



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 04:32 am GMT

PDB ID : 4R3O
Title : Human Constitutive 20S Proteasome
Authors : Sacchettini, J.C.; Harshbarger, W.H.
Deposited on : 2014-08-16
Resolution : 2.60 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
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

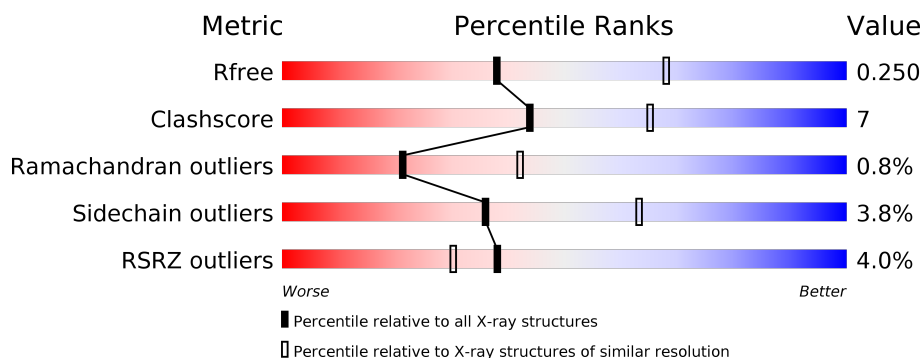
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.






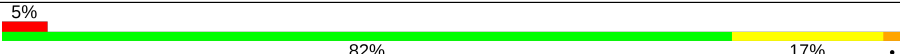
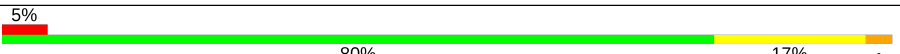
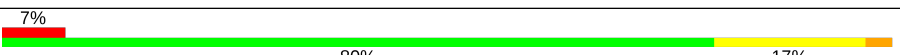
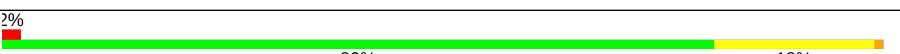
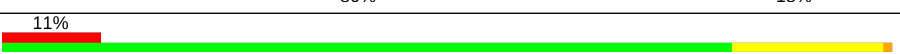

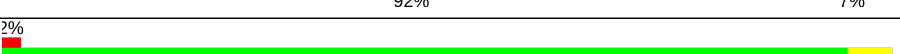
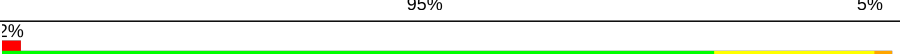
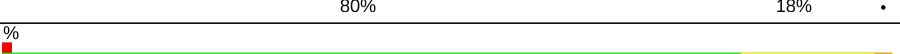
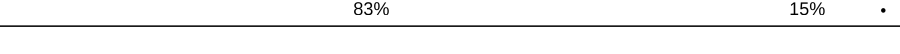
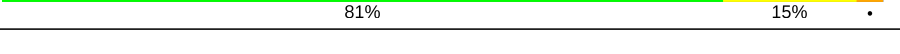
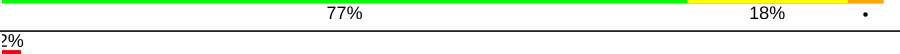







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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	244	<div> <div>3%</div> <div>76%</div> <div>22%</div> <div>•</div> </div>
1	O	244	<div> <div>9%</div> <div>83%</div> <div>16%</div> <div>•</div> </div>
2	B	233	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>
2	P	233	<div> <div>2%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>
3	C	250	<div> <div>5%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>
3	Q	250	<div> <div>7%</div> <div>84%</div> <div>15%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	243	
4	R	243	
5	E	234	
5	S	234	
6	F	238	
6	T	238	
7	G	245	
7	U	245	
8	H	202	
8	V	202	
9	I	220	
9	W	220	
10	J	204	
10	X	204	
11	K	199	
11	Y	199	
12	L	201	
12	Z	201	
13	1	213	
13	M	213	
14	2	217	
14	N	217	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47831 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			
1	O	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1707	1081	287	334	5			
2	P	233	Total	C	N	O	S	0	0	0
			1712	1085	287	334	6			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			1912	1204	329	371	8			
3	Q	250	Total	C	N	O	S	0	0	0
			1913	1203	330	372	8			

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1724	1068	312	339	5			
4	R	243	Total	C	N	O	S	0	0	0
			1691	1051	309	327	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	S	234	Total	C	N	O	S	0	0	0
			1716	1102	290	313	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	T	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	U	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	V	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	W	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			

- 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
			1585	1010	262	294	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	Y	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	Z	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1641	1036	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1644	1039	282	313	10			

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1676	1057	287	320	12			
14	2	217	Total	C	N	O	S	0	0	0
			1678	1058	290	318	12			

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	O	0	0
			2	2		
15	D	4	Total	O	0	0
			4	4		

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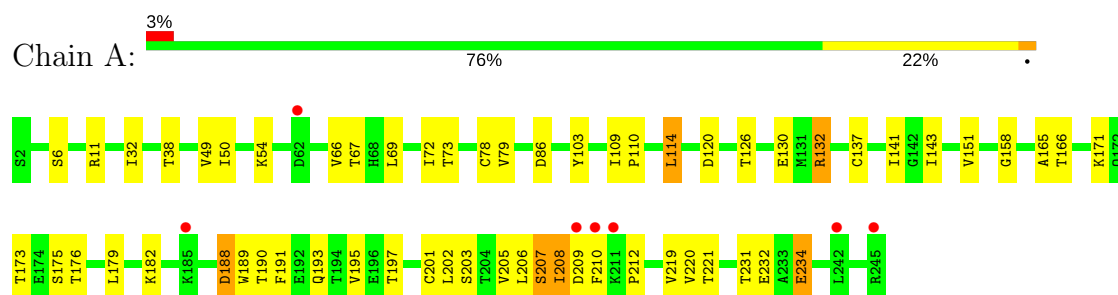
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	E	8	Total 8	O 8	0	0
15	F	19	Total 19	O 19	0	0
15	G	1	Total 1	O 1	0	0
15	K	9	Total 9	O 9	0	0
15	L	8	Total 8	O 8	0	0
15	M	34	Total 34	O 34	0	0
15	N	11	Total 11	O 11	0	0
15	O	1	Total 1	O 1	0	0
15	P	24	Total 24	O 24	0	0
15	Q	10	Total 10	O 10	0	0
15	R	5	Total 5	O 5	0	0
15	W	17	Total 17	O 17	0	0
15	X	25	Total 25	O 25	0	0
15	Y	3	Total 3	O 3	0	0
15	Z	4	Total 4	O 4	0	0

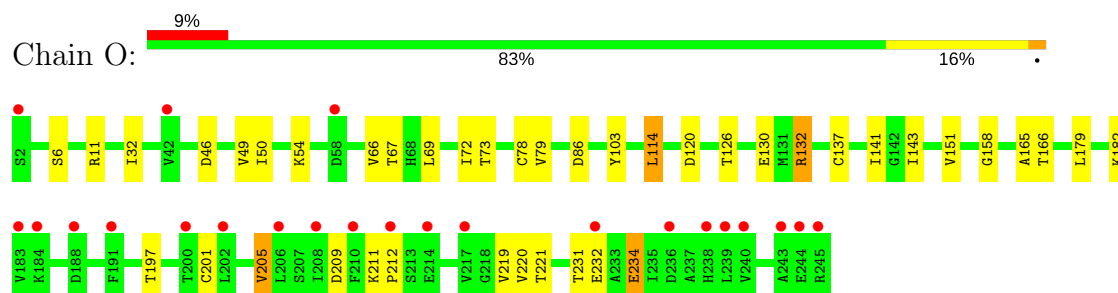
3 Residue-property plots [i](#)

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.

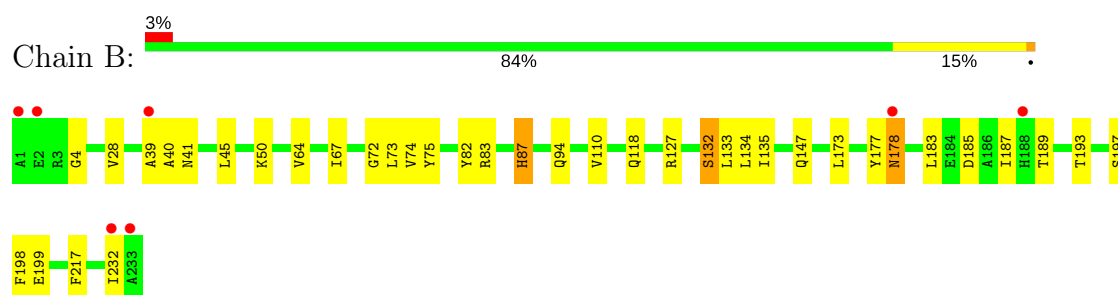
- Molecule 1: Proteasome subunit alpha type-6



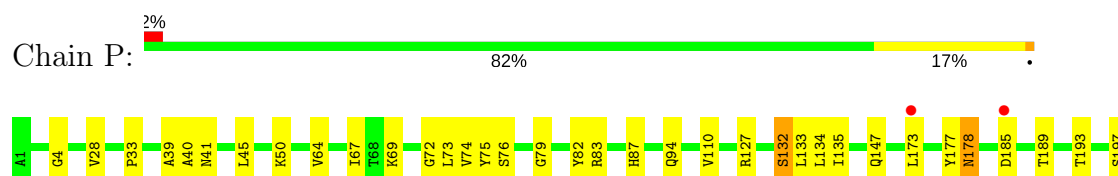
- Molecule 1: Proteasome subunit alpha type-6

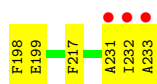


- Molecule 2: Proteasome subunit alpha type-2

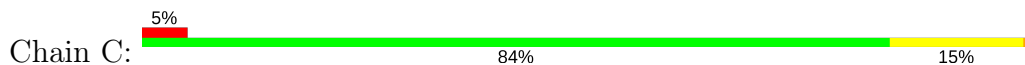


- Molecule 2: Proteasome subunit alpha type-2

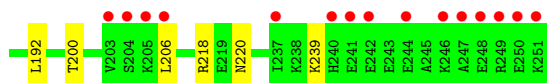
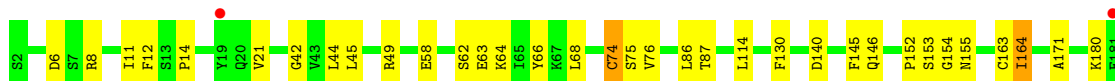
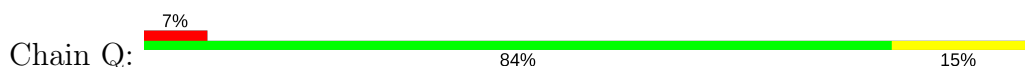




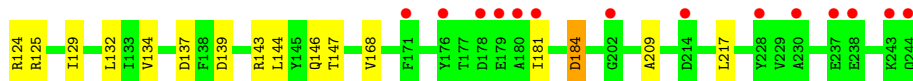
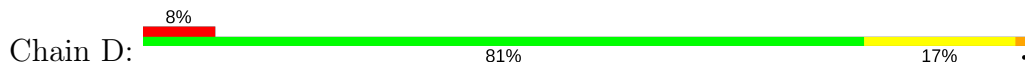
• Molecule 3: Proteasome subunit alpha type-4



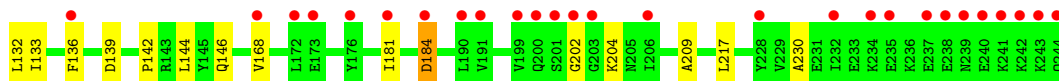
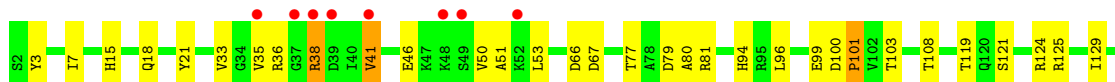
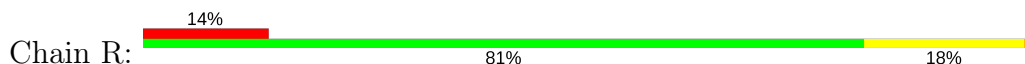
• Molecule 3: Proteasome subunit alpha type-4



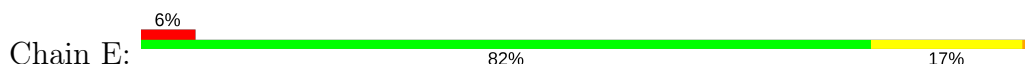
• Molecule 4: Proteasome subunit alpha type-7

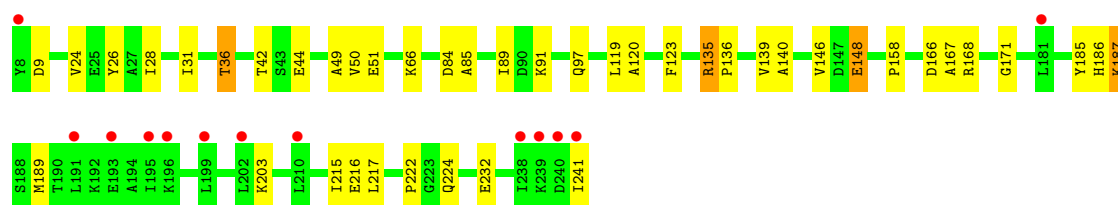


• Molecule 4: Proteasome subunit alpha type-7

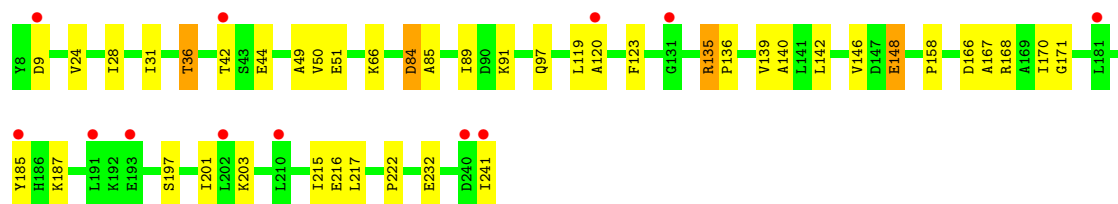
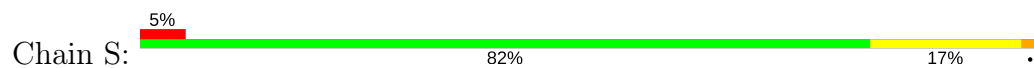


