 (3%)	51	84
13	M	178/180 (99%)	167 (94%)	11 (6%)	23	64
13	a	178/180 (99%)	167 (94%)	11 (6%)	23	64
14	N	155/155 (100%)	134 (86%)	21 (14%)	5	22
14	b	155/155 (100%)	134 (86%)	21 (14%)	5	22
All	All	5180/5358 (97%)	4838 (93%)	342 (7%)	21	61

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	ARG
1	A	19	VAL
1	A	28	VAL
1	A	67	ILE
1	A	83	ARG
1	A	201	GLN
2	B	43	LEU
2	B	49	ARG
2	B	51	ILE
2	B	75	VAL

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Mol	Chain	Res	Type
2	B	97	LEU
2	B	163	ILE
2	B	177	ASP
2	B	179	LYS
2	B	184	THR
2	B	191	LEU
2	B	217	ARG
2	B	234	GLN
2	B	240	GLU
2	B	243	GLU
3	C	4	ARG
3	C	39	ILE
3	C	46	LYS
3	C	56	ARG
3	C	76	THR
3	C	124	ARG
3	C	138	ASP
3	C	145	GLN
3	C	162	ARG
3	C	177	ASP
3	C	195	LEU
3	C	220	ASN
3	C	223	GLU
3	C	236	GLU
4	D	140	GLU
4	D	162	ILE
4	D	201	LYS
4	D	228	GLU
5	E	35	LEU
5	E	98	ARG
5	E	163	GLN
5	E	184	LEU
5	E	204	THR
5	E	206	ASN
6	F	30	VAL
6	F	39	ILE
6	F	66	LEU
6	F	129	ARG
6	F	181	MET
6	F	205	LYS
6	F	214	SER
6	F	230	ASP

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Mol	Chain	Res	Type
7	G	80	THR
7	G	113	LEU
7	G	140	ILE
7	G	178	LEU
7	G	209	PHE
7	G	220	THR
7	G	222	GLU
8	H	6	LEU
8	H	7	VAL
8	H	12	VAL
8	H	21	THR
8	H	34	ILE
8	H	40	LYS
8	H	56	THR
8	H	58	MET
8	H	65	LEU
8	H	68	LEU
8	H	70	THR
8	H	72	ARG
8	H	73	GLU
8	H	80	THR
8	H	89	ARG
8	H	106	ASN
8	H	113	VAL
8	H	119	TYR
8	H	121	ARG
8	H	122	LEU
8	H	127	LEU
8	H	137	LEU
8	H	147	THR
8	H	153	GLU
8	H	155	LEU
8	H	163	ILE
8	H	173	VAL
8	H	185	LEU
8	H	187	ARG
8	H	191	THR
8	H	193	THR
8	H	194	GLU
8	H	197	GLN
8	H	198	ARG
8	H	201	ARG

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Mol	Chain	Res	Type
8	H	216	VAL
9	I	21	ILE
9	I	33	MET
9	I	84	TYR
9	I	108	ILE
9	I	115	THR
9	I	116	PHE
9	I	120	ILE
9	I	131	VAL
9	I	144	GLN
9	I	166	ILE
9	I	171	LEU
9	I	192	ASP
10	J	1	MET
10	J	143	LEU
11	K	8	PHE
11	K	13	ILE
11	K	17	ASP
11	K	24	SER
11	K	29	LEU
11	K	35	ILE
11	K	40	TYR
11	K	70	ASN
11	K	73	ARG
11	K	75	SER
11	K	88	LEU
11	K	91	ARG
11	K	97	MET
11	K	100	MET
11	K	102	CYS
11	K	133	THR
11	K	146	ASP
11	K	147	LEU
11	K	158	ARG
11	K	176	MET
11	K	182	ASP
11	K	185	VAL
11	K	190	SER
12	L	31	GLU
12	L	133	ASP
12	L	162	GLU
12	L	166	LEU

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Mol	Chain	Res	Type
12	L	173	ARG
13	M	3	ASN
13	M	35	ARG
13	M	39	ILE
13	M	44	ARG
13	M	46	ASN
13	M	49	THR
13	M	94	ARG
13	M	100	ARG
13	M	109	THR
13	M	152	GLU
13	M	168	LEU
14	N	16	SER
14	N	24	THR
14	N	26	VAL
14	N	28	ASN
14	N	37	LEU
14	N	77	LEU
14	N	82	VAL
14	N	91	ARG
14	N	95	LEU
14	N	100	VAL
14	N	104	ASP
14	N	115	MET
14	N	118	MET
14	N	143	LYS
14	N	146	MET
14	N	152	ARG
14	N	160	THR
14	N	165	ARG
14	N	191	ASP
14	N	193	LEU
14	N	199	GLU
1	O	2	LYS
1	O	3	ARG
1	O	19	VAL
1	O	28	VAL
1	O	67	ILE
1	O	83	ARG
1	O	201	GLN
2	P	43	LEU
2	P	49	ARG

