Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:09 AM GMT

PDB ID	:	3NZW
Title	:	Crystal structure of the yeast 20S proteasome in complex with 2b
Authors	:	Groll, M.; Gallastegui, N.; Marechal, X.; Le Ravalec, V.; Basse, N.; Richy, N.; Genin, E.; Huber, R.; Moroder, M.; Vidal, V.; Reboud-Ravaux, M.
Deposited on	:	2010-07-17
Resolution	:	2.50 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:

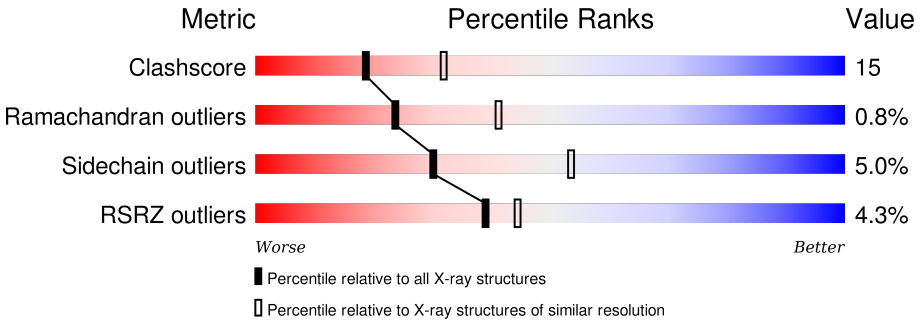
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	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	250	78% 20% •
1	O	250	4% 79% 18% •
2	B	258	3% 60% 30% • 5%
2	P	258	7% 61% 29% • 5%
3	C	254	7% 56% 37% • 5%
3	Q	254	20% 57% 36% • 5%
4	D	260	4% 70% 21% • 7%

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Mol	Chain	Length	Quality of chain
4	R	260	6% 68% 23% 7%
5	E	234	11% 61% 32% 6%
5	S	234	15% 62% 32% 6%
6	F	288	2% 59% 23% 15%
6	T	288	6% 59% 23% 15%
7	G	252	3% 66% 28%
7	U	252	2% 65% 30%
8	H	261	% 60% 25% 15%
8	V	261	60% 25% 15%
9	I	205	% 74% 24%
9	W	205	% 76% 22%
10	J	198	3% 71% 27%
10	X	198	5% 70% 28%
11	K	287	2% 56% 15% 26%
11	Y	287	2% 55% 16% 26%
12	L	241	2% 64% 26% 8%
12	Z	241	2% 62% 27% 8%
13	1	266	62% 23% 12%
13	M	266	61% 25% 12%
14	2	215	70% 19% 9%
14	N	215	71% 18% 9%
15	3	5	60% 40%
15	4	5	60% 40%

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
16	MES	K	212	-	-	-	X
16	MES	Y	212	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51030 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 Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

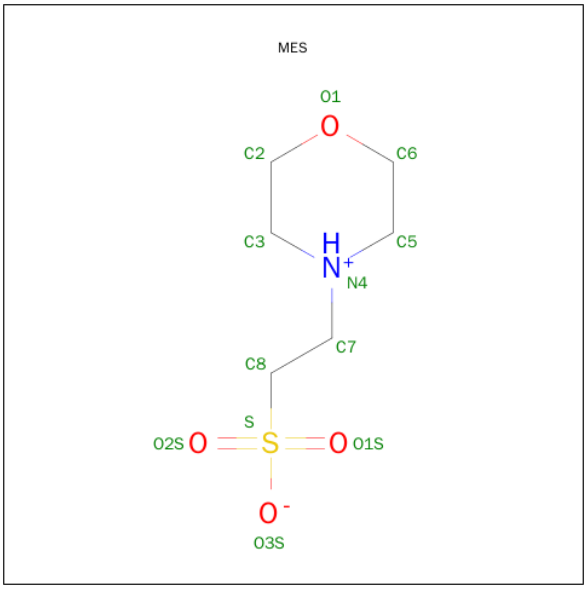
- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called TMC-95A mimic ligand 2b.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	5	Total	C	N	O	0	0	0
			55	42	5	8			
15	4	5	Total	C	N	O	0	0	0
			55	42	5	8			

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	58	Total	O	0	0
			58	58		
17	B	37	Total	O	0	0
			37	37		
17	C	43	Total	O	0	0
			43	43		
17	D	37	Total	O	0	0
			37	37		
17	E	23	Total	O	0	0
			23	23		
17	F	48	Total	O	0	0
			48	48		
17	G	64	Total	O	0	0
			64	64		
17	H	51	Total	O	0	0
			51	51		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	I	67	Total O 67 67	0	0
17	J	54	Total O 54 54	0	0
17	K	52	Total O 52 52	0	0
17	L	56	Total O 56 56	0	0
17	M	71	Total O 71 71	0	0
17	N	55	Total O 55 55	0	0
17	O	33	Total O 33 33	0	0
17	P	29	Total O 29 29	0	0
17	Q	27	Total O 27 27	0	0
17	R	29	Total O 29 29	0	0
17	S	22	Total O 22 22	0	0
17	T	39	Total O 39 39	0	0
17	U	60	Total O 60 60	0	0
17	V	47	Total O 47 47	0	0
17	W	64	Total O 64 64	0	0
17	X	50	Total O 50 50	0	0
17	Y	50	Total O 50 50	0	0
17	Z	51	Total O 51 51	0	0
17	1	75	Total O 75 75	0	0
17	2	61	Total O 61 61	0	0
17	3	2	Total O 2 2	0	0

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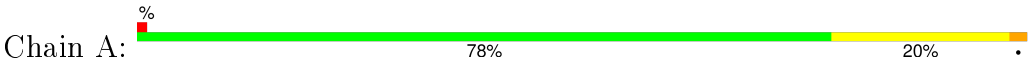
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	4	3	Total O 3 3	0	0

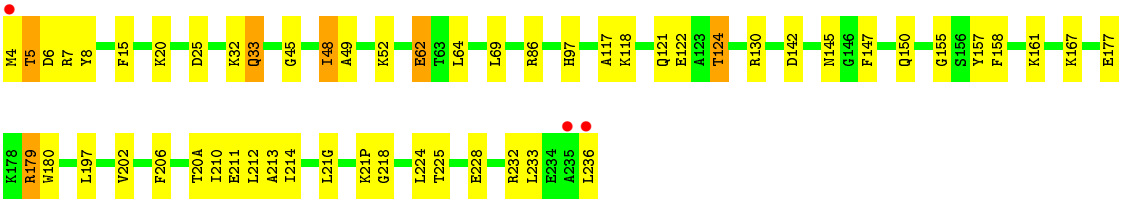
3 Residue-property plots (i)

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 Y7

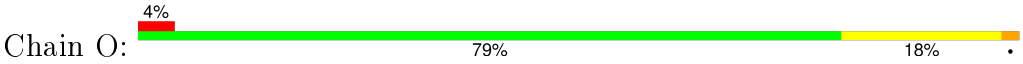
Chain A:

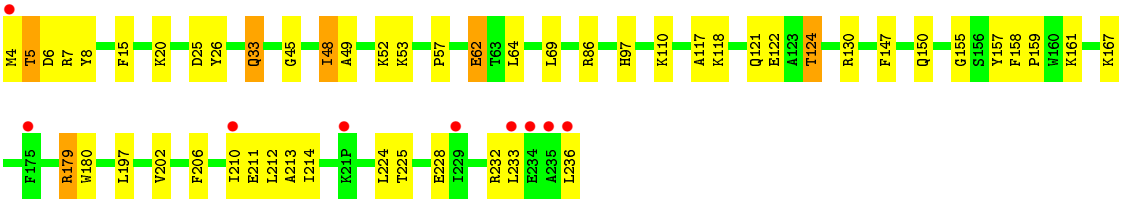




- Molecule 1: Proteasome component Y7

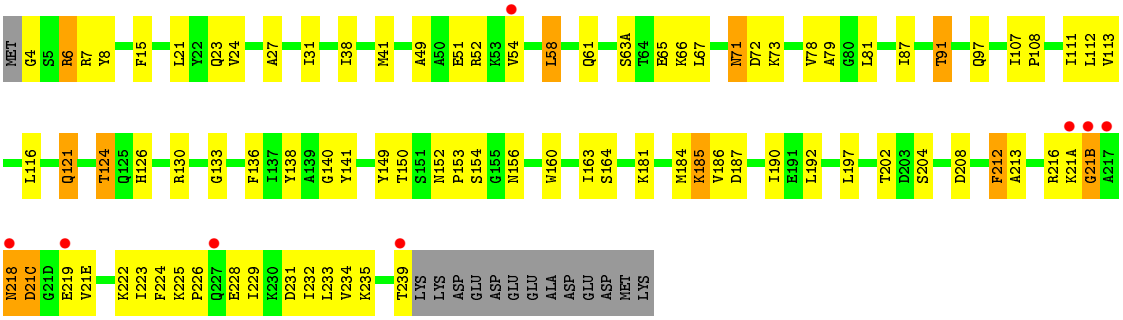
Chain O:





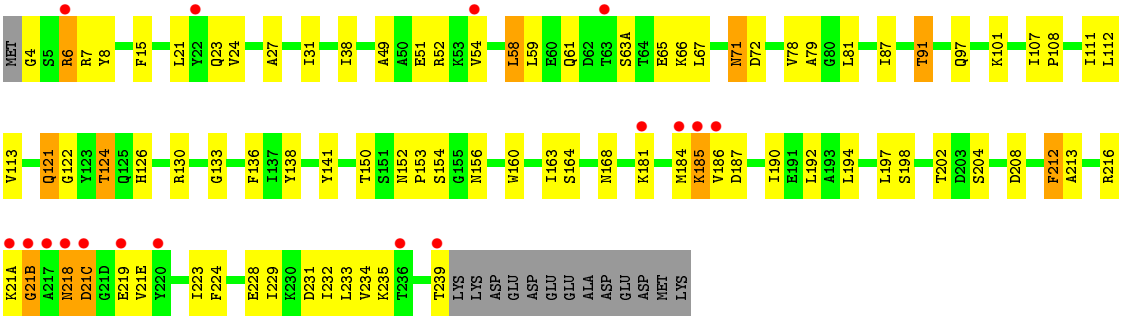
- Molecule 2: Proteasome component Y13

Chain B:



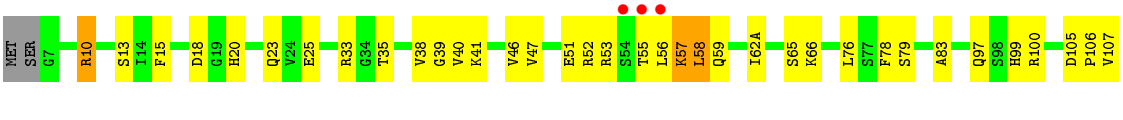
- Molecule 2: Proteasome component Y13

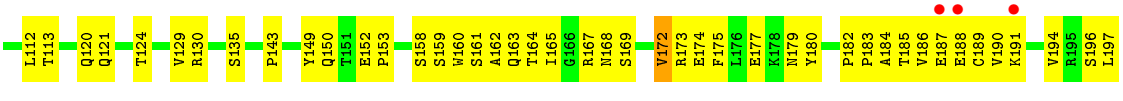
Chain P:

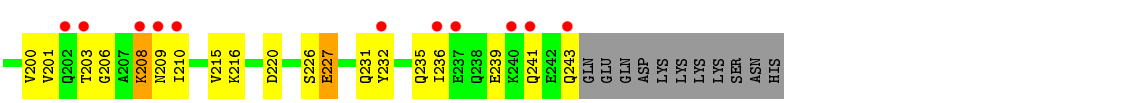


• Molecule 3: Proteasome component PRE6

Chain C:

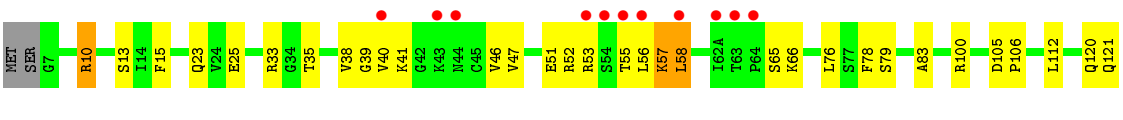


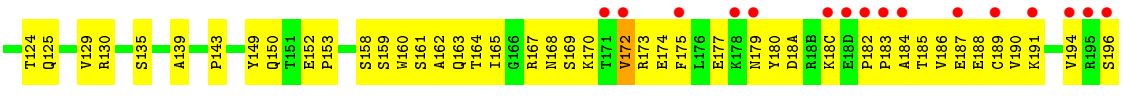


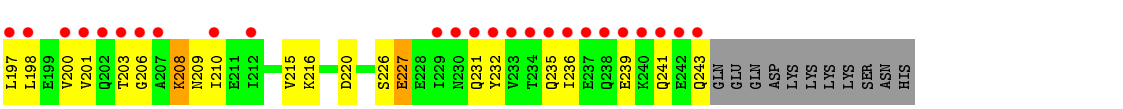


• Molecule 3: Proteasome component PRE6

Chain Q:

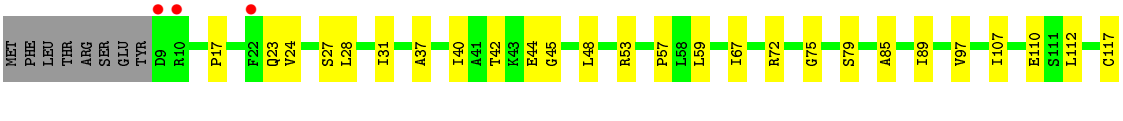


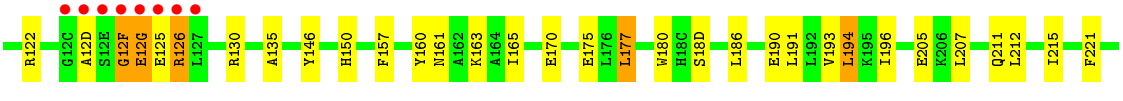




• Molecule 4: Proteasome component PUP2

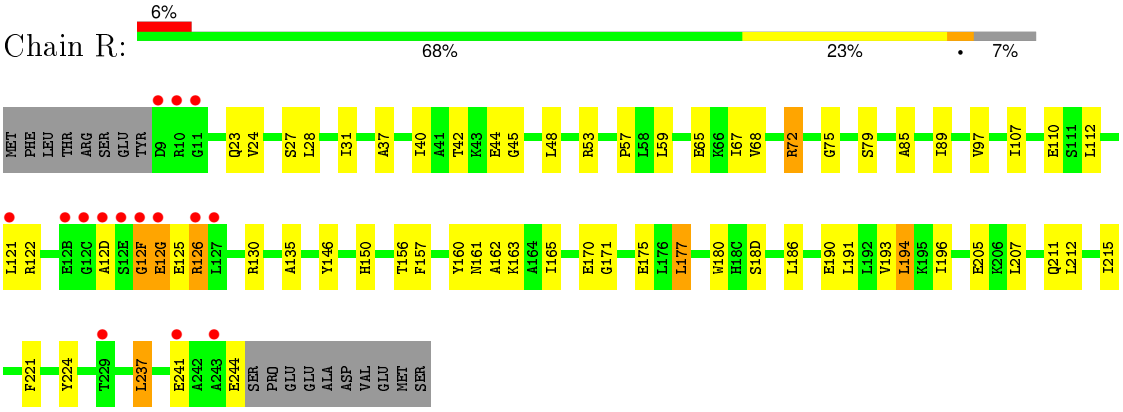
Chain D:





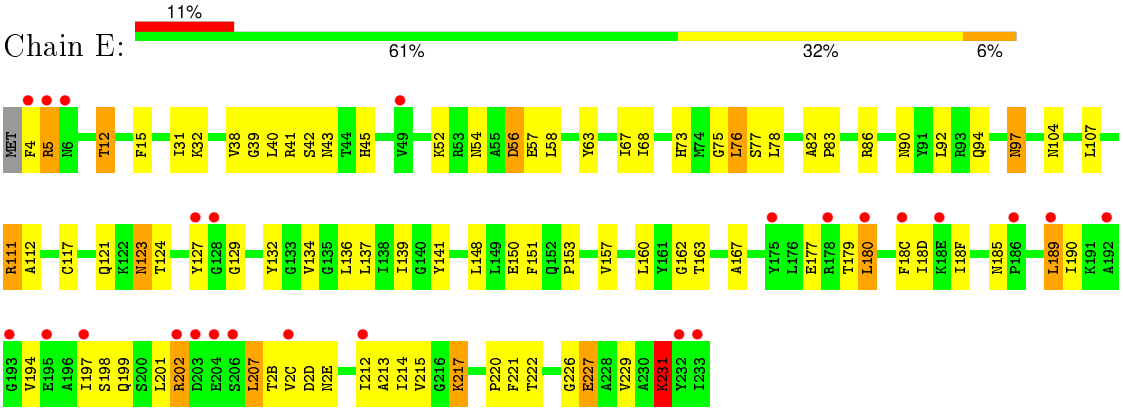
• Molecule 4: Proteasome component PUP2

Chain R:



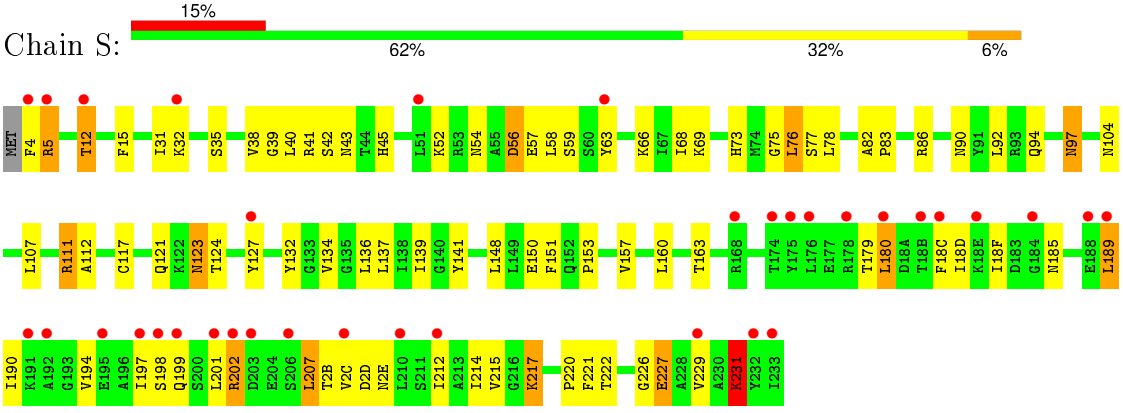
• Molecule 5: Proteasome component PRE5

Chain E:



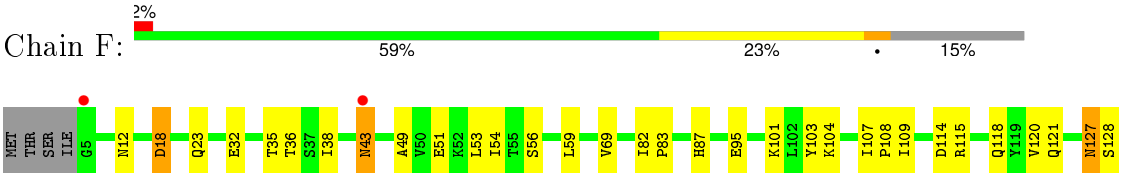
• Molecule 5: Proteasome component PRE5

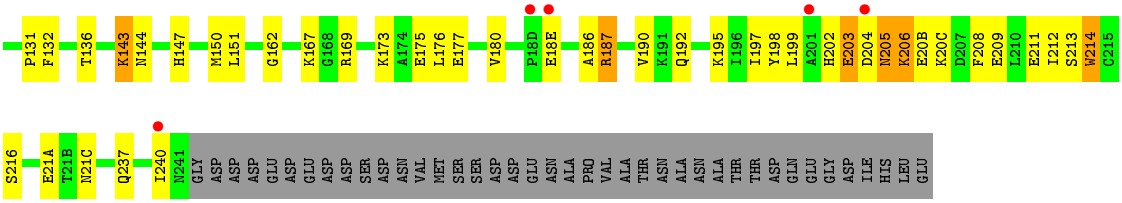
Chain S:



• Molecule 6: Proteasome component C1

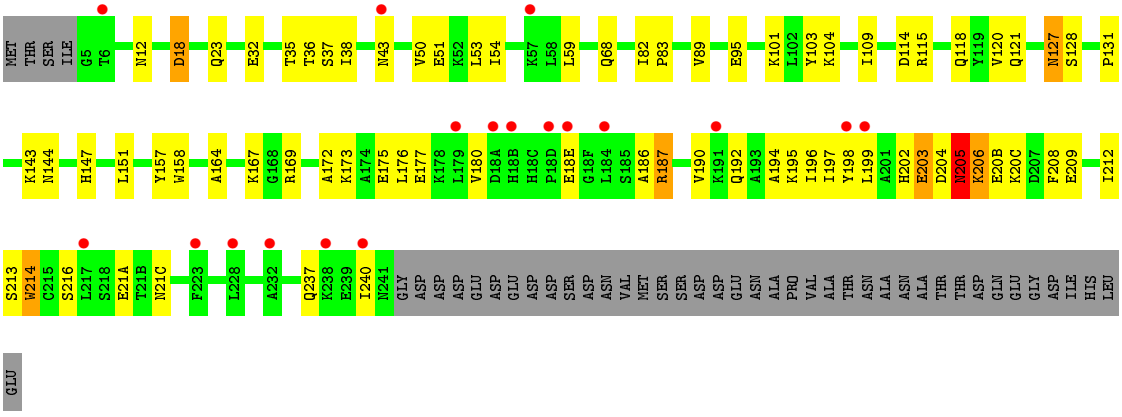
Chain F:





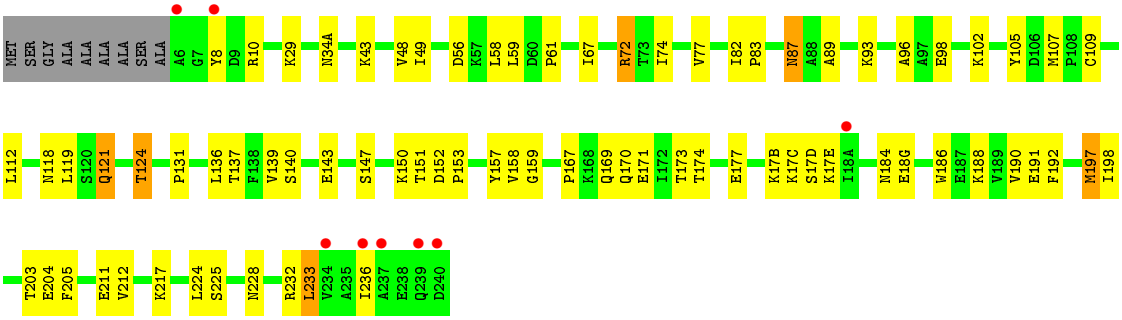
• Molecule 6: Proteasome component C1

Chain T:



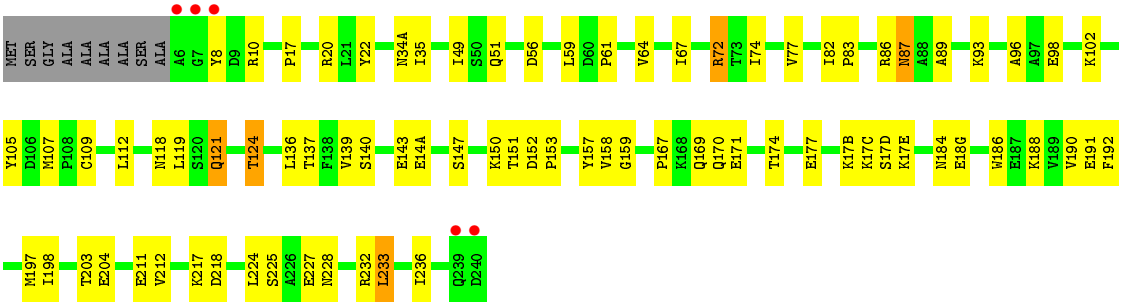
• Molecule 7: Proteasome component C7-alpha

Chain G:



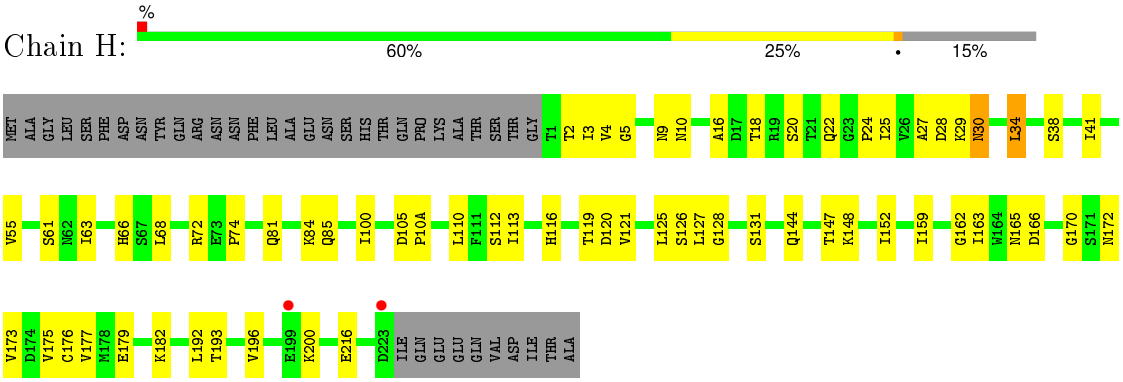
• Molecule 7: Proteasome component C7-alpha

Chain U:



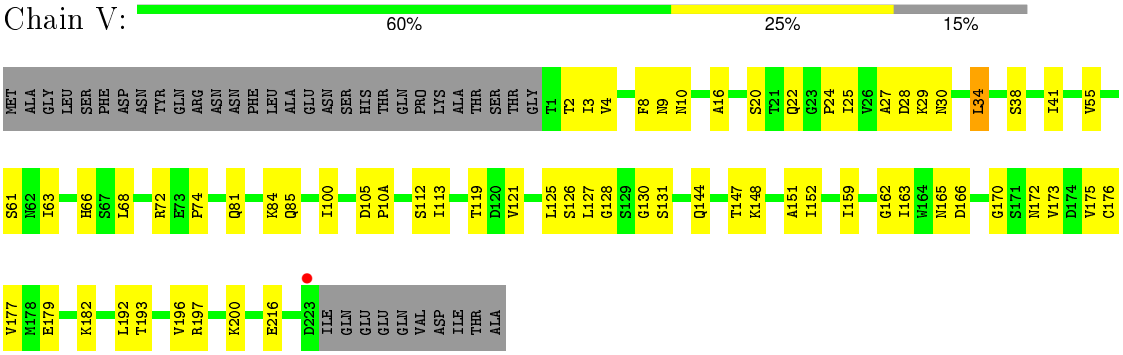
• Molecule 8: Proteasome component PUP1

Chain H:



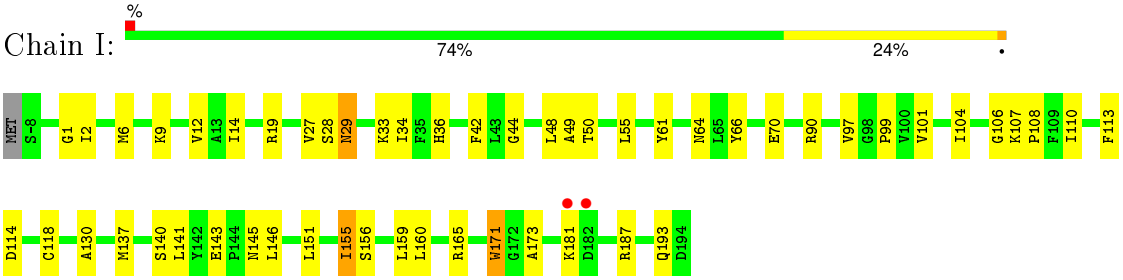
• Molecule 8: Proteasome component PUP1

Chain V:



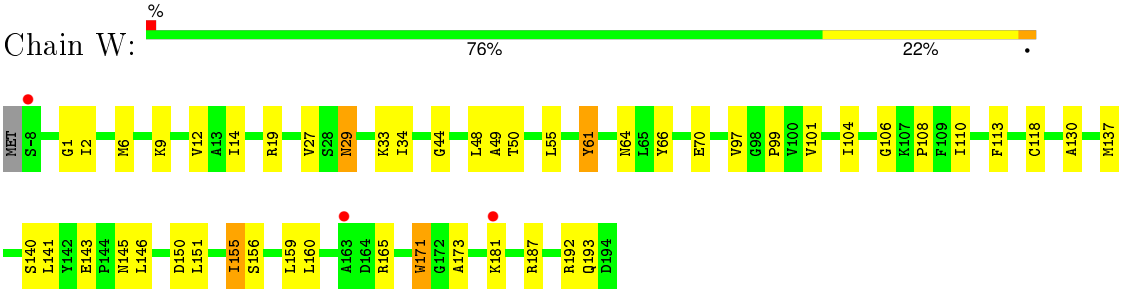
• Molecule 9: Proteasome component PUP3

Chain I:



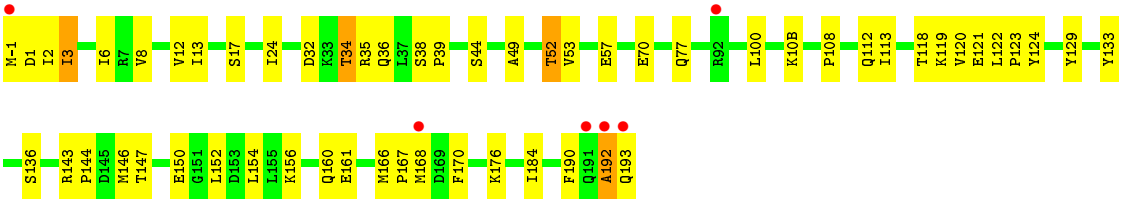
• Molecule 9: Proteasome component PUP3

Chain W:

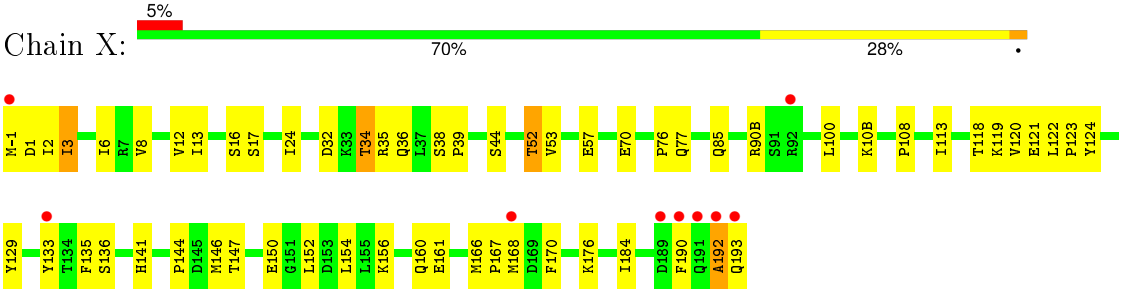


• Molecule 10: Proteasome component C11

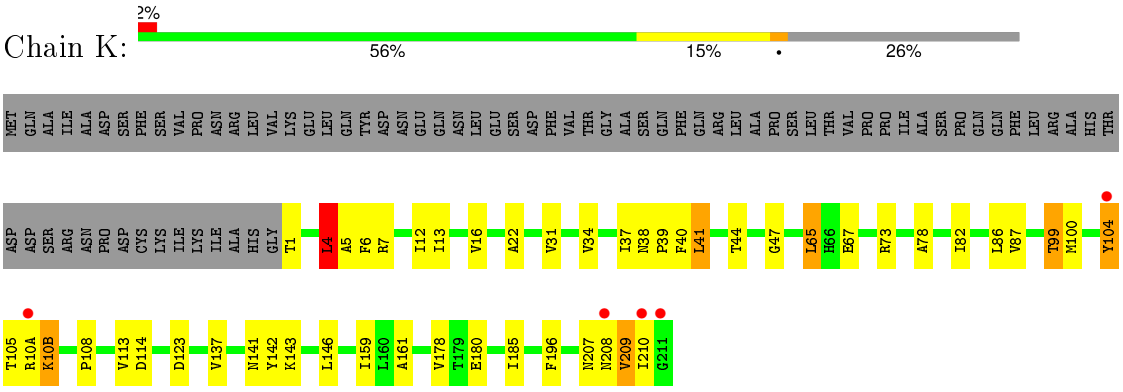
Chain J:



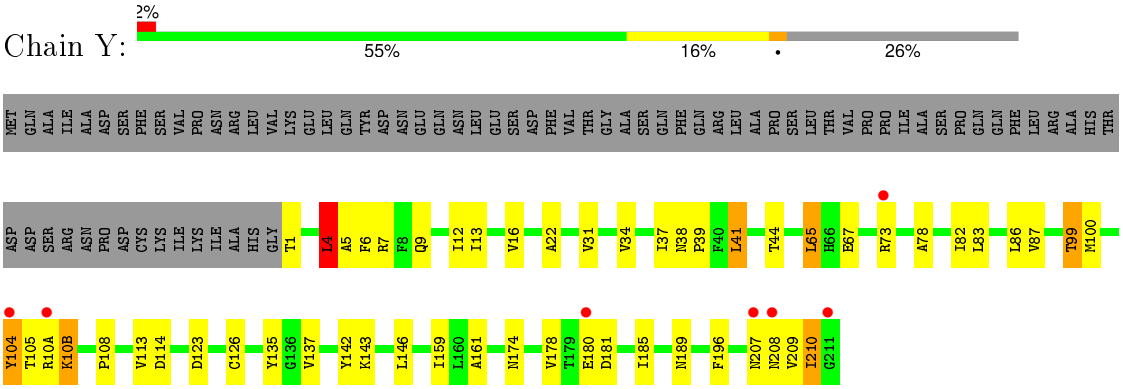
• Molecule 10: Proteasome component C11



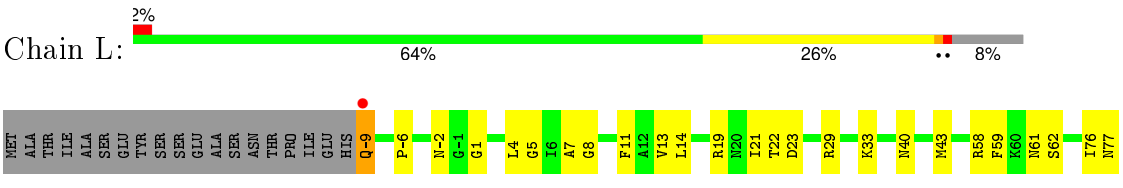
• Molecule 11: Proteasome component PRE2

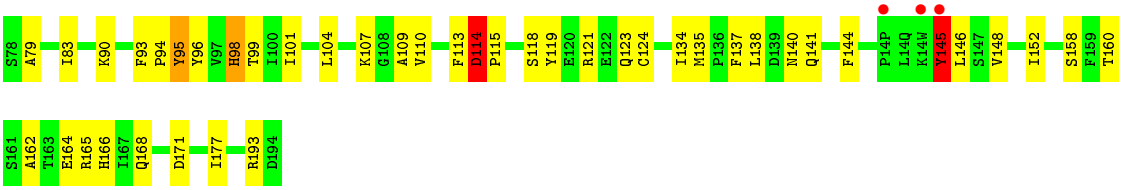


• Molecule 11: Proteasome component PRE2



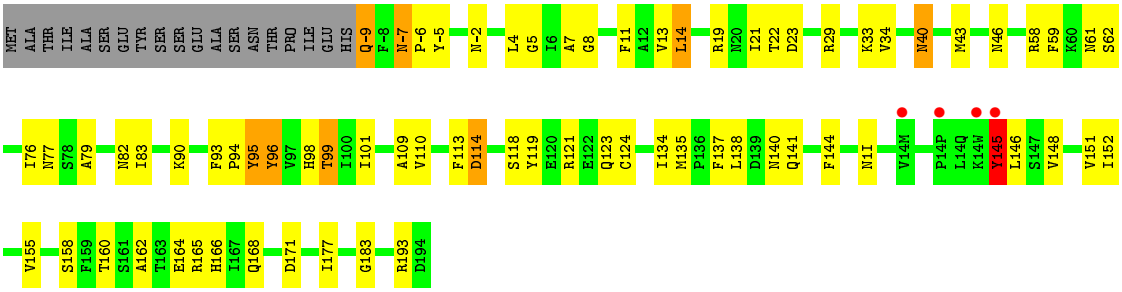
• Molecule 12: Proteasome component C5





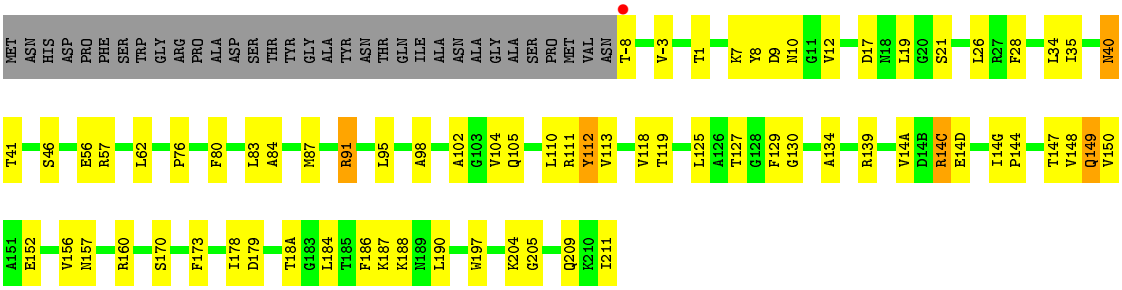
• Molecule 12: Proteasome component C5

Chain Z:



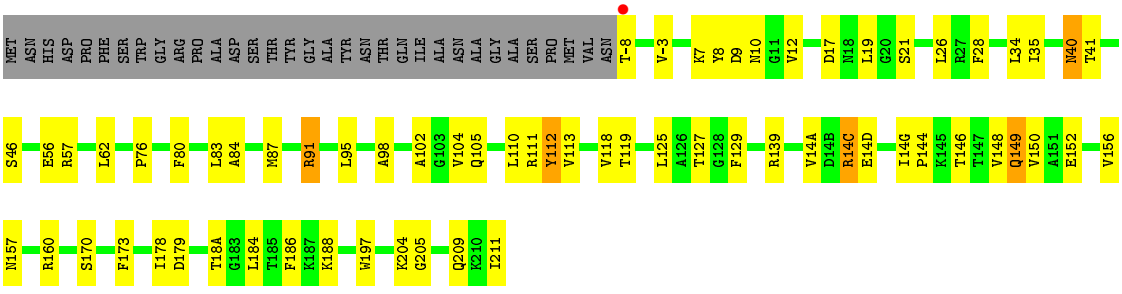
• Molecule 13: Proteasome component PRE4

Chain M:



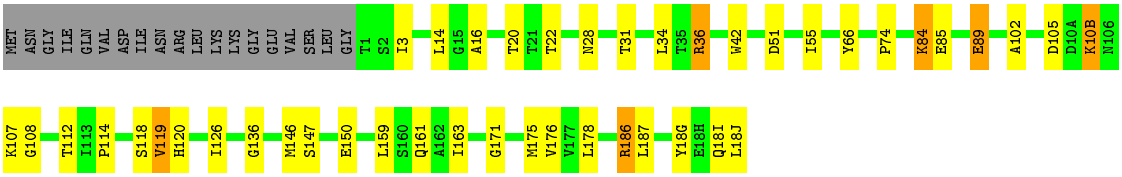
• Molecule 13: Proteasome component PRE4

Chain 1:



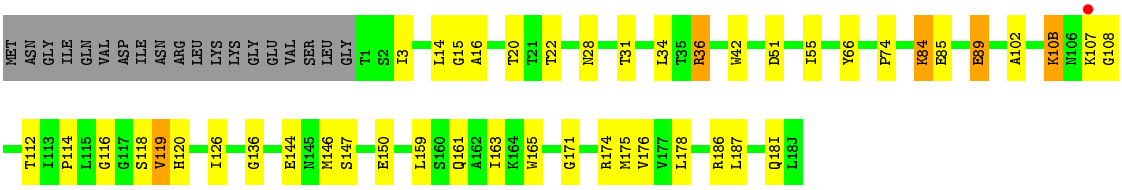
• Molecule 14: Proteasome component PRE3

Chain N:



• Molecule 14: Proteasome component PRE3

Chain 2:



• Molecule 15: TMC-95A mimic ligand 2b

Chain 3:

• Molecule 15: TMC-95A mimic ligand 2b

Chain 4:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.30Å 300.01Å 144.51Å 90.00° 112.92° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 49.51 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.50) 98.0 (49.51-2.51)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.240 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 354720 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	51030	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: TY5, RE0, BOC, MES, ABN