• Molecule 5: Proteasome subunit alpha type-5

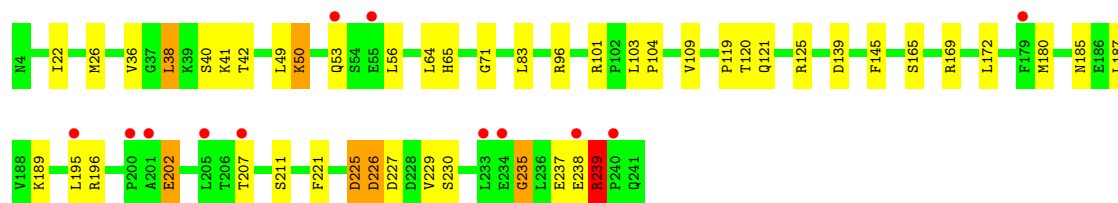
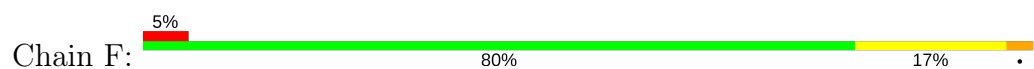




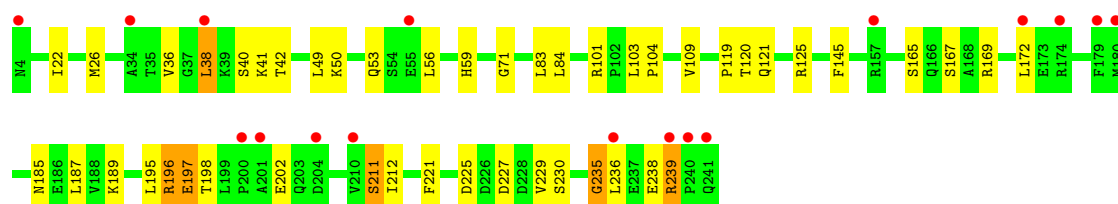
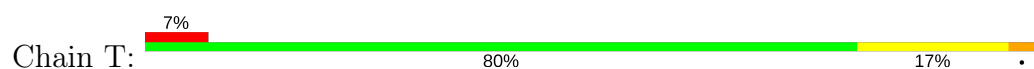
- Molecule 5: Proteasome subunit alpha type-5



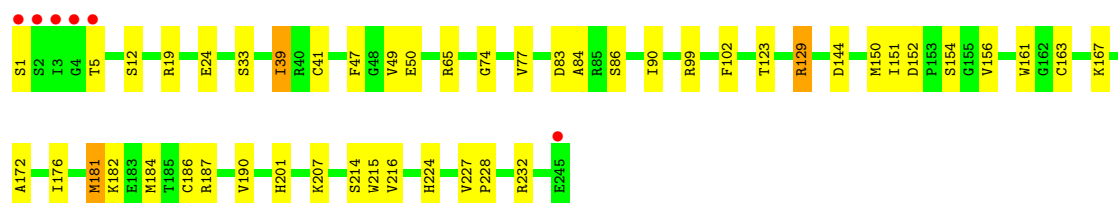
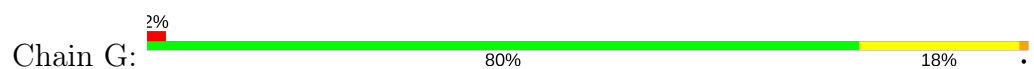
- Molecule 6: Proteasome subunit alpha type-1



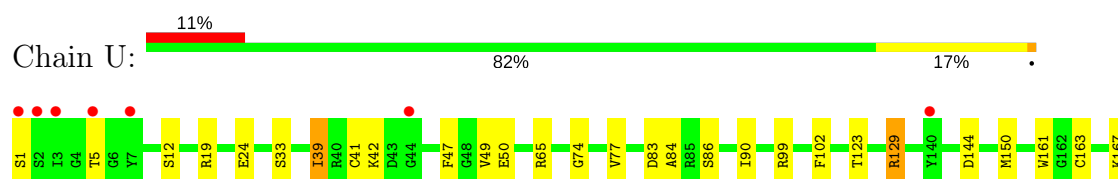
- Molecule 6: Proteasome subunit alpha type-1



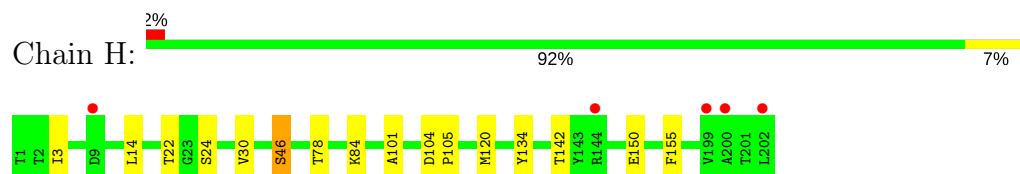
- Molecule 7: Proteasome subunit alpha type-3



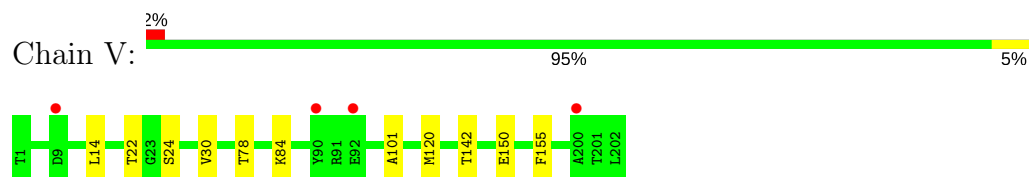
- Molecule 7: Proteasome subunit alpha type-3



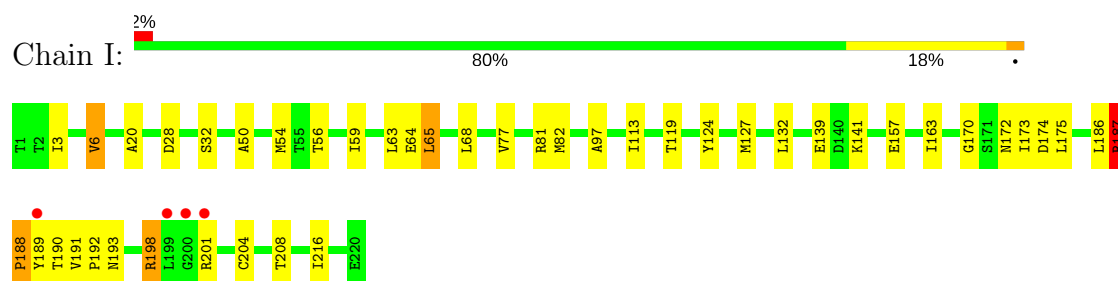
• Molecule 8: Proteasome subunit beta type-6



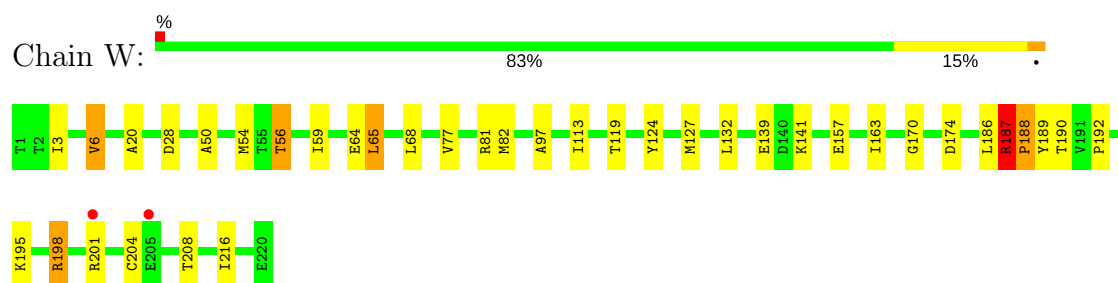
• Molecule 8: Proteasome subunit beta type-6



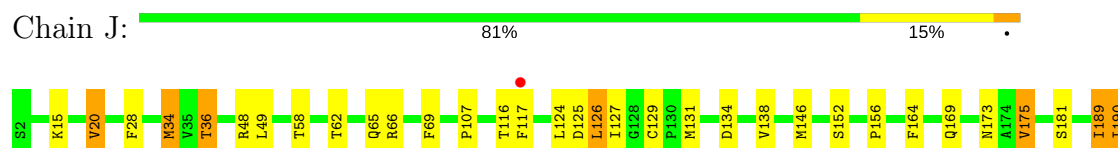
• Molecule 9: Proteasome subunit beta type-7



• Molecule 9: Proteasome subunit beta type-7



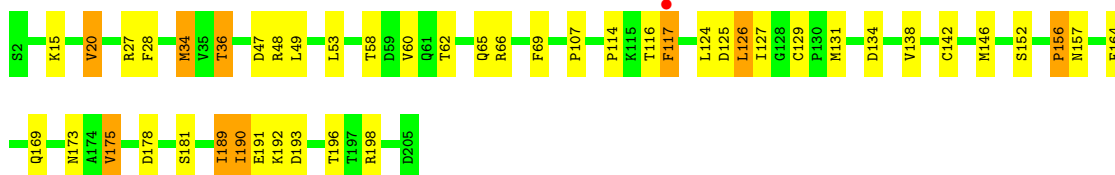
• Molecule 10: Proteasome subunit beta type-3





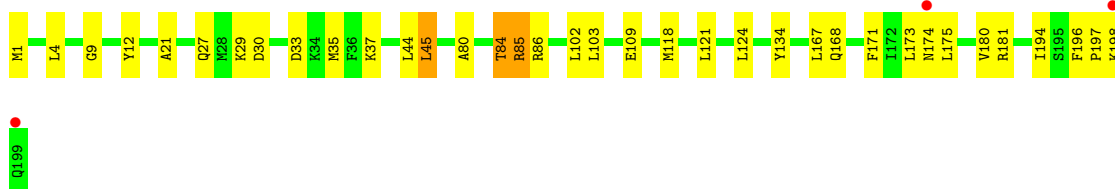
• Molecule 10: Proteasome subunit beta type-3

Chain X: 77% 18% .



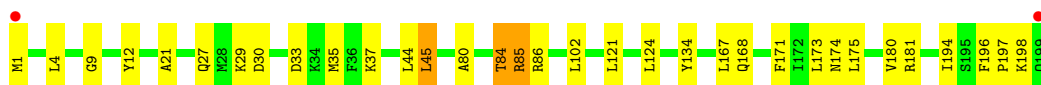
• Molecule 11: Proteasome subunit beta type-2

Chain K: 2% 82% 17% .



• Molecule 11: Proteasome subunit beta type-2

Chain Y: 83% 15% .



• Molecule 12: Proteasome subunit beta type-5

Chain L: 82% 17% .

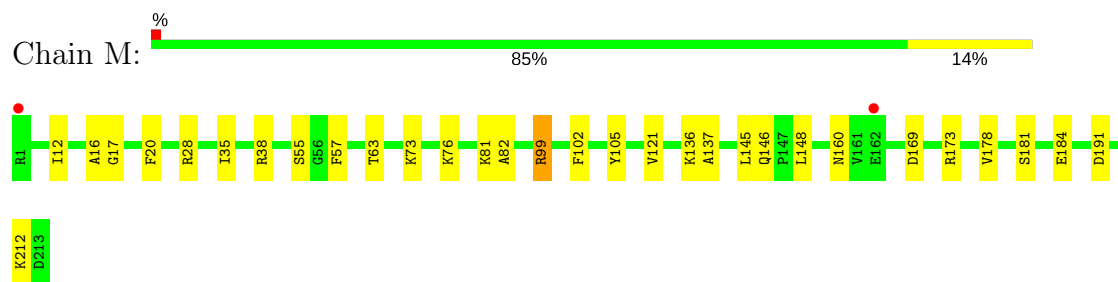


• Molecule 12: Proteasome subunit beta type-5

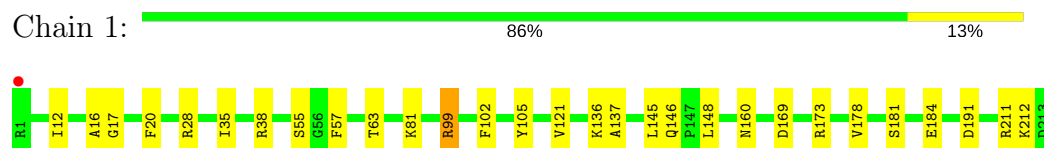
Chain Z: 85% 13% .