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Mol	Chain	Res	Type
2	P	51	ILE
2	P	75	VAL
2	P	97	LEU
2	P	116	ILE
2	P	163	ILE
2	P	177	ASP
2	P	179	LYS
2	P	184	THR
2	P	191	LEU
2	P	217	ARG
2	P	234	GLN
2	P	240	GLU
2	P	243	GLU
3	Q	4	ARG
3	Q	39	ILE
3	Q	46	LYS
3	Q	56	ARG
3	Q	76	THR
3	Q	124	ARG
3	Q	138	ASP
3	Q	145	GLN
3	Q	162	ARG
3	Q	177	ASP
3	Q	195	LEU
3	Q	220	ASN
3	Q	223	GLU
3	Q	236	GLU
4	R	140	GLU
4	R	162	ILE
4	R	201	LYS
4	R	207	ILE
4	R	228	GLU
5	S	35	LEU
5	S	98	ARG
5	S	163	GLN
5	S	184	LEU
5	S	204	THR
5	S	206	ASN
6	T	30	VAL
6	T	39	ILE
6	T	66	LEU
6	T	129	ARG

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Mol	Chain	Res	Type
6	T	181	MET
6	T	205	LYS
6	T	214	SER
6	T	230	ASP
7	U	80	THR
7	U	113	LEU
7	U	140	ILE
7	U	178	LEU
7	U	209	PHE
7	U	220	THR
7	U	222	GLU
8	V	6	LEU
8	V	7	VAL
8	V	12	VAL
8	V	21	THR
8	V	34	ILE
8	V	40	LYS
8	V	56	THR
8	V	58	MET
8	V	65	LEU
8	V	68	LEU
8	V	70	THR
8	V	72	ARG
8	V	73	GLU
8	V	80	THR
8	V	89	ARG
8	V	106	ASN
8	V	113	VAL
8	V	119	TYR
8	V	121	ARG
8	V	122	LEU
8	V	127	LEU
8	V	137	LEU
8	V	147	THR
8	V	153	GLU
8	V	155	LEU
8	V	163	ILE
8	V	173	VAL
8	V	185	LEU
8	V	187	ARG
8	V	191	THR
8	V	193	THR

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Mol	Chain	Res	Type
8	V	194	GLU
8	V	197	GLN
8	V	198	ARG
8	V	201	ARG
8	V	216	VAL
9	W	21	ILE
9	W	33	MET
9	W	84	TYR
9	W	108	ILE
9	W	115	THR
9	W	116	PHE
9	W	120	ILE
9	W	131	VAL
9	W	144	GLN
9	W	166	ILE
9	W	171	LEU
9	W	192	ASP
10	X	1	MET
10	X	143	LEU
11	Y	8	PHE
11	Y	13	ILE
11	Y	17	ASP
11	Y	24	SER
11	Y	29	LEU
11	Y	35	ILE
11	Y	40	TYR
11	Y	70	ASN
11	Y	73	ARG
11	Y	75	SER
11	Y	88	LEU
11	Y	91	ARG
11	Y	97	MET
11	Y	100	MET
11	Y	102	CYS
11	Y	133	THR
11	Y	146	ASP
11	Y	147	LEU
11	Y	158	ARG
11	Y	176	MET
11	Y	182	ASP
11	Y	185	VAL
11	Y	190	SER

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Mol	Chain	Res	Type
12	Z	31	GLU
12	Z	133	ASP
12	Z	162	GLU
12	Z	166	LEU
12	Z	173	ARG
13	a	3	ASN
13	a	35	ARG
13	a	39	ILE
13	a	44	ARG
13	a	46	ASN
13	a	49	THR
13	a	94	ARG
13	a	100	ARG
13	a	109	THR
13	a	152	GLU
13	a	168	LEU
14	b	16	SER
14	b	24	THR
14	b	26	VAL
14	b	28	ASN
14	b	37	LEU
14	b	77	LEU
14	b	82	VAL
14	b	91	ARG
14	b	95	LEU
14	b	100	VAL
14	b	104	ASP
14	b	115	MET
14	b	118	MET
14	b	143	LYS
14	b	146	MET
14	b	152	ARG
14	b	160	THR
14	b	165	ARG
14	b	191	ASP
14	b	193	LEU
14	b	199	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS