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	0.36	0/1952	0.62	0/2642
1	O	0.35	0/1952	0.62	0/2642
2	B	0.35	0/1934	0.62	0/2618
2	P	0.36	0/1934	0.62	0/2618
3	C	0.35	0/1919	0.61	0/2598
3	Q	0.33	0/1919	0.61	0/2598
4	D	0.34	0/1886	0.61	0/2541
4	R	0.34	0/1886	0.61	0/2541
5	E	0.34	0/1823	0.58	0/2463
5	S	0.35	0/1823	0.58	0/2463
6	F	0.35	0/1936	0.60	0/2614
6	T	0.36	0/1936	0.61	0/2614
7	G	0.39	0/1959	0.62	0/2652
7	U	0.38	0/1959	0.62	0/2652
8	H	0.37	0/1715	0.66	0/2326
8	V	0.36	0/1715	0.66	0/2326
9	I	0.39	0/1611	0.66	0/2174
9	W	0.39	0/1611	0.67	0/2174
10	J	0.38	0/1613	0.66	0/2173
10	X	0.38	0/1613	0.66	0/2173
11	K	0.45	1/1681 (0.1%)	0.69	2/2274 (0.1%)
11	Y	0.38	0/1681	0.68	2/2274 (0.1%)
12	L	0.38	0/1795	0.70	2/2420 (0.1%)
12	Z	0.37	0/1795	0.68	1/2420 (0.0%)
13	1	0.38	0/1855	0.66	1/2514 (0.0%)
13	M	0.36	0/1855	0.66	1/2514 (0.0%)
14	2	0.38	0/1541	0.64	1/2087 (0.0%)
14	N	0.38	0/1541	0.64	1/2087 (0.0%)
15	3	0.88	0/4	0.73	0/4
15	4	0.91	0/4	0.76	0/4
All	All	0.37	1/50448 (0.0%)	0.64	11/68200 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	47	GLY	C-N	-6.42	1.21	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	114	ASP	O-C-N	-6.93	107.94	121.10
11	K	4	LEU	CA-CB-CG	6.18	129.50	115.30
11	Y	4	LEU	CA-CB-CG	6.07	129.25	115.30
13	1	95	LEU	N-CA-C	-5.71	95.58	111.00
13	M	95	LEU	N-CA-C	-5.60	95.89	111.00
11	Y	22	ALA	N-CA-C	-5.43	96.34	111.00
12	L	95	TYR	N-CA-C	-5.32	96.62	111.00
11	K	22	ALA	N-CA-C	-5.31	96.65	111.00
14	2	22	THR	N-CA-C	-5.26	96.80	111.00
12	Z	95	TYR	N-CA-C	-5.22	96.90	111.00
14	N	22	THR	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

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	1915	0	1926	50	0
1	O	1915	0	1926	50	0
2	B	1904	0	1901	80	0
2	P	1904	0	1901	75	0
3	C	1890	0	1900	87	0
3	Q	1890	0	1900	84	0
4	D	1861	0	1836	46	0
4	R	1861	0	1836	50	0
5	E	1795	0	1797	87	0
5	S	1795	0	1797	86	0
6	F	1896	0	1886	60	0
6	T	1896	0	1886	59	0
7	G	1921	0	1910	70	0
7	U	1921	0	1910	78	0
8	H	1684	0	1688	50	0
8	V	1684	0	1688	50	0
9	I	1581	0	1574	47	0
9	W	1581	0	1574	43	0
10	J	1585	0	1590	68	0
10	X	1585	0	1590	80	0
11	K	1644	0	1595	54	0
11	Y	1644	0	1595	56	0
12	L	1757	0	1711	51	0
12	Z	1757	0	1711	57	0
13	1	1824	0	1832	55	0
13	M	1824	0	1832	60	0
14	2	1512	0	1481	38	0
14	N	1512	0	1481	36	0
15	3	55	0	45	4	0
15	4	55	0	45	4	0
16	K	12	0	13	1	0
16	Y	12	0	13	1	0
17	1	75	0	0	2	0
17	2	61	0	0	3	0
17	3	2	0	0	0	0
17	4	3	0	0	0	0
17	A	58	0	0	1	0
17	B	37	0	0	2	0
17	C	43	0	0	2	0
17	D	37	0	0	1	0
17	E	23	0	0	2	0
17	F	48	0	0	3	0
17	G	64	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	H	51	0	0	3	0
17	I	67	0	0	4	0
17	J	54	0	0	2	0
17	K	52	0	0	2	0
17	L	56	0	0	2	0
17	M	71	0	0	2	0
17	N	55	0	0	2	0
17	O	33	0	0	1	0
17	P	29	0	0	1	0
17	Q	27	0	0	3	0
17	R	29	0	0	3	0
17	S	22	0	0	1	0
17	T	39	0	0	1	0
17	U	60	0	0	6	0
17	V	47	0	0	2	0
17	W	64	0	0	3	0
17	X	50	0	0	11	0
17	Y	50	0	0	6	0
17	Z	51	0	0	3	0
All	All	51030	0	49370	1527	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 15.