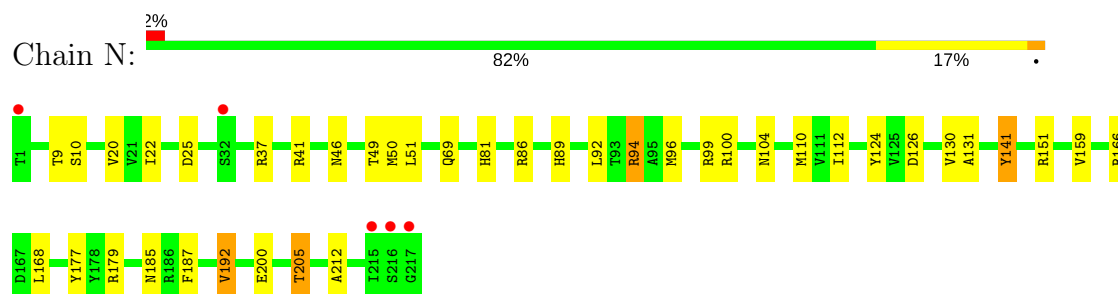
• Molecule 13: Proteasome subunit beta type-1



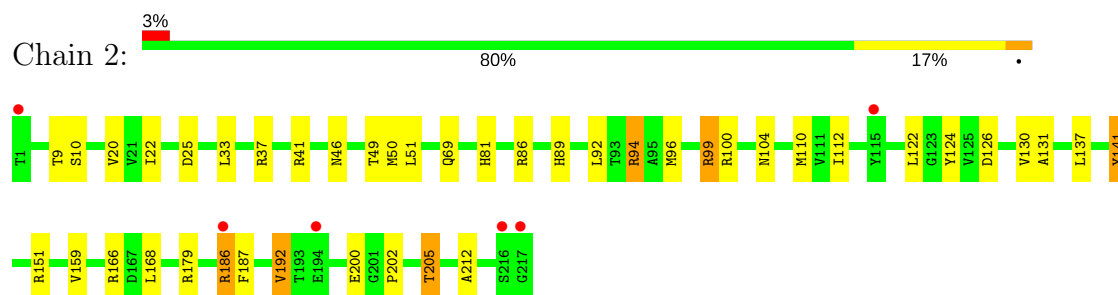
- Molecule 13: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.23Å 205.06Å 163.13Å 90.00° 106.37° 90.00°	Depositor
Resolution (Å)	36.34 – 2.60 49.42 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.34-2.60) 87.9 (49.42-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.45 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.244 0.217 , 0.250	Depositor DCC
R_{free} test set	11447 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	47831	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.73% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/1878	0.45	0/2549
1	O	0.24	0/1878	0.42	0/2549
2	B	0.25	0/1742	0.42	0/2372
2	P	0.25	0/1747	0.43	0/2378
3	C	0.24	0/1942	0.43	0/2628
3	Q	0.24	0/1943	0.43	0/2629
4	D	0.23	0/1748	0.44	0/2386
4	R	0.23	0/1716	0.44	0/2347
5	E	0.25	0/1786	0.42	0/2419
5	S	0.24	0/1743	0.42	0/2333
6	F	0.29	0/1885	0.46	1/2552 (0.0%)
6	T	0.25	0/1885	0.44	0/2552
7	G	0.26	0/1920	0.42	0/2591
7	U	0.27	0/1920	0.44	0/2591
8	H	0.27	0/1535	0.43	0/2078
8	V	0.26	0/1535	0.44	0/2078
9	I	0.32	1/1670 (0.1%)	0.49	1/2265 (0.0%)
9	W	0.28	0/1670	0.45	0/2265
10	J	0.26	0/1614	0.45	0/2177
10	X	0.26	0/1614	0.45	0/2177
11	K	0.24	0/1603	0.44	0/2174
11	Y	0.25	0/1603	0.44	0/2174
12	L	0.28	0/1579	0.45	0/2134
12	Z	0.25	0/1582	0.45	0/2138
13	1	0.28	0/1674	0.45	0/2257
13	M	0.31	0/1671	0.46	0/2253
14	2	0.25	0/1711	0.44	0/2319
14	N	0.25	0/1709	0.44	0/2317
All	All	0.26	1/48503 (0.0%)	0.44	2/65682 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	188	PRO	N-CD	5.13	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	F	239	ARG	C-N-CD	6.04	141.09	128.40
9	I	187	ARG	C-N-CD	5.11	139.14	128.40

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	1845	0	1805	52	0
1	O	1845	0	1805	27	0
2	B	1707	0	1591	25	0
2	P	1712	0	1605	33	0
3	C	1912	0	1851	21	0
3	Q	1913	0	1848	23	0
4	D	1724	0	1525	25	0
4	R	1691	0	1468	27	0
5	E	1759	0	1707	32	0
5	S	1716	0	1707	25	0
6	F	1850	0	1822	46	0
6	T	1850	0	1822	42	0
7	G	1885	0	1845	28	0
7	U	1885	0	1845	28	0
8	H	1509	0	1473	12	0
8	V	1509	0	1473	10	0
9	I	1643	0	1644	40	0
9	W	1643	0	1644	34	0
10	J	1585	0	1598	24	0
10	X	1585	0	1598	29	0
11	K	1570	0	1547	23	0
11	Y	1570	0	1547	21	0
12	L	1548	0	1499	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1551	0	1508	19	0
13	1	1644	0	1627	20	0
13	M	1641	0	1618	26	0
14	2	1678	0	1640	28	0
14	N	1676	0	1633	29	0
15	A	2	0	0	0	0
15	D	4	0	0	0	0
15	E	8	0	0	6	0
15	F	19	0	0	9	0
15	G	1	0	0	0	0
15	K	9	0	0	1	0
15	L	8	0	0	1	0
15	M	34	0	0	3	0
15	N	11	0	0	0	0
15	O	1	0	0	0	0
15	P	24	0	0	10	0
15	Q	10	0	0	1	0
15	R	5	0	0	2	0
15	W	17	0	0	1	0
15	X	25	0	0	3	0
15	Y	3	0	0	0	0
15	Z	4	0	0	0	0
All	All	47831	0	46295	680	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 7.