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Mol	Chain	Res	Type
1	A	111	GLN
1	A	139	ASN
1	A	165	ASN
1	A	206	ASN
2	B	39	ASN
2	B	87	ASN
2	B	94	GLN
2	B	122	GLN
2	B	154	ASN
3	C	22	GLN
3	C	91	GLN
3	C	220	ASN
4	D	106	GLN
4	D	174	GLN
4	D	196	GLN
4	D	213	GLN
5	E	2	GLN
5	E	143	GLN
7	G	89	GLN
7	G	126	GLN
8	H	66	HIS
8	H	106	ASN
8	H	109	GLN
8	H	143	GLN
9	I	6	ASN
9	I	39	GLN
9	I	64	GLN
9	I	144	GLN
10	J	27	GLN
10	J	61	GLN
10	J	174	ASN
11	K	53	GLN
11	K	70	ASN
11	K	117	ASN
11	K	145	GLN
12	L	8	ASN
12	L	108	ASN
12	L	131	GLN
12	L	146	GLN
12	L	163	HIS
13	M	46	ASN
13	M	104	ASN

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Mol	Chain	Res	Type
13	M	108	ASN
13	M	157	GLN
14	N	28	ASN
14	N	38	HIS
14	N	81	ASN
14	N	157	ASN
14	N	164	ASN
1	O	87	HIS
1	O	111	GLN
1	O	139	ASN
1	O	206	ASN
2	P	39	ASN
2	P	87	ASN
2	P	94	GLN
2	P	122	GLN
2	P	154	ASN
3	Q	22	GLN
3	Q	91	GLN
3	Q	220	ASN
4	R	106	GLN
4	R	174	GLN
4	R	196	GLN
4	R	213	GLN
5	S	143	GLN
7	U	89	GLN
7	U	126	GLN
7	U	171	GLN
8	V	66	HIS
8	V	106	ASN
8	V	109	GLN
8	V	143	GLN
9	W	6	ASN
9	W	39	GLN
9	W	64	GLN
9	W	80	GLN
9	W	144	GLN
10	X	27	GLN
10	X	61	GLN
10	X	174	ASN
11	Y	10	HIS
11	Y	38	ASN
11	Y	70	ASN

