Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:29 PM GMT

PDB ID	:	4EU2
Title	:	Crystal structure of 20s proteasome with novel inhibitor K-7174
Authors	:	Kikuchi, J.; Shibayama, N.; Yamada, S.; Wada, T.; Nobuyoshi, M.; Izumi, T.; Akutsu, M.; Kano, Y.; Ohki, M.; Sugiyama, K.; Park, S.-Y.; Furukawa, Y.
Deposited on	:	2012-04-25
Resolution	:	2.51 Å(reported)

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

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

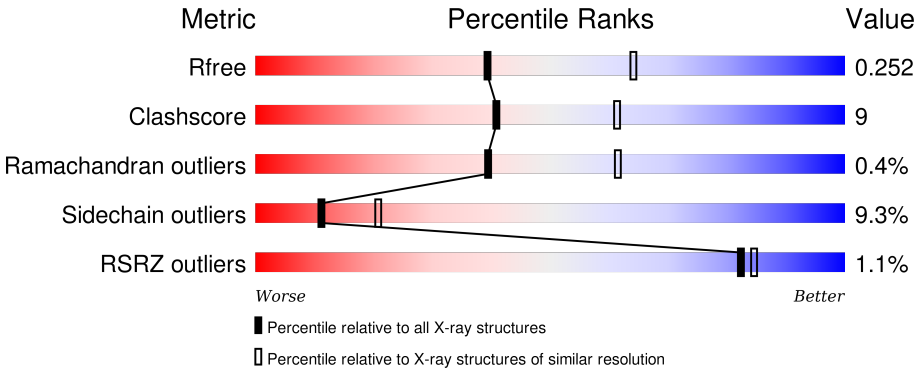
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	241	% 75% 22% •
1	O	241	70% 27% •
2	B	250	84% 14% •
2	P	250	67% 30% •
3	C	244	% 76% 23% •

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Mol	Chain	Length	Quality of chain
3	Q	244	2% 72% 25%
4	D	241	74% 23%
4	R	241	5% 70% 26%
5	E	242	2% 72% 24%
5	S	242	4% 70% 24% 5%
6	F	233	2% 70% 26%
6	T	233	3% 64% 30% 6%
7	G	244	76% 22%
7	U	244	72% 25%
8	H	196	74% 23%
8	V	196	79% 19%
9	I	222	80% 20%
9	W	222	73% 24%
10	J	204	78% 21%
10	X	204	82% 16%
11	K	198	75% 21%
11	Y	198	77% 19%
12	L	212	84% 13%
12	Z	212	85% 11%
13	1	222	75% 22%
13	M	222	76% 23%
14	2	233	74% 23%
14	N	233	78% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	WPI	H	300	-	-	-	X
15	WPI	I	301	-	-	-	X
15	WPI	L	301	-	-	-	X
15	WPI	V	201	-	-	-	X
15	WPI	W	301	-	-	-	X
15	WPI	Z	301	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50701 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 component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1903	1212	319	364	8			
1	O	241	Total	C	N	O	S	0	0	0
			1903	1212	319	364	8			

- Molecule 2 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1906	1213	314	375	4			
2	P	249	Total	C	N	O	S	0	0	0
			1906	1213	314	375	4			

- Molecule 3 is a protein called Proteasome component Y13.

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

- Molecule 4 is a protein called Proteasome component PRE6.

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

- Molecule 5 is a protein called Proteasome component PUP2.

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

- Molecule 6 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			
6	T	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

- Molecule 7 is a protein called Proteasome component C1.

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

- Molecule 8 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
8	V	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 9 is a protein called Proteasome component PUP1.

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

- Molecule 10 is a protein called Proteasome component PUP3.

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

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

- Molecule 11 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			
11	Y	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			

- Molecule 12 is a protein called Proteasome component PRE2.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 13 is a protein called Proteasome component C5.

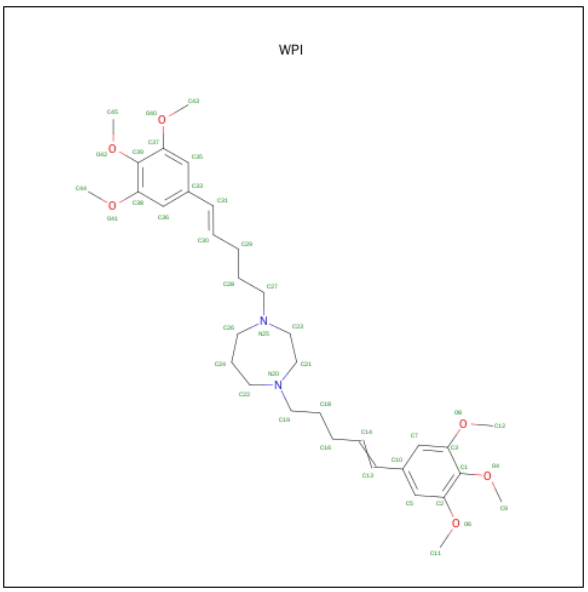
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	1	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called Proteasome component PRE4.

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

- Molecule 15 is 1,4-BIS[(4E)-5-(3,4,5-TRIMETHOXYPHENYL)PENT-4-EN-1-YL]-1,4-DIA

ZEPANE (three-letter code: WPI) (formula: $C_{33}H_{48}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total C N O 41 33 2 6	0	0
15	I	1	Total C N O 41 33 2 6	0	0
15	L	1	Total C N O 41 33 2 6	0	0
15	V	1	Total C N O 41 33 2 6	0	0
15	W	1	Total C N O 41 33 2 6	0	0
15	Z	1	Total C N O 41 33 2 6	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	47	Total O 47 47	0	0
16	B	27	Total O 27 27	0	0
16	C	34	Total O 34 34	0	0
16	D	35	Total O 35 35	0	0
16	E	30	Total O 30 30	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	F	18	Total O 18 18	0	0
16	G	36	Total O 36 36	0	0
16	H	34	Total O 34 34	0	0
16	I	29	Total O 29 29	0	0
16	J	47	Total O 47 47	0	0
16	K	34	Total O 34 34	0	0
16	L	46	Total O 46 46	0	0
16	M	51	Total O 51 51	0	0
16	N	44	Total O 44 44	0	0
16	O	33	Total O 33 33	0	0
16	P	32	Total O 32 32	0	0
16	Q	33	Total O 33 33	0	0
16	R	18	Total O 18 18	0	0
16	S	23	Total O 23 23	0	0
16	T	19	Total O 19 19	0	0
16	U	38	Total O 38 38	0	0
16	V	47	Total O 47 47	0	0
16	W	36	Total O 36 36	0	0
16	X	36	Total O 36 36	0	0
16	Y	49	Total O 49 49	0	0
16	Z	41	Total O 41 41	0	0

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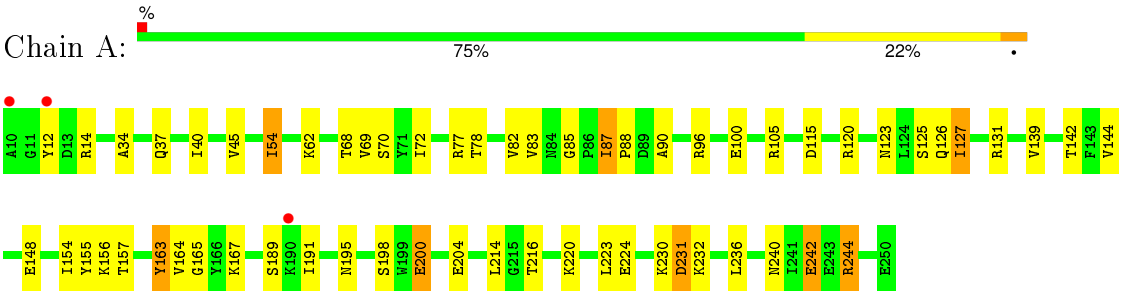
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	1	41	Total O 41 41	0	0
16	2	51	Total O 51 51	0	0

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.

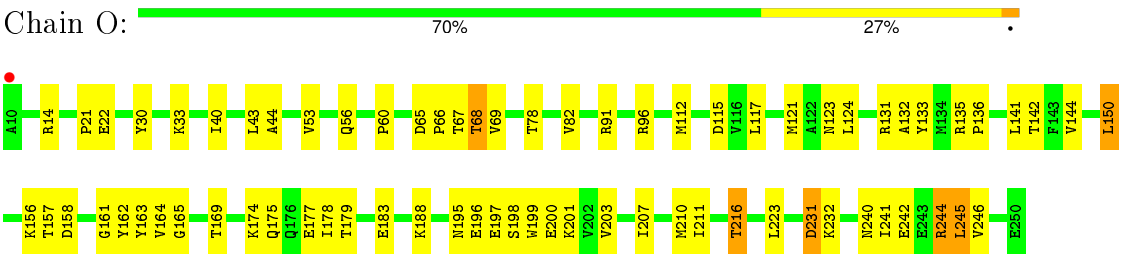
- Molecule 1: Proteasome component C7-alpha

Chain A:



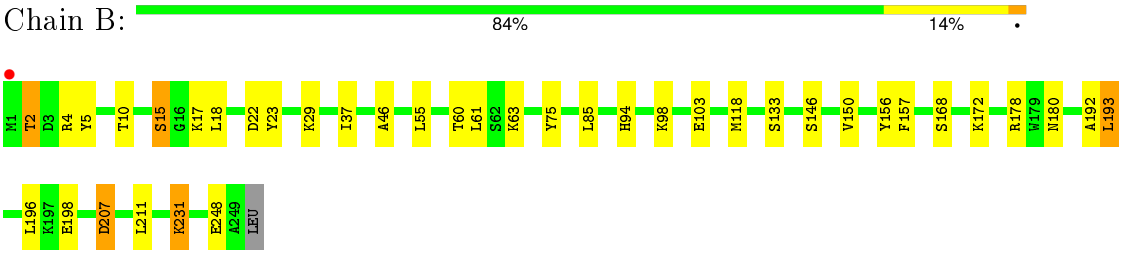
- Molecule 1: Proteasome component C7-alpha

Chain O:



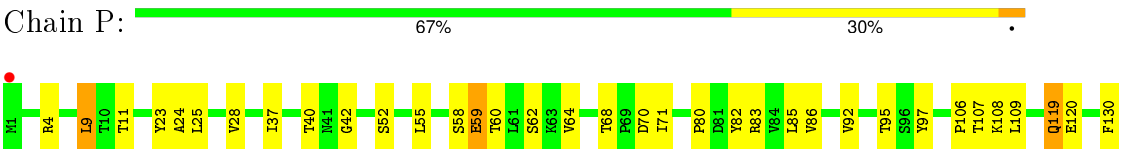
- Molecule 2: Proteasome component Y7

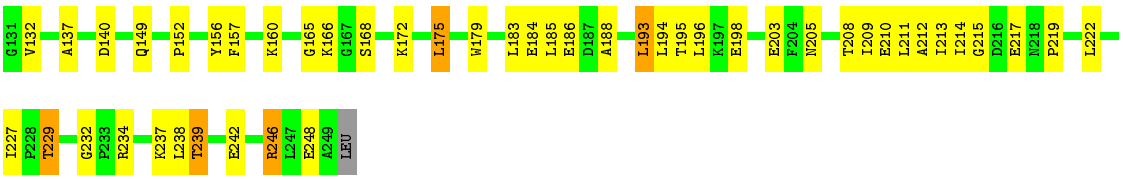
Chain B:



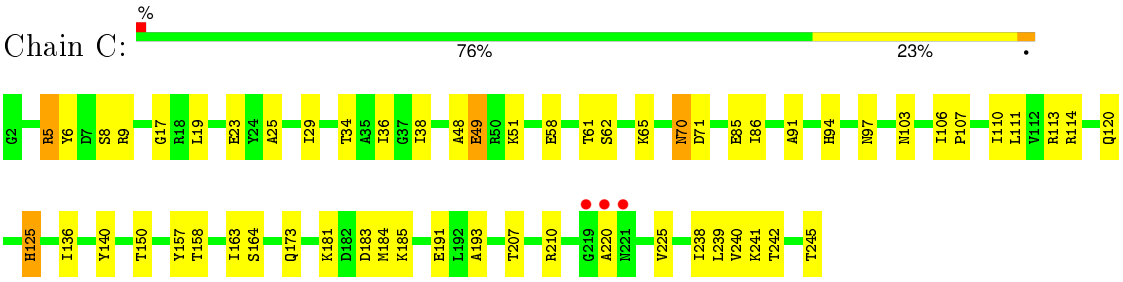
- Molecule 2: Proteasome component Y7

Chain P:

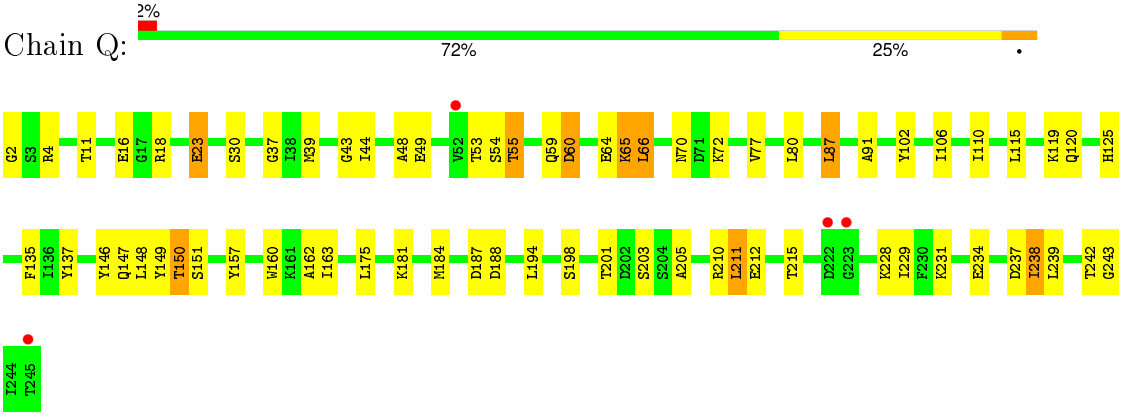




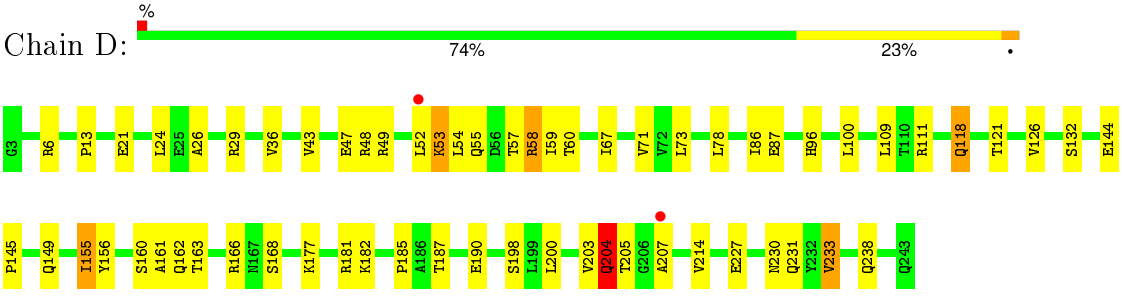
• Molecule 3: Proteasome component Y13



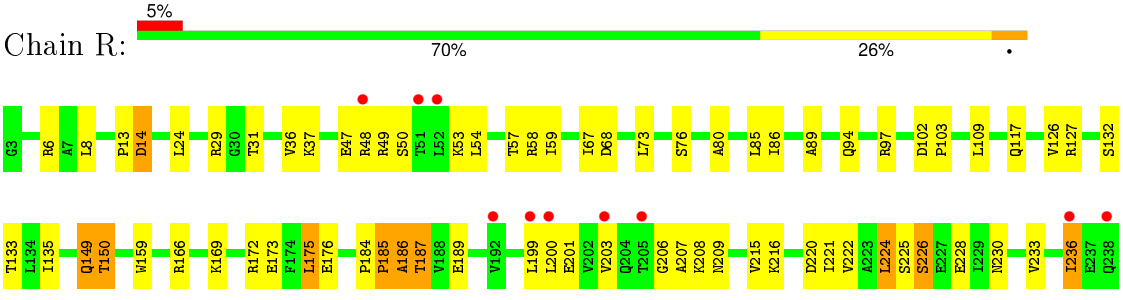
• Molecule 3: Proteasome component Y13



• Molecule 4: Proteasome component PRE6

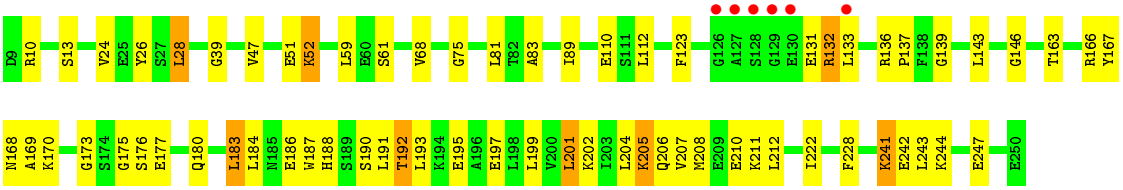


• Molecule 4: Proteasome component PRE6



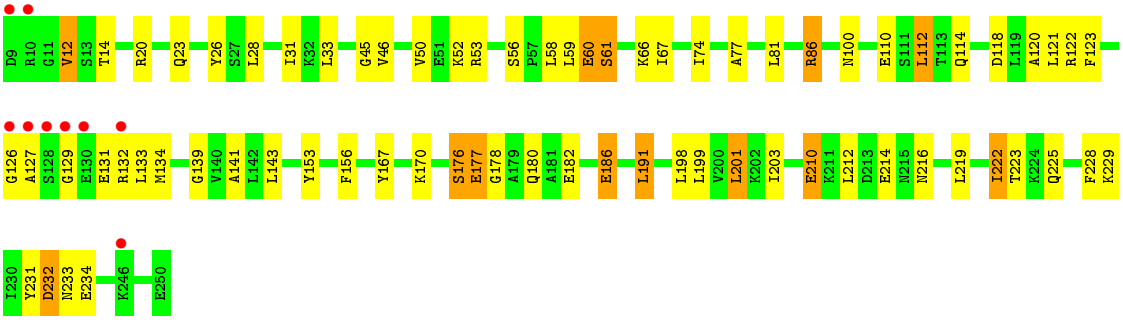
• Molecule 5: Proteasome component PUP2

Chain E:



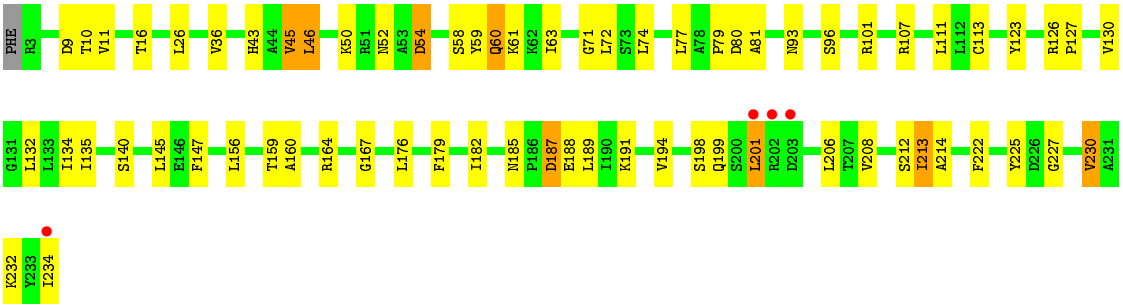
• Molecule 5: Proteasome component PUP2

Chain S:



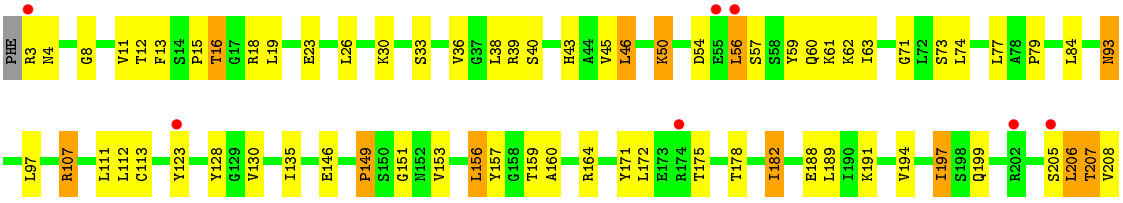
• Molecule 6: Proteasome component PRE5

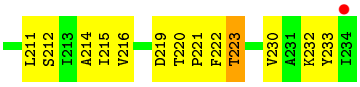
Chain F:



• Molecule 6: Proteasome component PRE5

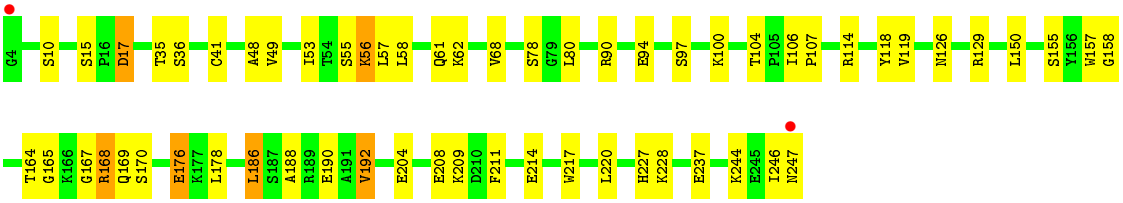
Chain T:





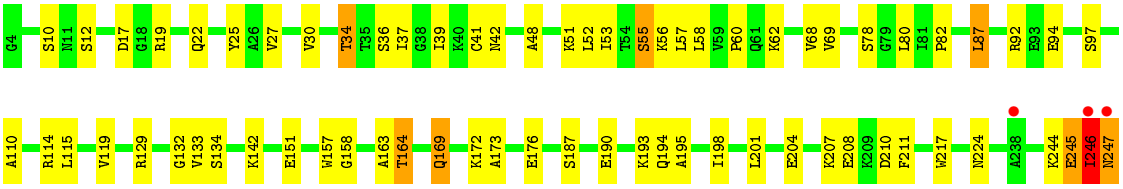
• Molecule 7: Proteasome component C1

Chain G:



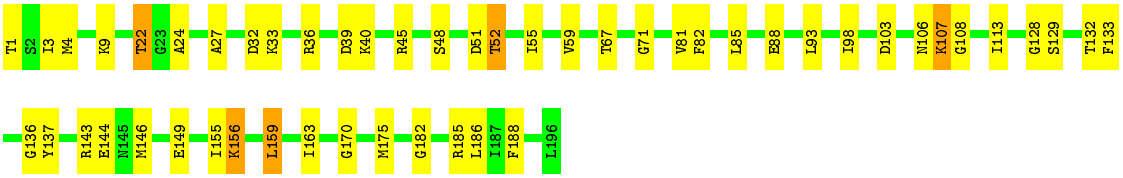
• Molecule 7: Proteasome component C1

Chain U:



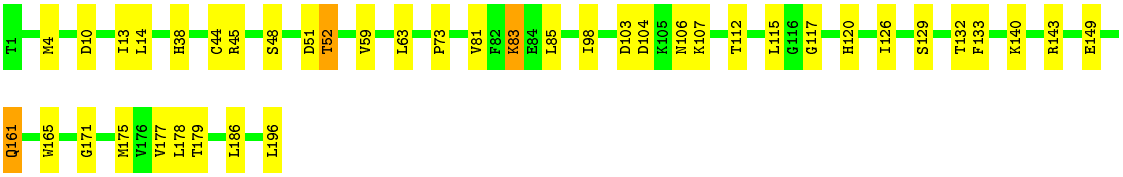
• Molecule 8: Proteasome component PRE3

Chain H:



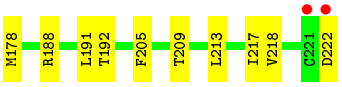
• Molecule 8: Proteasome component PRE3

Chain V:



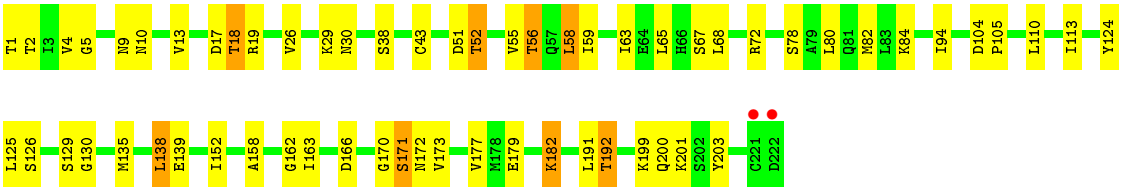
• Molecule 9: Proteasome component PUP1

Chain I:



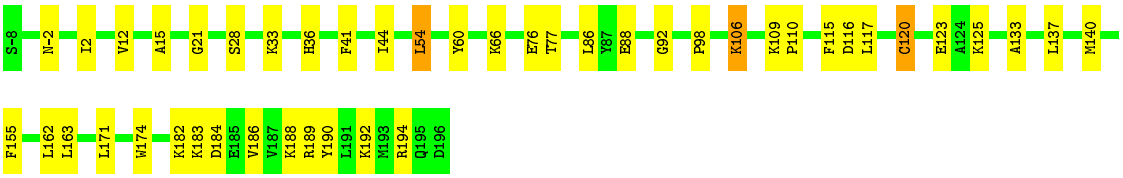
• Molecule 9: Proteasome component PUP1

Chain W:



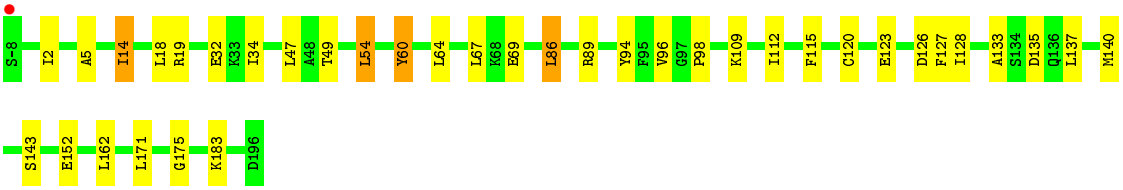
• Molecule 10: Proteasome component PUP3

Chain J:



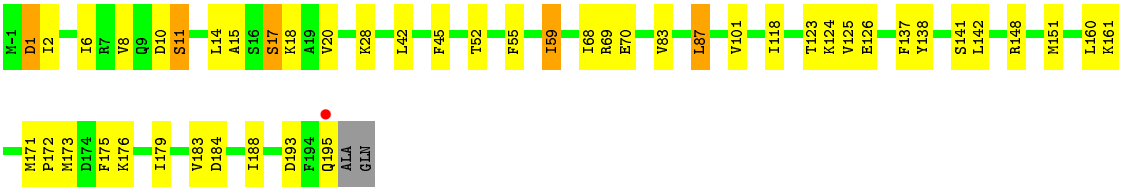
• Molecule 10: Proteasome component PUP3

Chain X:



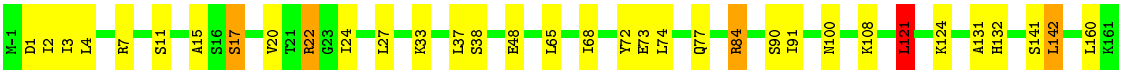
• Molecule 11: Proteasome component C11

Chain K:



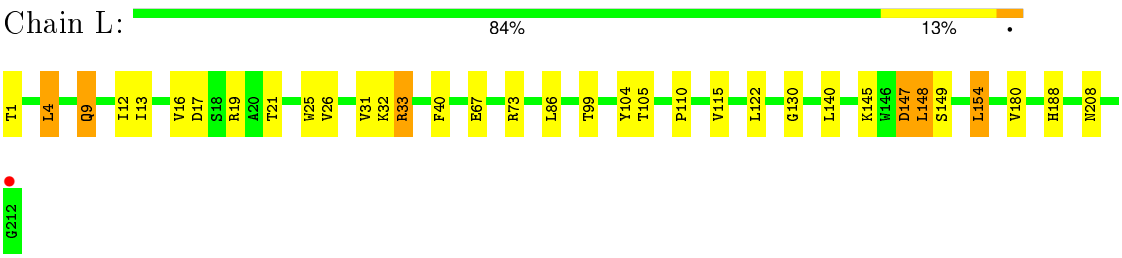
• Molecule 11: Proteasome component C11

Chain Y:



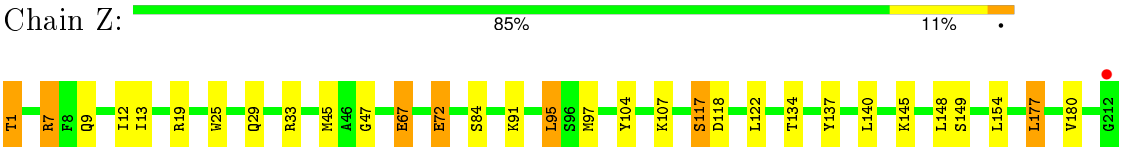
• Molecule 12: Proteasome component PRE2

Chain L:



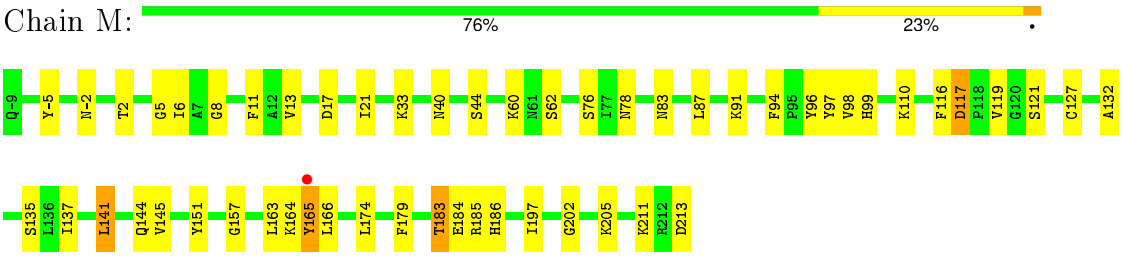
• Molecule 12: Proteasome component PRE2

Chain Z:



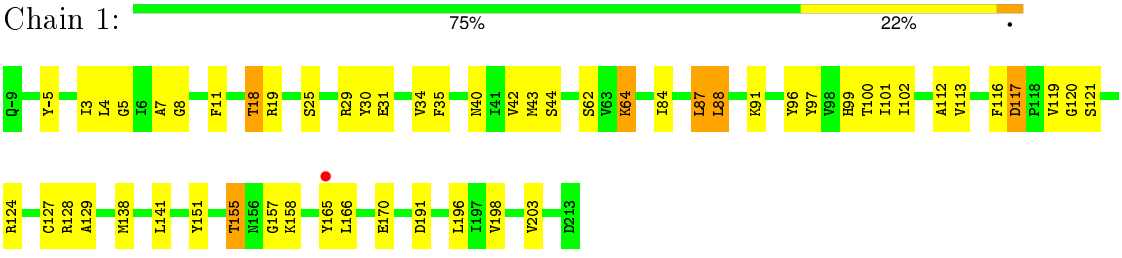
• Molecule 13: Proteasome component C5

Chain M:



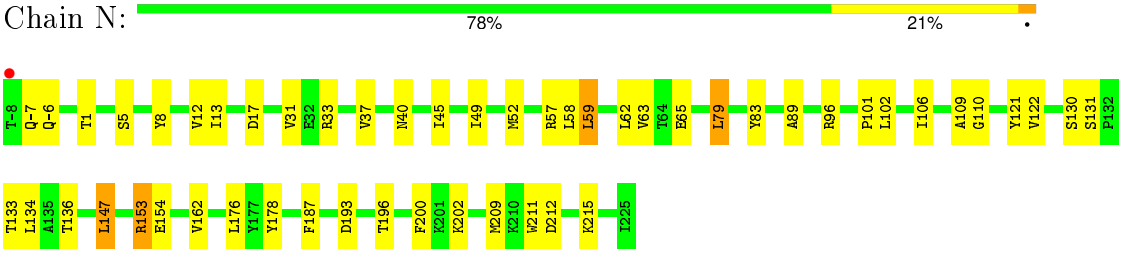
• Molecule 13: Proteasome component C5

Chain 1:



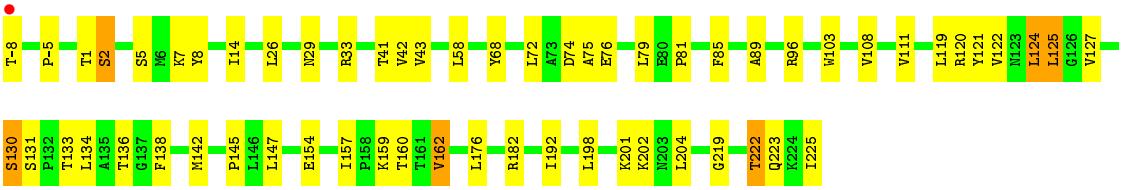
• Molecule 14: Proteasome component PRE4

Chain N:



• Molecule 14: Proteasome component PRE4

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.26Å 301.36Å 143.96Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	45.70 – 2.51 47.42 – 2.51	Depositor EDS
% Data completeness (in resolution range)	87.6 (45.70-2.51) 87.6 (47.42-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.202 , 0.255 0.202 , 0.252	Depositor DCC
R_{free} test set	15842 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 32.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 313767 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	50701	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.45	0/1941	0.62	0/2629
1	O	0.47	0/1941	0.59	0/2629
2	B	0.45	0/1943	0.59	0/2631
2	P	0.43	0/1943	0.57	0/2631
3	C	0.43	0/1935	0.58	0/2618
3	Q	0.44	0/1935	0.59	0/2618
4	D	0.41	0/1920	0.58	0/2598
4	R	0.42	0/1920	0.56	0/2598
5	E	0.45	0/1887	0.59	0/2541
5	S	0.41	0/1887	0.58	0/2541
6	F	0.40	0/1811	0.55	0/2447
6	T	0.41	0/1811	0.59	0/2447
7	G	0.42	0/1937	0.54	0/2614
7	U	0.43	0/1937	0.57	0/2614
8	H	0.45	0/1541	0.60	0/2087
8	V	0.46	0/1541	0.59	0/2087
9	I	0.45	0/1716	0.62	0/2326
9	W	0.43	0/1716	0.58	0/2326
10	J	0.44	0/1611	0.58	0/2174
10	X	0.47	0/1611	0.62	0/2174
11	K	0.44	0/1598	0.58	0/2154
11	Y	0.46	0/1598	0.63	1/2154 (0.0%)
12	L	0.46	0/1683	0.61	0/2277
12	Z	0.42	0/1683	0.58	0/2277
13	1	0.42	0/1795	0.60	0/2420
13	M	0.45	0/1795	0.61	0/2420
14	2	0.47	0/1855	0.62	0/2514
14	N	0.44	0/1855	0.61	0/2514
All	All	0.44	0/50346	0.59	1/68060 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	121	LEU	CA-CB-CG	6.17	129.49	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1903	0	1898	45	0
1	O	1903	0	1898	47	0
2	B	1906	0	1918	25	0
2	P	1906	0	1918	44	0
3	C	1905	0	1901	33	0
3	Q	1905	0	1901	43	0
4	D	1891	0	1900	38	0
4	R	1891	0	1900	44	0
5	E	1862	0	1836	37	0
5	S	1862	0	1836	42	0
6	F	1784	0	1788	39	0
6	T	1784	0	1788	44	0
7	G	1897	0	1886	29	0
7	U	1897	0	1886	45	0
8	H	1512	0	1481	40	0
8	V	1512	0	1481	27	0
9	I	1685	0	1688	24	0
9	W	1685	0	1688	35	0
10	J	1581	0	1574	21	0
10	X	1581	0	1574	18	0
11	K	1570	0	1577	27	0
11	Y	1570	0	1577	26	0
12	L	1646	0	1595	22	0
12	Z	1646	0	1595	21	0
13	1	1757	0	1711	36	0
13	M	1757	0	1711	27	0
14	2	1824	0	1832	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1824	0	1832	30	0
15	H	41	0	48	5	0
15	I	41	0	48	7	0
15	L	41	0	48	5	0
15	V	41	0	48	11	0
15	W	41	0	48	3	0
15	Z	41	0	48	9	0
16	1	41	0	0	1	0
16	2	51	0	0	2	0
16	A	47	0	0	0	0
16	B	27	0	0	0	0
16	C	34	0	0	0	0
16	D	35	0	0	0	0
16	E	30	0	0	0	0
16	F	18	0	0	0	0
16	G	36	0	0	0	0
16	H	34	0	0	1	0
16	I	29	0	0	0	0
16	J	47	0	0	0	0
16	K	34	0	0	1	0
16	L	46	0	0	0	0
16	M	51	0	0	0	0
16	N	44	0	0	1	0
16	O	33	0	0	1	0
16	P	32	0	0	0	0
16	Q	33	0	0	0	0
16	R	18	0	0	0	0
16	S	23	0	0	1	0
16	T	19	0	0	0	0
16	U	38	0	0	0	0
16	V	47	0	0	0	0
16	W	36	0	0	0	0
16	X	36	0	0	0	0
16	Y	49	0	0	1	0
16	Z	41	0	0	1	0
All	All	50701	0	49458	854	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 9.