All (680) 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)
9:W:187:ARG:HB3	9:W:188:PRO:CD	1.57	1.28
9:W:187:ARG:HB3	9:W:188:PRO:HD2	1.13	1.11
9:W:187:ARG:CB	9:W:188:PRO:CD	2.35	1.05
6:T:196:ARG:HD3	6:T:239:ARG:HE	1.21	1.03
6:F:189:LYS:HD3	15:F:317:HOH:O	1.63	0.99
2:P:233:ALA:HB1	15:P:323:HOH:O	1.65	0.97
12:L:201:GLY:HA2	15:L:306:HOH:O	1.65	0.95
1:A:207:SER:O	1:A:208:ILE:HD13	1.68	0.93
6:F:96:ARG:HD2	13:M:73:LYS:NZ	1.84	0.92
6:F:180:MET:HG2	15:F:316:HOH:O	1.68	0.91
14:2:186:ARG:HE	14:2:202:PRO:HB3	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:O	1:A:207:SER:N	2.04	0.90
12:L:38:ASN:ND2	12:L:40:TYR:CZ	2.40	0.90
9:I:32:SER:HB2	9:I:187:ARG:NH2	1.87	0.88
6:F:96:ARG:HD2	13:M:73:LYS:HZ2	1.39	0.88
2:P:231:ALA:HA	15:P:307:HOH:O	1.75	0.87
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.54	0.87
9:I:32:SER:CA	9:I:187:ARG:HH21	1.90	0.84
9:W:187:ARG:CB	9:W:188:PRO:HD3	2.06	0.83
11:K:1:MET:HE1	11:K:134:TYR:H	1.44	0.83
11:Y:1:MET:HE1	11:Y:134:TYR:H	1.44	0.83
1:A:171:LYS:HB3	1:A:205:VAL:HG21	1.59	0.83
6:F:207:THR:HB	6:F:226:ASP:O	1.79	0.82
9:I:32:SER:HA	9:I:187:ARG:HH21	1.45	0.82
5:E:186:HIS:HA	15:E:306:HOH:O	1.81	0.81
6:F:50:LYS:HE2	6:F:211:SER:OG	1.80	0.81
9:W:187:ARG:HG3	9:W:188:PRO:HD3	1.62	0.80
5:E:186:HIS:HB2	15:E:302:HOH:O	1.82	0.80
6:F:40:SER:HB3	15:F:307:HOH:O	1.81	0.80
9:I:172:ASN:CG	9:I:191:VAL:HG22	2.03	0.79
1:A:67:THR:HG22	1:A:69:LEU:H	1.48	0.78
6:T:196:ARG:HD3	6:T:239:ARG:NE	1.96	0.78
6:T:239:ARG:O	6:T:239:ARG:HD2	1.82	0.78
1:A:171:LYS:HB3	1:A:205:VAL:CG2	2.12	0.78
9:I:172:ASN:OD1	9:I:191:VAL:HG13	1.83	0.78
2:P:110:VAL:HG22	2:P:135:ILE:HD12	1.66	0.78
2:B:110:VAL:HG22	2:B:135:ILE:HD12	1.66	0.77
9:W:187:ARG:CG	9:W:188:PRO:HD3	2.14	0.77
9:I:172:ASN:OD1	9:I:191:VAL:HG22	1.84	0.77
10:J:28:PHE:HB3	10:J:36:THR:HG22	1.65	0.77
6:T:239:ARG:H	6:T:239:ARG:NH1	1.80	0.77
1:O:67:THR:HG22	1:O:69:LEU:H	1.48	0.77
10:X:28:PHE:HB3	10:X:36:THR:HG22	1.66	0.76
11:Y:44:LEU:HD11	11:Y:102:LEU:HD12	1.67	0.76
11:K:44:LEU:HD11	11:K:102:LEU:HD12	1.67	0.75
3:Q:8:ARG:HB3	3:Q:11:ILE:HD12	1.67	0.75
4:R:204:LYS:CB	15:R:303:HOH:O	2.32	0.75
3:C:8:ARG:HB3	3:C:11:ILE:HD12	1.67	0.75
1:A:206:LEU:O	1:A:207:SER:OG	2.04	0.75
14:2:186:ARG:HE	14:2:202:PRO:CB	1.99	0.74
5:E:84:ASP:OD2	5:E:135:ARG:NH2	2.20	0.74
6:F:96:ARG:CD	13:M:73:LYS:NZ	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:ASP:OD2	4:D:143:ARG:NH1	2.21	0.73
5:E:42:THR:HG22	5:E:44:GLU:H	1.53	0.73
5:S:42:THR:HG22	5:S:44:GLU:H	1.52	0.73
7:U:83:ASP:OD2	7:U:129:ARG:NH2	2.22	0.72
6:F:65:HIS:HB2	15:F:305:HOH:O	1.87	0.72
1:A:158:GLY:O	2:B:83:ARG:NH2	2.23	0.71
7:U:186:CYS:HB3	7:U:215:TRP:HZ3	1.54	0.71
7:G:83:ASP:OD2	7:G:129:ARG:NH2	2.23	0.71
6:F:237:GLU:CB	15:F:312:HOH:O	2.38	0.71
12:L:38:ASN:ND2	12:L:40:TYR:CE1	2.59	0.70
10:X:116:THR:O	10:X:192:LYS:NZ	2.23	0.70
10:J:116:THR:O	10:J:192:LYS:NZ	2.24	0.70
6:T:120:THR:O	7:U:129:ARG:NH1	2.24	0.70
9:I:32:SER:CB	9:I:187:ARG:NH2	2.54	0.70
6:T:104:PRO:HB3	14:2:81:HIS:HD2	1.56	0.70
6:T:196:ARG:CD	6:T:239:ARG:HE	2.00	0.69
10:X:65:GLN:OE1	11:Y:86:ARG:NH2	2.24	0.69
11:Y:33:ASP:OD2	11:Y:181:ARG:NH2	2.26	0.69
1:O:132:ARG:HG2	7:U:12:SER:HA	1.75	0.69
1:A:132:ARG:HG2	7:G:12:SER:HA	1.74	0.69
2:P:69:LYS:HD2	15:P:314:HOH:O	1.93	0.69
7:U:1:SER:HA	7:U:19:ARG:HH12	1.56	0.69
6:F:104:PRO:HB3	14:N:81:HIS:HD2	1.58	0.69
7:G:1:SER:HA	7:G:19:ARG:HH12	1.57	0.68
11:K:33:ASP:OD2	11:K:181:ARG:NH2	2.25	0.68
1:A:202:LEU:O	1:A:205:VAL:CG1	2.42	0.68
1:A:202:LEU:O	1:A:205:VAL:HG12	1.94	0.67
2:P:67:ILE:HD11	2:P:73:LEU:HD12	1.74	0.67
12:L:115:ASP:HB2	12:L:119:ASN:HB2	1.76	0.67
6:F:120:THR:O	7:G:129:ARG:NH1	2.24	0.67
1:A:49:VAL:HG22	1:A:219:VAL:HG23	1.76	0.67
14:N:212:ALA:HA	8:V:30:VAL:HG21	1.75	0.67
2:B:67:ILE:HD11	2:B:73:LEU:HD12	1.75	0.67
6:F:225:ASP:O	6:F:226:ASP:HB2	1.93	0.66
2:B:94:GLN:HG3	9:I:65:LEU:HD13	1.78	0.66
1:A:171:LYS:HG3	1:A:205:VAL:HG22	1.76	0.66
14:N:51:LEU:HD11	14:N:110:MET:HB3	1.78	0.66
8:H:30:VAL:HG21	14:2:212:ALA:HA	1.76	0.66
14:2:51:LEU:HD13	14:2:112:ILE:HG12	1.76	0.66
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.78	0.66
9:I:172:ASN:OD1	9:I:191:VAL:CG1	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:115:ASP:HB2	12:Z:119:ASN:HB2	1.78	0.66
14:2:51:LEU:HD11	14:2:110:MET:HB3	1.78	0.66
14:N:51:LEU:HD13	14:N:112:ILE:HG12	1.76	0.66
2:P:50:LYS:NZ	2:P:199:GLU:O	2.28	0.66
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.78	0.65
5:S:84:ASP:OD2	5:S:135:ARG:NH2	2.30	0.65
1:A:130:GLU:HG2	2:B:4:GLY:HA2	1.77	0.65
13:M:137:ALA:H	13:M:146:GLN:HE21	1.44	0.65
6:F:96:ARG:CD	13:M:73:LYS:HZ1	2.08	0.65
1:O:158:GLY:O	2:P:83:ARG:NH2	2.29	0.65
10:J:65:GLN:OE1	11:K:86:ARG:NH2	2.28	0.65
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.77	0.65
13:1:137:ALA:H	13:1:146:GLN:HE21	1.45	0.65
5:E:31:ILE:HD13	5:E:140:ALA:HB2	1.77	0.65
9:I:172:ASN:OD1	9:I:191:VAL:CG2	2.45	0.65
10:J:125:ASP:HB2	10:J:129:CYS:H	1.61	0.65
6:F:225:ASP:HA	6:F:229:VAL:HG23	1.78	0.64
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.78	0.64
1:A:201:CYS:O	1:A:205:VAL:HG12	1.98	0.64
2:P:94:GLN:HG3	9:W:65:LEU:HD13	1.80	0.64
9:I:32:SER:CA	9:I:187:ARG:NH2	2.61	0.64
1:O:49:VAL:HG22	1:O:219:VAL:HG23	1.79	0.64
13:1:148:LEU:HD23	13:1:178:VAL:HG12	1.78	0.64
5:E:49:ALA:HB2	5:E:217:LEU:HD23	1.80	0.64
2:B:50:LYS:NZ	2:B:199:GLU:O	2.29	0.64
9:I:163:ILE:HG23	9:I:170:GLY:HA2	1.79	0.64
5:S:49:ALA:HB2	5:S:217:LEU:HD23	1.80	0.63
9:W:141:LYS:NZ	9:W:157:GLU:OE2	2.26	0.63
10:X:125:ASP:HB2	10:X:129:CYS:H	1.62	0.63
4:D:38:ARG:NE	4:D:181:ILE:O	2.31	0.63
13:M:148:LEU:HD23	13:M:178:VAL:HG12	1.79	0.63
6:T:167:SER:HB3	6:T:197:GLU:HG2	1.80	0.63
4:R:38:ARG:NE	4:R:181:ILE:O	2.31	0.63
9:W:190:THR:HG22	9:W:192:PRO:HD3	1.81	0.62
11:Y:21:ALA:HB3	11:Y:29:LYS:HB3	1.80	0.62
6:F:196:ARG:HD3	6:F:239:ARG:CZ	2.29	0.62
12:L:38:ASN:HB2	12:L:41:LEU:HB2	1.82	0.62
6:F:225:ASP:HA	6:F:229:VAL:CG2	2.30	0.62
11:K:21:ALA:HB3	11:K:29:LYS:HB3	1.81	0.62
13:1:99:ARG:NH1	13:1:102:PHE:O	2.33	0.62
1:O:120:ASP:OD1	2:P:83:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:9:THR:O	14:2:41:ARG:NH2	2.33	0.61
1:O:6:SER:HB2	1:O:11:ARG:HH11	1.62	0.61
1:A:132:ARG:NH1	7:G:123:THR:O	2.33	0.61
14:N:9:THR:O	14:N:41:ARG:NH2	2.34	0.61
2:P:39:ALA:O	2:P:41:ASN:N	2.33	0.61
1:O:130:GLU:HG2	2:P:4:GLY:HA2	1.82	0.61
9:I:141:LYS:NZ	9:I:157:GLU:OE2	2.26	0.61
9:I:175:LEU:HD12	9:I:189:TYR:CE1	2.35	0.61
1:A:6:SER:HB2	1:A:11:ARG:HH11	1.63	0.61
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.83	0.61
7:U:227:VAL:O	7:U:232:ARG:NH1	2.34	0.61
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.83	0.61
13:M:99:ARG:NH1	13:M:102:PHE:O	2.33	0.61
10:J:34:MET:O	12:Z:166:ARG:NH1	2.34	0.61
6:T:104:PRO:HB3	14:2:81:HIS:CD2	2.36	0.60
6:F:180:MET:CG	15:F:316:HOH:O	2.37	0.60
1:O:132:ARG:NH1	7:U:123:THR:O	2.34	0.60
7:U:186:CYS:HB3	7:U:215:TRP:CZ3	2.36	0.60
6:F:189:LYS:CD	15:F:317:HOH:O	2.34	0.60
7:G:99:ARG:NH1	14:N:69:GLN:OE1	2.31	0.60
6:T:239:ARG:H	6:T:239:ARG:HH11	1.47	0.60
9:W:204:CYS:HB3	9:W:208:THR:HG21	1.84	0.60
12:Z:38:ASN:ND2	12:Z:40:TYR:CZ	2.66	0.60
1:A:202:LEU:C	1:A:205:VAL:HG12	2.22	0.60
2:B:39:ALA:O	2:B:41:ASN:N	2.35	0.60
9:I:32:SER:CB	9:I:187:ARG:HH21	2.15	0.60
1:A:203:SER:O	1:A:207:SER:CA	2.49	0.60
6:T:103:LEU:HD12	6:T:104:PRO:HD2	1.83	0.59
9:I:204:CYS:HB3	9:I:208:THR:HG21	1.84	0.59
10:X:47:ASP:HA	15:X:317:HOH:O	2.02	0.59
12:Z:10:HIS:HD2	12:Z:149:VAL:HG23	1.67	0.59
3:C:62:SER:OG	3:C:63:GLU:N	2.35	0.59
5:E:168:ARG:NH1	6:F:53:GLN:OE1	2.35	0.59
6:T:36:VAL:HG13	6:T:172:LEU:HD11	1.84	0.59
4:R:209:ALA:HB1	4:R:217:LEU:HD11	1.84	0.59
12:L:166:ARG:NH1	10:X:34:MET:O	2.35	0.59
12:L:10:HIS:HD2	12:L:149:VAL:HG23	1.68	0.59
4:D:209:ALA:HB1	4:D:217:LEU:HD11	1.84	0.58
4:R:230:ALA:HA	15:R:301:HOH:O	2.02	0.58
11:Y:4:LEU:HD22	11:Y:45:LEU:HD12	1.85	0.58
11:K:4:LEU:HD22	11:K:45:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:237:GLU:O	6:F:239:ARG:N	2.37	0.58
6:T:212:ILE:HD12	6:T:229:VAL:HG22	1.85	0.58
5:E:148:GLU:OE2	13:M:81:LYS:NZ	2.34	0.58
9:I:174:ASP:OD2	9:I:187:ARG:NE	2.36	0.58
12:L:97:MET:HB3	12:L:116:SER:HB3	1.86	0.58
3:Q:68:LEU:HD11	3:Q:74:CYS:HB3	1.86	0.58
6:F:104:PRO:HB3	14:N:81:HIS:CD2	2.38	0.58
6:F:40:SER:CB	15:F:307:HOH:O	2.43	0.58
2:P:74:VAL:HG23	2:P:134:LEU:HB2	1.86	0.58
1:O:126:THR:HG22	2:P:127:ARG:HH21	1.69	0.58
1:A:120:ASP:OD1	2:B:83:ARG:NH1	2.37	0.57
7:G:227:VAL:O	7:G:232:ARG:NH1	2.35	0.57
1:O:54:LYS:NZ	1:O:66:VAL:O	2.37	0.57
3:Q:62:SER:OG	3:Q:63:GLU:N	2.35	0.57
6:T:165:SER:OG	6:T:169:ARG:NH2	2.37	0.57
7:U:99:ARG:NH1	14:2:69:GLN:OE1	2.33	0.57
12:Z:38:ASN:HB2	12:Z:41:LEU:HB2	1.86	0.57
6:F:165:SER:OG	6:F:169:ARG:NH2	2.37	0.57
3:C:68:LEU:HD11	3:C:74:CYS:HB3	1.86	0.57
6:T:121:GLN:HG3	7:U:129:ARG:HG3	1.87	0.57
10:X:189:ILE:HG23	10:X:196:THR:HB	1.85	0.57
6:T:239:ARG:O	6:T:239:ARG:NH1	2.32	0.57
5:S:148:GLU:OE2	13:1:81:LYS:NZ	2.37	0.57
2:B:74:VAL:HG23	2:B:134:LEU:HB2	1.86	0.57
6:F:36:VAL:HG13	6:F:172:LEU:HD11	1.85	0.57
4:D:80:ALA:HA	4:D:129:ILE:HD13	1.86	0.57
10:J:189:ILE:HG23	10:J:196:THR:HB	1.85	0.57
1:A:54:LYS:NZ	1:A:66:VAL:O	2.37	0.57
5:E:51:GLU:HA	5:E:215:ILE:HG22	1.87	0.57
10:J:20:VAL:HG12	10:J:190:ILE:HG12	1.86	0.57
4:R:119:THR:O	5:S:135:ARG:NH1	2.38	0.57
2:B:45:LEU:HD13	2:B:74:VAL:HG22	1.87	0.57
6:F:103:LEU:HD12	6:F:104:PRO:HD2	1.85	0.57
4:D:119:THR:O	5:E:135:ARG:NH1	2.38	0.56
13:1:63:THR:OG1	14:2:94:ARG:NH2	2.37	0.56
1:A:126:THR:HG22	2:B:127:ARG:HH21	1.70	0.56
3:C:154:GLY:O	4:D:81:ARG:NH2	2.36	0.56
13:M:38:ARG:NE	13:M:191:ASP:OD1	2.34	0.56
12:Z:97:MET:HB3	12:Z:116:SER:HB3	1.88	0.56
6:F:121:GLN:HG3	7:G:129:ARG:HG3	1.87	0.56
14:N:99:ARG:NH1	14:N:104:ASN:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:51:GLU:HA	5:S:215:ILE:HG22	1.88	0.56
9:W:6:VAL:HG23	9:W:124:TYR:HB3	1.87	0.56
13:M:38:ARG:HG3	15:M:305:HOH:O	2.04	0.56
13:1:38:ARG:NE	13:1:191:ASP:OD1	2.34	0.56
10:X:20:VAL:HG12	10:X:190:ILE:HG12	1.87	0.56
1:A:202:LEU:HA	1:A:205:VAL:CG1	2.36	0.56
6:T:227:ASP:O	6:T:230:SER:OG	2.24	0.56
11:Y:85:ARG:HG3	11:Y:124:LEU:HB2	1.88	0.56
1:A:182:LYS:HD3	1:A:197:THR:HG23	1.86	0.56
2:P:45:LEU:HD13	2:P:74:VAL:HG22	1.88	0.56
9:I:6:VAL:HG23	9:I:124:TYR:HB3	1.88	0.56
4:R:100:ASP:OD2	12:Z:107:ARG:NH2	2.39	0.56
4:R:80:ALA:HA	4:R:129:ILE:HD13	1.88	0.55
11:K:85:ARG:HG3	11:K:124:LEU:HB2	1.88	0.55
14:2:99:ARG:NH1	14:2:104:ASN:O	2.37	0.55
5:E:224:GLN:HB2	15:E:304:HOH:O	2.07	0.55
1:A:132:ARG:HB3	7:G:12:SER:O	2.06	0.55
7:U:50:GLU:OE2	7:U:201:HIS:ND1	2.38	0.55
1:A:173:THR:O	1:A:176:THR:OG1	2.24	0.55
1:O:182:LYS:HD3	1:O:197:THR:HG23	1.87	0.55
2:P:76:SER:HA	15:P:310:HOH:O	2.05	0.55
5:S:168:ARG:NH1	6:T:53:GLN:OE1	2.40	0.55
1:A:32:ILE:HD13	1:A:137:CYS:HB2	1.90	0.54
13:1:28:ARG:NE	13:1:191:ASP:OD2	2.35	0.54
3:Q:155:ASN:OD1	4:R:77:THR:OG1	2.24	0.54
6:T:40:SER:HB3	6:T:187:LEU:HD22	1.90	0.54
6:F:227:ASP:O	6:F:230:SER:OG	2.25	0.54
13:1:191:ASP:O	13:1:212:LYS:NZ	2.38	0.54
1:A:6:SER:HB2	1:A:11:ARG:NH1	2.22	0.54
13:M:191:ASP:O	13:M:212:LYS:NZ	2.38	0.54
7:G:50:GLU:OE2	7:G:201:HIS:ND1	2.39	0.54
9:I:174:ASP:CG	9:I:187:ARG:HG2	2.28	0.54
5:E:232:GLU:N	5:E:232:GLU:OE2	2.38	0.54
5:E:36:THR:HA	5:E:171:GLY:HA3	1.90	0.53
14:N:185:ASN:OD1	14:N:205:THR:OG1	2.20	0.53
2:P:33:PRO:HB3	15:P:309:HOH:O	2.08	0.53
1:A:207:SER:O	1:A:208:ILE:CD1	2.50	0.53
6:F:225:ASP:N	6:F:225:ASP:OD2	2.38	0.53
12:L:105:ASP:OD1	12:L:106:LYS:N	2.40	0.53
6:F:40:SER:HB3	6:F:187:LEU:HD22	1.90	0.53
12:Z:105:ASP:OD1	12:Z:106:LYS:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:ILE:HD13	1:O:137:CYS:HB2	1.91	0.53
3:Q:239:LYS:HG3	15:Q:308:HOH:O	2.08	0.53
4:D:184:ASP:N	4:D:184:ASP:OD1	2.40	0.53
1:O:6:SER:HB2	1:O:11:ARG:NH1	2.22	0.53
4:R:184:ASP:N	4:R:184:ASP:OD1	2.40	0.53
6:F:225:ASP:CA	6:F:229:VAL:HG23	2.39	0.53
3:Q:154:GLY:O	4:R:81:ARG:NH2	2.36	0.53
1:O:103:TYR:O	9:W:81:ARG:NH1	2.42	0.52
3:Q:49:ARG:NH2	3:Q:58:GLU:OE2	2.31	0.52
13:M:63:THR:OG1	14:N:94:ARG:NH2	2.43	0.52
5:E:85:ALA:HB2	5:E:139:VAL:HG21	1.91	0.52
10:J:15:LYS:NZ	10:J:134:ASP:OD1	2.41	0.52
5:S:85:ALA:HB2	5:S:139:VAL:HG21	1.91	0.52
10:X:15:LYS:NZ	10:X:134:ASP:OD1	2.42	0.52
5:E:167:ALA:HB3	6:F:56:LEU:HD13	1.90	0.52
11:K:109:GLU:HA	15:K:201:HOH:O	2.10	0.52
6:T:196:ARG:C	6:T:198:THR:H	2.13	0.52
3:Q:45:LEU:HD13	3:Q:75:SER:HB2	1.92	0.52
10:J:62:THR:OG1	11:K:85:ARG:NH2	2.43	0.52
8:V:84:LYS:HG3	8:V:120:MET:HB2	1.92	0.52
2:B:185:ASP:O	2:B:189:THR:HG22	2.10	0.52
3:C:45:LEU:HD13	3:C:75:SER:HB2	1.92	0.52
11:K:37:LYS:HD2	11:K:37:LYS:H	1.74	0.52
1:O:50:ILE:HG21	1:O:79:VAL:HB	1.92	0.51
3:C:49:ARG:NH2	3:C:58:GLU:OE2	2.31	0.51
14:N:177:TYR:CZ	14:N:185:ASN:HB2	2.45	0.51
7:U:47:PHE:HB2	7:U:214:SER:HB2	1.93	0.51
8:V:142:THR:HB	8:V:155:PHE:HE1	1.75	0.51
8:H:142:THR:HB	8:H:155:PHE:HE1	1.75	0.51
5:S:36:THR:HA	5:S:171:GLY:HA3	1.92	0.51
14:2:9:THR:OG1	14:2:10:SER:N	2.44	0.51
1:A:50:ILE:HG21	1:A:79:VAL:HB	1.93	0.51
7:G:186:CYS:O	7:G:190:VAL:HG23	2.10	0.51
9:W:56:THR:CG2	15:W:313:HOH:O	2.57	0.51
6:T:212:ILE:CD1	6:T:229:VAL:HG13	2.41	0.51
3:C:21:VAL:HG11	3:C:153:SER:HB3	1.93	0.51
7:G:47:PHE:HB2	7:G:214:SER:HB2	1.93	0.51
3:Q:21:VAL:HG11	3:Q:153:SER:HB3	1.93	0.51
6:T:196:ARG:CD	6:T:239:ARG:NE	2.67	0.51
10:X:114:PRO:HG2	15:X:312:HOH:O	2.11	0.51
13:1:16:ALA:HB2	13:1:121:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:224:GLN:CB	15:E:304:HOH:O	2.59	0.51
14:2:166:ARG:NH2	14:2:200:GLU:OE1	2.42	0.50
7:G:74:GLY:HA3	7:G:224:HIS:CD2	2.46	0.50
5:S:24:VAL:O	5:S:28:ILE:HG12	2.11	0.50
7:U:74:GLY:HA3	7:U:224:HIS:CD2	2.46	0.50
11:Y:37:LYS:HD2	11:Y:37:LYS:H	1.75	0.50
13:1:169:ASP:OD2	13:1:173:ARG:NH2	2.44	0.50
13:M:169:ASP:OD2	13:M:173:ARG:NH2	2.44	0.50
8:H:84:LYS:HG3	8:H:120:MET:HB2	1.94	0.50
9:I:20:ALA:HB3	9:I:28:ASP:HB3	1.94	0.50
11:K:80:ALA:O	11:K:84:THR:HG23	2.11	0.50
9:I:173:ILE:O	9:I:189:TYR:N	2.40	0.50
9:W:20:ALA:HB3	9:W:28:ASP:HB3	1.94	0.50
11:Y:80:ALA:O	11:Y:84:THR:HG23	2.11	0.50
4:D:12:PRO:HA	5:E:26:TYR:CD1	2.47	0.50
2:P:94:GLN:HE21	2:P:94:GLN:HA	1.77	0.50
5:E:24:VAL:O	5:E:28:ILE:HG12	2.12	0.49
9:I:190:THR:O	9:I:192:PRO:HD3	2.12	0.49
1:O:132:ARG:HB3	7:U:12:SER:O	2.12	0.49
2:P:185:ASP:O	2:P:189:THR:HG22	2.11	0.49
10:X:66:ARG:O	10:X:69:PHE:HB3	2.12	0.49
1:A:202:LEU:O	1:A:205:VAL:HG13	2.12	0.49
10:J:66:ARG:O	10:J:69:PHE:HB3	2.12	0.49
13:M:16:ALA:HB2	13:M:121:VAL:HG23	1.94	0.49
9:W:186:LEU:HD13	9:W:189:TYR:HD1	1.77	0.49
2:B:173:LEU:HD21	2:B:193:THR:HG21	1.94	0.49
9:I:216:ILE:HD13	10:J:196:THR:HG23	1.93	0.49
7:U:186:CYS:O	7:U:190:VAL:HG23	2.12	0.49
4:R:94:HIS:ND1	4:R:101:PRO:O	2.41	0.49
2:B:94:GLN:HA	2:B:94:GLN:HE21	1.76	0.49
4:D:94:HIS:ND1	4:D:101:PRO:O	2.42	0.49
7:G:86:SER:O	7:G:90:ILE:HD12	2.12	0.49
9:W:97:ALA:HB1	9:W:127:MET:HE2	1.94	0.49
12:Z:20:ALA:HB2	12:Z:31:VAL:HG21	1.93	0.49
2:P:173:LEU:HD21	2:P:193:THR:HG21	1.94	0.49
5:S:232:GLU:N	5:S:232:GLU:OE2	2.38	0.49
2:P:94:GLN:HG2	15:P:319:HOH:O	2.12	0.49
9:W:189:TYR:O	9:W:190:THR:OG1	2.25	0.49
13:1:12:ILE:HD12	13:1:55:SER:HB2	1.95	0.48
1:A:72:ILE:HG21	1:A:114:LEU:HD11	1.94	0.48
9:W:216:ILE:HD13	10:X:196:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:66:ASP:OD1	4:D:67:ASP:N	2.41	0.48
10:J:107:PRO:HG2	10:J:124:LEU:HB2	1.95	0.48
6:T:41:LYS:HG3	6:T:42:THR:HG23	1.95	0.48
6:T:40:SER:OG	6:T:41:LYS:N	2.45	0.48
9:I:175:LEU:HD12	9:I:189:TYR:CD1	2.49	0.48
11:Y:1:MET:CE	11:Y:134:TYR:H	2.22	0.48
5:E:166:ASP:HB3	5:E:185:TYR:CE2	2.49	0.48
6:F:202:GLU:HG3	6:F:202:GLU:H	1.40	0.48
4:R:79:ASP:OD2	4:R:125:ARG:NH2	2.47	0.48
10:X:107:PRO:HG2	10:X:124:LEU:HB2	1.95	0.48
5:E:66:LYS:N	5:E:216:GLU:OE2	2.45	0.48
8:H:3:ILE:HD13	8:H:46:SER:HB3	1.94	0.48
9:I:113:ILE:HG12	9:I:119:THR:HG22	1.94	0.48
13:M:12:ILE:HD12	13:M:55:SER:HB2	1.96	0.48
14:N:126:ASP:HB2	14:N:130:VAL:HB	1.94	0.48
5:S:66:LYS:N	5:S:216:GLU:OE2	2.45	0.48
6:F:40:SER:OG	6:F:41:LYS:N	2.46	0.48
14:N:9:THR:OG1	14:N:10:SER:N	2.45	0.48