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Mol	Chain	Res	Type
11	Y	117	ASN
11	Y	145	GLN
12	Z	8	ASN
12	Z	77	HIS
12	Z	108	ASN
12	Z	131	GLN
12	Z	146	GLN
12	Z	163	HIS
13	a	46	ASN
13	a	104	ASN
13	a	108	ASN
13	a	157	GLN
13	a	208	ASN
14	b	28	ASN
14	b	38	HIS
14	b	157	ASN
14	b	164	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 47 ligands modelled in this entry, 47 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/234 (98%)	0.00	5 (2%) 65 50	58, 92, 140, 157	0
1	O	230/234 (98%)	0.00	5 (2%) 65 50	59, 90, 134, 147	0
2	B	248/261 (95%)	-0.07	8 (3%) 51 36	55, 86, 155, 209	0
2	P	248/261 (95%)	0.00	12 (4%) 34 21	56, 88, 149, 188	0
3	C	238/248 (95%)	0.07	8 (3%) 49 34	50, 89, 165, 230	0
3	Q	238/248 (95%)	0.16	9 (3%) 44 29	54, 99, 172, 252	0
4	D	233/241 (96%)	-0.09	0 100 100	49, 83, 136, 175	0
4	R	233/241 (96%)	-0.01	3 (1%) 79 67	59, 95, 151, 191	0
5	E	238/263 (90%)	-0.00	7 (2%) 55 41	53, 85, 135, 172	0
5	S	238/263 (90%)	-0.03	7 (2%) 55 41	49, 80, 136, 160	0
6	F	244/255 (95%)	0.01	5 (2%) 68 54	54, 91, 138, 160	0
6	T	244/255 (95%)	-0.02	6 (2%) 61 47	49, 81, 125, 141	0
7	G	243/246 (98%)	0.06	5 (2%) 67 52	62, 98, 157, 198	0
7	U	243/246 (98%)	0.01	9 (3%) 45 30	59, 88, 137, 166	0
8	H	219/234 (93%)	-0.24	4 (1%) 71 58	39, 72, 123, 151	0
8	V	219/234 (93%)	-0.22	5 (2%) 64 49	36, 70, 116, 147	0
9	I	204/205 (99%)	-0.33	0 100 100	42, 61, 103, 127	0
9	W	204/205 (99%)	-0.30	0 100 100	46, 65, 107, 132	0
10	J	196/201 (97%)	-0.35	1 (0%) 91 87	45, 62, 89, 113	0
10	X	196/201 (97%)	-0.28	1 (0%) 91 87	47, 65, 98, 118	0
11	K	201/204 (98%)	-0.38	2 (0%) 84 75	34, 59, 92, 104	0
11	Y	201/204 (98%)	-0.31	0 100 100	39, 65, 99, 111	0
12	L	213/213 (100%)	-0.27	0 100 100	43, 61, 90, 118	0
12	Z	213/213 (100%)	-0.34	1 (0%) 91 87	44, 57, 88, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.39	1 (0%) 91 87	42, 61, 94, 108	0
13	a	216/219 (98%)	-0.40	0 100 100	41, 57, 87, 117	0
14	N	199/199 (100%)	-0.40	0 100 100	35, 63, 92, 102	0
14	b	199/199 (100%)	-0.36	0 100 100	37, 64, 92, 101	0
All	All	6244/6446 (96%)	-0.15	104 (1%) 73 60	34, 75, 138, 252	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	1	SER	7.4
6	F	1	SER	7.2
5	E	238	GLN	6.7
7	U	1	SER	6.7
6	F	2	SER	6.5
6	T	5	THR	6.2
7	G	1	SER	5.8
5	S	238	GLN	5.3
7	G	2	ARG	5.3
3	Q	232	GLU	5.3
7	U	2	ARG	5.1
2	B	248	ARG	4.9
2	P	244	ALA	4.9
2	P	203	SER	4.5
5	E	237	PRO	4.3
6	T	4	GLY	4.3
3	C	212	ARG	4.2
3	Q	236	GLU	4.1
1	A	180	ASP	3.6
3	C	181	GLU	3.6
2	P	202	VAL	3.5
3	Q	206	GLU	3.4
8	H	199	ALA	3.4
5	E	50	GLN	3.3
5	S	198	ALA	3.3
2	P	248	ARG	3.2
8	H	195	PRO	3.2
10	X	195	ALA	3.2
2	P	247	GLU	3.2
5	S	199	GLU	3.2
5	S	237	PRO	3.2
2	P	208	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	P	1	SER	3.1
3	C	45	GLU	3.1
8	V	197	GLN	3.1
6	T	3	ILE	3.1
1	O	1	ALA	3.0
3	C	49	VAL	3.0
1	A	52	LYS	3.0
3	Q	45	GLU	3.0
1	O	197	SER	3.0
3	Q	233	LYS	3.0
2	B	244	ALA	2.9
1	O	3	ARG	2.9
5	S	201	ASP	2.8
6	F	5	THR	2.8
10	J	195	ALA	2.8
6	T	2	SER	2.8
3	Q	235	LYS	2.8
7	U	146	GLN	2.8
2	B	202	VAL	2.7
3	C	222	GLU	2.7
4	R	123	GLY	2.7
7	U	5	SER	2.7
12	Z	1	ARG	2.6