All (854) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:165:GLY:H	2:P:60:THR:HG21	1.14	1.09
7:U:245:GLU:O	7:U:246:ILE:HG22	1.56	1.04
7:U:246:ILE:O	7:U:246:ILE:HG13	1.60	0.99
8:V:45:ARG:HD2	8:V:52:THR:HG23	1.48	0.94
3:Q:70:ASN:HB3	3:Q:72:LYS:H	1.40	0.87
8:H:40:LYS:HE2	8:H:182:GLY:HA2	1.57	0.86
6:T:50:LYS:HB2	6:T:59:TYR:HB3	1.58	0.85
4:R:215:VAL:HG12	4:R:221:ILE:HG12	1.61	0.82
9:W:18:THR:HG23	9:W:30:ASN:HA	1.62	0.82
7:G:36:SER:HB3	7:G:49:VAL:HG23	1.61	0.81
7:U:245:GLU:O	7:U:246:ILE:CG2	2.30	0.80
7:U:246:ILE:CG1	7:U:246:ILE:O	2.33	0.77
1:A:54:ILE:HD11	1:A:223:LEU:HD22	1.67	0.77
2:P:68:THR:HG22	2:P:70:ASP:H	1.50	0.76
14:2:43:VAL:HG22	14:2:108:VAL:HG22	1.67	0.75
4:D:121:THR:HG22	5:E:136:ARG:HH21	1.49	0.75
12:Z:91:LYS:HE3	15:Z:301:WPI:H8	1.68	0.75
6:T:33:SER:HB3	6:T:62:LYS:HE3	1.68	0.75
9:I:205:PHE:HB3	9:I:209:THR:HG21	1.67	0.75
8:H:45:ARG:HD2	8:H:52:THR:HG23	1.68	0.75
13:1:198:VAL:HG22	13:1:203:VAL:HG22	1.70	0.74
13:1:155:THR:HG23	13:1:158:LYS:H	1.53	0.73
1:O:165:GLY:N	2:P:60:THR:HG21	1.98	0.73
3:C:125:HIS:HB3	4:D:126:VAL:HG12	1.70	0.73
4:R:47:GLU:OE1	4:R:166:ARG:NH2	2.21	0.73
3:Q:125:HIS:HB3	4:R:126:VAL:HG12	1.72	0.72
3:Q:49:GLU:OE2	3:Q:210:ARG:NH2	2.23	0.71
9:I:3:ILE:HG13	9:I:99:ILE:HD12	1.72	0.71
13:M:165:TYR:HD2	13:M:166:LEU:H	1.38	0.71
13:M:213:ASP:OD1	9:W:19:ARG:NH2	2.23	0.71
4:R:216:LYS:HB2	4:R:220:ASP:HB3	1.72	0.71
7:U:80:LEU:HD12	7:U:132:GLY:HA3	1.71	0.70
7:U:245:GLU:C	7:U:246:ILE:CG2	2.59	0.70
9:W:18:THR:HG22	9:W:171:SER:HB2	1.72	0.70
14:N:1:THR:O	14:N:33:ARG:NH2	2.25	0.70
5:S:222:ILE:HG22	5:S:228:PHE:HD1	1.57	0.69
12:L:145:LYS:HB2	12:L:148:LEU:HD13	1.75	0.69
6:F:198:SER:HA	6:F:201:LEU:HD22	1.74	0.68
5:S:182:GLU:HB3	5:S:203:ILE:HD13	1.73	0.68
13:1:117:ASP:HB3	13:1:119:VAL:H	1.59	0.68
1:A:220:LYS:HB3	1:A:242:GLU:HG2	1.74	0.68
2:P:64:VAL:HG11	2:P:212:ALA:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:128:GLY:HA2	15:H:300:WPI:H48	1.75	0.67
4:R:73:LEU:HD12	4:R:135:ILE:HG12	1.76	0.67
8:H:1:THR:HG23	15:H:300:WPI:H53	1.76	0.67
5:E:180:GLN:NE2	6:F:54:ASP:OD1	2.27	0.67
2:P:186:GLU:OE2	2:P:246:ARG:NH2	2.25	0.67
14:2:124:LEU:HD13	14:2:125:LEU:HD13	1.77	0.67
8:H:103:ASP:HB2	8:H:106:ASN:HB2	1.76	0.67
2:B:94:HIS:HA	2:B:98:LYS:HB3	1.77	0.66
4:D:162:GLN:OE1	4:D:163:THR:N	2.26	0.66
2:P:106:PRO:HG2	2:P:109:LEU:HB2	1.77	0.66
4:D:207:ALA:HB2	4:D:233:VAL:HG21	1.78	0.66
1:A:87:ILE:HD12	1:A:88:PRO:HD3	1.76	0.65
2:P:59:GLU:CD	2:P:59:GLU:H	1.99	0.65
1:A:157:THR:HG22	1:A:163:TYR:HB2	1.77	0.65
11:K:15:ALA:HB2	11:K:160:LEU:HD21	1.77	0.65
4:D:53:LYS:O	4:D:54:LEU:HB2	1.96	0.65
9:I:46:ALA:HB1	15:I:301:WPI:H45	1.79	0.65
12:Z:1:THR:OG1	15:Z:301:WPI:H46	1.97	0.64
2:P:239:THR:HG23	2:P:242:GLU:HB2	1.79	0.64
12:Z:1:THR:HG21	12:Z:33:ARG:CZ	2.27	0.64
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.78	0.64
8:V:129:SER:HA	15:V:201:WPI:H52	1.78	0.64
5:S:31:ILE:HD13	5:S:141:ALA:HB2	1.79	0.64
10:J:117:LEU:HD23	10:J:117:LEU:H	1.63	0.64
4:D:200:LEU:HD11	4:D:233:VAL:HG12	1.79	0.64
7:U:94:GLU:HG2	7:U:114:ARG:HB3	1.78	0.64
1:A:78:THR:HG22	1:A:231:ASP:HA	1.78	0.64
8:H:1:THR:HB	8:H:33:LYS:HZ3	1.61	0.64
9:I:46:ALA:HA	15:I:301:WPI:H51	1.78	0.64
13:M:179:PHE:O	13:M:183:THR:HG22	1.98	0.64
7:U:247:ASN:ND2	7:U:247:ASN:C	2.51	0.64
13:1:117:ASP:HB2	13:1:121:SER:H	1.63	0.63
2:P:68:THR:HB	2:P:71:ILE:HB	1.79	0.63
11:K:137:PHE:HB3	12:Z:134:THR:HG21	1.80	0.63
8:H:45:ARG:HH11	8:H:52:THR:CG2	2.12	0.63
6:F:77:LEU:HD12	6:F:79:PRO:HD2	1.81	0.63
13:1:18:THR:HG21	13:1:30:TYR:CD1	2.33	0.63
14:2:111:VAL:HG23	14:2:192:ILE:HG22	1.80	0.63
3:Q:48:ALA:HB1	3:Q:65:LYS:HD3	1.80	0.63
1:A:220:LYS:HD3	1:A:242:GLU:HG3	1.80	0.62
14:N:89:ALA:HA	14:N:122:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:44:CYS:HB2	8:V:98:ILE:HB	1.80	0.62
4:D:118:GLN:O	4:D:121:THR:HB	1.99	0.62
2:P:213:ILE:HG23	2:P:238:LEU:HD11	1.81	0.62
11:Y:169:LYS:HG3	11:Y:170:ARG:HG2	1.82	0.62
7:U:246:ILE:O	7:U:247:ASN:CB	2.48	0.61
1:A:87:ILE:HG12	7:G:157:TRP:CZ2	2.36	0.61
9:W:199:LYS:NZ	10:X:143:SER:O	2.33	0.61
7:G:94:GLU:HG2	7:G:114:ARG:HB3	1.82	0.61
10:X:14:ILE:HG23	10:X:34:ILE:HD13	1.81	0.61
12:L:21:THR:HG22	12:L:26:VAL:HA	1.83	0.61
9:W:58:LEU:HD23	9:W:59:ILE:HD12	1.82	0.61
8:H:136:GLY:HA2	8:V:161:GLN:HG3	1.81	0.61
12:L:13:ILE:HD12	12:L:154:LEU:HD13	1.83	0.61
2:P:4:ARG:HH22	5:S:126:GLY:HA3	1.65	0.61
10:X:126:ASP:OD1	10:X:127:PHE:N	2.29	0.61
1:A:204:GLU:OE2	1:A:244:ARG:NH1	2.33	0.61
1:A:82:VAL:HG12	1:A:142:THR:HB	1.81	0.61
4:R:97:ARG:HD3	4:R:103:PRO:HG3	1.81	0.61
3:Q:234:GLU:O	3:Q:238:ILE:HG22	2.01	0.60
13:1:19:ARG:NE	13:1:191:ASP:OD2	2.32	0.60
8:V:13:ILE:HG12	8:V:177:VAL:HG13	1.83	0.60
9:W:4:VAL:HG12	9:W:126:SER:HB3	1.83	0.60
8:H:36:ARG:HD2	14:2:225:ILE:HD11	1.82	0.60
1:O:123:ASN:OD1	2:P:83:ARG:NH1	2.34	0.60
15:V:201:WPI:H6	14:2:182:ARG:HG3	1.84	0.60
11:Y:91:ILE:HG12	11:Y:121:LEU:HB2	1.83	0.60
7:G:169:GLN:CD	7:G:169:GLN:H	2.06	0.60
7:G:119:VAL:HG21	7:G:150:LEU:HD21	1.84	0.59
1:O:203:VAL:O	1:O:207:ILE:HG12	2.03	0.59
6:T:156:LEU:HD23	7:U:58:LEU:HA	1.85	0.59
3:Q:184:MET:HG2	3:Q:188:ASP:HB2	1.85	0.59
5:S:52:LYS:NZ	5:S:61:SER:O	2.35	0.59
3:Q:160:TRP:CD2	3:Q:163:ILE:HD13	2.37	0.59
10:X:18:LEU:HD12	10:X:175:GLY:HA3	1.85	0.59
5:E:192:THR:CG2	5:E:195:GLU:H	2.16	0.59
12:L:147:ASP:OD2	12:L:147:ASP:N	2.35	0.59
3:C:91:ALA:HB1	3:C:111:LEU:HD11	1.84	0.58
8:H:156:LYS:HE3	8:H:188:PHE:CD1	2.37	0.58
8:H:22:THR:HG22	8:H:27:ALA:HB2	1.84	0.58
14:N:178:TYR:HD2	9:W:139:GLU:HG3	1.68	0.58
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:205:ASN:H	2:P:208:THR:HG22	1.68	0.58
10:J:12:VAL:HG13	10:J:110:PRO:HB3	1.85	0.58
7:U:37:ILE:HD11	7:U:48:ALA:HB3	1.85	0.58
4:D:187:THR:HG22	4:D:190:GLU:HB2	1.84	0.58
4:D:121:THR:CG2	5:E:136:ARG:HH21	2.17	0.58
3:Q:60:ASP:OD1	3:Q:60:ASP:N	2.22	0.58
8:V:115:LEU:HD13	15:V:201:WPI:H47	1.85	0.58
14:2:89:ALA:HA	14:2:122:VAL:HG21	1.84	0.58
8:H:32:ASP:OD2	8:H:185:ARG:NH2	2.36	0.58
6:F:134:ILE:HB	6:F:145:LEU:HB2	1.85	0.58
3:Q:181:LYS:H	3:Q:184:MET:HE2	1.68	0.58
6:T:43:HIS:HB3	6:T:215:ILE:HD11	1.85	0.58
3:Q:2:GLY:HA3	6:T:123:TYR:CE1	2.39	0.58
11:K:11:SER:HB3	11:K:184:ASP:HB3	1.85	0.57
6:T:63:ILE:HG21	6:T:214:ALA:HB2	1.85	0.57
13:1:7:ALA:HB2	13:1:113:VAL:HG23	1.87	0.57
3:Q:44:ILE:HD11	3:Q:146:TYR:HB3	1.86	0.57
8:V:59:VAL:HG22	8:V:81:VAL:HG12	1.86	0.57
4:R:14:ASP:N	4:R:14:ASP:OD2	2.34	0.57
2:P:42:GLY:HA3	2:P:185:LEU:HD13	1.85	0.57
13:M:165:TYR:HD2	13:M:166:LEU:N	2.01	0.57
3:Q:119:LYS:NZ	3:Q:151:SER:OG	2.38	0.57
2:P:227:ILE:HG22	2:P:229:THR:HG23	1.86	0.57
1:O:177:GLU:OE1	1:O:177:GLU:N	2.38	0.57
5:S:81:LEU:HD12	5:S:139:GLY:HA3	1.87	0.57
9:I:104:ASP:HB2	9:I:105:PRO:HD2	1.87	0.57
1:A:70:SER:HA	1:A:224:GLU:OE2	2.05	0.57
9:I:128:GLY:HA2	15:I:301:WPI:H42	1.86	0.57
4:D:187:THR:HG23	4:D:190:GLU:H	1.70	0.57
11:K:59:ILE:HG13	11:K:83:VAL:HG22	1.87	0.57
7:U:69:VAL:HG22	7:U:92:ARG:HG3	1.87	0.56
3:C:70:ASN:OD1	3:C:71:ASP:N	2.37	0.56
13:1:43:MET:HG3	13:1:102:ILE:HG22	1.86	0.56
12:Z:118:ASP:OD1	15:Z:301:WPI:H16	2.04	0.56
9:I:128:GLY:O	9:I:131:SER:HB2	2.05	0.56
15:V:201:WPI:H6	14:2:182:ARG:CD	2.36	0.56
3:Q:64:GLU:HG3	3:Q:65:LYS:HG2	1.87	0.56
8:V:4:MET:HB3	8:V:126:ILE:HG22	1.87	0.56
4:R:48:ARG:NH1	4:R:208:LYS:HE2	2.20	0.56
5:S:127:ALA:HB3	5:S:132:ARG:HD2	1.87	0.56
8:H:1:THR:OG1	15:H:300:WPI:H46	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:22:ARG:HG3	11:Y:27:LEU:HD12	1.87	0.56
11:Y:84:ARG:HG3	11:Y:124:LYS:HB3	1.88	0.56
12:L:130:GLY:HA2	15:L:301:WPI:H42	1.87	0.56
14:N:17:ASP:O	14:N:33:ARG:NH1	2.34	0.56
1:O:131:ARG:HD3	1:O:133:TYR:HE2	1.71	0.56
1:A:100:GLU:HG2	1:A:120:ARG:HG2	1.88	0.56
6:F:72:LEU:HD22	6:F:132:LEU:HD22	1.88	0.56
4:D:203:VAL:HG12	4:D:205:THR:H	1.71	0.56
5:S:167:TYR:CE1	5:S:170:LYS:HD3	2.41	0.56
5:S:176:SER:O	5:S:180:GLN:N	2.24	0.56
5:E:68:VAL:HG21	5:E:89:ILE:HD13	1.88	0.55
13:1:8:GLY:HA3	13:1:11:PHE:CE2	2.41	0.55
4:D:26:ALA:HB1	4:D:78:LEU:HD13	1.88	0.55
5:S:186:GLU:HG2	5:S:199:LEU:HD11	1.86	0.55
2:P:222:LEU:HD13	2:P:232:GLY:HA2	1.89	0.55
12:Z:12:ILE:HB	12:Z:180:VAL:HB	1.89	0.55
10:J:15:ALA:HB1	10:J:162:LEU:HD22	1.88	0.55
13:1:166:LEU:HD23	13:1:170:GLU:HG2	1.88	0.55
15:V:201:WPI:H6	14:2:182:ARG:NE	2.21	0.55
14:2:131:SER:HB3	14:2:133:THR:O	2.06	0.55
10:X:96:VAL:HG23	10:X:98:PRO:HD3	1.89	0.55
5:E:166:ARG:HB3	6:F:58:SER:HB3	1.87	0.55
5:E:192:THR:HG22	5:E:195:GLU:H	1.71	0.55
11:K:28:LYS:HD3	12:L:122:LEU:HD22	1.87	0.55
8:H:136:GLY:CA	8:V:161:GLN:HG3	2.37	0.55
6:F:72:LEU:HB3	6:F:134:ILE:HD13	1.89	0.55
4:R:175:LEU:HB3	5:S:58:LEU:HD11	1.88	0.55
3:Q:106:ILE:HD11	3:Q:110:ILE:HG22	1.88	0.55
9:W:67:SER:HB2	9:W:72:ARG:O	2.06	0.55
15:V:201:WPI:H6	14:2:182:ARG:HE	1.70	0.55
6:T:107:ARG:NH2	14:2:68:TYR:O	2.39	0.55
10:X:98:PRO:HB2	10:X:115:PHE:CD2	2.42	0.55
14:N:178:TYR:CD2	9:W:139:GLU:HG3	2.42	0.55
11:K:1:ASP:N	11:K:1:ASP:OD1	2.36	0.55
13:1:91:LYS:HD3	13:1:96:TYR:CE2	2.42	0.54
10:X:2:ILE:HG21	10:X:133:ALA:HB3	1.87	0.54
5:S:74:ILE:HD13	5:S:112:LEU:HD22	1.88	0.54
8:H:82:PHE:HB3	8:H:113:ILE:HD13	1.89	0.54
1:A:220:LYS:HD3	1:A:242:GLU:CG	2.37	0.54
15:L:301:WPI:C45	15:L:301:WPI:H51	2.37	0.54
1:O:199:TRP:O	1:O:203:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:45:VAL:HG22	6:T:215:ILE:HD13	1.90	0.54
4:R:149:GLN:HG2	4:R:159:TRP:NE1	2.22	0.54
6:F:46:LEU:HD22	6:F:135:ILE:HG12	1.90	0.54
13:1:127:CYS:SG	13:1:141:LEU:HD23	2.48	0.54
4:D:155:ILE:HD12	5:E:83:ALA:HB2	1.90	0.54
13:M:117:ASP:HB3	13:M:119:VAL:H	1.73	0.54
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.90	0.54
4:R:226:SER:O	4:R:230:ASN:N	2.37	0.54
6:T:182:ILE:HD11	6:T:188:GLU:HB3	1.89	0.54
8:V:45:ARG:HH11	8:V:52:THR:CG2	2.20	0.54
12:Z:97:MET:N	12:Z:117:SER:OG	2.39	0.53
11:Y:2:ILE:H	11:Y:17:SER:HB3	1.73	0.53
6:T:128:TYR:O	6:T:149:PRO:HB3	2.07	0.53
2:P:160:LYS:HD3	2:P:179:TRP:CZ3	2.44	0.53
6:T:206:LEU:HD12	6:T:206:LEU:H	1.72	0.53
13:M:76:SER:OG	13:M:78:ASN:OD1	2.23	0.53
7:U:247:ASN:C	7:U:247:ASN:HD22	2.12	0.53
3:C:9:ARG:HD3	4:D:6:ARG:CZ	2.39	0.53
1:O:179:THR:HG23	2:P:55:LEU:HD12	1.91	0.53
13:M:141:LEU:O	13:M:145:VAL:HB	2.09	0.53
8:H:48:SER:O	8:H:52:THR:HB	2.08	0.53
11:K:148:ARG:HB2	11:K:151:MET:HG3	1.90	0.53
11:Y:15:ALA:HB2	11:Y:160:LEU:HD21	1.91	0.53
11:K:193:ASP:N	11:K:193:ASP:OD1	2.42	0.53
11:K:183:VAL:HG22	11:K:188:ILE:HG12	1.91	0.52
13:M:99:HIS:HD2	13:M:116:PHE:O	1.92	0.52
5:S:12:VAL:HG22	5:S:23:GLN:HG3	1.92	0.52
4:R:29:ARG:HB2	4:R:29:ARG:CZ	2.38	0.52
9:I:174:ASP:OD2	9:I:188:ARG:NH1	2.37	0.52
6:F:50:LYS:HB3	6:F:59:TYR:HB3	1.90	0.52
1:O:161:GLY:O	2:P:83:ARG:NH2	2.40	0.52
4:D:58:ARG:HD3	4:D:59:ILE:HG23	1.91	0.52
2:B:118:MET:HE3	2:B:150:VAL:HG22	1.92	0.52
3:C:25:ALA:O	3:C:29:ILE:HG13	2.09	0.52
3:C:238:ILE:HA	3:C:241:LYS:HB2	1.92	0.52
16:1:306:HOH:O	14:2:-8:THR:HG23	2.09	0.52
2:B:15:SER:OG	2:B:17:LYS:HG2	2.09	0.52
8:V:115:LEU:CD1	15:V:201:WPI:H47	2.39	0.52
7:G:35:THR:HB	7:G:167:GLY:H	1.75	0.52
3:C:36:ILE:HD13	3:C:164:SER:HB3	1.92	0.52
5:S:77:ALA:HB3	5:S:143:LEU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:176:LEU:HA	6:F:179:PHE:CE2	2.45	0.52
4:R:184:PRO:O	4:R:186:ALA:N	2.43	0.52
13:M:13:VAL:HG12	13:M:197:ILE:HG13	1.91	0.52
4:R:207:ALA:HB2	4:R:233:VAL:HG21	1.91	0.52
10:X:112:ILE:HD12	10:X:128:ILE:HG12	1.91	0.52
9:W:172:ASN:HD22	9:W:192:THR:HA	1.75	0.52
4:R:97:ARG:HH11	4:R:103:PRO:HG3	1.76	0.51
5:S:177:GLU:OE2	5:S:178:GLY:N	2.34	0.51
5:S:45:GLY:HA2	5:S:153:TYR:CE1	2.45	0.51
7:U:94:GLU:HG3	7:U:114:ARG:HH11	1.75	0.51
1:A:105:ARG:HH22	14:2:222:THR:HG23	1.74	0.51
7:U:245:GLU:C	7:U:246:ILE:HG23	2.30	0.51
4:R:172:ARG:O	4:R:176:GLU:HG2	2.09	0.51
1:O:91:ARG:HD2	16:O:317:HOH:O	2.09	0.51
6:F:101:ARG:HG3	14:N:83:TYR:CZ	2.45	0.51
14:N:45:ILE:HD12	14:N:52:MET:HG3	1.92	0.51
13:M:17:ASP:OD1	13:M:33:LYS:NZ	2.43	0.51
12:L:17:ASP:OD2	12:L:33:ARG:NH2	2.44	0.51
4:R:31:THR:HG21	4:R:49:ARG:HG2	1.92	0.51
3:C:245:THR:OXT	3:C:245:THR:HG23	2.11	0.51
11:Y:48:GLU:HG2	15:Z:301:WPI:H6	1.92	0.51
1:O:207:ILE:HD12	1:O:223:LEU:HD13	1.93	0.51
13:M:137:ILE:HG22	13:M:141:LEU:HD22	1.93	0.51
4:R:185:PRO:O	4:R:187:THR:N	2.43	0.51
6:F:63:ILE:HG21	6:F:214:ALA:HB2	1.93	0.51
1:O:44:ALA:HB2	1:O:53:VAL:HG12	1.92	0.51
13:1:18:THR:HG22	13:1:31:GLU:H	1.74	0.51
1:O:242:GLU:O	1:O:246:VAL:HG12	2.11	0.51
14:2:42:VAL:HG23	14:2:192:ILE:HD11	1.93	0.51
6:T:232:LYS:HE3	6:T:233:TYR:CE2	2.45	0.51
14:N:8:TYR:CE1	14:N:162:VAL:HG22	2.46	0.51
6:T:46:LEU:HD22	6:T:135:ILE:HG12	1.93	0.51
9:W:172:ASN:ND2	9:W:192:THR:HG22	2.25	0.51
12:L:12:ILE:HB	12:L:180:VAL:HB	1.92	0.51
5:E:188:HIS:CE1	5:E:191:LEU:HG	2.46	0.51
14:2:1:THR:O	14:2:33:ARG:NH2	2.44	0.51
9:W:110:LEU:HG	9:W:125:LEU:HD12	1.92	0.51
6:T:159:THR:OG1	6:T:160:ALA:N	2.43	0.51
1:A:62:LYS:HE3	7:G:176:GLU:HG2	1.93	0.51
3:Q:238:ILE:O	3:Q:238:ILE:HG12	2.10	0.51
8:V:112:THR:HG22	8:V:120:HIS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:156:LEU:HD13	6:F:159:THR:HB	1.93	0.51
3:Q:91:ALA:HB2	3:Q:115:LEU:HD22	1.93	0.50
12:Z:19:ARG:HH21	12:Z:29:GLN:HE22	1.57	0.50
13:1:84:ILE:HG22	13:1:88:LEU:HD22	1.94	0.50
3:C:173:GLN:HE21	4:D:52:LEU:HD12	1.76	0.50
9:W:1:THR:HB	15:W:301:WPI:H52	1.93	0.50