6:F:71:GLY:HA3	6:F:221:PHE:CZ	2.49	0.48
13:M:28:ARG:NE	13:M:191:ASP:OD2	2.35	0.48
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.95	0.48
3:Q:86:LEU:HD22	3:Q:114:LEU:HD11	1.95	0.48
12:L:20:ALA:HB2	12:L:31:VAL:HG21	1.95	0.48
14:2:126:ASP:HB2	14:2:130:VAL:HB	1.95	0.48
9:I:187:ARG:HA	9:I:188:PRO:HA	1.61	0.48
4:R:66:ASP:OD1	4:R:67:ASP:N	2.42	0.48
4:D:79:ASP:OD2	4:D:125:ARG:NH2	2.47	0.47
6:F:64:LEU:HA	15:F:315:HOH:O	2.12	0.47
9:I:97:ALA:HB1	9:I:127:MET:HE2	1.96	0.47
1:O:72:ILE:HG21	1:O:114:LEU:HD11	1.95	0.47
14:2:124:TYR:O	14:2:131:ALA:HA	2.14	0.47
4:D:121:SER:HB2	4:D:124:ARG:HD2	1.96	0.47
6:F:41:LYS:HG3	6:F:42:THR:HG23	1.96	0.47
5:S:166:ASP:HB3	5:S:185:TYR:CE2	2.48	0.47
6:T:71:GLY:HA3	6:T:221:PHE:CZ	2.50	0.47
1:A:165:ALA:HB1	1:A:179:LEU:HD13	1.95	0.47
14:N:177:TYR:CE1	14:N:185:ASN:HB2	2.48	0.47
1:O:165:ALA:HB1	1:O:179:LEU:HD13	1.95	0.47
5:E:31:ILE:HD11	5:E:158:PRO:CD	2.45	0.47
4:D:100:ASP:OD2	12:L:107:ARG:NH2	2.47	0.47
13:1:145:LEU:HD22	13:1:178:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:LEU:HD22	4:D:144:LEU:HD11	1.97	0.47
4:R:132:LEU:HD22	4:R:144:LEU:HD11	1.97	0.47
14:N:141:TYR:HE2	8:V:24:SER:HB2	1.80	0.47
9:W:113:ILE:HG12	9:W:119:THR:HG22	1.95	0.47
9:I:64:GLU:O	9:I:68:LEU:HB2	2.13	0.47
7:U:86:SER:O	7:U:90:ILE:HD12	2.14	0.47
9:W:64:GLU:O	9:W:68:LEU:HB2	2.14	0.47
10:X:62:THR:OG1	11:Y:85:ARG:NH2	2.45	0.47
14:N:124:TYR:O	14:N:131:ALA:HA	2.14	0.47
2:P:33:PRO:CB	15:P:309:HOH:O	2.63	0.47
12:Z:38:ASN:ND2	12:Z:40:TYR:CE1	2.83	0.47
1:A:202:LEU:CA	1:A:205:VAL:HG12	2.45	0.47
7:G:215:TRP:HE1	7:G:228:PRO:HD2	1.80	0.47
6:T:211:SER:OG	6:T:225:ASP:OD1	2.32	0.47
1:A:175:SER:OG	1:A:201:CYS:SG	2.69	0.46
5:S:31:ILE:HD11	5:S:158:PRO:CD	2.46	0.46
11:Y:168:GLN:NE2	11:Y:175:LEU:O	2.35	0.46
3:C:66:TYR:CG	3:C:87:THR:HG21	2.51	0.46
9:I:198:ARG:NH2	10:J:152:SER:O	2.49	0.46
13:M:35:ILE:O	14:N:151:ARG:NH2	2.42	0.46
1:O:50:ILE:HG12	1:O:141:ILE:HD13	1.98	0.46
11:K:196:PHE:O	11:K:198:LYS:N	2.48	0.46
11:K:35:MET:HG2	11:K:45:LEU:HD13	1.97	0.46
6:T:196:ARG:O	6:T:198:THR:N	2.48	0.46
7:U:215:TRP:HE1	7:U:228:PRO:HD2	1.80	0.46
1:A:143:ILE:HG12	1:A:220:VAL:HG22	1.97	0.46
2:P:231:ALA:CA	15:P:307:HOH:O	2.47	0.46
9:W:198:ARG:NH2	10:X:152:SER:O	2.47	0.46
3:C:130:PHE:O	3:C:152:PRO:HB3	2.16	0.46
8:H:24:SER:HB2	14:2:141:TYR:HE2	1.81	0.46
13:M:184:GLU:HG3	9:W:195:LYS:HE2	1.98	0.46
14:N:212:ALA:HA	8:V:30:VAL:CG2	2.44	0.46
4:R:121:SER:HB2	4:R:124:ARG:HD2	1.97	0.46
13:1:38:ARG:NH2	13:1:212:LYS:O	2.49	0.46
1:A:103:TYR:O	9:I:81:ARG:NH1	2.47	0.46
2:B:75:TYR:HB3	2:B:82:TYR:CD1	2.51	0.46
13:M:145:LEU:HD22	13:M:178:VAL:HB	1.98	0.46
3:C:86:LEU:HD22	3:C:114:LEU:HD11	1.98	0.46
11:K:168:GLN:NE2	11:K:175:LEU:O	2.36	0.46
11:Y:196:PHE:O	11:Y:198:LYS:N	2.49	0.46
1:A:208:ILE:O	1:A:209:ASP:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:143:ILE:HG12	1:O:220:VAL:HG22	1.98	0.45
12:Z:40:TYR:CZ	12:Z:73:ARG:HG2	2.51	0.45
9:W:59:ILE:HD12	9:W:82:MET:HB3	1.97	0.45
7:U:49:VAL:HG11	7:U:65:ARG:HB2	1.98	0.45
5:S:123:PHE:CE2	5:S:136:PRO:HG3	2.52	0.45
6:T:185:ASN:OD1	6:T:189:LYS:HE3	2.17	0.45
10:X:114:PRO:CG	15:X:312:HOH:O	2.64	0.45
13:M:136:LYS:HA	13:M:146:GLN:NE2	2.31	0.45
3:Q:66:TYR:CG	3:Q:87:THR:HG21	2.51	0.45
1:A:203:SER:O	1:A:207:SER:HA	2.17	0.45
2:B:177:TYR:O	2:B:178:ASN:ND2	2.47	0.45
7:G:49:VAL:HG11	7:G:65:ARG:HB2	1.99	0.45
2:P:75:TYR:HB3	2:P:82:TYR:CD1	2.52	0.45
4:R:38:ARG:CZ	4:R:38:ARG:H	2.30	0.45
11:Y:35:MET:HG2	11:Y:45:LEU:HD13	1.98	0.45
1:A:38:THR:HG21	1:A:171:LYS:HB2	1.99	0.45
5:E:50:VAL:HG11	5:E:66:LYS:HB2	1.99	0.45
11:K:1:MET:CE	11:K:134:TYR:H	2.23	0.45
14:N:89:HIS:HA	14:N:112:ILE:HD12	1.99	0.45
15:M:324:HOH:O	9:W:198:ARG:HA	2.15	0.45
7:G:152:ASP:OD1	7:G:154:SER:OG	2.25	0.45
3:Q:130:PHE:O	3:Q:152:PRO:HB3	2.16	0.45
13:M:38:ARG:NH2	13:M:212:LYS:O	2.50	0.45
3:Q:14:PRO:HA	4:R:21:TYR:CE1	2.52	0.45
2:B:28:VAL:HG11	2:B:132:SER:HB2	1.99	0.44
3:C:11:ILE:HG23	4:D:18:GLN:HE22	1.81	0.44
13:M:160:ASN:O	13:M:160:ASN:ND2	2.47	0.44
13:1:136:LYS:HA	13:1:146:GLN:NE2	2.32	0.44
4:D:38:ARG:CZ	4:D:38:ARG:H	2.31	0.44
12:L:37:ILE:HG23	12:L:60:ALA:HB2	1.99	0.44
1:A:188:ASP:O	1:A:190:THR:HG23	2.17	0.44
7:G:215:TRP:CD1	7:G:227:VAL:HA	2.53	0.44
10:J:58:THR:OG1	11:K:121:LEU:O	2.30	0.44
5:S:50:VAL:HG11	5:S:66:LYS:HB2	1.99	0.44
1:A:50:ILE:HG12	1:A:141:ILE:HD13	2.00	0.44
2:P:231:ALA:CB	15:P:307:HOH:O	2.65	0.44
10:X:48:ARG:HA	10:X:190:ILE:HD12	1.98	0.44
2:B:118:GLN:HG3	3:C:81:SER:HB2	1.98	0.44
3:C:171:ALA:HB2	3:C:200:THR:HG21	1.99	0.44
2:P:28:VAL:HG11	2:P:132:SER:HB2	1.99	0.44
6:T:50:LYS:HB3	6:T:59:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:138:VAL:HG11	10:X:146:MET:HB3	2.00	0.44
12:Z:13:ILE:HG13	12:Z:152:ALA:HB1	2.00	0.44
14:2:89:HIS:HA	14:2:112:ILE:HD12	1.99	0.44
1:A:171:LYS:HD3	1:A:171:LYS:HA	1.78	0.44
1:A:212:PRO:HB2	1:A:232:GLU:HG3	1.99	0.44
7:G:102:PHE:HD1	8:H:78:THR:HG23	1.81	0.44
14:N:187:PHE:CE1	14:N:205:THR:HG23	2.52	0.44
2:P:177:TYR:O	2:P:178:ASN:ND2	2.48	0.44
6:T:22:ILE:O	6:T:26:MET:HG2	2.17	0.44
10:X:126:LEU:HD13	10:X:127:ILE:HG23	1.99	0.44
10:X:62:THR:O	10:X:66:ARG:HG3	2.17	0.44
13:1:160:ASN:ND2	13:1:160:ASN:O	2.47	0.44
1:A:171:LYS:CG	1:A:205:VAL:HG22	2.45	0.44
4:D:36:ARG:HA	4:D:41:VAL:HG12	1.99	0.44
6:F:139:ASP:HB2	14:N:81:HIS:CE1	2.52	0.44
10:J:62:THR:O	10:J:66:ARG:HG3	2.18	0.44
14:N:166:ARG:NH2	14:N:200:GLU:OE1	2.42	0.44
7:U:33:SER:O	7:U:167:LYS:HG3	2.18	0.44
12:Z:75:SER:HB2	12:Z:105:ASP:OD2	2.18	0.44
12:Z:38:ASN:ND2	12:Z:40:TYR:OH	2.50	0.44
3:C:197:LEU:HA	3:C:197:LEU:HD12	1.80	0.44
4:D:33:VAL:HG11	4:D:168:VAL:HG11	1.99	0.44
5:E:146:VAL:HG11	5:E:222:PRO:HA	2.00	0.44
5:E:203:LYS:HE2	5:E:241:ILE:HD11	1.99	0.44
6:F:189:LYS:HE2	6:F:235:GLY:O	2.17	0.44
10:J:48:ARG:HA	10:J:190:ILE:HD12	1.98	0.44
1:O:201:CYS:O	1:O:205:VAL:HB	2.17	0.44
4:R:33:VAL:HG11	4:R:168:VAL:HG11	2.00	0.44
4:R:36:ARG:HA	4:R:41:VAL:HG12	1.99	0.44
5:S:203:LYS:HE2	5:S:241:ILE:HD11	1.99	0.44
9:W:3:ILE:HD11	9:W:127:MET:HB2	2.00	0.44
9:W:28:ASP:HB2	10:X:131:MET:SD	2.58	0.44
12:L:67:GLU:HA	12:L:72:GLU:O	2.17	0.44
9:W:174:ASP:OD1	9:W:187:ARG:O	2.35	0.44
5:E:123:PHE:CE2	5:E:136:PRO:HG3	2.53	0.43
5:E:85:ALA:O	5:E:89:ILE:HG12	2.18	0.43
11:K:180:VAL:HG21	11:K:194:ILE:HG12	1.99	0.43
14:N:92:LEU:O	14:N:96:MET:HG2	2.18	0.43
7:U:215:TRP:CD1	7:U:227:VAL:HA	2.52	0.43
10:X:164:PHE:CE1	10:X:198:ARG:HD2	2.53	0.43
6:F:119:PRO:HB3	6:F:125:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:59:ILE:HD12	9:I:82:MET:HB3	1.98	0.43
14:N:20:VAL:HB	14:N:192:VAL:HG23	1.99	0.43
2:P:72:GLY:HA3	2:P:217:PHE:CE1	2.53	0.43
2:B:87:HIS:C	2:B:87:HIS:HD1	2.21	0.43
3:C:140:ASP:OD2	3:C:146:GLN:NE2	2.41	0.43
4:D:43:LEU:HD12	4:D:72:ALA:HB2	1.99	0.43
8:H:24:SER:HB2	14:2:141:TYR:CE2	2.54	0.43
11:K:1:MET:N	11:K:173:LEU:HD13	2.33	0.43
14:N:141:TYR:CE2	8:V:24:SER:HB2	2.53	0.43
2:P:64:VAL:HG12	2:P:217:PHE:HZ	1.83	0.43
5:S:146:VAL:HG11	5:S:222:PRO:HA	2.01	0.43
11:Y:1:MET:N	11:Y:173:LEU:HD13	2.33	0.43
14:2:20:VAL:HB	14:2:192:VAL:HG23	1.99	0.43
3:C:42:GLY:HA2	3:C:145:PHE:CE1	2.53	0.43
7:U:39:ILE:HD11	7:U:181:MET:HB3	2.00	0.43
10:X:169:GLN:O	10:X:173:ASN:ND2	2.49	0.43
13:1:35:ILE:O	14:2:151:ARG:NH2	2.44	0.43
2:B:72:GLY:HA3	2:B:217:PHE:CE1	2.53	0.43
6:F:185:ASN:OD1	6:F:189:LYS:HE3	2.19	0.43
6:F:22:ILE:O	6:F:26:MET:HG2	2.18	0.43
10:J:138:VAL:HG11	10:J:146:MET:HB3	2.01	0.43
14:N:25:ASP:HA	14:N:187:PHE:HA	2.00	0.43
1:O:211:LYS:HE2	1:O:211:LYS:HB3	1.73	0.43
1:O:212:PRO:HB2	1:O:232:GLU:HG3	2.00	0.43
6:T:239:ARG:N	6:T:239:ARG:HH11	2.16	0.43
14:2:187:PHE:CE1	14:2:205:THR:HG23	2.54	0.43
9:I:63:LEU:HD23	9:I:63:LEU:HA	1.80	0.43
12:L:13:ILE:HG13	12:L:152:ALA:HB1	2.01	0.43
3:Q:171:ALA:HB2	3:Q:200:THR:HG21	2.00	0.43
6:T:189:LYS:HE2	6:T:235:GLY:O	2.19	0.43
12:L:160:ILE:O	12:L:164:THR:HG23	2.18	0.43
6:T:196:ARG:C	6:T:198:THR:N	2.72	0.43
10:X:116:THR:HB	10:X:117:PHE:H	1.63	0.43
12:L:75:SER:HB2	12:L:105:ASP:OD2	2.19	0.43
5:S:85:ALA:O	5:S:89:ILE:HG12	2.18	0.43
6:T:49:LEU:HB2	6:T:195:LEU:HD11	2.01	0.43
6:T:239:ARG:C	6:T:239:ARG:HH11	2.20	0.43
10:J:164:PHE:CE1	10:J:198:ARG:HD2	2.53	0.43
9:W:50:ALA:O	9:W:54:MET:HG2	2.19	0.43
11:Y:180:VAL:HG21	11:Y:194:ILE:HG12	2.00	0.43
13:1:181:SER:O	13:1:184:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:175:VAL:HG22	10:J:181:SER:HB3	2.01	0.43
14:2:92:LEU:O	14:2:96:MET:HG2	2.19	0.42
3:C:155:ASN:OD1	4:D:77:THR:OG1	2.31	0.42
3:Q:140:ASP:OD2	3:Q:146:GLN:NE2	2.41	0.42
10:X:58:THR:OG1	11:Y:121:LEU:O	2.27	0.42
1:A:109:ILE:HA	1:A:110:PRO:HD3	1.92	0.42
1:A:188:ASP:O	1:A:190:THR:N	2.52	0.42
6:T:119:PRO:HB3	6:T:125:ARG:HH11	1.83	0.42
9:W:174:ASP:CG	9:W:187:ARG:O	2.57	0.42
7:G:150:MET:HG3	7:G:163:CYS:SG	2.60	0.42
9:I:139:GLU:OE1	14:2:179:ARG:NH2	2.42	0.42
9:I:3:ILE:HD11	9:I:127:MET:HB2	2.01	0.42
11:K:30:ASP:N	11:K:30:ASP:OD1	2.52	0.42
2:P:197:SER:O	2:P:199:GLU:N	2.52	0.42
3:Q:6:ASP:OD2	4:R:3:TYR:OH	2.32	0.42
1:A:86:ASP:OD2	1:A:132:ARG:NH2	2.52	0.42
2:B:183:LEU:O	2:B:187:ILE:HG13	2.19	0.42
2:B:64:VAL:HG12	2:B:217:PHE:HZ	1.84	0.42
6:F:49:LEU:HB2	6:F:195:LEU:HD11	2.01	0.42
9:I:193:ASN:HB3	13:1:211:ARG:NH2	2.34	0.42
7:U:102:PHE:HD1	8:V:78:THR:HG23	1.84	0.42
1:A:191:PHE:CE1	1:A:219:VAL:HG21	2.54	0.42
5:E:224:GLN:HA	15:E:304:HOH:O	2.19	0.42
7:G:33:SER:O	7:G:167:LYS:HG3	2.19	0.42
7:G:77:VAL:HG11	7:G:84:ALA:HB1	2.00	0.42
9:I:175:LEU:HD12	9:I:189:TYR:CZ	2.55	0.42
12:L:38:ASN:ND2	12:L:40:TYR:OH	2.51	0.42
5:S:91:LYS:HE3	5:S:119:LEU:HD21	2.02	0.42
1:A:234:GLU:HG2	1:A:234:GLU:H	1.59	0.42
7:G:161:TRP:CE2	7:G:182:LYS:HE2	2.55	0.42
8:H:104:ASP:HA	8:H:105:PRO:HD3	1.94	0.42
9:I:28:ASP:HB2	10:J:131:MET:SD	2.60	0.42
7:U:77:VAL:HG11	7:U:84:ALA:HB1	2.01	0.42
14:N:179:ARG:NH2	9:W:139:GLU:OE1	2.44	0.42
3:C:163:CYS:SG	3:C:164:ILE:N	2.93	0.42
3:C:48:GLU:OE2	3:C:50:ARG:NE	2.48	0.42
6:T:212:ILE:HD11	6:T:229:VAL:HG13	2.01	0.42
6:T:196:ARG:CZ	6:T:239:ARG:HG2	2.49	0.42
10:X:175:VAL:HG22	10:X:181:SER:HB3	2.01	0.42
14:2:25:ASP:HA	14:2:187:PHE:HA	2.01	0.42
4:D:43:LEU:HD22	4:D:134:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:43:GLY:HA3	12:L:56:GLU:OE1	2.20	0.42
11:Y:167:LEU:HA	11:Y:167:LEU:HD23	1.90	0.42
11:Y:30:ASP:N	11:Y:30:ASP:OD1	2.52	0.42
5:E:97:GLN:HB3	12:L:61:ARG:HG3	2.01	0.42
1:O:234:GLU:H	1:O:234:GLU:HG2	1.60	0.42
1:O:46:ASP:N	1:O:46:ASP:OD1	2.53	0.42
3:Q:63:GLU:HG2	3:Q:64:LYS:HG3	2.02	0.42
7:U:150:MET:HG3	7:U:163:CYS:SG	2.60	0.42
14:2:122:LEU:HG	14:2:137:LEU:HD12	2.01	0.41
14:2:22:ILE:HB	14:2:50:MET:HE3	2.01	0.41
10:J:169:GLN:O	10:J:173:ASN:ND2	2.51	0.41
7:U:161:TRP:CE2	7:U:182:LYS:HE2	2.55	0.41
6:F:109:VAL:HG21	6:F:145:PHE:CG	2.55	0.41
7:G:39:ILE:HD11	7:G:181:MET:HB3	2.02	0.41
10:J:126:LEU:HD13	10:J:127:ILE:HG23	2.01	0.41
13:M:181:SER:O	13:M:184:GLU:HB2	2.21	0.41
2:P:133:LEU:O	2:P:147:GLN:HA	2.20	0.41
3:Q:163:CYS:SG	3:Q:164:ILE:N	2.93	0.41
13:1:17:GLY:HA3	13:1:20:PHE:CE1	2.55	0.41
2:B:133:LEU:O	2:B:147:GLN:HA	2.19	0.41
3:C:63:GLU:HG2	3:C:64:LYS:HG3	2.02	0.41
7:G:19:ARG:NH2	7:G:24:GLU:OE1	2.52	0.41
9:I:50:ALA:HB2	10:J:129:CYS:HB2	2.02	0.41
11:K:9:GLY:HA3	11:K:12:TYR:CE1	2.55	0.41
13:M:17:GLY:HA3	13:M:20:PHE:CE1	2.55	0.41
3:Q:11:ILE:HG23	4:R:18:GLN:HE22	1.84	0.41
4:R:51:ALA:C	4:R:53:LEU:H	2.24	0.41
6:T:109:VAL:HG21	6:T:145:PHE:CG	2.55	0.41
13:1:57:PHE:HB3	13:1:105:TYR:HB3	2.02	0.41
3:C:193:ALA:O	3:C:197:LEU:HB2	2.20	0.41
1:O:86:ASP:OD2	1:O:132:ARG:NH2	2.53	0.41
4:R:136:PHE:CZ	4:R:142:PRO:HB3	2.56	0.41
2:B:197:SER:O	2:B:199:GLU:N	2.53	0.41
2:P:69:LYS:CE	15:P:314:HOH:O	2.67	0.41
3:Q:42:GLY:HA2	3:Q:145:PHE:CE1	2.56	0.41
7:U:171:ALA:O	7:U:174:THR:OG1	2.29	0.41
9:W:68:LEU:HA	9:W:68:LEU:HD12	1.95	0.41
4:D:51:ALA:C	4:D:53:LEU:H	2.24	0.41
5:E:186:HIS:O	5:E:189:MET:HG3	2.21	0.41
5:E:187:LYS:N	15:E:306:HOH:O	2.53	0.41
6:F:38:LEU:HD13	6:F:187:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:PRO:HA	5:E:26:TYR:CE1	2.56	0.41
13:M:82:ALA:HA	15:M:332:HOH:O	2.21	0.41
8:H:84:LYS:HB3	8:H:84:LYS:HE3	1.82	0.41
11:K:102:LEU:HG	11:K:118:MET:HB2	2.02	0.41
11:K:167:LEU:HA	11:K:167:LEU:HD23	1.92	0.41
13:M:57:PHE:HB3	13:M:105:TYR:HB3	2.02	0.41
3:Q:11:ILE:HG12	4:R:7:ILE:HG23	2.03	0.41
3:Q:164:ILE:HD13	3:Q:164:ILE:HA	1.90	0.41
4:R:108:THR:HG23	4:R:133:ILE:HD12	2.03	0.41
10:X:53:LEU:HB2	10:X:60:VAL:HG13	2.02	0.41
12:Z:12:VAL:HG11	12:Z:102:CYS:HB3	2.03	0.41
9:I:172:ASN:CB	9:I:191:VAL:HG22	2.51	0.41
10:J:15:LYS:HZ2	10:J:134:ASP:HA	1.85	0.41
12:L:8:PHE:N	12:L:8:PHE:CD1	2.89	0.41
6:T:84:LEU:HD23	6:T:84:LEU:HA	1.93	0.41
9:I:50:ALA:O	9:I:54:MET:HG2	2.20	0.41
12:L:12:VAL:HG11	12:L:102:CYS:HB3	2.03	0.41
12:L:15:ALA:HB2	12:L:176:LEU:HD13	2.03	0.41
12:L:8:PHE:HD1	12:L:8:PHE:H	1.69	0.41
2:P:94:GLN:HA	2:P:94:GLN:NE2	2.36	0.41
7:U:19:ARG:NH2	7:U:24:GLU:OE1	2.53	0.41
11:Y:1:MET:HE1	11:Y:134:TYR:N	2.25	0.41
12:Z:160:ILE:O	12:Z:164:THR:HG23	2.19	0.41
2:B:94:GLN:NE2	2:B:94:GLN:HA	2.36	0.41
6:F:71:GLY:HA3	6:F:221:PHE:CE1	2.56	0.41
7:G:172:ALA:O	7:G:176:ILE:HG13	2.21	0.41
3:Q:12:PHE:HB2	4:R:18:GLN:OE1	2.21	0.41
5:S:142:LEU:HG	5:S:170:ILE:HD13	2.03	0.41
7:U:185:THR:O	7:U:189:ILE:HG12	2.20	0.41
8:H:30:VAL:CG2	14:2:212:ALA:HA	2.45	0.40
1:A:191:PHE:O	1:A:195:VAL:HG23	2.21	0.40
4:D:115:LYS:NZ	4:D:147:THR:OG1	2.48	0.40
5:E:91:LYS:HE3	5:E:119:LEU:HD21	2.03	0.40
7:G:151:ILE:HA	7:G:156:VAL:O	2.21	0.40
7:G:41:CYS:HB2	7:G:184:MET:O	2.20	0.40
4:R:96:LEU:HD23	4:R:96:LEU:HA	1.87	0.40
8:V:14:LEU:HD21	8:V:101:ALA:CB	2.50	0.40
8:V:84:LYS:HE3	8:V:84:LYS:HB3	1.82	0.40
12:Z:43:GLY:HA3	12:Z:56:GLU:OE1	2.21	0.40
6:T:38:LEU:HD13	6:T:187:LEU:HG	2.03	0.40
11:K:45:LEU:HB2	11:K:103:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:9:GLY:HA3	11:Y:12:TYR:CE1	2.56	0.40
4:D:96:LEU:HA	4:D:96:LEU:HD23	1.88	0.40
9:W:65:LEU:HA	9:W:65:LEU:HD12	1.89	0.40
10:X:156:PRO:HB2	10:X:157:ASN:H	1.75	0.40
10:X:142:CYS:HB3	10:X:178:ASP:HB2	2.03	0.40
1:A:190:THR:H	1:A:193:GLN:HB3	1.86	0.40
8:H:134:TYR:CE1	14:2:33:LEU:HD13	2.56	0.40
14:N:22:ILE:HB	14:N:50:MET:HE3	2.02	0.40
14:N:25:ASP:O	14:N:41:ARG:HD3	2.22	0.40
2:P:79:GLY:O	2:P:82:TYR:HB3	2.22	0.40
5:S:197:SER:O	5:S:201:ILE:HG13	2.22	0.40
5:S:97:GLN:HB3	12:Z:61:ARG:HG3	2.02	0.40
12:Z:8:PHE:CD1	12:Z:8:PHE:N	2.89	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	242/244 (99%)	230 (95%)	7 (3%)	5 (2%)	8	14
1	O	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	36	60
2	B	231/233 (99%)	210 (91%)	18 (8%)	3 (1%)	13	27
2	P	231/233 (99%)	209 (90%)	19 (8%)	3 (1%)	13	27
3	C	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	36	60
3	Q	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	36	60
4	D	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	14	30
4	R	241/243 (99%)	222 (92%)	15 (6%)	4 (2%)	10	20
5	E	232/234 (99%)	220 (95%)	10 (4%)	2 (1%)	19	38
5	S	232/234 (99%)	220 (95%)	10 (4%)	2 (1%)	19	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	236/238 (99%)	223 (94%)	9 (4%)	4 (2%)	10	20
6	T	236/238 (99%)	224 (95%)	9 (4%)	3 (1%)	13	27
7	G	243/245 (99%)	233 (96%)	8 (3%)	2 (1%)	21	42
7	U	243/245 (99%)	234 (96%)	7 (3%)	2 (1%)	21	42
8	H	200/202 (99%)	196 (98%)	4 (2%)	0	100	100
8	V	200/202 (99%)	196 (98%)	4 (2%)	0	100	100
9	I	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
9	W	218/220 (99%)	208 (95%)	8 (4%)	2 (1%)	19	38
10	J	202/204 (99%)	189 (94%)	11 (5%)	2 (1%)	17	35
10	X	202/204 (99%)	189 (94%)	11 (5%)	2 (1%)	17	35
11	K	197/199 (99%)	188 (95%)	7 (4%)	2 (1%)	17	35
11	Y	197/199 (99%)	188 (95%)	7 (4%)	2 (1%)	17	35
12	L	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
12	Z	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
13	1	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
13	M	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
14	2	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	31	56
14	N	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	31	56
All	All	6230/6286 (99%)	5913 (95%)	269 (4%)	48 (1%)	21	42