All (1527) 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)
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.08	1.14
7:G:96:ALA:HA	7:G:107:MET:HE2	1.34	1.09
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.11	1.08
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.15	1.08
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.15	1.06
7:U:96:ALA:HA	7:U:107:MET:HE2	1.33	1.06
11:K:207:ASN:ND2	10:X:144:PRO:HG3	1.73	1.04
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	1.74	1.03
10:J:133:TYR:HD1	17:Y:593:HOH:O	1.42	1.01
2:B:15:PHE:H	3:C:23:GLN:HE22	1.07	1.00
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	1.58	1.00
9:W:27:VAL:HG13	17:X:622:HOH:O	1.58	1.00
11:K:208:ASN:ND2	9:W:29:ASN:HD21	1.58	1.00
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.09	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:207:LEU:HD23	5:S:207:LEU:H	1.31	0.95
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.48	0.94
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.06	0.94
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.32	0.94
2:P:202:THR:HG22	2:P:204:SER:H	1.30	0.93
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.51	0.93
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.07	0.93
5:E:207:LEU:H	5:E:207:LEU:HD23	1.31	0.93
3:C:163:GLN:NE2	3:C:164:THR:H	1.67	0.92
2:B:202:THR:HG22	2:B:204:SER:H	1.31	0.92
9:I:29:ASN:HD21	11:Y:208:ASN:HD22	1.13	0.92
11:K:208:ASN:HD22	9:W:29:ASN:HD21	1.12	0.92
3:C:185:THR:HG22	3:C:187:GLU:H	1.33	0.92
3:C:163:GLN:HE21	3:C:164:THR:N	1.67	0.91
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.68	0.91
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.06	0.90
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.68	0.90
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.34	0.90
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.35	0.88
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.55	0.88
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.74	0.88
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.36	0.88
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.54	0.88
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.84	0.88
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.57	0.87
3:Q:65:SER:HB2	17:Q:303:HOH:O	1.74	0.87
1:O:15:PHE:H	2:P:23:GLN:HE22	1.23	0.86
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.58	0.86
5:E:15:PHE:H	6:F:23:GLN:HE22	1.24	0.86
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.58	0.86
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.41	0.86
5:S:15:PHE:H	6:T:23:GLN:HE22	1.19	0.85
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.89	0.85
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.75	0.85
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.84	0.85
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.56	0.84
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.57	0.84
3:C:185:THR:HB	3:C:188:GLU:HG2	1.58	0.84
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.42	0.84
9:I:29:ASN:ND2	11:Y:208:ASN:ND2	2.26	0.83
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.88	0.83
11:K:208:ASN:ND2	9:W:29:ASN:ND2	2.26	0.83
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.61	0.83
6:F:35:THR:HG21	6:F:51:GLU:O	1.79	0.82
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.62	0.82
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.61	0.82
1:A:15:PHE:H	2:B:23:GLN:HE22	1.28	0.82
6:T:35:THR:HG21	6:T:51:GLU:O	1.79	0.82
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.25	0.81
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.62	0.81
10:J:133:TYR:HE1	17:X:876:HOH:O	1.63	0.81
3:C:163:GLN:HE21	3:C:164:THR:H	0.87	0.81
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.77	0.81
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.79	0.80
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.62	0.80
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.64	0.80
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.62	0.80
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.12	0.80
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.97	0.79
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.11	0.79
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.64	0.79
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.65	0.79
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.83	0.78
12:L:114:ASP:HB3	12:L:118:SER:HB3	1.65	0.78
10:J:24:ILE:O	10:X:133:TYR:OH	2.02	0.78
10:J:-1:MET:HG2	10:J:1:ASP:H	1.50	0.77
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.29	0.77
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.81	0.77
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.31	0.77
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.67	0.77
11:Y:1:THR:HB	16:Y:212:MES:O2S	1.84	0.77
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.65	0.77
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.82	0.77
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.66	0.76
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.99	0.76
5:S:12:THR:HG21	5:S:124:THR:HA	1.68	0.76
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.49	0.76
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.67	0.76
2:P:124:THR:CG2	3:Q:130:ARG:HH21	1.98	0.76
5:E:12:THR:HG21	5:E:124:THR:HA	1.68	0.75
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.01	0.75
11:Y:210:ILE:HB	17:Y:1226:HOH:O	1.85	0.75
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.35	0.75
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.01	0.75
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.16	0.74
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.69	0.74
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.68	0.74
10:X:-1:MET:HG2	10:X:1:ASP:H	1.51	0.74
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.35	0.74
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.69	0.74
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.87	0.74
5:E:207:LEU:H	5:E:207:LEU:CD2	2.01	0.74
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.87	0.74
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.02	0.74
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.70	0.74
10:J:133:TYR:OH	10:X:24:ILE:O	2.05	0.73
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.17	0.73
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.88	0.73
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.97	0.73
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.53	0.73
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.70	0.73
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.69	0.73
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.85	0.73
5:S:207:LEU:H	5:S:207:LEU:CD2	2.01	0.73
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.23	0.73
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.36	0.73
12:Z:114:ASP:HB3	12:Z:118:SER:HB3	1.68	0.73
5:S:198:SER:HA	5:S:201:LEU:HG	1.70	0.73
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.36	0.73
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.38	0.72
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.19	0.72
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.90	0.72
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.02	0.72
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.71	0.72
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.70	0.72
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.71	0.72
11:K:99:THR:HG22	11:K:113:VAL:O	1.89	0.72
2:B:71:ASN:ND2	2:B:72:ASP:H	1.88	0.71
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.19	0.71
14:2:107:LYS:HG2	14:2:108:GLY:H	1.55	0.71
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.54	0.71
14:2:51:ASP:O	14:2:55:ILE:HG12	1.88	0.71
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.38	0.71
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.72	0.71
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.26	0.71
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.72	0.71
12:L:166:HIS:HD2	12:L:168:GLN:H	1.37	0.71
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.70	0.70
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.20	0.70
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.56	0.70
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.06	0.70
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.26	0.70
1:O:4:MET:SD	1:O:5:THR:N	2.59	0.70
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.36	0.70
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.55	0.70
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.06	0.70
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.74	0.70
4:R:121:LEU:HB2	17:R:853:HOH:O	1.90	0.70
14:N:51:ASP:O	14:N:55:ILE:HG12	1.90	0.70
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.56	0.70
7:U:86:ARG:HD2	17:U:248:HOH:O	1.90	0.70
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.55	0.70
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.26	0.70
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.72	0.70
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.03	0.70
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.55	0.70
3:C:15:PHE:H	4:D:23:GLN:HE22	1.39	0.70
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.55	0.70
5:E:198:SER:HA	5:E:201:LEU:HG	1.71	0.70
4:R:186:LEU:O	4:R:190:GLU:HG3	1.92	0.70
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.21	0.70
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.56	0.70
10:J:168:MET:HE3	10:X:168:MET:HE3	1.73	0.69
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.56	0.69
2:P:121:GLN:O	2:P:124:THR:HB	1.91	0.69
13:M:40:ASN:H	13:M:40:ASN:HD22	1.39	0.69
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	1.92	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.69
8:H:38:SER:OG	8:H:41:ILE:HD13	1.93	0.69
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.75	0.69
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:LEU:O	4:D:190:GLU:HG3	1.94	0.68
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	1.91	0.68
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.06	0.68
2:P:71:ASN:ND2	2:P:72:ASP:H	1.91	0.68
3:C:232:TYR:O	3:C:236:ILE:HG12	1.94	0.68
14:N:107:LYS:HG2	14:N:108:GLY:H	1.56	0.68
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.76	0.68
5:S:123:ASN:N	5:S:123:ASN:HD22	1.92	0.68
13:1:40:ASN:HD22	13:1:40:ASN:H	1.39	0.68
3:C:185:THR:HG22	3:C:187:GLU:N	2.08	0.67
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.75	0.67
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.58	0.67
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.90	0.67
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.07	0.67
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.60	0.67
7:U:96:ALA:CA	7:U:107:MET:HE2	2.19	0.67
3:Q:232:TYR:O	3:Q:236:ILE:HG12	1.94	0.67
8:V:38:SER:OG	8:V:41:ILE:HD13	1.94	0.67
10:J:-1:MET:HG2	10:J:1:ASP:N	2.09	0.67
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.77	0.67
1:A:4:MET:SD	1:A:5:THR:N	2.58	0.67
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.08	0.67
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.76	0.67
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.77	0.67
7:U:59:LEU:O	7:U:61:PRO:HD3	1.95	0.67
10:X:-1:MET:HG2	10:X:1:ASP:N	2.10	0.67
7:U:198:ILE:HG23	7:U:203:THR:O	1.95	0.67
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.77	0.67
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.59	0.67
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.42	0.66
7:G:96:ALA:HA	7:G:107:MET:CE	2.21	0.66
3:C:41:LYS:HG2	3:C:161:SER:O	1.96	0.66
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.43	0.66
10:J:133:TYR:CE1	17:X:876:HOH:O	2.43	0.66
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.77	0.66
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.11	0.66
2:B:6:ARG:HB2	5:E:127:TYR:OH	1.96	0.66
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.78	0.66
14:2:144:GLU:HG2	17:2:1115:HOH:O	1.95	0.66
7:G:59:LEU:O	7:G:61:PRO:HD3	1.95	0.66
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:237:GLN:O	6:F:240:ILE:HG22	1.97	0.65
9:W:6:MET:HE3	9:W:155:ILE:HA	1.78	0.65
6:T:237:GLN:O	6:T:240:ILE:HG22	1.96	0.65
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.78	0.65
5:S:207:LEU:N	5:S:207:LEU:HD23	2.08	0.65
11:K:99:THR:HG22	11:K:113:VAL:HB	1.78	0.65
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.32	0.65
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.77	0.65
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.61	0.65
12:L:98:HIS:HD2	17:L:199:HOH:O	1.79	0.65
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.77	0.65
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.11	0.65
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.79	0.65
6:T:203:GLU:O	6:T:206:LYS:HD2	1.96	0.65
7:G:198:ILE:HG23	7:G:203:THR:O	1.96	0.65
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.79	0.65
11:K:208:ASN:HB3	17:K:776:HOH:O	1.97	0.65
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.12	0.65
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.79	0.65
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.10	0.65
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.43	0.65
8:V:81:GLN:O	8:V:85:GLN:HG3	1.96	0.64
5:S:226:GLY:O	5:S:229:VAL:HG22	1.98	0.64
6:T:54:ILE:HG12	6:T:208:PHE:HA	1.79	0.64
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.78	0.64
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.08	0.64