3:Q:66:LEU:HD22	3:Q:212:GLU:HB3	1.93	0.50
6:T:50:LYS:HB3	6:T:60:GLN:O	2.11	0.50
14:2:121:TYR:HE1	14:2:136:THR:HG22	1.75	0.50
4:D:96:HIS:CD2	4:D:100:LEU:HD13	2.47	0.50
3:C:136:ILE:HG12	3:C:150:THR:HG22	1.92	0.50
2:B:10:THR:HG22	2:B:18:LEU:HD22	1.94	0.50
8:H:67:THR:HA	8:H:71:GLY:O	2.12	0.50
3:Q:11:THR:O	4:R:127:ARG:HD3	2.11	0.50
11:Y:185:LYS:HG2	16:Y:217:HOH:O	2.11	0.50
11:Y:108:LYS:HE2	11:Y:185:LYS:O	2.12	0.50
5:E:51:GLU:HG3	5:E:208:MET:HG2	1.94	0.50
14:2:119:LEU:O	14:2:130:SER:OG	2.24	0.50
5:S:120:ALA:C	5:S:122:ARG:H	2.15	0.50
1:O:200:GLU:O	1:O:203:VAL:HG22	2.12	0.50
5:E:173:GLY:O	5:E:176:SER:OG	2.29	0.50
1:O:132:ALA:HB2	2:P:9:LEU:HD21	1.94	0.50
5:S:234:GLU:CD	5:S:234:GLU:H	2.15	0.50
1:O:40:ILE:HG23	1:O:56:GLN:HB2	1.92	0.50
10:X:5:ALA:HB2	10:X:14:ILE:HG13	1.93	0.50
7:U:246:ILE:O	7:U:247:ASN:OD1	2.30	0.49
9:W:52:THR:O	9:W:56:THR:HB	2.12	0.49
13:1:3:ILE:HG13	13:1:101:ILE:HD12	1.92	0.49
5:E:52:LYS:NZ	5:E:61:SER:O	2.45	0.49
14:N:200:PHE:HE2	14:N:202:LYS:HG3	1.77	0.49
9:I:148:LYS:HD2	9:I:177:VAL:HG11	1.94	0.49
13:M:151:TYR:CD1	13:M:157:GLY:HA2	2.47	0.49
14:2:5:SER:HB3	14:2:14:ILE:HG13	1.93	0.49
6:F:11:VAL:O	7:G:129:ARG:HB3	2.12	0.49
6:T:54:ASP:HB3	6:T:56:LEU:H	1.77	0.49
12:Z:95:LEU:HB2	16:Z:403:HOH:O	2.12	0.49
1:O:21:PRO:HA	2:P:23:TYR:CD1	2.47	0.49
13:1:3:ILE:HD12	13:1:44:SER:HB3	1.94	0.49
11:Y:100:ASN:HB3	11:Y:132:HIS:CG	2.47	0.49
5:E:146:GLY:HA2	5:E:222:ILE:HG12	1.92	0.49
13:M:151:TYR:CG	13:M:157:GLY:HA2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:90:ARG:HG2	7:G:118:TYR:CD2	2.47	0.49
1:O:82:VAL:HG13	1:O:142:THR:HB	1.95	0.49
5:E:202:LYS:HE2	5:E:206:GLN:OE1	2.12	0.49
2:P:210:GLU:HG2	2:P:237:LYS:HE2	1.93	0.49
6:T:171:TYR:HB2	6:T:199:GLN:HG3	1.93	0.49
4:D:87:GLU:OE2	11:K:69:ARG:NH1	2.45	0.49
14:2:85:PHE:CZ	14:2:120:ARG:HG2	2.47	0.49
5:E:169:ALA:HB1	5:E:183:LEU:HG	1.93	0.49
6:F:167:GLY:HA3	6:F:199:GLN:O	2.13	0.49
3:C:17:GLY:O	4:D:29:ARG:NH2	2.42	0.49
3:Q:150:THR:O	3:Q:157:TYR:HA	2.13	0.49
3:Q:215:THR:HG22	3:Q:228:LYS:HB3	1.95	0.49
8:V:48:SER:HB3	8:V:51:ASP:HB2	1.95	0.48
14:N:45:ILE:HG12	14:N:106:ILE:HG13	1.95	0.48
9:I:222:ASP:OD2	10:J:66:LYS:NZ	2.45	0.48
1:O:78:THR:HG22	1:O:231:ASP:HA	1.95	0.48
3:Q:18:ARG:HB3	3:Q:23:GLU:OE1	2.13	0.48
7:U:246:ILE:O	7:U:247:ASN:CG	2.51	0.48
11:Y:17:SER:HB2	11:Y:175:PHE:HB2	1.95	0.48
2:B:63:LYS:HG3	2:B:75:TYR:CE2	2.48	0.48
1:O:150:LEU:HD22	9:W:72:ARG:NH2	2.27	0.48
5:S:46:VAL:HG23	5:S:153:TYR:HB3	1.95	0.48
3:C:163:ILE:HG13	3:C:164:SER:N	2.29	0.48
5:E:193:LEU:O	5:E:197:GLU:HG3	2.12	0.48
1:O:162:TYR:CE1	2:P:80:PRO:HD3	2.48	0.48
13:1:117:ASP:HB2	13:1:121:SER:N	2.27	0.48
8:V:161:GLN:HE21	8:V:165:TRP:HE1	1.62	0.48
6:T:215:ILE:HD12	6:T:216:VAL:H	1.79	0.48
8:V:38:HIS:CE1	8:V:73:PRO:HD2	2.47	0.48
11:K:14:LEU:HD12	11:K:42:LEU:HD23	1.96	0.48
7:U:39:ILE:HD12	7:U:195:ALA:HB2	1.95	0.48
5:S:214:GLU:HG3	5:S:233:ASN:HB3	1.96	0.48
3:C:5:ARG:HD2	3:C:6:TYR:CZ	2.48	0.48
1:A:88:PRO:HG3	7:G:155:SER:N	2.28	0.48
5:S:45:GLY:HA2	5:S:153:TYR:CD1	2.48	0.48
2:B:63:LYS:HG3	2:B:75:TYR:HE2	1.78	0.48
7:U:53:ILE:HG13	7:U:211:PHE:HA	1.95	0.48
1:A:165:GLY:HA3	2:B:60:THR:HG21	1.96	0.48
1:A:156:LYS:O	1:A:163:TYR:HA	2.14	0.48
3:Q:231:LYS:HB2	3:Q:234:GLU:HG3	1.94	0.48
7:U:68:VAL:HG12	16:2:304:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:89:ALA:HB1	4:R:109:LEU:HD11	1.95	0.48
12:L:40:PHE:HB3	12:L:73:ARG:HH21	1.79	0.48
6:F:213:ILE:HG23	6:F:225:TYR:HB2	1.95	0.48
10:J:76:GLU:N	10:J:76:GLU:OE1	2.37	0.48
7:U:246:ILE:O	7:U:247:ASN:HB3	2.13	0.48
1:A:82:VAL:CG1	1:A:142:THR:HB	2.44	0.48
6:T:45:VAL:HG23	6:T:189:LEU:HD23	1.95	0.48
6:F:43:HIS:HB2	6:F:189:LEU:HD23	1.96	0.48
7:G:41:CYS:HB2	7:G:186:LEU:O	2.14	0.48
11:K:118:ILE:HA	11:K:123:THR:O	2.14	0.48
6:T:77:LEU:HD12	6:T:79:PRO:HD2	1.95	0.48
9:W:179:GLU:HB3	9:W:182:LYS:HG3	1.95	0.47
12:Z:118:ASP:OD2	15:Z:301:WPI:H21	2.15	0.47
4:D:47:GLU:OE2	4:D:166:ARG:NH2	2.47	0.47
14:N:12:VAL:HG21	14:N:109:ALA:HB1	1.96	0.47
5:S:232:ASP:OD2	5:S:232:ASP:N	2.44	0.47
3:Q:148:LEU:HB3	3:Q:160:TRP:O	2.14	0.47
3:C:140:TYR:CD2	3:C:225:VAL:HG21	2.49	0.47
5:E:175:GLY:HA3	5:E:207:VAL:HG11	1.95	0.47
9:W:5:GLY:O	9:W:124:TYR:HA	2.13	0.47
11:K:2:ILE:H	11:K:17:SER:HB3	1.78	0.47
6:F:52:ASN:ND2	6:F:54:ASP:O	2.48	0.47
6:F:50:LYS:HE2	6:F:212:SER:HB2	1.97	0.47
2:B:103:GLU:OE2	10:J:77:THR:OG1	2.30	0.47
6:T:151:GLY:O	7:U:82:PRO:HG3	2.14	0.47
7:G:55:SER:OG	7:G:56:LYS:N	2.47	0.47
1:A:115:ASP:HB3	1:A:155:TYR:CZ	2.49	0.47
5:E:168:ASN:HB3	5:E:187:TRP:CZ2	2.50	0.47
11:K:45:PHE:HB3	11:K:101:VAL:HG12	1.96	0.47
9:I:147:THR:HG23	9:I:150:GLU:OE1	2.14	0.47
8:H:129:SER:H	15:H:300:WPI:H47	1.79	0.47
8:H:1:THR:HB	8:H:33:LYS:NZ	2.30	0.47
6:T:182:ILE:HG12	6:T:182:ILE:O	2.14	0.47
14:N:63:VAL:HG22	14:N:79:LEU:HD23	1.96	0.47
5:S:121:LEU:HA	5:S:123:PHE:CE2	2.50	0.47
1:A:87:ILE:HA	1:A:90:ALA:HB3	1.96	0.47
4:R:159:TRP:CZ2	5:S:59:LEU:HD12	2.49	0.47
1:O:68:THR:HG21	7:U:158:GLY:HA3	1.96	0.47
3:Q:54:SER:OG	3:Q:55:THR:N	2.48	0.47
12:L:99:THR:HG22	12:L:115:VAL:O	2.14	0.47
3:Q:239:LEU:HD12	3:Q:239:LEU:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:171:MET:HE2	11:K:173:MET:HB2	1.97	0.47
7:G:188:ALA:O	7:G:192:VAL:HG12	2.15	0.47
1:O:141:LEU:O	1:O:156:LYS:HA	2.14	0.47
9:W:26:VAL:HG11	9:W:29:LYS:HG2	1.97	0.47
14:N:17:ASP:OD1	14:N:33:ARG:NH1	2.47	0.47
6:F:107:ARG:O	6:F:111:LEU:HG	2.14	0.47
6:F:132:LEU:HD12	6:F:147:PHE:CD2	2.50	0.47
9:W:172:ASN:ND2	9:W:192:THR:HA	2.29	0.47
1:A:68:THR:HG21	7:G:158:GLY:H	1.80	0.47
14:2:7:LYS:HD2	14:2:157:ILE:HD13	1.96	0.47
11:Y:167:LEU:O	11:Y:171:MET:HB2	2.15	0.47
8:H:137:TYR:CE1	8:V:140:LYS:HG3	2.50	0.47
9:W:152:ILE:HD11	9:W:177:VAL:HG21	1.97	0.47
8:H:51:ASP:O	8:H:55:ILE:HG13	2.15	0.46
4:R:53:LYS:O	4:R:54:LEU:HB2	2.14	0.46
5:E:75:GLY:HA3	5:E:228:PHE:CE1	2.50	0.46
7:U:194:GLN:O	7:U:198:ILE:HG13	2.15	0.46
13:1:34:VAL:HG12	13:1:196:LEU:HD22	1.97	0.46
5:S:219:LEU:HB3	5:S:231:TYR:CD2	2.51	0.46
6:T:36:VAL:HG22	6:T:160:ALA:HB2	1.96	0.46
5:E:132:ARG:HB3	5:E:133:LEU:H	1.54	0.46
15:L:301:WPI:H51	15:L:301:WPI:O42	2.15	0.46
10:X:47:LEU:HG	10:X:49:THR:HG22	1.97	0.46
3:C:150:THR:O	3:C:157:TYR:HA	2.14	0.46
5:E:205:LYS:NZ	5:E:247:GLU:OE1	2.48	0.46
8:V:48:SER:O	8:V:52:THR:HB	2.16	0.46
8:H:55:ILE:HD11	8:H:93:LEU:HD13	1.98	0.46
12:L:9:GLN:NE2	12:L:148:LEU:O	2.44	0.46
11:K:118:ILE:HG12	11:K:124:LYS:HB2	1.98	0.46
3:Q:102:TYR:CE1	11:Y:74:LEU:HD21	2.50	0.46
8:H:48:SER:HB3	8:H:51:ASP:HB2	1.95	0.46
6:F:54:ASP:N	6:F:54:ASP:OD2	2.48	0.46
1:O:203:VAL:HG21	1:O:244:ARG:HD3	1.97	0.46
8:H:156:LYS:HE3	8:H:188:PHE:CE1	2.50	0.46
3:C:106:ILE:HD11	3:C:110:ILE:HG22	1.97	0.46
3:C:94:HIS:CD2	3:C:114:ARG:HG2	2.51	0.46
5:E:81:LEU:HD12	5:E:139:GLY:HA3	1.98	0.46
14:2:142:MET:O	14:2:145:PRO:HD2	2.16	0.46
2:P:175:LEU:HD22	2:P:195:THR:HG21	1.98	0.46
4:R:169:LYS:HE3	4:R:169:LYS:HB2	1.70	0.46
3:C:163:ILE:HG13	3:C:164:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:171:MET:HE1	11:K:175:PHE:HD2	1.81	0.46
10:J:-2:ASN:HA	10:J:21:GLY:O	2.15	0.46
8:H:132:THR:O	8:V:133:PHE:HA	2.16	0.46
2:P:109:LEU:HA	2:P:109:LEU:HD12	1.73	0.46
5:S:191:LEU:HD21	5:S:199:LEU:HD22	1.97	0.46
4:R:67:ILE:HG21	4:R:109:LEU:HD21	1.97	0.46
13:M:185:ARG:HH21	9:W:29:LYS:HE2	1.81	0.46
14:N:37:VAL:HG21	14:N:59:LEU:HG	1.98	0.46
12:L:1:THR:HB	15:L:301:WPI:C36	2.46	0.46
3:C:240:VAL:HA	3:C:245:THR:HA	1.98	0.46
10:J:115:PHE:HA	10:J:120:CYS:O	2.15	0.46
10:J:2:ILE:HG21	10:J:133:ALA:HB3	1.99	0.46
14:N:193:ASP:HB3	14:N:196:THR:OG1	2.16	0.46
7:U:187:SER:HB2	7:U:190:GLU:HB2	1.97	0.46
10:X:98:PRO:HB2	10:X:115:PHE:HD2	1.80	0.45
6:F:179:PHE:HA	6:F:182:ILE:HG13	1.97	0.45
9:W:9:ASN:OD1	9:W:10:ASN:N	2.50	0.45
1:A:34:ALA:O	1:A:37:GLN:HG2	2.16	0.45
2:B:85:LEU:HA	2:B:85:LEU:HD12	1.79	0.45
12:Z:47:GLY:HA2	15:Z:301:WPI:H40	1.98	0.45
1:O:69:VAL:HA	7:U:157:TRP:CZ3	2.52	0.45
2:B:207:ASP:N	2:B:207:ASP:OD1	2.50	0.45
2:B:193:LEU:HA	2:B:193:LEU:HD12	1.78	0.45
4:D:53:LYS:HE2	4:D:54:LEU:HD12	1.98	0.45
15:V:201:WPI:H6	14:2:182:ARG:CG	2.45	0.45
4:R:159:TRP:CH2	5:S:56:SER:HB3	2.51	0.45
5:E:205:LYS:HG3	5:E:212:LEU:HB3	1.98	0.45
10:X:19:ARG:HD3	10:X:171:LEU:O	2.16	0.45
6:T:16:THR:HB	6:T:18:ARG:HG3	1.98	0.45
3:C:113:ARG:NH2	11:K:70:GLU:OE2	2.49	0.45
3:C:191:GLU:HG2	3:C:242:THR:HG22	1.97	0.45
3:Q:147:GLN:HG2	4:R:59:ILE:HG21	1.96	0.45
12:L:154:LEU:HD21	12:L:188:HIS:CG	2.52	0.45
12:L:25:TRP:CH2	13:M:135:SER:HA	2.51	0.45
4:R:37:LYS:NZ	5:S:60:GLU:OE2	2.50	0.45
3:Q:201:THR:HG22	3:Q:203:SER:HB3	1.96	0.45
9:I:137:VAL:HG21	9:I:161:ALA:HB2	1.98	0.45
2:B:5:TYR:OH	7:G:126:ASN:ND2	2.42	0.45
9:I:2:THR:OG1	9:I:130:GLY:HA3	2.16	0.45
11:Y:38:SER:HB3	11:Y:73:GLU:HG3	1.99	0.45
2:P:24:ALA:O	2:P:28:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:VAL:HG12	4:D:161:ALA:HB1	1.97	0.45
11:Y:171:MET:HE3	11:Y:171:MET:HB3	1.89	0.45
6:F:36:VAL:HG22	6:F:160:ALA:HB2	1.97	0.45
1:O:117:LEU:O	1:O:121:MET:HG2	2.17	0.45
2:B:37:ILE:HD12	2:B:192:ALA:HB2	1.98	0.45
5:S:210:GLU:HB3	5:S:216:ASN:ND2	2.32	0.45
8:V:129:SER:HA	15:V:201:WPI:C45	2.45	0.45
9:W:135:MET:O	9:W:139:GLU:HB2	2.16	0.45
2:P:196:LEU:HD13	2:P:209:ILE:HD12	1.98	0.45
3:C:38:ILE:HD12	3:C:193:ALA:HB2	1.98	0.45
7:U:51:LYS:HB3	7:U:51:LYS:HE2	1.62	0.45
1:O:14:ARG:HD3	1:O:14:ARG:HA	1.74	0.45
8:H:129:SER:H	15:H:300:WPI:C43	2.29	0.45
15:W:301:WPI:H32	15:W:301:WPI:H37	1.79	0.45
14:2:8:TYR:CZ	14:2:162:VAL:HG13	2.52	0.45
5:E:39:GLY:HA2	5:E:47:VAL:O	2.17	0.45
4:R:133:THR:O	4:R:149:GLN:HA	2.17	0.45
7:G:48:ALA:HA	7:G:214:GLU:O	2.17	0.45
4:D:73:LEU:HD22	4:D:86:ILE:HG12	1.99	0.45
1:O:240:ASN:O	1:O:244:ARG:HG2	2.16	0.45
2:B:150:VAL:HG23	2:B:156:TYR:HB3	1.99	0.45
4:D:55:GLN:NE2	4:D:60:THR:HG21	2.32	0.45
1:A:214:LEU:HB3	1:A:216:THR:HG22	1.99	0.45
8:H:155:ILE:HB	8:H:175:MET:HE1	1.99	0.45
9:I:173:VAL:HB	9:I:191:LEU:HB2	1.99	0.45
15:Z:301:WPI:H37	15:Z:301:WPI:H33	1.52	0.44
6:T:46:LEU:HB2	6:T:214:ALA:HB3	1.99	0.44
1:O:231:ASP:O	1:O:232:LYS:HB2	2.17	0.44
3:Q:120:GLN:HG3	4:R:80:ALA:HB1	1.99	0.44
10:J:188:LYS:HE2	10:J:190:TYR:CE2	2.52	0.44
7:G:94:GLU:HG3	7:G:114:ARG:HH11	1.83	0.44
1:O:135:ARG:HG3	1:O:136:PRO:O	2.17	0.44
5:E:241:LYS:O	5:E:244:LYS:HG2	2.17	0.44
5:S:86:ARG:HD3	5:S:86:ARG:HA	1.75	0.44
8:H:182:GLY:HA3	16:H:403:HOH:O	2.17	0.44
12:Z:7:ARG:HB3	12:Z:12:ILE:HG12	1.99	0.44
3:Q:137:TYR:HB2	3:Q:149:TYR:HB2	1.99	0.44
14:N:211:TRP:CH2	8:V:171:GLY:HA2	2.52	0.44
10:X:89:ARG:HG3	10:X:94:TYR:CE2	2.52	0.44
2:P:165:GLY:O	2:P:168:SER:HB3	2.17	0.44
3:C:239:LEU:HD23	3:C:239:LEU:HA	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:THR:HG23	4:D:168:SER:HB2	1.98	0.44
9:I:1:THR:OG1	15:I:301:WPI:H50	2.16	0.44
3:C:107:PRO:HD2	3:C:110:ILE:HD12	1.98	0.44
14:N:153:ARG:NH2	16:N:320:HOH:O	2.50	0.44
8:H:133:PHE:HA	8:V:132:THR:O	2.17	0.44
11:K:18:LYS:HG2	11:K:179:ILE:HG13	1.99	0.44
7:U:110:ALA:O	7:U:114:ARG:HG2	2.18	0.44
13:1:29:ARG:NH1	13:1:191:ASP:OD1	2.44	0.44
1:O:131:ARG:HD3	1:O:133:TYR:CE2	2.52	0.44
13:M:132:ALA:HB1	13:M:186:HIS:CE1	2.52	0.44
12:L:19:ARG:O	12:L:33:ARG:NH2	2.49	0.44
12:L:31:VAL:HG12	12:L:33:ARG:HG2	1.98	0.44
1:O:135:ARG:HB3	7:U:12:SER:OG	2.17	0.44
6:T:146:GLU:O	6:T:153:VAL:HA	2.17	0.44
10:J:182:LYS:HE2	10:J:182:LYS:HB3	1.72	0.44
4:R:236:ILE:O	4:R:240:LYS:HB2	2.18	0.44
12:Z:1:THR:H3	15:Z:301:WPI:H47	1.83	0.44
9:I:128:GLY:CA	15:I:301:WPI:H42	2.47	0.44
4:R:175:LEU:HA	4:R:175:LEU:HD12	1.80	0.44
2:B:17:LYS:HE3	2:B:22:ASP:OD2	2.17	0.44
6:F:176:LEU:HD13	7:G:57:LEU:HD23	2.00	0.44
11:K:171:MET:HA	11:K:172:PRO:HD3	1.89	0.44
12:Z:25:TRP:HH2	13:1:138:MET:HB2	1.83	0.44
3:C:19:LEU:O	3:C:23:GLU:HG2	2.18	0.44
11:Y:3:ILE:HD13	11:Y:3:ILE:HA	1.73	0.44
7:G:56:LYS:HD3	7:G:56:LYS:HA	1.63	0.44
12:Z:145:LYS:HB2	12:Z:148:LEU:HD13	2.00	0.44
9:W:51:ASP:HB3	9:W:94:ILE:HG23	2.00	0.44
2:B:196:LEU:HA	2:B:196:LEU:HD12	1.77	0.44
8:H:149:GLU:CD	8:H:149:GLU:H	2.20	0.44
11:Y:142:LEU:HG	11:Y:162:LEU:HD23	1.99	0.44
14:N:17:ASP:HA	14:N:187:PHE:CB	2.48	0.44
2:P:106:PRO:HA	2:P:140:ASP:HB3	2.00	0.44
14:N:131:SER:HB3	14:N:133:THR:O	2.18	0.44
1:A:127:ILE:HD13	1:A:131:ARG:HD2	2.00	0.44
5:E:123:PHE:CE2	5:E:137:PRO:HG3	2.53	0.44
3:Q:77:VAL:HG22	3:Q:135:PHE:CE1	2.53	0.44
13:M:205:LYS:HE3	13:M:205:LYS:HB2	1.60	0.44
1:A:105:ARG:HH22	14:2:222:THR:CG2	2.31	0.43
7:U:201:LEU:O	7:U:204:GLU:HG2	2.18	0.43
4:R:200:LEU:HA	4:R:203:VAL:HG12	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:13:PHE:HB2	7:U:22:GLN:OE1	2.18	0.43
8:H:59:VAL:HG22	8:H:81:VAL:HG12	2.00	0.43
14:N:-7:GLN:NE2	14:N:101:PRO:O	2.51	0.43
12:Z:67:GLU:HG3	12:Z:72:GLU:O	2.18	0.43
6:F:185:ASN:ND2	6:F:188:GLU:HB2	2.32	0.43
13:M:40:ASN:OD1	13:M:202:GLY:HA2	2.18	0.43
10:X:152:GLU:CD	10:X:152:GLU:H	2.20	0.43
10:J:33:LYS:HB3	10:J:44:ILE:O	2.18	0.43
14:N:209:MET:HE2	14:N:211:TRP:HE1	1.82	0.43
7:U:87:LEU:HD11	7:U:119:VAL:HG22	1.99	0.43
6:T:194:VAL:O	6:T:197:ILE:HG22	2.18	0.43
6:F:80:ASP:OD1	6:F:126:ARG:NH1	2.49	0.43
8:V:107:LYS:HE3	8:V:107:LYS:HB2	1.83	0.43
10:J:54:LEU:HA	10:J:54:LEU:HD12	1.73	0.43
9:W:129:SER:HB3	15:W:301:WPI:C44	2.49	0.43
1:A:115:ASP:N	1:A:115:ASP:OD2	2.52	0.43
2:P:196:LEU:HA	2:P:196:LEU:HD23	1.82	0.43
4:R:13:PRO:HA	5:S:26:TYR:CD1	2.54	0.43