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	PRO
5	E	120	ALA
6	F	238	GLU
7	G	207	LYS
10	J	156	PRO
4	R	101	PRO
5	S	120	ALA
7	U	207	LYS
9	W	187	ARG
10	X	156	PRO
1	A	188	ASP
1	A	189	TRP
2	B	40	ALA

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Mol	Chain	Res	Type
2	B	198	PHE
4	D	46	GLU
4	D	50	VAL
10	J	117	PHE
2	P	40	ALA
2	P	198	PHE
2	P	232	ILE
4	R	46	GLU
4	R	50	VAL
6	T	197	GLU
10	X	117	PHE
1	A	210	PHE
2	B	232	ILE
6	F	226	ASP
6	F	235	GLY
6	T	235	GLY
14	2	46	ASN
1	A	207	SER
6	F	50	LYS
11	K	197	PRO
14	N	46	ASN
6	T	238	GLU
11	Y	197	PRO
3	C	206	LEU
11	K	174	ASN
1	O	209	ASP
3	Q	206	LEU
5	S	187	LYS
9	W	188	PRO
11	Y	174	ASN
5	E	187	LYS
7	U	216	VAL
7	G	216	VAL
1	A	208	ILE
4	R	202	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/208 (93%)	185 (96%)	8 (4%)	33	60
1	O	193/208 (93%)	184 (95%)	9 (5%)	29	54
2	B	163/190 (86%)	160 (98%)	3 (2%)	62	83
2	P	165/190 (87%)	162 (98%)	3 (2%)	62	83
3	C	193/210 (92%)	184 (95%)	9 (5%)	29	54
3	Q	193/210 (92%)	185 (96%)	8 (4%)	33	60
4	D	152/207 (73%)	141 (93%)	11 (7%)	16	32
4	R	142/207 (69%)	133 (94%)	9 (6%)	20	40
5	E	189/196 (96%)	185 (98%)	4 (2%)	56	80
5	S	189/196 (96%)	184 (97%)	5 (3%)	49	75
6	F	198/204 (97%)	192 (97%)	6 (3%)	44	71
6	T	198/204 (97%)	190 (96%)	8 (4%)	34	61
7	G	195/202 (96%)	189 (97%)	6 (3%)	43	70
7	U	195/202 (96%)	188 (96%)	7 (4%)	38	65
8	H	155/157 (99%)	152 (98%)	3 (2%)	60	82
8	V	155/157 (99%)	153 (99%)	2 (1%)	71	88
9	I	177/181 (98%)	168 (95%)	9 (5%)	26	50
9	W	177/181 (98%)	169 (96%)	8 (4%)	30	56
10	J	172/173 (99%)	162 (94%)	10 (6%)	22	44
10	X	172/173 (99%)	161 (94%)	11 (6%)	19	39
11	K	164/170 (96%)	159 (97%)	5 (3%)	44	71
11	Y	164/170 (96%)	159 (97%)	5 (3%)	44	71
12	L	153/156 (98%)	148 (97%)	5 (3%)	41	68
12	Z	154/156 (99%)	148 (96%)	6 (4%)	35	62
13	1	175/178 (98%)	174 (99%)	1 (1%)	87	96
13	M	174/178 (98%)	172 (99%)	2 (1%)	76	90
14	2	175/179 (98%)	163 (93%)	12 (7%)	17	34
14	N	175/179 (98%)	165 (94%)	10 (6%)	23	45
All	All	4900/5222 (94%)	4715 (96%)	185 (4%)	36	63