1:A:97:HIS:HD2	8:H:61:SER:OG	1.81	0.64
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.28	0.64
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.44	0.64
8:V:172:ASN:HD22	8:V:193:THR:HA	1.63	0.64
3:Q:170:LYS:HB2	17:Q:833:HOH:O	1.97	0.64
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.61	0.64
5:E:226:GLY:O	5:E:229:VAL:HG22	1.98	0.64
8:H:172:ASN:HD22	8:H:193:THR:HA	1.63	0.64
5:E:123:ASN:HD22	5:E:123:ASN:N	1.94	0.64
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.80	0.63
11:K:99:THR:CG2	11:K:113:VAL:HB	2.29	0.63
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	1.99	0.63
2:P:87:ILE:O	2:P:91:THR:HG23	1.98	0.63
5:E:207:LEU:HD23	5:E:207:LEU:N	2.08	0.63
17:B:565:HOH:O	3:C:33:ARG:HD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:211:ILE:HD11	14:2:36:ARG:HD2	1.80	0.63
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.80	0.63
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.97	0.63
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.33	0.63
6:F:203:GLU:O	6:F:206:LYS:HD2	1.99	0.63
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	1.99	0.63
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.80	0.63
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.28	0.63
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.80	0.63
7:G:233:LEU:O	7:G:236:ILE:HG13	1.99	0.63
5:E:227:GLU:CD	5:E:227:GLU:H	2.01	0.63
4:R:53:ARG:HG2	4:R:53:ARG:O	1.99	0.63
1:A:121:GLN:O	1:A:124:THR:HB	1.99	0.62
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.47	0.62
2:P:185:LYS:HD3	2:P:186:VAL:N	2.14	0.62
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.00	0.62
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.80	0.62
5:S:227:GLU:CD	5:S:227:GLU:H	2.01	0.62
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.00	0.62
1:O:121:GLN:O	1:O:124:THR:HB	1.99	0.62
2:B:202:THR:HG22	2:B:204:SER:N	2.11	0.61
2:B:185:LYS:HD3	2:B:186:VAL:N	2.15	0.61
11:K:31:VAL:HG11	15:3:5:ABN:C3	2.30	0.61
1:O:97:HIS:HD2	8:V:61:SER:OG	1.83	0.61
7:U:233:LEU:O	7:U:236:ILE:HG13	2.00	0.61
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.35	0.61
8:H:81:GLN:O	8:H:85:GLN:HG3	1.99	0.61
13:1:149:GLN:H	13:1:149:GLN:NE2	1.98	0.61
6:F:54:ILE:HG12	6:F:208:PHE:HA	1.82	0.61
6:T:186:ALA:O	6:T:190:VAL:HG23	2.00	0.61
13:M:149:GLN:NE2	13:M:149:GLN:H	1.99	0.61
13:1:41:THR:OG1	13:1:76:PRO:HG3	1.99	0.61
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.82	0.61
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.31	0.61
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.01	0.61
6:T:54:ILE:HD11	6:T:209:GLU:HB2	1.82	0.61
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.83	0.61
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.83	0.61
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.15	0.61
10:X:2:ILE:O	10:X:3:ILE:HD12	2.00	0.61
2:B:87:ILE:O	2:B:91:THR:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.30	0.61
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.83	0.60
10:J:112:GLN:NE2	17:J:898:HOH:O	2.34	0.60
10:X:136:SER:N	17:X:203:HOH:O	2.29	0.60
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.02	0.60
11:Y:181:ASP:N	17:Y:812:HOH:O	2.34	0.60
2:B:71:ASN:HD22	2:B:72:ASP:H	1.49	0.60
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.82	0.60
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	2.01	0.60
6:T:176:LEU:O	6:T:180:VAL:HG23	2.01	0.60
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.83	0.60
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.13	0.60
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.67	0.60
3:C:65:SER:HB2	17:C:274:HOH:O	2.02	0.60
7:U:186:TRP:O	7:U:190:VAL:HG23	2.02	0.60
10:X:156:LYS:O	10:X:160:GLN:HG3	2.02	0.60
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.67	0.60
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.37	0.60
6:F:186:ALA:O	6:F:190:VAL:HG23	2.01	0.60
10:J:2:ILE:O	10:J:3:ILE:HD12	2.02	0.60
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.32	0.60
3:C:186:VAL:O	3:C:190:VAL:HG23	2.02	0.60
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.83	0.60
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.67	0.60
11:Y:31:VAL:HG11	15:4:5:ABN:C3	2.32	0.60
9:I:6:MET:HE3	9:I:155:ILE:HD12	1.84	0.60
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.17	0.60
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.23	0.60
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.37	0.59
7:G:186:TRP:O	7:G:190:VAL:HG23	2.01	0.59
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.83	0.59
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.83	0.59
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.31	0.59
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.02	0.59
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.85	0.59
10:X:3:ILE:HB	17:X:1164:HOH:O	2.02	0.59
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.82	0.59
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.37	0.59
5:S:132:TYR:O	5:S:153:PRO:HB3	2.02	0.59
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.67	0.59
14:2:10(B):LYS:C	14:2:10(B):LYS:HD3	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:144:PRO:CG	11:Y:207:ASN:HD21	1.99	0.59
10:J:133:TYR:HE2	10:J:166:MET:SD	2.26	0.59
2:B:15:PHE:H	3:C:23:GLN:NE2	1.89	0.59
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.03	0.59
11:K:104:TYR:CE1	11:K:180:GLU:OE2	2.56	0.59
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.85	0.59
10:J:6:ILE:CD1	10:J:154:LEU:HD23	2.33	0.59
11:K:141:ASN:HD21	10:X:141:HIS:HE1	1.50	0.59
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.67	0.59
5:S:194:VAL:O	5:S:197:ILE:HG22	2.03	0.59
7:G:77:VAL:CG1	7:G:137:THR:HB	2.33	0.59
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.49	0.59
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.03	0.59
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.02	0.59
7:U:121:GLN:O	7:U:124:THR:HB	2.03	0.59
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.68	0.59
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.50	0.59
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.00	0.58
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.02	0.58
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.85	0.58
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.84	0.58
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.38	0.58
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.03	0.58
4:D:53:ARG:HG2	4:D:53:ARG:O	2.02	0.58
5:E:194:VAL:O	5:E:197:ILE:HG22	2.03	0.58
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.18	0.58
7:U:77:VAL:CG1	7:U:137:THR:HB	2.32	0.58
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.84	0.58
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.34	0.58
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.68	0.58
2:P:202:THR:HG22	2:P:204:SER:N	2.10	0.58
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.04	0.58
5:S:73:HIS:HE1	5:S:107:LEU:O	1.86	0.58
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.18	0.58
2:P:71:ASN:HD22	2:P:72:ASP:H	1.51	0.58
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.33	0.58
5:S:160:LEU:HD13	5:S:163:THR:HB	1.85	0.58
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.86	0.58
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.17	0.58
11:K:141:ASN:HD21	10:X:141:HIS:CE1	2.21	0.58
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.85	0.58
5:S:227:GLU:N	5:S:227:GLU:CD	2.57	0.58
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.84	0.58
5:E:160:LEU:HD13	5:E:163:THR:HB	1.85	0.58
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.04	0.58
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.50	0.58
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.85	0.58
14:N:34:LEU:CD1	14:N:176:VAL:HG23	2.33	0.58
7:U:8:TYR:C	7:U:10:ARG:H	2.07	0.58
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.16	0.58
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.04	0.58
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.67	0.58
8:H:148:LYS:O	8:H:152:ILE:HG12	2.04	0.58
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.85	0.58
12:L:79:ALA:O	12:L:83:ILE:HG12	2.04	0.58
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.29	0.57
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.86	0.57
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.86	0.57
9:I:90:ARG:HD2	17:I:1159:HOH:O	2.04	0.57
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.86	0.57
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.34	0.57
9:W:192:ARG:HG3	17:W:201:HOH:O	2.03	0.57
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.04	0.57
3:Q:241:GLN:C	3:Q:243:GLN:H	2.07	0.57
8:V:148:LYS:O	8:V:152:ILE:HG12	2.03	0.57
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.04	0.57
10:J:168:MET:HE1	10:X:167:PRO:CB	2.32	0.57
10:J:52:THR:CG2	10:J:53:VAL:N	2.67	0.57
3:C:191:LYS:HG3	3:C:236:ILE:HD11	1.85	0.57
12:Z:79:ALA:O	12:Z:83:ILE:HG12	2.04	0.57
6:F:176:LEU:O	6:F:180:VAL:HG23	2.04	0.57
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.87	0.57
2:P:108:PRO:HB2	2:P:111:ILE:HD13	1.86	0.57
10:J:146:MET:HE3	10:J:150:GLU:HB3	1.87	0.57
10:J:167:PRO:CB	10:X:168:MET:HE1	2.31	0.57
3:Q:191:LYS:HG3	3:Q:236:ILE:HD11	1.87	0.57
12:L:145:TYR:CD1	12:L:146:LEU:N	2.72	0.57
10:J:136:SER:HB2	11:Y:161:ALA:HB1	1.87	0.57
10:X:52:THR:CG2	10:X:53:VAL:N	2.68	0.57
4:D:112:LEU:C	4:D:112:LEU:HD13	2.24	0.57
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.73	0.57
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.70	0.57
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.85	0.57
6:F:95:GLU:HG2	6:F:115:ARG:CB	2.32	0.57
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.87	0.57
11:K:161:ALA:HB1	10:X:136:SER:HB2	1.86	0.56
11:K:67:GLU:OE2	17:K:959:HOH:O	2.17	0.56
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.05	0.56
3:C:241:GLN:C	3:C:243:GLN:H	2.07	0.56
10:X:133:TYR:HE2	10:X:166:MET:SD	2.27	0.56
5:E:132:TYR:O	5:E:153:PRO:HB3	2.04	0.56
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.40	0.56
10:J:136:SER:N	17:J:198:HOH:O	2.31	0.56
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.70	0.56
3:C:46:VAL:O	3:C:215:VAL:HG12	2.04	0.56
11:Y:104:TYR:CE1	11:Y:180:GLU:OE2	2.57	0.56
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.05	0.56
1:O:48:ILE:HD12	1:O:48:ILE:O	2.04	0.56
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.87	0.56
5:E:73:HIS:HE1	5:E:107:LEU:O	1.88	0.56
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.41	0.56
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.85	0.56
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.05	0.56
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.36	0.56
13:M:150:VAL:HG21	17:M:1069:HOH:O	2.06	0.56
4:R:112:LEU:C	4:R:112:LEU:HD13	2.26	0.56
13:1:46:SER:OG	13:1:98:ALA:HB3	2.06	0.56
13:M:17:ASP:HA	13:M:173:PHE:CB	2.36	0.56
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.05	0.56
8:V:113:ILE:HG13	8:V:119:THR:HG22	1.88	0.56
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.04	0.56
10:J:52:THR:HG23	10:J:53:VAL:N	2.20	0.56
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.87	0.56
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.41	0.56
13:1:152:GLU:O	13:1:156:VAL:HG23	2.06	0.56
5:E:227:GLU:CD	5:E:227:GLU:N	2.58	0.55
1:A:48:ILE:O	1:A:48:ILE:HD12	2.05	0.55
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.88	0.55
10:J:156:LYS:O	10:J:160:GLN:HG3	2.06	0.55
2:B:108:PRO:HB2	2:B:111:ILE:HD13	1.87	0.55
2:B:181:LYS:O	2:B:184:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:27:VAL:O	17:I:510:HOH:O	2.18	0.55
2:P:112:LEU:HD23	2:P:112:LEU:C	2.26	0.55
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.88	0.55
12:L:96:TYR:CD1	15:3:2:TY5:H49	2.41	0.55
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.87	0.55
7:U:227:GLU:HG2	17:U:1255:HOH:O	2.06	0.55
10:X:44:SER:OG	10:X:100:LEU:HB2	2.06	0.55
2:P:231:ASP:O	2:P:235:LYS:HG2	2.07	0.55
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.05	0.55
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.21	0.55
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.07	0.55
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.21	0.55
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.89	0.55
12:L:135:MET:CE	9:W:165:ARG:NH2	2.69	0.55
7:U:67:ILE:HD13	7:U:211:GLU:CD	2.27	0.55
10:J:168:MET:CE	10:X:168:MET:CE	2.85	0.55
3:C:35:THR:HB	3:C:51:GLU:HG3	1.89	0.55
3:C:41:LYS:HD3	3:C:161:SER:HA	1.88	0.55
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.41	0.55
10:J:44:SER:OG	10:J:100:LEU:HB2	2.07	0.55
3:C:235:GLN:O	3:C:239:GLU:HG2	2.07	0.55
7:G:8:TYR:C	7:G:10:ARG:H	2.08	0.55
14:2:34:LEU:CD1	14:2:176:VAL:HG23	2.34	0.55
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.88	0.55
5:S:41:ARG:NH1	5:S:42:SER:O	2.39	0.55
10:X:52:THR:HG23	10:X:53:VAL:N	2.22	0.55
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.88	0.55
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.89	0.55
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.88	0.55
3:C:57:LYS:O	3:C:58:LEU:HB2	2.07	0.54
14:N:36:ARG:HD2	13:1:211:ILE:HD11	1.88	0.54
13:M:46:SER:OG	13:M:98:ALA:HB3	2.07	0.54
12:Z:96:TYR:CD1	15:4:2:TY5:H49	2.42	0.54
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.89	0.54
10:X:36:GLN:HG3	10:X:184:ILE:CD1	2.37	0.54
7:G:96:ALA:CA	7:G:107:MET:HE2	2.23	0.54
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.89	0.54
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.08	0.54