7:G:246:ILE:HG13	7:G:247:ASN:OD1	2.19	0.43
2:P:149:GLN:O	2:P:156:TYR:HA	2.19	0.43
4:R:94:GLN:HG3	11:Y:65:LEU:HB2	2.00	0.43
6:F:187:ASP:N	6:F:187:ASP:OD2	2.51	0.43
9:W:162:GLY:O	9:W:166:ASP:HB3	2.19	0.43
11:K:184:ASP:HB2	16:K:205:HOH:O	2.18	0.43
13:M:185:ARG:NH2	9:W:29:LYS:HE2	2.33	0.43
14:N:133:THR:HG21	14:N:147:LEU:HB3	2.01	0.43
10:J:36:HIS:HB3	10:J:41:PHE:CD1	2.53	0.43
6:T:15:PRO:HA	7:U:25:TYR:CG	2.53	0.43
12:L:4:LEU:HD13	12:L:140:LEU:HD11	2.00	0.43
7:G:208:GLU:HG2	7:G:209:LYS:HG2	2.00	0.43
8:H:4:MET:SD	8:H:159:LEU:HD13	2.58	0.43
3:Q:87:LEU:HD12	3:Q:87:LEU:HA	1.72	0.43
4:D:238:GLN:HG2	4:D:238:GLN:H	1.70	0.43
5:E:13:SER:HB3	6:F:126:ARG:HG2	2.00	0.43
4:D:67:ILE:HG21	4:D:109:LEU:HD21	2.01	0.43
3:C:49:GLU:OE2	3:C:210:ARG:NH2	2.51	0.43
5:S:53:ARG:HA	16:S:303:HOH:O	2.19	0.43
9:W:138:LEU:HD12	9:W:138:LEU:HA	1.89	0.43
2:P:203:GLU:O	2:P:208:THR:HG21	2.19	0.43
3:Q:43:GLY:HA2	3:Q:146:TYR:CE1	2.53	0.43
6:T:130:VAL:O	6:T:149:PRO:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:191:LYS:HA	6:F:194:VAL:HG12	2.01	0.43
14:N:62:LEU:HA	14:N:62:LEU:HD12	1.72	0.43
4:R:73:LEU:HD22	4:R:86:ILE:HG12	2.00	0.43
1:A:240:ASN:O	1:A:244:ARG:HG2	2.18	0.43
3:Q:181:LYS:O	3:Q:184:MET:HB2	2.19	0.43
14:2:119:LEU:HG	14:2:134:LEU:HD12	2.00	0.43
2:B:46:ALA:HB1	2:B:196:LEU:HD22	2.01	0.43
4:D:13:PRO:HA	5:E:26:TYR:CD1	2.53	0.43
1:A:77:ARG:HH22	8:H:39:ASP:CG	2.22	0.43
6:F:227:GLY:O	6:F:230:VAL:HG12	2.19	0.43
13:1:-5:TYR:CD1	13:1:97:TYR:HB2	2.54	0.43
11:Y:4:LEU:HD23	11:Y:131:ALA:HB2	2.00	0.43
5:S:131:GLU:HB3	5:S:133:LEU:HG	2.00	0.43
2:P:193:LEU:HA	2:P:193:LEU:HD12	1.86	0.43
13:1:88:LEU:HD23	13:1:120:GLY:HA2	2.01	0.43
12:Z:13:ILE:HD12	12:Z:154:LEU:HD23	1.99	0.43
3:Q:242:THR:HG22	3:Q:243:GLY:H	1.84	0.43
6:F:201:LEU:HD21	6:F:206:LEU:HG	2.01	0.43
6:T:46:LEU:HG	6:T:73:SER:HB3	1.99	0.43
11:Y:171:MET:HA	11:Y:172:PRO:HD3	1.88	0.43
3:Q:120:GLN:CG	4:R:80:ALA:HB1	2.49	0.43
6:F:126:ARG:HD2	6:F:127:PRO:O	2.19	0.43
5:E:167:TYR:CZ	5:E:170:LYS:HD3	2.54	0.43
7:G:165:GLY:O	7:G:168:ARG:HB3	2.19	0.43
2:P:40:THR:HG23	2:P:183:LEU:O	2.19	0.43
1:A:198:SER:OG	1:A:200:GLU:HG2	2.18	0.43
1:A:69:VAL:HA	7:G:157:TRP:CZ3	2.53	0.42
4:R:48:ARG:HB3	4:R:209:ASN:HA	2.01	0.42
10:X:54:LEU:HA	10:X:54:LEU:HD12	1.62	0.42
4:R:117:GLN:OE1	4:R:150:THR:HG23	2.19	0.42
13:1:100:THR:HB	13:1:116:PHE:HB2	2.00	0.42
8:V:112:THR:CG2	8:V:120:HIS:HB2	2.49	0.42
4:D:55:GLN:HE21	4:D:60:THR:HG21	1.84	0.42
14:N:121:TYR:HB2	14:N:134:LEU:HD13	2.01	0.42
7:U:78:SER:HB2	7:U:164:THR:HG23	2.01	0.42
1:O:211:ILE:HG23	1:O:216:THR:O	2.19	0.42
9:I:110:LEU:HG	9:I:125:LEU:HD12	2.01	0.42
7:G:15:SER:OG	7:G:17:ASP:OD2	2.28	0.42
7:G:53:ILE:HG13	7:G:211:PHE:HA	2.00	0.42
1:O:174:LYS:O	1:O:178:ILE:HG13	2.19	0.42
10:J:106:LYS:HE3	10:J:106:LYS:HB3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:188:LYS:HE2	1:O:188:LYS:HB3	1.78	0.42
11:Y:20:VAL:HG11	12:Z:122:LEU:HD11	2.01	0.42
13:1:116:PHE:HA	13:1:121:SER:O	2.19	0.42
4:R:73:LEU:HD12	4:R:135:ILE:CG1	2.47	0.42
1:A:72:ILE:HG13	1:A:224:GLU:OE1	2.20	0.42
13:1:91:LYS:HD3	13:1:96:TYR:CZ	2.54	0.42
1:O:158:ASP:OD2	1:O:162:TYR:HB2	2.20	0.42
5:E:175:GLY:HA3	5:E:207:VAL:CG1	2.49	0.42
6:T:71:GLY:HA3	6:T:222:PHE:CZ	2.54	0.42
3:Q:211:LEU:HA	3:Q:211:LEU:HD12	1.89	0.42
6:T:46:LEU:HA	6:T:46:LEU:HD12	1.85	0.42
11:K:20:VAL:HG11	12:L:122:LEU:HD11	2.01	0.42
3:C:241:LYS:HE2	3:C:241:LYS:HB3	1.79	0.42
8:H:107:LYS:HB3	8:H:108:GLY:H	1.65	0.42
8:V:175:MET:HB2	8:V:186:LEU:HB2	2.02	0.42
14:N:40:ASN:O	14:N:110:GLY:HA3	2.19	0.42
4:D:230:ASN:O	4:D:233:VAL:HG23	2.20	0.42
3:Q:39:MET:HG3	3:Q:44:ILE:HD13	2.01	0.42
10:X:49:THR:O	11:Y:84:ARG:NH2	2.52	0.42
3:C:173:GLN:HE21	4:D:52:LEU:CD1	2.32	0.42
1:A:123:ASN:O	1:A:127:ILE:HG23	2.19	0.42
13:1:4:LEU:HD13	13:1:129:ALA:HB2	2.01	0.42
6:T:207:THR:HG22	6:T:208:VAL:H	1.85	0.42
13:1:35:PHE:O	13:1:42:VAL:HA	2.19	0.42
15:I:301:WPI:H19	15:I:301:WPI:H12	1.56	0.42
14:2:1:THR:OG1	14:2:2:SER:N	2.51	0.42
14:2:-5:PRO:HD3	14:2:103:TRP:CE2	2.54	0.42
4:D:181:ARG:NH2	5:E:59:LEU:O	2.52	0.42
3:C:183:ASP:OD2	3:C:183:ASP:N	2.52	0.42
9:I:128:GLY:C	15:I:301:WPI:H42	2.40	0.42
3:Q:2:GLY:HA3	6:T:123:TYR:CZ	2.54	0.42
11:Y:84:ARG:HG3	11:Y:124:LYS:CB	2.49	0.42
13:1:5:GLY:O	13:1:127:CYS:HA	2.19	0.42
5:E:24:VAL:O	5:E:28:LEU:HD22	2.20	0.42
13:M:-2:ASN:HA	13:M:21:ILE:O	2.20	0.42
6:T:93:ASN:HA	6:T:93:ASN:HD22	1.66	0.42
1:O:241:ILE:HG22	1:O:245:LEU:HD22	2.01	0.42
14:2:41:THR:OG1	14:2:81:PRO:HG3	2.20	0.42
2:P:37:ILE:HD12	2:P:188:ALA:O	2.20	0.42
3:C:185:LYS:HB3	3:C:185:LYS:HE2	1.81	0.42
2:P:205:ASN:H	2:P:208:THR:CG2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:242:THR:HG22	3:Q:243:GLY:N	2.34	0.42
9:I:213:LEU:HD21	10:J:192:LYS:HG3	2.01	0.42
14:2:201:LYS:HB3	14:2:204:LEU:HD11	2.01	0.42
4:D:144:GLU:HA	4:D:145:PRO:HD2	1.95	0.42
6:F:71:GLY:HA3	6:F:222:PHE:CE1	2.55	0.42
14:N:212:ASP:OD1	14:N:215:LYS:HE3	2.20	0.42
5:S:222:ILE:O	5:S:222:ILE:HG13	2.18	0.42
1:A:87:ILE:HG13	1:A:87:ILE:H	1.54	0.42
5:E:168:ASN:HB3	5:E:187:TRP:CE2	2.55	0.42
5:S:210:GLU:HB3	5:S:216:ASN:HD21	1.84	0.42
8:H:175:MET:HB2	8:H:186:LEU:HB2	2.02	0.42
1:O:65:ASP:HA	1:O:66:PRO:HD3	1.86	0.42
1:A:12:TYR:C	1:A:14:ARG:H	2.22	0.42
9:I:63:ILE:HD13	9:I:63:ILE:HA	1.88	0.42
1:A:232:LYS:HA	1:A:232:LYS:HD2	1.84	0.42
14:2:202:LYS:HB3	14:2:202:LYS:HE3	1.88	0.42
10:X:60:TYR:CD2	10:X:60:TYR:C	2.93	0.42
1:A:85:GLY:HA3	1:A:139:VAL:HG12	2.02	0.42
5:S:67:ILE:HG22	5:S:228:PHE:HZ	1.84	0.42
2:P:222:LEU:HD12	2:P:222:LEU:HA	1.86	0.42
9:W:2:THR:OG1	9:W:130:GLY:HA3	2.20	0.42
9:W:201:LYS:HB3	9:W:203:TYR:CZ	2.55	0.42
9:I:8:PHE:HB3	9:I:151:ALA:HB2	2.02	0.42
5:E:201:LEU:HA	5:E:201:LEU:HD12	1.90	0.42
2:B:61:LEU:HA	2:B:61:LEU:HD13	1.80	0.41
5:E:186:GLU:HB3	5:E:199:LEU:HD11	2.01	0.41
11:K:138:TYR:OH	11:Y:24:ILE:HG12	2.20	0.41
2:P:82:TYR:O	2:P:86:VAL:HG23	2.20	0.41
7:U:55:SER:OG	7:U:56:LYS:N	2.53	0.41
2:B:231:LYS:HB2	2:B:231:LYS:HE3	1.85	0.41
7:U:169:GLN:H	7:U:169:GLN:CD	2.24	0.41
9:W:173:VAL:HB	9:W:191:LEU:HB2	2.01	0.41
13:M:91:LYS:HD3	13:M:96:TYR:CE2	2.55	0.41
12:Z:1:THR:H3	15:Z:301:WPI:C43	2.34	0.41
1:A:236:LEU:HB3	1:A:240:ASN:HB2	2.01	0.41
7:U:37:ILE:HG22	7:U:163:ALA:HB2	2.01	0.41
6:T:93:ASN:ND2	13:1:64:LYS:HE3	2.35	0.41
1:A:144:VAL:HG12	1:A:154:ILE:HG12	2.02	0.41
1:A:167:LYS:HG2	2:B:55:LEU:O	2.20	0.41
9:I:218:VAL:HB	10:J:186:VAL:HG12	2.01	0.41
13:M:-5:TYR:CE1	13:M:97:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:164:VAL:HG12	1:O:165:GLY:O	2.20	0.41
13:1:117:ASP:HB3	13:1:119:VAL:N	2.32	0.41
7:U:37:ILE:HG22	7:U:163:ALA:CB	2.50	0.41
6:F:45:VAL:CG1	6:F:189:LEU:HG	2.50	0.41
11:Y:1:ASP:CG	11:Y:33:LYS:HE2	2.40	0.41
4:D:43:VAL:HG22	4:D:214:VAL:HG22	2.02	0.41
2:P:137:ALA:O	2:P:214:ILE:HG13	2.21	0.41
14:N:31:VAL:HG11	14:N:49:ILE:HD13	2.01	0.41
6:F:46:LEU:HD13	6:F:135:ILE:HG23	2.03	0.41
4:R:29:ARG:NH1	4:R:29:ARG:HB2	2.35	0.41
11:K:171:MET:CE	11:K:173:MET:HB2	2.50	0.41
8:V:83:LYS:HG2	8:V:117:GLY:O	2.19	0.41
7:G:78:SER:OG	7:G:164:THR:HG23	2.20	0.41
2:P:119:GLN:HG3	2:P:120:GLU:N	2.32	0.41
1:O:30:TYR:O	1:O:33:LYS:HB3	2.20	0.41
11:K:176:LYS:NZ	11:Y:169:LYS:HA	2.35	0.41
4:R:68:ASP:OD1	4:R:97:ARG:NH2	2.53	0.41
12:L:17:ASP:O	12:L:33:ARG:HG3	2.21	0.41
3:Q:37:GLY:O	3:Q:162:ALA:HA	2.21	0.41
8:V:129:SER:CA	15:V:201:WPI:H52	2.47	0.41
12:L:12:ILE:HG13	12:L:110:PRO:HB3	2.02	0.41
2:B:55:LEU:HA	2:B:55:LEU:HD12	1.77	0.41
9:W:104:ASP:HB2	9:W:105:PRO:HD2	2.01	0.41
11:K:55:PHE:CZ	11:K:87:LEU:HD13	2.55	0.41
14:N:5:SER:HB2	14:N:13:ILE:O	2.19	0.41
10:J:86:LEU:HD11	10:J:98:PRO:HG2	2.02	0.41
13:1:151:TYR:CG	13:1:157:GLY:HA2	2.56	0.41
7:U:173:ALA:O	7:U:176:GLU:HB2	2.20	0.41
7:U:27:VAL:O	7:U:30:VAL:HB	2.20	0.41
6:T:211:LEU:HB3	6:T:230:VAL:HG21	2.02	0.41
3:C:58:GLU:O	3:C:62:SER:HB2	2.20	0.41
14:2:122:VAL:HA	14:2:127:VAL:O	2.21	0.41
1:O:179:THR:O	1:O:183:GLU:HG3	2.21	0.41
2:B:60:THR:C	2:B:61:LEU:HD22	2.41	0.41
6:T:12:THR:HG23	7:U:22:GLN:HE22	1.84	0.41
7:U:169:GLN:H	7:U:169:GLN:NE2	2.18	0.41
13:M:96:TYR:HB3	13:M:98:VAL:HG22	2.03	0.41
6:T:157:TYR:OH	7:U:60:PRO:HD2	2.20	0.41
5:S:114:GLN:NE2	5:S:118:ASP:OD1	2.54	0.41
12:Z:177:LEU:HA	12:Z:177:LEU:HD12	1.87	0.41
3:Q:184:MET:HG2	3:Q:188:ASP:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:167:TYR:CG	5:S:170:LYS:HB2	2.55	0.41
6:T:19:LEU:O	6:T:23:GLU:HG3	2.20	0.41
8:H:24:ALA:HB3	14:2:138:PHE:HE2	1.86	0.41
6:T:39:ARG:NH1	6:T:40:SER:O	2.54	0.41
2:B:2:THR:O	2:B:4:ARG:HD3	2.20	0.41
9:W:138:LEU:HD13	9:W:158:ALA:HB2	2.02	0.41
14:N:121:TYR:HE1	14:N:136:THR:HG22	1.85	0.41
8:V:14:LEU:O	8:V:175:MET:HA	2.20	0.41
8:H:3:ILE:HD12	8:H:98:ILE:HD12	2.03	0.41
1:A:189:SER:HB3	1:A:191:ILE:HG12	2.02	0.41
14:N:-6:GLN:HG3	14:N:-6:GLN:O	2.21	0.41
14:2:219:GLY:HA3	14:2:223:GLN:HB3	2.03	0.41
13:M:6:ILE:HG13	13:M:127:CYS:HB2	2.03	0.41
4:D:111:ARG:HB3	4:D:111:ARG:HE	1.61	0.41
10:J:155:PHE:CE1	10:J:189:ARG:HD2	2.56	0.41
8:H:45:ARG:HB3	8:H:52:THR:CG2	2.51	0.41
2:P:97:TYR:CE1	2:P:109:LEU:HD23	2.56	0.41
3:Q:160:TRP:CE3	3:Q:163:ILE:HD13	2.56	0.41
13:M:5:GLY:HA2	13:M:13:VAL:O	2.21	0.41
12:L:16:VAL:HG21	12:L:33:ARG:HB2	2.03	0.41
1:O:245:LEU:HA	1:O:245:LEU:HD12	1.82	0.41
10:J:28:SER:HB2	11:K:125:VAL:HG21	2.03	0.41
1:A:148:GLU:HB3	1:A:230:LYS:NZ	2.36	0.41
2:B:168:SER:O	2:B:172:LYS:HB2	2.21	0.41
7:U:17:ASP:OD1	7:U:19:ARG:HD3	2.20	0.41
5:S:201:LEU:HD12	5:S:212:LEU:HD21	2.03	0.41
14:2:160:THR:HA	16:2:330:HOH:O	2.20	0.41
2:B:23:TYR:N	2:B:23:TYR:CD1	2.88	0.41
13:1:99:HIS:HE1	13:1:128:ARG:HD2	1.87	0.40
1:A:83:VAL:HG11	1:A:90:ALA:CB	2.51	0.40
6:F:156:LEU:HD23	7:G:58:LEU:HA	2.01	0.40
8:H:143:ARG:NH2	8:H:146:MET:HE3	2.36	0.40
13:M:8:GLY:HA3	13:M:11:PHE:CZ	2.56	0.40
9:W:78:SER:O	9:W:82:MET:HG3	2.21	0.40
7:G:106:ILE:HA	7:G:107:PRO:HD3	1.94	0.40
7:U:193:LYS:HB2	7:U:193:LYS:HE3	1.81	0.40
12:Z:33:ARG:O	12:Z:45:MET:N	2.52	0.40
9:I:46:ALA:O	9:I:97:TYR:HB2	2.21	0.40
4:D:203:VAL:O	4:D:204:GLN:HG2	2.20	0.40
5:E:243:LEU:O	5:E:247:GLU:HB2	2.21	0.40
1:A:77:ARG:HA	1:A:77:ARG:HD2	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:221:PRO:O	6:T:223:THR:OG1	2.38	0.40
4:D:149:GLN:O	4:D:156:TYR:HA	2.21	0.40
13:1:87:LEU:HD12	13:1:87:LEU:HA	1.83	0.40
1:A:40:ILE:HD13	1:A:40:ILE:HA	1.87	0.40
10:X:86:LEU:HD12	10:X:86:LEU:HA	1.88	0.40
13:1:99:HIS:HD2	13:1:116:PHE:O	2.03	0.40
1:A:78:THR:CG2	1:A:231:ASP:HA	2.50	0.40
1:O:53:VAL:HG13	1:O:144:VAL:HG11	2.02	0.40
12:L:73:ARG:CZ	12:L:105:THR:HG22	2.52	0.40
1:O:178:ILE:H	1:O:178:ILE:HG13	1.69	0.40
4:D:48:ARG:HG2	4:D:49:ARG:H	1.86	0.40
13:1:112:ALA:HB2	13:1:124:ARG:NH2	2.37	0.40
3:C:97:ASN:OD1	10:J:60:TYR:HE1	2.05	0.40
2:P:217:GLU:O	2:P:219:PRO:HD3	2.21	0.40
5:E:163:THR:HG23	6:F:60:GLN:NE2	2.36	0.40
9:I:172:ASN:OD1	9:I:192:THR:HG22	2.20	0.40
7:G:68:VAL:HB	7:G:227:HIS:HD1	1.87	0.40
15:V:201:WPI:H1	15:V:201:WPI:H8	1.75	0.40
1:O:82:VAL:CG1	1:O:142:THR:HB	2.52	0.40
4:R:236:ILE:HG12	4:R:236:ILE:H	1.72	0.40
5:S:14:THR:HG21	6:T:8:GLY:O	2.20	0.40
13:M:184:GLU:OE1	13:M:211:LYS:NZ	2.42	0.40
1:O:196:GLU:HG2	1:O:201:LYS:HB2	2.03	0.40
4:R:224:LEU:HB3	4:R:228:GLU:OE2	2.22	0.40
15:L:301:WPI:H51	15:L:301:WPI:H54	2.03	0.40
5:S:143:LEU:HA	5:S:156:PHE:O	2.22	0.40
13:1:-5:TYR:CE1	13:1:97:TYR:HB2	2.57	0.40
2:P:215:GLY:O	2:P:234:ARG:NH1	2.53	0.40
3:C:48:ALA:HB1	3:C:65:LYS:HE3	2.03	0.40
5:S:50:VAL:HG21	5:S:66:LYS:HB2	2.02	0.40
2:P:130:PHE:O	2:P:152:PRO:HB3	2.21	0.40
4:R:24:LEU:HD23	4:R:24:LEU:HA	1.96	0.40
1:O:124:LEU:HA	1:O:124:LEU:HD23	1.81	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	239/241 (99%)	229 (96%)	9 (4%)	1 (0%)	39	61
1	O	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	24	41
2	B	247/250 (99%)	230 (93%)	17 (7%)	0	100	100
2	P	247/250 (99%)	236 (96%)	9 (4%)	2 (1%)	24	41
3	C	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	24	41
3	Q	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	24	41
4	D	239/241 (99%)	224 (94%)	13 (5%)	2 (1%)	24	41
4	R	239/241 (99%)	225 (94%)	11 (5%)	3 (1%)	15	26
5	E	240/242 (99%)	228 (95%)	10 (4%)	2 (1%)	24	41
5	S	240/242 (99%)	222 (92%)	16 (7%)	2 (1%)	24	41
6	F	230/233 (99%)	217 (94%)	13 (6%)	0	100	100
6	T	230/233 (99%)	219 (95%)	10 (4%)	1 (0%)	39	61
7	G	242/244 (99%)	234 (97%)	8 (3%)	0	100	100
7	U	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	24	41
8	H	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
8	V	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
9	I	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
9	W	220/222 (99%)	215 (98%)	4 (2%)	1 (0%)	34	55
10	J	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	34	55
10	X	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
11	K	194/198 (98%)	185 (95%)	8 (4%)	1 (0%)	34	55
11	Y	194/198 (98%)	185 (95%)	9 (5%)	0	100	100
12	L	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	Z	210/212 (99%)	200 (95%)	10 (5%)	0	100	100
13	1	220/222 (99%)	210 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	220/222 (99%)	208 (94%)	12 (6%)	0	100 100
14	2	231/233 (99%)	218 (94%)	12 (5%)	1 (0%)	39 61
14	N	231/233 (99%)	221 (96%)	10 (4%)	0	100 100
All	All	6300/6364 (99%)	6002 (95%)	273 (4%)	25 (0%)	39 61