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
1	A	78	CYS
1	A	114	LEU
1	A	132	ARG
1	A	166	THR
1	A	221	THR
1	A	231	THR
1	A	234	GLU
2	B	87	HIS
2	B	132	SER
2	B	178	ASN
3	C	44	LEU
3	C	74	CYS
3	C	76	VAL
3	C	164	ILE
3	C	180	LYS
3	C	192	LEU
3	C	197	LEU
3	C	218	ARG
3	C	220	ASN
4	D	15	HIS
4	D	35	VAL
4	D	38	ARG
4	D	41	VAL
4	D	43	LEU
4	D	56	GLU
4	D	99	GLU
4	D	103	THR
4	D	139	ASP
4	D	146	GLN
4	D	184	ASP
5	E	9	ASP
5	E	36	THR
5	E	135	ARG
5	E	148	GLU
6	F	38	LEU
6	F	83	LEU
6	F	101	ARG
6	F	202	GLU
6	F	225	ASP
6	F	239	ARG
7	G	5	THR
7	G	39	ILE

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Mol	Chain	Res	Type
7	G	129	ARG
7	G	144	ASP
7	G	181	MET
7	G	187	ARG
8	H	22	THR
8	H	46	SER
8	H	150	GLU
9	I	6	VAL
9	I	56	THR
9	I	65	LEU
9	I	77	VAL
9	I	132	LEU
9	I	186	LEU
9	I	187	ARG
9	I	198	ARG
9	I	201	ARG
10	J	20	VAL
10	J	34	MET
10	J	36	THR
10	J	49	LEU
10	J	126	LEU
10	J	175	VAL
10	J	189	ILE
10	J	190	ILE
10	J	191	GLU
10	J	193	ASP
11	K	27	GLN
11	K	45	LEU
11	K	84	THR
11	K	85	ARG
11	K	171	PHE
12	L	8	PHE
12	L	82	LEU
12	L	87	VAL
12	L	115	ASP
12	L	138	VAL
13	M	76	LYS
13	M	99	ARG
14	N	37	ARG
14	N	49	THR
14	N	86	ARG
14	N	94	ARG