2	P	201	ASP	2.6
6	T	143	ASN	2.6
3	Q	212	ARG	2.6
7	G	243	GLU	2.5
5	E	215	ASP	2.5
2	B	1	SER	2.5
3	Q	220	ASN	2.5
1	O	201	GLN	2.5
6	F	207	LYS	2.5
8	V	195	PRO	2.5
5	E	235	GLU	2.5
8	V	181	GLY	2.5
3	C	178	ASP	2.5
2	P	13	PRO	2.4
8	V	196	VAL	2.4
7	U	185	LYS	2.4
3	C	203	LYS	2.4
5	E	199	GLU	2.4
7	U	56	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	213	ASP	2.3
8	V	23	ASP	2.3
6	F	199	ILE	2.3
7	U	210	LYS	2.3
7	U	232	ALA	2.3
1	A	3	ARG	2.3
2	P	204	LYS	2.3
7	G	5	SER	2.2
5	S	5	ASN	2.2
7	U	58	LYS	2.2
2	B	207	ALA	2.2
5	S	197	PRO	2.2
7	G	10	ARG	2.2
1	A	201	GLN	2.2
13	M	206	GLN	2.1
8	H	197	GLN	2.1
1	O	2	LYS	2.1
2	P	207	ALA	2.1
11	K	9	GLN	2.1
2	B	204	LYS	2.1
11	K	22	ALA	2.1
4	R	204	ALA	2.1
8	H	201	ARG	2.1
2	P	14	GLU	2.1
4	R	232	ASP	2.0
2	B	247	GLU	2.0
1	A	1	ALA	2.0
2	B	245	LYS	2.0
3	Q	238	ASN	2.0
5	E	234	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
16	CL	S	262	1/1	0.98	0.23	0.73	30,30,30,30	0
16	CL	N	202	1/1	0.94	0.20	0.69	24,24,24,24	0
17	K	H	236	1/1	0.92	0.19	0.35	30,30,30,30	0
16	CL	V	236	1/1	0.98	0.20	0.16	27,27,27,27	0
16	CL	R	234	1/1	0.87	0.18	0.04	56,56,56,56	0
16	CL	G	246	1/1	0.83	0.18	-0.11	28,28,28,28	0
16	CL	A	235	1/1	0.96	0.22	-0.58	23,23,23,23	0
16	CL	b	203	1/1	0.93	0.15	-0.78	23,23,23,23	0
16	CL	Q	248	1/1	0.97	0.22	-0.94	34,34,34,34	0
16	CL	N	203	1/1	0.94	0.17	-1.11	33,33,33,33	0
16	CL	H	237	1/1	0.99	0.13	-1.21	29,29,29,29	0
16	CL	K	207	1/1	0.97	0.08	-1.47	27,27,27,27	0
17	K	T	255	1/1	0.82	0.10	-1.71	40,40,40,40	0
17	K	Y	206	1/1	0.95	0.10	-1.81	29,29,29,29	0
16	CL	E	263	1/1	0.99	0.10	-1.82	42,42,42,42	0
17	K	D	234	1/1	0.92	0.11	-2.02	42,42,42,42	0
17	K	b	202	1/1	0.95	0.12	-2.10	30,30,30,30	0
17	K	E	262	1/1	0.90	0.08	-2.12	46,46,46,46	0
16	CL	V	237	1/1	1.00	0.13	-2.29	20,20,20,20	0
16	CL	U	246	1/1	0.72	0.15	-2.34	30,30,30,30	0
16	CL	D	235	1/1	0.98	0.12	-2.43	41,41,41,41	0
15	IOD	E	261	1/1	0.99	0.07	-2.50	92,92,92,92	0
16	CL	Q	249	1/1	0.97	0.20	-	35,35,35,35	0
17	K	C	249	1/1	0.95	0.12	-	36,36,36,36	0
16	CL	M	220	1/1	0.96	0.16	-	31,31,31,31	0
16	CL	a	221	1/1	0.99	0.06	-	20,20,20,20	0
17	K	F	255	1/1	0.90	0.09	-	48,48,48,48	0
15	IOD	N	201	1/1	0.99	0.24	-	168,168,168,168	0
15	IOD	b	201	1/1	0.99	0.09	-	82,82,82,82	0
15	IOD	I	205	1/1	0.99	0.06	-	79,79,79,79	0
16	CL	Z	214	1/1	0.97	0.06	-	24,24,24,24	0
15	IOD	V	235	1/1	0.99	0.03	-	68,68,68,68	0
15	IOD	O	234	1/1	0.99	0.06	-	83,83,83,83	0
15	IOD	C	248	1/1	0.99	0.07	-	86,86,86,86	0
17	K	K	206	1/1	0.94	0.12	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	CL	P	261	1/1	0.94	0.07	-	27,27,27,27	0
15	IOD	H	235	1/1	0.99	0.03	-	59,59,59,59	0
16	CL	a	220	1/1	0.96	0.19	-	41,41,41,41	0
16	CL	L	214	1/1	0.98	0.13	-	28,28,28,28	0
15	IOD	Y	205	1/1	1.00	0.07	-	69,69,69,69	0
15	IOD	b	200	1/1	0.99	0.10	-	30,30,30,30	0
16	CL	B	261	1/1	0.96	0.09	-	34,34,34,34	0
15	IOD	A	234	1/1	0.99	0.11	-	76,76,76,76	0
15	IOD	K	205	1/1	1.00	0.02	-	64,64,64,64	0
15	IOD	W	205	1/1	0.99	0.09	-	83,83,83,83	0
15	IOD	N	200	1/1	0.99	0.03	-	49,49,49,49	0
17	K	S	261	1/1	0.91	0.12	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.