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	131	GLU
5	E	132	ARG
7	U	246	ILE
4	R	185	PRO
4	R	186	ALA
9	W	171	SER
4	D	185	PRO
4	D	204	GLN
11	K	8	VAL
1	O	60	PRO
1	A	195	ASN
3	C	70	ASN
3	C	220	ALA
2	P	52	SER
2	P	166	LYS
3	Q	4	ARG
5	S	134	MET
10	J	92	GLY
3	Q	205	ALA
7	U	34	THR
14	2	75	ALA
1	O	195	ASN
4	R	206	GLY
5	S	129	GLY
6	T	149	PRO

5.3.2 Protein sidechains (i)

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	205/205 (100%)	192 (94%)	13 (6%)	22 40
1	O	205/205 (100%)	186 (91%)	19 (9%)	11 21
2	B	208/209 (100%)	194 (93%)	14 (7%)	20 37
2	P	208/209 (100%)	183 (88%)	25 (12%)	6 12
3	C	203/203 (100%)	188 (93%)	15 (7%)	17 31
3	Q	203/203 (100%)	183 (90%)	20 (10%)	10 18
4	D	213/213 (100%)	196 (92%)	17 (8%)	15 28
4	R	213/213 (100%)	189 (89%)	24 (11%)	7 13
5	E	198/198 (100%)	180 (91%)	18 (9%)	12 22
5	S	198/198 (100%)	176 (89%)	22 (11%)	8 14
6	F	191/192 (100%)	168 (88%)	23 (12%)	6 12
6	T	191/192 (100%)	156 (82%)	35 (18%)	2 3
7	G	201/201 (100%)	179 (89%)	22 (11%)	8 15
7	U	201/201 (100%)	172 (86%)	29 (14%)	4 7
8	H	162/162 (100%)	153 (94%)	9 (6%)	26 47
8	V	162/162 (100%)	148 (91%)	14 (9%)	13 24
9	I	181/181 (100%)	169 (93%)	12 (7%)	21 38
9	W	181/181 (100%)	162 (90%)	19 (10%)	8 16
10	J	172/172 (100%)	156 (91%)	16 (9%)	11 21
10	X	172/172 (100%)	156 (91%)	16 (9%)	11 21
11	K	174/175 (99%)	160 (92%)	14 (8%)	15 28
11	Y	174/175 (99%)	157 (90%)	17 (10%)	10 19
12	L	169/169 (100%)	157 (93%)	12 (7%)	18 34
12	Z	169/169 (100%)	155 (92%)	14 (8%)	14 26
13	1	185/185 (100%)	175 (95%)	10 (5%)	27 49
13	M	185/185 (100%)	168 (91%)	17 (9%)	11 21
14	2	199/199 (100%)	180 (90%)	19 (10%)	11 20
14	N	199/199 (100%)	187 (94%)	12 (6%)	24 43
All	All	5322/5328 (100%)	4825 (91%)	497 (9%)	11 21