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Mol	Chain	Res	Type
14	N	100	ARG
14	N	141	TYR
14	N	159	VAL
14	N	168	LEU
14	N	192	VAL
14	N	205	THR
1	O	73	THR
1	O	78	CYS
1	O	114	LEU
1	O	132	ARG
1	O	166	THR
1	O	205	VAL
1	O	221	THR
1	O	231	THR
1	O	234	GLU
2	P	87	HIS
2	P	132	SER
2	P	178	ASN
3	Q	44	LEU
3	Q	74	CYS
3	Q	76	VAL
3	Q	164	ILE
3	Q	180	LYS
3	Q	192	LEU
3	Q	218	ARG
3	Q	220	ASN
4	R	15	HIS
4	R	35	VAL
4	R	38	ARG
4	R	41	VAL
4	R	99	GLU
4	R	103	THR
4	R	139	ASP
4	R	146	GLN
4	R	184	ASP
5	S	9	ASP
5	S	36	THR
5	S	84	ASP
5	S	135	ARG
5	S	148	GLU
6	T	38	LEU
6	T	83	LEU

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Mol	Chain	Res	Type
6	T	101	ARG
6	T	196	ARG
6	T	202	GLU
6	T	211	SER
6	T	236	LEU
6	T	239	ARG
7	U	5	THR
7	U	39	ILE
7	U	41	CYS
7	U	42	LYS
7	U	129	ARG
7	U	144	ASP
7	U	181	MET
8	V	22	THR
8	V	150	GLU
9	W	6	VAL
9	W	56	THR
9	W	65	LEU
9	W	77	VAL
9	W	132	LEU
9	W	187	ARG
9	W	198	ARG
9	W	201	ARG
10	X	20	VAL
10	X	27	ARG
10	X	34	MET
10	X	36	THR
10	X	49	LEU
10	X	126	LEU
10	X	175	VAL
10	X	189	ILE
10	X	190	ILE
10	X	191	GLU
10	X	193	ASP
11	Y	27	GLN
11	Y	45	LEU
11	Y	84	THR
11	Y	85	ARG
11	Y	171	PHE
12	Z	8	PHE
12	Z	73	ARG
12	Z	82	LEU

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Mol	Chain	Res	Type
12	Z	87	VAL
12	Z	115	ASP
12	Z	138	VAL
13	1	99	ARG
14	2	37	ARG
14	2	49	THR
14	2	86	ARG
14	2	94	ARG
14	2	99	ARG
14	2	100	ARG
14	2	141	TYR
14	2	159	VAL
14	2	168	LEU
14	2	186	ARG
14	2	192	VAL
14	2	205	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
12	L	10	HIS
13	M	146	GLN
14	N	81	HIS
12	Z	10	HIS
12	Z	38	ASN
13	1	146	GLN
14	2	81	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	244/244 (100%)	0.13	7 (2%)	51	44	55, 89, 135, 176	0
1	O	244/244 (100%)	0.43	23 (9%)	8	5	57, 97, 148, 214	0
2	B	233/233 (100%)	0.12	7 (3%)	50	43	56, 83, 130, 210	0
2	P	233/233 (100%)	0.20	5 (2%)	63	58	57, 83, 129, 215	0
3	C	250/250 (100%)	0.21	13 (5%)	27	20	57, 87, 147, 232	0
3	Q	250/250 (100%)	0.34	17 (6%)	17	12	54, 89, 157, 228	0
4	D	243/243 (100%)	0.42	20 (8%)	11	8	55, 95, 177, 238	0
4	R	243/243 (100%)	0.60	35 (14%)	2	1	53, 98, 190, 261	0
5	E	234/234 (100%)	0.27	13 (5%)	24	18	51, 90, 134, 187	0
5	S	234/234 (100%)	0.30	12 (5%)	28	21	50, 91, 134, 178	0
6	F	238/238 (100%)	0.31	12 (5%)	29	22	50, 79, 125, 199	0
6	T	238/238 (100%)	0.33	17 (7%)	16	11	54, 82, 130, 246	0
7	G	245/245 (100%)	0.20	6 (2%)	59	52	59, 85, 131, 198	0
7	U	245/245 (100%)	0.59	28 (11%)	5	3	61, 92, 145, 222	0
8	H	202/202 (100%)	0.16	5 (2%)	57	50	53, 69, 111, 212	0
8	V	202/202 (100%)	0.16	4 (1%)	65	59	50, 70, 113, 171	0
9	I	220/220 (100%)	0.09	4 (1%)	68	63	51, 67, 109, 169	0
9	W	220/220 (100%)	0.07	2 (0%)	84	81	48, 67, 114, 157	0
10	J	204/204 (100%)	0.04	1 (0%)	90	89	47, 66, 99, 150	0
10	X	204/204 (100%)	0.00	1 (0%)	90	89	46, 65, 96, 141	0
11	K	199/199 (100%)	0.06	3 (1%)	73	69	47, 70, 103, 207	0
11	Y	199/199 (100%)	0.09	2 (1%)	82	79	49, 70, 101, 171	0
12	L	201/201 (100%)	0.02	1 (0%)	90	89	41, 66, 100, 140	0
12	Z	201/201 (100%)	-0.08	1 (0%)	90	89	46, 66, 101, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	213/213 (100%)	-0.10	1 (0%) 90 89	42, 63, 92, 149	0
13	M	213/213 (100%)	-0.06	2 (0%) 84 81	44, 61, 94, 137	0
14	2	217/217 (100%)	0.07	6 (2%) 53 46	42, 69, 101, 167	0
14	N	217/217 (100%)	0.12	5 (2%) 60 54	42, 64, 102, 192	0
All	All	6286/6286 (100%)	0.19	253 (4%) 38 30	41, 77, 135, 261	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	233	ALA	17.1
2	P	232	ILE	13.8
11	K	199	GLN	13.6
2	B	233	ALA	12.7
6	T	240	PRO	12.6
4	R	244	GLN	10.0
4	R	48	LYS	9.4
2	B	232	ILE	9.2
4	R	242	LYS	9.1
14	2	217	GLY	9.1
1	O	245	ARG	8.3
3	Q	247	ALA	8.1
11	Y	199	GLN	6.7
8	H	202	LEU	6.7
4	R	201	SER	6.6
8	H	200	ALA	6.6
4	R	239	ASN	6.5
5	E	241	ILE	6.3
3	Q	250	GLU	6.2
14	N	215	ILE	6.2
4	R	238	GLU	6.2
4	D	244	GLN	6.1
7	G	3	ILE	6.1
4	R	243	LYS	5.5
5	E	191	LEU	5.4
13	1	1	ARG	5.3
3	Q	251	LYS	5.1
7	U	5	THR	5.0
1	O	239	LEU	4.9
4	R	203	GLY	4.8
4	R	232	ILE	4.8
4	D	39	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
7	U	2	SER	4.7
7	U	215	TRP	4.7
7	U	241	GLU	4.7
6	T	241	GLN	4.6
6	F	240	PRO	4.5
7	U	3	ILE	4.5
3	Q	205	LYS	4.4
4	D	38	ARG	4.3
4	D	181	ILE	4.2
4	D	228	TYR	4.2
5	E	8	TYR	4.2
4	R	240	GLU	4.1
3	C	204	SER	4.1
13	M	1	ARG	4.0
5	S	241	ILE	4.0
5	E	238	ILE	4.0
2	B	1	ALA	4.0
8	H	144	ARG	3.9
6	T	236	LEU	3.9
4	D	243	LYS	3.9
4	R	241	LYS	3.9
4	D	238	GLU	3.9
3	C	203	VAL	3.8
4	R	202	GLY	3.8
4	R	38	ARG	3.8
10	J	117	PHE	3.7
1	O	236	ASP	3.7
4	R	181	ILE	3.7
3	Q	249	ARG	3.7
7	U	235	ALA	3.7
3	Q	203	VAL	3.7
14	N	216	SER	3.6
14	2	216	SER	3.6
5	S	191	LEU	3.5
7	G	1	SER	3.5
7	U	236	GLU	3.5
14	N	217	GLY	3.5
1	O	210	PHE	3.4
3	C	249	ARG	3.4
1	O	243	ALA	3.4
7	U	240	LYS	3.4
1	O	202	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
7	U	1	SER	3.3
3	C	181	GLU	3.3
4	R	206	ILE	3.3
1	O	212	PRO	3.3
1	O	188	ASP	3.2
2	P	231	ALA	3.2
6	F	200	PRO	3.2
14	2	194	GLU	3.2
4	D	48	LYS	3.2
9	I	201	ARG	3.2
12	L	201	GLY	3.1
4	R	237	GLU	3.1
10	X	117	PHE	3.1
4	D	214	ASP	3.1
4	R	37	GLY	3.1
3	C	238	LYS	3.1
6	F	201	ALA	3.1
4	D	178	ASP	3.0
1	O	240	VAL	3.0
3	C	197	LEU	3.0
1	O	238	HIS	3.0
1	A	210	PHE	3.0
3	Q	206	LEU	3.0
6	T	200	PRO	3.0
4	R	235	GLU	3.0
8	H	199	VAL	3.0
6	T	201	ALA	2.9
3	C	247	ALA	2.9
5	E	196	LYS	2.9
1	O	214	GLU	2.9
7	U	176	ILE	2.9
3	Q	244	GLU	2.9
4	R	234	LYS	2.9
4	D	180	ALA	2.9
6	T	157	ARG	2.9
7	U	181	MET	2.9
12	Z	200	SER	2.8
4	D	179	GLU	2.8
5	S	185	TYR	2.8
5	E	195	ILE	2.8
5	S	202	LEU	2.8
2	B	39	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
4	R	49	SER	2.8
4	R	176	TYR	2.8
1	O	191	PHE	2.8
1	A	209	ASP	2.8
7	U	209	PHE	2.8
4	R	39	ASP	2.8
9	W	205	GLU	2.7
7	U	243	LEU	2.7
4	R	172	LEU	2.7
14	2	115	TYR	2.7
1	O	217	VAL	2.7
6	T	174	ARG	2.7
1	O	184	LYS	2.7
4	R	228	TYR	2.7
3	C	246	LYS	2.7
5	S	181	LEU	2.7
7	U	140	TYR	2.7
4	D	237	GLU	2.7
7	U	208	ALA	2.6
7	G	5	THR	2.6
2	P	173	LEU	2.6
5	S	120	ALA	2.6
3	Q	181	GLU	2.6
4	R	190	LEU	2.6
4	D	171	PHE	2.6
1	A	211	LYS	2.6
6	T	4	ASN	2.6
4	R	199	VAL	2.6
4	D	49	SER	2.6
11	Y	1	MET	2.6
3	Q	204	SER	2.6
3	Q	242	GLU	2.5
4	D	47	LYS	2.5
6	T	179	PHE	2.5
1	O	200	THR	2.5
1	A	242	LEU	2.5
3	Q	241	GLU	2.5
2	B	188	HIS	2.5
6	F	205	LEU	2.5
6	T	38	LEU	2.5
6	F	234	GLU	2.5
6	F	179	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	7	ILE	2.5
2	B	2	GLU	2.5
6	F	53	GLN	2.5
7	U	193	VAL	2.5
8	V	9	ASP	2.5
7	U	7	TYR	2.4
6	F	207	THR	2.4
9	I	189	TYR	2.4
8	V	200	ALA	2.4
6	F	55	GLU	2.4
2	B	178	ASN	2.4
5	E	239	LYS	2.4
6	F	233	LEU	2.4
7	U	211	LEU	2.4
7	U	197	ILE	2.4
4	R	136	PHE	2.4
4	D	176	TYR	2.4
1	O	183	VAL	2.4
3	Q	248	GLU	2.4
7	U	175	GLU	2.4
1	O	208	ILE	2.4
3	Q	237	ILE	2.4
7	U	225	GLU	2.3
4	R	35	VAL	2.3
9	I	199	LEU	2.3
3	C	242	GLU	2.3
5	S	131	GLY	2.3
11	K	174	ASN	2.3
4	R	41	VAL	2.3
3	Q	246	LYS	2.3
7	G	245	GLU	2.3
1	O	42	VAL	2.3
4	R	168	VAL	2.3
5	E	210	LEU	2.3
3	C	205	LYS	2.3
4	R	200	GLN	2.3
4	R	191	VAL	2.3
1	A	245	ARG	2.3
9	W	201	ARG	2.3
5	E	193	GLU	2.3
5	E	199	LEU	2.3
7	U	200	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
6	T	204	ASP	2.3
1	O	2	SER	2.3
6	T	172	LEU	2.3
7	U	219	LEU	2.3
5	S	42	THR	2.3
2	P	185	ASP	2.3
7	U	190	VAL	2.3
1	O	244	GLU	2.2
3	C	233	VAL	2.2
6	F	238	GLU	2.2
3	Q	19	TYR	2.2
1	O	206	LEU	2.2
4	R	52	LYS	2.2
14	2	1	THR	2.2
6	T	210	VAL	2.2
7	U	189	ILE	2.2
14	N	1	THR	2.2
6	T	239	ARG	2.2
5	E	202	LEU	2.2
5	E	240	ASP	2.2
5	S	240	ASP	2.2
6	T	55	GLU	2.2
7	U	184	MET	2.2
7	G	4	GLY	2.2
5	S	210	LEU	2.1
7	U	44	GLY	2.1
4	R	173	GLU	2.1
4	D	202	GLY	2.1
9	I	200	GLY	2.1
11	K	198	LYS	2.1
5	S	193	GLU	2.1
8	V	90	TYR	2.1
5	S	9	ASP	2.1
7	G	2	SER	2.1
5	E	181	LEU	2.1
6	T	34	ALA	2.1
1	A	62	ASP	2.1
1	O	232	GLU	2.1
6	F	195	LEU	2.1
14	N	32	SER	2.1
3	C	235	GLN	2.0
6	T	180	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	185	LYS	2.0
8	V	92	GLU	2.0
8	H	9	ASP	2.0
3	Q	240	HIS	2.0
13	M	162	GLU	2.0
3	C	179	TYR	2.0
1	O	58	ASP	2.0
4	D	230	ALA	2.0
4	R	184	ASP	2.0
14	2	186	ARG	2.0
7	U	182	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.