All (497) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	54	ILE
1	A	87	ILE
1	A	96	ARG
1	A	125	SER
1	A	126	GLN
1	A	127	ILE
1	A	163	TYR
1	A	164	VAL
1	A	200	GLU
1	A	231	ASP
1	A	242	GLU
1	A	244	ARG
2	B	2	THR
2	B	15	SER
2	B	29	LYS
2	B	133	SER
2	B	146	SER
2	B	157	PHE
2	B	178	ARG
2	B	180	ASN
2	B	193	LEU
2	B	198	GLU
2	B	207	ASP
2	B	211	LEU
2	B	231	LYS
2	B	248	GLU
3	C	5	ARG
3	C	8	SER
3	C	34	THR
3	C	49	GLU
3	C	51	LYS
3	C	61	THR
3	C	85	GLU
3	C	86	ILE
3	C	103	ASN
3	C	120	GLN
3	C	125	HIS
3	C	158	THR
3	C	181	LYS
3	C	184	MET
3	C	207	THR
4	D	21	GLU

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Mol	Chain	Res	Type
4	D	24	LEU
4	D	53	LYS
4	D	57	THR
4	D	58	ARG
4	D	71	VAL
4	D	118	GLN
4	D	132	SER
4	D	155	ILE
4	D	160	SER
4	D	177	LYS
4	D	182	LYS
4	D	198	SER
4	D	204	GLN
4	D	227	GLU
4	D	231	GLN
4	D	233	VAL
5	E	10	ARG
5	E	28	LEU
5	E	52	LYS
5	E	110	GLU
5	E	112	LEU
5	E	143	LEU
5	E	177	GLU
5	E	183	LEU
5	E	184	LEU
5	E	190	SER
5	E	192	THR
5	E	201	LEU
5	E	204	LEU
5	E	205	LYS
5	E	210	GLU
5	E	211	LYS
5	E	241	LYS
5	E	242	GLU
6	F	9	ASP
6	F	10	THR
6	F	16	THR
6	F	26	LEU
6	F	45	VAL
6	F	46	LEU
6	F	54	ASP
6	F	60	GLN

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Mol	Chain	Res	Type
6	F	61	LYS
6	F	74	LEU
6	F	93	ASN
6	F	96	SER
6	F	113	CYS
6	F	123	TYR
6	F	140	SER
6	F	164	ARG
6	F	187	ASP
6	F	201	LEU
6	F	208	VAL
6	F	213	ILE
6	F	230	VAL
6	F	232	LYS
6	F	234	ILE
7	G	10	SER
7	G	17	ASP
7	G	56	LYS
7	G	61	GLN
7	G	62	LYS
7	G	80	LEU
7	G	97	SER
7	G	100	LYS
7	G	104	THR
7	G	168	ARG
7	G	170	SER
7	G	176	GLU
7	G	178	LEU
7	G	186	LEU
7	G	190	GLU
7	G	192	VAL
7	G	204	GLU
7	G	217	TRP
7	G	220	LEU
7	G	228	LYS
7	G	237	GLU
7	G	244	LYS
8	H	9	LYS
8	H	22	THR
8	H	52	THR
8	H	85	LEU
8	H	88	GLU

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Mol	Chain	Res	Type
8	H	107	LYS
8	H	144	GLU
8	H	156	LYS
8	H	159	LEU
9	I	13	VAL
9	I	38	SER
9	I	43	CYS
9	I	55	VAL
9	I	77	VAL
9	I	78	SER
9	I	87	LEU
9	I	113	ILE
9	I	144	GLN
9	I	167	LEU
9	I	178	MET
9	I	217	ILE
10	J	54	LEU
10	J	88	GLU
10	J	106	LYS
10	J	109	LYS
10	J	116	ASP
10	J	120	CYS
10	J	123	GLU
10	J	125	LYS
10	J	137	LEU
10	J	140	MET
10	J	163	LEU
10	J	171	LEU
10	J	174	TRP
10	J	183	LYS
10	J	184	ASP
10	J	194	ARG
11	K	1	ASP
11	K	6	ILE
11	K	10	ASP
11	K	11	SER
11	K	17	SER
11	K	52	THR
11	K	59	ILE
11	K	68	ILE
11	K	87	LEU
11	K	126	GLU

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Mol	Chain	Res	Type
11	K	141	SER
11	K	142	LEU
11	K	161	LYS
11	K	195	GLN
12	L	4	LEU
12	L	9	GLN
12	L	32	LYS
12	L	33	ARG
12	L	67	GLU
12	L	86	LEU
12	L	104	TYR
12	L	147	ASP
12	L	148	LEU
12	L	149	SER
12	L	154	LEU
12	L	208	ASN
13	M	2	THR
13	M	44	SER
13	M	60	LYS
13	M	62	SER
13	M	83	ASN
13	M	87	LEU
13	M	94	PHE
13	M	110	LYS
13	M	117	ASP
13	M	121	SER
13	M	141	LEU
13	M	144	GLN
13	M	163	LEU
13	M	164	LYS
13	M	165	TYR
13	M	174	LEU
13	M	183	THR
14	N	57	ARG
14	N	58	LEU
14	N	59	LEU
14	N	65	GLU
14	N	79	LEU
14	N	96	ARG
14	N	102	LEU
14	N	130	SER
14	N	147	LEU

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Mol	Chain	Res	Type
14	N	153	ARG
14	N	154	GLU
14	N	176	LEU
1	O	22	GLU
1	O	43	LEU
1	O	67	THR
1	O	68	THR
1	O	96	ARG
1	O	112	MET
1	O	115	ASP
1	O	150	LEU
1	O	157	THR
1	O	163	TYR
1	O	169	THR
1	O	175	GLN
1	O	197	GLU
1	O	198	SER
1	O	210	MET
1	O	216	THR
1	O	231	ASP
1	O	244	ARG
1	O	245	LEU
2	P	9	LEU
2	P	11	THR
2	P	25	LEU
2	P	58	SER
2	P	59	GLU
2	P	62	SER
2	P	85	LEU
2	P	92	VAL
2	P	95	THR
2	P	107	THR
2	P	108	LYS
2	P	119	GLN
2	P	132	VAL
2	P	157	PHE
2	P	172	LYS
2	P	175	LEU
2	P	184	GLU
2	P	193	LEU
2	P	194	LEU
2	P	198	GLU

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Mol	Chain	Res	Type
2	P	211	LEU
2	P	229	THR
2	P	239	THR
2	P	246	ARG
2	P	248	GLU
3	Q	16	GLU
3	Q	23	GLU
3	Q	30	SER
3	Q	53	THR
3	Q	55	THR
3	Q	59	GLN
3	Q	60	ASP
3	Q	65	LYS
3	Q	66	LEU
3	Q	80	LEU
3	Q	87	LEU
3	Q	150	THR
3	Q	175	LEU
3	Q	187	ASP
3	Q	194	LEU
3	Q	198	SER
3	Q	211	LEU
3	Q	229	ILE
3	Q	237	ASP
3	Q	238	ILE
4	R	6	ARG
4	R	8	LEU
4	R	14	ASP
4	R	36	VAL
4	R	50	SER
4	R	57	THR
4	R	58	ARG
4	R	76	SER
4	R	85	LEU
4	R	102	ASP
4	R	132	SER
4	R	149	GLN
4	R	150	THR
4	R	173	GLU
4	R	175	LEU
4	R	187	THR
4	R	189	GLU

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Mol	Chain	Res	Type
4	R	199	LEU
4	R	201	GLU
4	R	222	VAL
4	R	224	LEU
4	R	225	SER
4	R	226	SER
4	R	236	ILE
5	S	12	VAL
5	S	20	ARG
5	S	28	LEU
5	S	33	LEU
5	S	60	GLU
5	S	61	SER
5	S	86	ARG
5	S	100	ASN
5	S	110	GLU
5	S	112	LEU
5	S	176	SER
5	S	177	GLU
5	S	186	GLU
5	S	191	LEU
5	S	198	LEU
5	S	201	LEU
5	S	210	GLU
5	S	222	ILE
5	S	223	THR
5	S	225	GLN
5	S	229	LYS
5	S	232	ASP
6	T	3	ARG
6	T	4	ASN
6	T	11	VAL
6	T	16	THR
6	T	26	LEU
6	T	30	LYS
6	T	38	LEU
6	T	46	LEU
6	T	50	LYS
6	T	56	LEU
6	T	57	SER
6	T	61	LYS
6	T	74	LEU

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Mol	Chain	Res	Type
6	T	84	LEU
6	T	93	ASN
6	T	97	LEU
6	T	107	ARG
6	T	111	LEU
6	T	112	LEU
6	T	113	CYS
6	T	156	LEU
6	T	164	ARG
6	T	172	LEU
6	T	175	THR
6	T	178	THR
6	T	182	ILE
6	T	191	LYS
6	T	197	ILE
6	T	205	SER
6	T	206	LEU
6	T	207	THR
6	T	212	SER
6	T	219	ASP
6	T	220	THR
6	T	223	THR
7	U	10	SER
7	U	34	THR
7	U	36	SER
7	U	41	CYS
7	U	42	ASN
7	U	52	LEU
7	U	55	SER
7	U	57	LEU
7	U	62	LYS
7	U	87	LEU
7	U	97	SER
7	U	115	LEU
7	U	129	ARG
7	U	133	VAL
7	U	134	SER
7	U	142	LYS
7	U	151	GLU
7	U	164	THR
7	U	169	GLN
7	U	172	LYS

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Mol	Chain	Res	Type
7	U	207	LYS
7	U	208	GLU
7	U	210	ASP
7	U	217	TRP
7	U	224	ASN
7	U	244	LYS
7	U	245	GLU
7	U	246	ILE
7	U	247	ASN
8	V	10	ASP
8	V	52	THR
8	V	63	LEU
8	V	83	LYS
8	V	85	LEU
8	V	103	ASP
8	V	104	ASP
8	V	106	ASN
8	V	143	ARG
8	V	149	GLU
8	V	161	GLN
8	V	178	LEU
8	V	179	THR
8	V	196	LEU
9	W	13	VAL
9	W	17	ASP
9	W	18	THR
9	W	38	SER
9	W	43	CYS
9	W	52	THR
9	W	55	VAL
9	W	56	THR
9	W	58	LEU
9	W	63	ILE
9	W	65	LEU
9	W	68	LEU
9	W	80	LEU
9	W	84	LYS
9	W	113	ILE
9	W	138	LEU
9	W	182	LYS
9	W	192	THR
9	W	200	GLN

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Mol	Chain	Res	Type
10	X	14	ILE
10	X	32	GLU
10	X	54	LEU
10	X	60	TYR
10	X	64	LEU
10	X	67	LEU
10	X	69	GLU
10	X	86	LEU
10	X	109	LYS
10	X	120	CYS
10	X	123	GLU
10	X	135	ASP
10	X	137	LEU
10	X	140	MET
10	X	162	LEU
10	X	183	LYS
11	Y	7	ARG
11	Y	11	SER
11	Y	17	SER
11	Y	22	ARG
11	Y	37	LEU
11	Y	68	ILE
11	Y	72	TYR
11	Y	77	GLN
11	Y	84	ARG
11	Y	90	SER
11	Y	121	LEU
11	Y	141	SER
11	Y	142	LEU
11	Y	169	LYS
11	Y	171	MET
11	Y	173	MET
11	Y	195	GLN
12	Z	1	THR
12	Z	7	ARG
12	Z	9	GLN
12	Z	67	GLU
12	Z	72	GLU
12	Z	84	SER
12	Z	95	LEU
12	Z	104	TYR
12	Z	107	LYS

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Mol	Chain	Res	Type
12	Z	117	SER
12	Z	137	TYR
12	Z	140	LEU
12	Z	149	SER
12	Z	177	LEU
13	1	18	THR
13	1	25	SER
13	1	40	ASN
13	1	62	SER
13	1	64	LYS
13	1	87	LEU
13	1	88	LEU
13	1	117	ASP
13	1	155	THR
13	1	165	TYR
14	2	2	SER
14	2	26	LEU
14	2	29	ASN
14	2	58	LEU
14	2	72	LEU
14	2	74	ASP
14	2	76	GLU
14	2	79	LEU
14	2	96	ARG
14	2	124	LEU
14	2	125	LEU
14	2	130	SER
14	2	147	LEU
14	2	154	GLU
14	2	159	LYS
14	2	162	VAL
14	2	176	LEU
14	2	198	LEU
14	2	222	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	94	HIS
3	C	173	GLN
7	G	169	GLN
12	L	133	GLN

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Mol	Chain	Res	Type
13	M	83	ASN
1	O	84	ASN
8	V	38	HIS
8	V	161	GLN
9	W	172	ASN
13	1	70	HIS
13	1	99	HIS

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

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	WPI	H	300	-	43,43,43	2.03	11 (25%)	53,55,55	3.06	24 (45%)
15	WPI	I	301	-	43,43,43	1.96	13 (30%)	53,55,55	2.92	24 (45%)
15	WPI	L	301	-	43,43,43	2.09	14 (32%)	53,55,55	2.67	20 (37%)
15	WPI	V	201	-	43,43,43	1.99	10 (23%)	53,55,55	2.97	20 (37%)
15	WPI	W	301	-	43,43,43	1.97	11 (25%)	53,55,55	2.57	18 (33%)
15	WPI	Z	301	-	43,43,43	2.02	11 (25%)	53,55,55	2.98	26 (49%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	WPI	H	300	-	-	0/28/39/39	0/3/3/3
15	WPI	I	301	-	-	0/28/39/39	0/3/3/3
15	WPI	L	301	-	-	0/28/39/39	0/3/3/3
15	WPI	V	201	-	-	0/28/39/39	0/3/3/3
15	WPI	W	301	-	-	1/28/39/39	0/3/3/3
15	WPI	Z	301	-	-	0/28/39/39	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	300	WPI	C22-N20	-3.00	1.42	1.46
15	V	201	WPI	C23-C21	-2.76	1.40	1.51
15	V	201	WPI	C22-N20	-2.67	1.43	1.46
15	H	300	WPI	C23-C21	-2.65	1.40	1.51
15	Z	301	WPI	C23-C21	-2.64	1.40	1.51
15	L	301	WPI	C23-C21	-2.63	1.40	1.51
15	L	301	WPI	C22-N20	-2.59	1.43	1.46
15	W	301	WPI	C23-C21	-2.58	1.41	1.51
15	I	301	WPI	C23-C21	-2.47	1.41	1.51
15	W	301	WPI	C22-N20	-2.29	1.43	1.46
15	I	301	WPI	C22-N20	-2.06	1.43	1.46
15	I	301	WPI	C35-C37	2.07	1.42	1.38
15	W	301	WPI	C23-N25	2.07	1.49	1.46
15	I	301	WPI	O6-C2	2.09	1.40	1.37
15	L	301	WPI	C37-C39	2.10	1.45	1.40
15	V	201	WPI	O8-C3	2.12	1.40	1.37
15	H	300	WPI	C5-C2	2.12	1.42	1.38
15	L	301	WPI	O41-C38	2.15	1.40	1.37
15	Z	301	WPI	O6-C2	2.15	1.40	1.37
15	I	301	WPI	O42-C39	2.22	1.42	1.38
15	I	301	WPI	C7-C3	2.23	1.42	1.38
15	W	301	WPI	C7-C3	2.23	1.42	1.38
15	W	301	WPI	C5-C2	2.25	1.42	1.38
15	I	301	WPI	C5-C2	2.25	1.42	1.38
15	Z	301	WPI	C5-C2	2.27	1.43	1.38
15	Z	301	WPI	O41-C38	2.29	1.40	1.37
15	L	301	WPI	O6-C2	2.31	1.40	1.37
15	V	201	WPI	C3-C1	2.40	1.45	1.40
15	L	301	WPI	C7-C3	2.48	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	301	WPI	C5-C2	2.49	1.43	1.38
15	H	300	WPI	O6-C2	2.50	1.41	1.37
15	I	301	WPI	O41-C38	2.50	1.41	1.37
15	H	300	WPI	C7-C3	2.50	1.43	1.38
15	W	301	WPI	C36-C38	2.54	1.43	1.38
15	Z	301	WPI	C7-C3	2.56	1.43	1.38
15	V	201	WPI	C33-C31	2.59	1.55	1.47
15	L	301	WPI	C33-C31	2.59	1.55	1.47
15	I	301	WPI	C36-C38	2.60	1.43	1.38
15	I	301	WPI	C10-C13	2.61	1.55	1.47
15	V	201	WPI	C10-C13	2.65	1.55	1.47
15	I	301	WPI	C33-C31	2.67	1.55	1.47
15	H	300	WPI	O42-C39	2.70	1.43	1.38
15	V	201	WPI	O4-C1	2.70	1.43	1.38
15	H	300	WPI	C33-C31	2.75	1.56	1.47
15	W	301	WPI	C10-C13	2.75	1.56	1.47
15	Z	301	WPI	O42-C39	2.75	1.43	1.38
15	L	301	WPI	C35-C37	2.76	1.43	1.38
15	Z	301	WPI	C33-C31	2.79	1.56	1.47
15	H	300	WPI	C10-C13	2.81	1.56	1.47
15	W	301	WPI	C35-C37	2.87	1.44	1.38
15	V	201	WPI	C7-C3	2.92	1.44	1.38
15	L	301	WPI	O42-C39	2.94	1.43	1.38
15	W	301	WPI	C33-C31	2.96	1.56	1.47
15	Z	301	WPI	C10-C13	3.04	1.57	1.47
15	L	301	WPI	C10-C13	3.09	1.57	1.47
15	Z	301	WPI	C36-C38	3.10	1.44	1.38
15	H	300	WPI	C36-C38	3.16	1.44	1.38
15	L	301	WPI	C36-C38	3.22	1.44	1.38
15	I	301	WPI	C13-C14	5.91	1.51	1.31
15	W	301	WPI	C13-C14	6.03	1.52	1.31
15	L	301	WPI	C31-C30	6.08	1.52	1.31
15	H	300	WPI	C13-C14	6.10	1.52	1.31
15	H	300	WPI	C31-C30	6.12	1.52	1.31
15	V	201	WPI	C13-C14	6.19	1.52	1.31
15	L	301	WPI	C13-C14	6.24	1.53	1.31
15	Z	301	WPI	C31-C30	6.24	1.53	1.31
15	Z	301	WPI	C13-C14	6.26	1.53	1.31
15	W	301	WPI	C31-C30	6.34	1.53	1.31
15	V	201	WPI	C31-C30	6.35	1.53	1.31
15	I	301	WPI	C31-C30	6.35	1.53	1.31

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	300	WPI	C29-C30-C31	-9.07	108.47	125.24
15	I	301	WPI	C16-C14-C13	-8.74	109.09	125.24
15	W	301	WPI	C16-C14-C13	-8.27	109.95	125.24
15	V	201	WPI	C16-C14-C13	-8.13	110.22	125.24
15	Z	301	WPI	C16-C14-C13	-7.69	111.03	125.24
15	H	300	WPI	C16-C14-C13	-7.62	111.16	125.24
15	I	301	WPI	C29-C30-C31	-7.31	111.72	125.24
15	L	301	WPI	C16-C14-C13	-7.19	111.96	125.24
15	L	301	WPI	C29-C30-C31	-6.95	112.38	125.24
15	V	201	WPI	C10-C13-C14	-6.71	108.40	127.01
15	W	301	WPI	C29-C30-C31	-6.62	113.01	125.24
15	Z	301	WPI	C33-C31-C30	-6.35	109.39	127.01
15	Z	301	WPI	C29-C30-C31	-6.30	113.59	125.24
15	V	201	WPI	C29-C30-C31	-6.25	113.69	125.24
15	V	201	WPI	O6-C2-C5	-6.11	113.78	124.21
15	Z	301	WPI	O40-C37-C35	-6.05	113.88	124.21
15	H	300	WPI	C10-C13-C14	-5.88	110.69	127.01
15	I	301	WPI	C10-C13-C14	-5.77	111.01	127.01
15	L	301	WPI	C33-C31-C30	-5.62	111.43	127.01
15	W	301	WPI	C10-C13-C14	-5.40	112.02	127.01
15	I	301	WPI	C33-C31-C30	-5.29	112.34	127.01
15	H	300	WPI	C33-C31-C30	-5.15	112.73	127.01
15	V	201	WPI	C33-C31-C30	-4.97	113.23	127.01
15	W	301	WPI	C33-C31-C30	-4.83	113.62	127.01
15	Z	301	WPI	C10-C13-C14	-4.82	113.63	127.01
15	L	301	WPI	C10-C13-C14	-4.71	113.94	127.01
15	H	300	WPI	O40-C37-C35	-3.56	118.13	124.21
15	H	300	WPI	O8-C3-C7	-3.39	118.43	124.21
15	I	301	WPI	O40-C37-C35	-3.00	119.08	124.21
15	L	301	WPI	O40-C37-C35	-2.96	119.16	124.21
15	H	300	WPI	C43-O40-C37	-2.93	113.09	117.54
15	H	300	WPI	C24-C26-N25	-2.92	109.54	115.38
15	L	301	WPI	O8-C3-C7	-2.88	119.29	124.21
15	I	301	WPI	O8-C3-C7	-2.87	119.31	124.21
15	H	300	WPI	O6-C2-C5	-2.86	119.32	124.21
15	I	301	WPI	O6-C2-C5	-2.78	119.46	124.21
15	V	201	WPI	O40-C37-C35	-2.71	119.58	124.21
15	V	201	WPI	O41-C38-C36	-2.65	119.69	124.21
15	V	201	WPI	O8-C3-C7	-2.62	119.74	124.21
15	Z	301	WPI	C37-C39-C38	-2.52	116.63	119.51
15	W	301	WPI	O41-C38-C36	-2.45	120.02	124.21
15	Z	301	WPI	C24-C26-N25	-2.44	110.50	115.38
15	Z	301	WPI	C43-O40-C37	-2.38	113.93	117.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Z	301	WPI	O41-C38-C36	-2.34	120.22	124.21
15	H	300	WPI	C37-C39-C38	-2.28	116.91	119.51
15	W	301	WPI	O8-C3-C7	-2.26	120.35	124.21
15	V	201	WPI	C24-C26-N25	-2.21	110.95	115.38
15	Z	301	WPI	C36-C38-C39	-2.18	117.69	120.23
15	W	301	WPI	O6-C2-C5	-2.15	120.53	124.21
15	L	301	WPI	C37-C39-C38	-2.12	117.09	119.51
15	L	301	WPI	O6-C2-C5	-2.11	120.61	124.21
15	I	301	WPI	O41-C38-C36	-2.05	120.71	124.21
15	Z	301	WPI	C18-C16-C14	2.00	122.94	112.45
15	W	301	WPI	C11-O6-C2	2.01	120.59	117.54
15	H	300	WPI	C24-C22-N20	2.03	119.43	115.38
15	W	301	WPI	C23-C21-N20	2.06	122.76	115.61
15	I	301	WPI	C11-O6-C2	2.09	120.72	117.54
15	W	301	WPI	C18-C19-N20	2.10	119.18	113.89
15	Z	301	WPI	C9-O4-C1	2.12	120.38	114.82
15	I	301	WPI	C24-C22-N20	2.14	119.66	115.38
15	I	301	WPI	C21-C23-N25	2.24	123.39	115.61
15	I	301	WPI	C23-C21-N20	2.27	123.48	115.61
15	Z	301	WPI	C11-O6-C2	2.31	121.04	117.54
15	L	301	WPI	C45-O42-C39	2.35	120.99	114.82
15	H	300	WPI	C23-C21-N20	2.38	123.88	115.61
15	I	301	WPI	C43-O40-C37	2.41	121.20	117.54
15	V	201	WPI	O40-C37-C39	2.43	119.65	115.26
15	H	300	WPI	C33-C36-C38	2.44	123.40	120.17
15	W	301	WPI	O41-C38-C39	2.44	119.67	115.26
15	Z	301	WPI	C12-O8-C3	2.45	121.25	117.54
15	L	301	WPI	C9-O4-C1	2.48	121.34	114.82
15	Z	301	WPI	O8-C3-C1	2.58	119.91	115.26
15	W	301	WPI	C9-O4-C1	2.58	121.60	114.82
15	L	301	WPI	C11-O6-C2	2.62	121.51	117.54
15	H	300	WPI	C11-O6-C2	2.63	121.53	117.54
15	W	301	WPI	O8-C3-C1	2.63	120.01	115.26
15	W	301	WPI	C21-C23-N25	2.64	124.77	115.61
15	I	301	WPI	O40-C37-C39	2.64	120.03	115.26
15	I	301	WPI	C9-O4-C1	2.70	121.91	114.82
15	V	201	WPI	C18-C19-N20	2.73	120.75	113.89
15	I	301	WPI	C33-C36-C38	2.73	123.78	120.17
15	Z	301	WPI	O6-C2-C1	2.75	120.22	115.26
15	H	300	WPI	C35-C37-C39	2.76	123.45	120.23
15	Z	301	WPI	C33-C36-C38	2.77	123.84	120.17
15	H	300	WPI	C44-O41-C38	2.79	121.77	117.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	301	WPI	O6-C2-C1	2.79	120.30	115.26
15	W	301	WPI	O6-C2-C1	2.80	120.32	115.26
15	H	300	WPI	O41-C38-C39	2.90	120.49	115.26
15	V	201	WPI	C28-C27-N25	2.92	121.24	113.89
15	V	201	WPI	C44-O41-C38	2.92	121.98	117.54
15	L	301	WPI	C12-O8-C3	2.95	122.02	117.54
15	Z	301	WPI	C24-C22-N20	2.97	121.32	115.38
15	L	301	WPI	O41-C38-C39	2.98	120.63	115.26
15	L	301	WPI	C18-C19-N20	2.99	121.41	113.89
15	L	301	WPI	C33-C36-C38	3.02	124.16	120.17
15	I	301	WPI	C18-C19-N20	3.04	121.53	113.89
15	V	201	WPI	C9-O4-C1	3.08	122.91	114.82
15	Z	301	WPI	C45-O42-C39	3.14	123.07	114.82
15	Z	301	WPI	C35-C37-C39	3.20	123.96	120.23
15	H	300	WPI	C45-O42-C39	3.21	123.25	114.82
15	I	301	WPI	O8-C3-C1	3.36	121.32	115.26
15	I	301	WPI	O41-C38-C39	3.38	121.35	115.26
15	L	301	WPI	O8-C3-C1	3.38	121.36	115.26
15	W	301	WPI	C28-C27-N25	3.42	122.49	113.89
15	I	301	WPI	O6-C2-C1	3.45	121.49	115.26
15	H	300	WPI	C28-C27-N25	3.51	122.72	113.89
15	H	300	WPI	O6-C2-C1	3.56	121.68	115.26
15	V	201	WPI	O41-C38-C39	3.69	121.92	115.26
15	V	201	WPI	O8-C3-C1	3.70	121.94	115.26
15	I	301	WPI	C28-C27-N25	3.72	123.25	113.89
15	Z	301	WPI	O41-C38-C39	3.78	122.08	115.26
15	Z	301	WPI	O40-C37-C39	3.81	122.14	115.26
15	Z	301	WPI	C18-C19-N20	3.89	123.67	113.89
15	V	201	WPI	C12-O8-C3	4.07	123.72	117.54
15	H	300	WPI	O8-C3-C1	4.41	123.22	115.26
15	L	301	WPI	C44-O41-C38	4.46	124.30	117.54
15	Z	301	WPI	C44-O41-C38	4.60	124.52	117.54
15	H	300	WPI	C12-O8-C3	4.76	124.76	117.54
15	L	301	WPI	C22-N20-C21	5.05	127.55	113.92
15	I	301	WPI	C44-O41-C38	5.20	125.43	117.54
15	H	300	WPI	C26-N25-C23	5.32	128.25	113.92
15	I	301	WPI	C26-N25-C23	5.88	129.79	113.92
15	V	201	WPI	C22-N20-C21	5.91	129.86	113.92
15	W	301	WPI	C22-N20-C21	5.95	129.96	113.92
15	I	301	WPI	C22-N20-C21	5.95	129.97	113.92
15	L	301	WPI	C26-N25-C23	6.00	130.09	113.92
15	Z	301	WPI	C26-N25-C23	6.08	130.31	113.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	V	201	WPI	O6-C2-C1	6.10	126.28	115.26
15	Z	301	WPI	C22-N20-C21	6.18	130.59	113.92
15	V	201	WPI	C26-N25-C23	6.31	130.94	113.92
15	W	301	WPI	C26-N25-C23	6.62	131.77	113.92
15	H	300	WPI	C22-N20-C21	7.02	132.84	113.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	W	301	WPI	C18-C19-N20-C22

There are no ring outliers.

6 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	300	WPI	5	0
15	I	301	WPI	7	0
15	L	301	WPI	5	0
15	V	201	WPI	11	0
15	W	301	WPI	3	0
15	Z	301	WPI	9	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	241/241 (100%)	-0.44	3 (1%)	81	83	18, 32, 60, 80	0
1	O	241/241 (100%)	-0.46	1 (0%)	93	93	20, 36, 61, 88	0
2	B	249/250 (99%)	-0.45	1 (0%)	93	93	21, 34, 63, 85	0
2	P	249/250 (99%)	-0.39	1 (0%)	93	93	21, 39, 69, 84	0
3	C	244/244 (100%)	-0.38	3 (1%)	81	83	19, 37, 72, 128	0
3	Q	244/244 (100%)	-0.31	4 (1%)	74	78	18, 37, 71, 110	0
4	D	241/241 (100%)	-0.30	2 (0%)	87	89	19, 39, 86, 96	0
4	R	241/241 (100%)	-0.05	12 (4%)	32	37	22, 45, 93, 116	0
5	E	242/242 (100%)	-0.25	6 (2%)	61	65	20, 40, 69, 122	0
5	S	242/242 (100%)	-0.20	9 (3%)	45	50	24, 44, 78, 139	0
6	F	232/233 (99%)	-0.18	4 (1%)	73	76	25, 45, 70, 99	0
6	T	232/233 (99%)	-0.05	8 (3%)	49	54	25, 47, 75, 96	0
7	G	244/244 (100%)	-0.37	2 (0%)	87	89	22, 40, 71, 85	0
7	U	244/244 (100%)	-0.25	3 (1%)	81	83	22, 40, 72, 83	0
8	H	196/196 (100%)	-0.66	0	100	100	19, 27, 46, 64	0
8	V	196/196 (100%)	-0.56	0	100	100	19, 28, 48, 63	0
9	I	222/222 (100%)	-0.50	2 (0%)	85	88	18, 31, 52, 105	0
9	W	222/222 (100%)	-0.53	2 (0%)	85	88	21, 33, 51, 100	0
10	J	204/204 (100%)	-0.52	0	100	100	17, 31, 51, 71	0
10	X	204/204 (100%)	-0.47	1 (0%)	91	92	17, 30, 52, 73	0
11	K	196/198 (98%)	-0.65	1 (0%)	91	92	18, 31, 48, 83	0
11	Y	196/198 (98%)	-0.59	2 (1%)	84	86	17, 31, 48, 85	0
12	L	212/212 (100%)	-0.63	1 (0%)	91	92	18, 28, 44, 64	0
12	Z	212/212 (100%)	-0.57	1 (0%)	91	92	20, 31, 50, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1	222/222 (100%)	-0.52	1 (0%)	91	92	18, 32, 58, 74	0
13	M	222/222 (100%)	-0.61	1 (0%)	91	92	18, 31, 52, 71	0
14	2	233/233 (100%)	-0.62	1 (0%)	93	93	18, 29, 44, 59	0
14	N	233/233 (100%)	-0.59	1 (0%)	93	93	17, 30, 48, 58	0
All	All	6356/6364 (99%)	-0.42	73 (1%)	82	84	17, 35, 68, 139	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	127	ALA	9.6
5	S	129	GLY	9.1
5	S	128	SER	7.8
2	B	1	MET	7.1
7	U	247	ASN	6.5
2	P	1	MET	6.5
1	A	10	ALA	6.0
4	R	205	THR	5.9
3	C	221	ASN	5.8
1	O	10	ALA	5.7
9	W	222	ASP	5.4
6	T	3	ARG	4.9
5	S	127	ALA	4.9
9	W	221	CYS	4.8
6	F	234	ILE	4.8
5	E	128	SER	4.6
9	I	222	ASP	4.6
3	C	220	ALA	4.5
4	D	207	ALA	4.3
5	E	129	GLY	4.2
6	T	234	ILE	4.0
4	D	52	LEU	4.0
9	I	221	CYS	3.9
11	K	195	GLN	3.9
3	Q	222	ASP	3.8
5	E	133	LEU	3.6
4	R	51	THR	3.5
4	R	200	LEU	3.5
7	G	4	GLY	3.4
11	Y	195	GLN	3.4
10	X	-8	SER	3.4
3	Q	223	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	219	GLY	3.2
4	R	238	GLN	3.2
5	E	130	GLU	3.2
5	S	130	GLU	3.2
5	S	9	ASP	3.1
7	U	246	ILE	3.1
4	R	236	ILE	3.0
6	T	174	ARG	2.9
4	R	52	LEU	2.9
6	T	123	TYR	2.8
14	N	-8	THR	2.8
4	R	203	VAL	2.7
3	Q	52	VAL	2.7
5	E	126	GLY	2.6
12	L	212	GLY	2.6
6	T	55	GLU	2.6
4	R	240	LYS	2.5
6	T	205	SER	2.5
3	Q	245	THR	2.5
14	2	-8	THR	2.5
13	M	165	TYR	2.4
6	F	203	ASP	2.3
6	T	202	ARG	2.3
7	U	238	ALA	2.3
5	S	246	LYS	2.3
7	G	247	ASN	2.3
4	R	199	LEU	2.3
13	1	165	TYR	2.3
12	Z	212	GLY	2.3
5	S	132	ARG	2.3
1	A	190	LYS	2.2
5	S	126	GLY	2.2
4	R	48	ARG	2.2
5	S	10	ARG	2.2
1	A	12	TYR	2.2
4	R	192	VAL	2.2
4	R	242	GLU	2.2
6	F	202	ARG	2.2
11	Y	192	ASP	2.1
6	F	201	LEU	2.1
6	T	56	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	WPI	W	301	41/41	0.62	0.63	33.46	46,99,128,133	0
15	WPI	I	301	41/41	0.62	0.53	17.32	46,94,124,133	0
15	WPI	H	300	41/41	0.70	0.58	14.88	40,78,102,107	0
15	WPI	V	201	41/41	0.77	0.40	10.37	38,67,81,90	0
15	WPI	Z	301	41/41	0.61	0.50	9.20	36,76,123,131	0
15	WPI	L	301	41/41	0.65	0.41	7.18	38,67,111,118	0

6.5 Other polymers (i)

There are no such residues in this entry.