11:K:142:TYR:O	11:K:143:LYS:HD2	2.06	0.54
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.37	0.54
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:GLU:OE1	3:C:227:GLU:N	2.40	0.54
13:1:17:ASP:HA	13:1:173:PHE:CB	2.37	0.54
5:E:15:PHE:H	6:F:23:GLN:NE2	2.01	0.54
8:V:84:LYS:HG3	8:V:85:GLN:N	2.23	0.54
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.90	0.54
12:Z:21:ILE:HD12	12:Z:21:ILE:C	2.28	0.54
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.89	0.54
7:G:67:ILE:HD13	7:G:211:GLU:CD	2.27	0.54
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.43	0.54
11:Y:135:TYR:HB2	17:Y:593:HOH:O	2.07	0.54
11:Y:210:ILE:HB	17:Y:1150:HOH:O	2.07	0.54
8:V:4:VAL:HG22	8:V:159:ILE:CD1	2.38	0.54
12:Z:114:ASP:CB	12:Z:118:SER:HB3	2.35	0.54
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.06	0.54
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.90	0.54
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.90	0.54
2:P:181:LYS:O	2:P:184:MET:HG3	2.07	0.54
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.43	0.54
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.06	0.54
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.43	0.54
14:2:107:LYS:HG2	14:2:108:GLY:N	2.22	0.54
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.90	0.54
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.08	0.54
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.72	0.54
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.08	0.53
8:H:84:LYS:HG3	8:H:85:GLN:N	2.22	0.53
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.08	0.53
11:K:12:ILE:HB	11:K:178:VAL:HB	1.90	0.53
13:M:152:GLU:O	13:M:156:VAL:HG23	2.08	0.53
3:C:52:ARG:HD2	3:C:208:LYS:O	2.09	0.53
13:1:35:ILE:HG12	13:1:56:GLU:HG2	1.91	0.53
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.90	0.53
10:J:168:MET:HE3	10:X:168:MET:CE	2.36	0.53
12:L:114:ASP:CB	12:L:118:SER:HB3	2.37	0.53
2:B:112:LEU:C	2:B:112:LEU:HD23	2.28	0.53
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.37	0.53
14:N:176:VAL:HG12	14:N:178:LEU:CD1	2.38	0.53
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.41	0.53
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.89	0.53
8:H:4:VAL:HG22	8:H:159:ILE:CD1	2.37	0.53
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.89	0.53
9:I:48:LEU:HG	9:I:50:THR:HG22	1.91	0.53
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.90	0.53
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.09	0.53
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.08	0.53
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.08	0.53
14:N:107:LYS:CG	14:N:108:GLY:H	2.21	0.53
7:G:121:GLN:O	7:G:124:THR:HB	2.07	0.53
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.09	0.53
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.09	0.53
4:R:79:SER:HB3	4:R:165:ILE:HD12	1.91	0.53
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.24	0.53
12:L:21:ILE:HD12	12:L:21:ILE:C	2.28	0.53
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.39	0.53
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.44	0.53
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.90	0.53
13:M:40:ASN:HD22	13:M:40:ASN:N	1.99	0.53
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.09	0.53
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.91	0.53
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.23	0.53
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.91	0.53
5:S:160:LEU:CD2	6:T:59:LEU:HD12	2.39	0.53
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.43	0.53
13:1:12:VAL:HG21	13:1:102:ALA:HB1	1.91	0.53
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.91	0.53
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.91	0.53
10:X:146:MET:HE3	10:X:150:GLU:HB3	1.91	0.53
14:N:107:LYS:HG2	14:N:108:GLY:N	2.23	0.52
1:A:150:GLN:O	1:A:157:TYR:HA	2.09	0.52
4:R:85:ALA:O	4:R:89:ILE:HG12	2.09	0.52
10:J:168:MET:HE2	10:X:168:MET:HE2	1.91	0.52
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.92	0.52
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.09	0.52
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.38	0.52
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.90	0.52
9:W:6:MET:HE3	9:W:155:ILE:HD12	1.92	0.52
12:Z:99:THR:HG23	17:Z:231:HOH:O	2.09	0.52
5:E:41:ARG:NH1	5:E:42:SER:O	2.42	0.52
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.90	0.52
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.91	0.52
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.44	0.52
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.60	0.52
7:U:96:ALA:HA	7:U:107:MET:CE	2.23	0.52
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.25	0.52
1:O:150:GLN:O	1:O:157:TYR:HA	2.10	0.52
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.09	0.52
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.24	0.52
9:I:6:MET:CE	9:I:155:ILE:HA	2.40	0.52
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.42	0.52
5:S:69:LYS:HB3	17:S:528:HOH:O	2.09	0.52
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.74	0.52
14:2:176:VAL:HG12	14:2:178:LEU:CD1	2.39	0.52
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.25	0.52
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.74	0.52
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.40	0.52
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.44	0.52
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.91	0.52
9:I:6:MET:HE3	9:I:155:ILE:HA	1.91	0.52
11:K:73:ARG:NH2	11:K:104:TYR:O	2.43	0.52
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.09	0.52
5:S:77:SER:OG	5:S:137:LEU:HB2	2.10	0.52
13:M:57:ARG:HH11	13:M:57:ARG:HG2	1.75	0.52
2:P:163:ILE:HG13	2:P:164:SER:N	2.25	0.52
4:D:175:GLU:HB3	4:D:196:ILE:HD13	1.92	0.52
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.25	0.52
4:R:175:GLU:HB3	4:R:196:ILE:HD13	1.92	0.52
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.92	0.52
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.92	0.52
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.92	0.52
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.75	0.52
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.93	0.51
3:Q:33:ARG:HH11	3:Q:33:ARG:HB2	1.75	0.51
9:W:143:GLU:CG	9:W:146:LEU:HD21	2.39	0.51
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.40	0.51
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.25	0.51
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.93	0.51
2:B:78:VAL:HG22	2:B:136:PHE:CE2	2.45	0.51
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.44	0.51
7:G:151:THR:HG22	7:G:157:TYR:CB	2.40	0.51
2:B:231:ASP:O	2:B:235:LYS:HG2	2.10	0.51
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:VAL:O	3:C:194:VAL:HG23	2.10	0.51
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.75	0.51
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.26	0.51
1:A:117:ALA:HB1	1:A:155:GLY:O	2.10	0.51
14:N:186:ARG:HD3	17:N:933:HOH:O	2.10	0.51
11:K:86:LEU:HD13	11:K:86:LEU:C	2.31	0.51
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.45	0.51
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.93	0.51
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.73	0.51
8:H:172:ASN:ND2	8:H:193:THR:HG22	2.26	0.51
11:K:104:TYR:HE1	11:K:180:GLU:OE2	1.93	0.51
7:U:77:VAL:HG12	7:U:137:THR:HB	1.91	0.51
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.93	0.51
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.10	0.51
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.51
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.92	0.51
3:C:66:LYS:HE2	3:C:78:PHE:CZ	2.46	0.51
13:M:35:ILE:HG12	13:M:56:GLU:HG2	1.92	0.51
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.76	0.51
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.75	0.51
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.26	0.51
8:H:116:HIS:HB2	17:H:324:HOH:O	2.11	0.51
10:J:133:TYR:CE2	10:J:166:MET:SD	3.04	0.51
7:G:77:VAL:HG12	7:G:137:THR:HB	1.93	0.51
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.46	0.51
10:J:-1:MET:CG	10:J:1:ASP:H	2.21	0.51
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.09	0.51
1:O:48:ILE:HD11	1:O:213:ALA:HB3	1.92	0.51
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.74	0.51
4:D:24:VAL:O	4:D:27:SER:HB3	2.11	0.51
7:U:87:ASN:HD22	7:U:87:ASN:C	2.14	0.51
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.08	0.51
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.21	0.51
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.26	0.51
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.76	0.51
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.10	0.51
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.92	0.51
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.93	0.51
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.11	0.51
5:S:54:ASN:ND2	5:S:56:ASP:O	2.40	0.51
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.26	0.51
1:A:97:HIS:CD2	8:H:61:SER:OG	2.61	0.51
10:X:2:ILE:HD13	10:X:170:PHE:CD2	2.46	0.51
3:C:169:SER:HA	3:C:172:VAL:CG1	2.41	0.51
8:V:128:GLY:O	8:V:131:SER:HB2	2.11	0.51
3:Q:66:LYS:HE2	3:Q:78:PHE:CZ	2.46	0.51
8:V:34:LEU:HB2	17:V:578:HOH:O	2.10	0.51
1:A:69:LEU:HD23	1:A:69:LEU:C	2.31	0.51
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.11	0.50
9:W:6:MET:CE	9:W:155:ILE:HA	2.40	0.50
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.93	0.50
11:K:7:ARG:HH11	11:K:108:PRO:HB2	1.76	0.50
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.41	0.50
3:C:168:ASN:O	3:C:172:VAL:HG12	2.11	0.50
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.11	0.50
2:B:27:ALA:O	2:B:31:ILE:HG12	2.11	0.50
13:1:57:ARG:HH11	13:1:57:ARG:HG2	1.76	0.50
7:U:228:ASN:HB3	17:U:242:HOH:O	2.10	0.50
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.41	0.50
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.75	0.50
3:C:112:LEU:HD13	3:C:112:LEU:O	2.11	0.50
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.42	0.50
4:D:85:ALA:O	4:D:89:ILE:HG12	2.12	0.50
6:F:127:ASN:HD22	6:F:127:ASN:C	2.14	0.50
7:U:35:ILE:HD11	17:U:1201:HOH:O	2.12	0.50
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.12	0.50
7:G:67:ILE:HD13	7:G:211:GLU:HG2	1.93	0.50
8:H:128:GLY:O	8:H:131:SER:HB2	2.10	0.50
1:O:117:ALA:HB1	1:O:155:GLY:O	2.11	0.50
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.47	0.50
13:1:146:THR:HA	17:1:323:HOH:O	2.12	0.50
3:C:175:PHE:O	3:C:179:ASN:HB2	2.12	0.50
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.76	0.50
3:C:158:SER:CB	4:D:59:LEU:HD21	2.41	0.50
10:X:6:ILE:HD11	10:X:154:LEU:HD23	1.94	0.50
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.12	0.50
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.42	0.50
5:E:18(D):ILE:O	5:E:18(D):ILE:HG12	2.10	0.50
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.75	0.50
4:R:170:GLU:OE1	4:R:170:GLU:N	2.44	0.50
7:U:83:PRO:HG2	17:U:557:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:9:LYS:HD3	9:W:145:ASN:HD22	1.77	0.50
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.93	0.50
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.42	0.50
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.93	0.50
2:P:27:ALA:O	2:P:31:ILE:HG12	2.11	0.50
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.32	0.50
7:G:228:ASN:HD22	7:G:228:ASN:N	2.10	0.50
9:W:48:LEU:HG	9:W:50:THR:HG22	1.93	0.50
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.93	0.50
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.47	0.50
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.47	0.50
10:J:6:ILE:HD11	10:J:154:LEU:HD23	1.94	0.50
5:E:160:LEU:CD2	6:F:59:LEU:HD12	2.42	0.50
12:L:113:PHE:CD1	12:L:113:PHE:N	2.80	0.50
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.46	0.50
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.76	0.50
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.94	0.50
5:S:134:VAL:O	5:S:153:PRO:HG3	2.11	0.50
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.10	0.50
12:L:-2:ASN:HA	12:L:21:ILE:O	2.12	0.50
5:E:139:ILE:HD12	5:E:215:VAL:HG12	1.93	0.50
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.94	0.50
3:Q:182:PRO:O	3:Q:184:ALA:N	2.45	0.50
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.93	0.50
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.47	0.50
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.39	0.50
6:F:35:THR:CG2	6:F:51:GLU:O	2.57	0.49
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.47	0.49
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.12	0.49
11:K:6:PHE:HA	11:K:123:ASP:O	2.12	0.49
3:C:185:THR:HG22	3:C:186:VAL:N	2.26	0.49
10:X:133:TYR:CE2	10:X:166:MET:SD	3.05	0.49
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.93	0.49
9:I:143:GLU:CG	9:I:146:LEU:HD21	2.41	0.49
6:T:127:ASN:HD22	6:T:127:ASN:C	2.14	0.49
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.42	0.49
14:N:105:ASP:HB2	17:N:775:HOH:O	2.12	0.49
1:O:69:LEU:HD23	1:O:69:LEU:C	2.32	0.49
14:N:147:SER:OG	14:N:150:GLU:HG3	2.12	0.49
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.93	0.49
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:160:LEU:HD23	6:T:59:LEU:HA	1.93	0.49
9:W:150:ASP:HA	17:W:1181:HOH:O	2.11	0.49
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.27	0.49
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.77	0.49
1:A:48:ILE:HD11	1:A:213:ALA:HB3	1.94	0.49
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.47	0.49
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.94	0.49
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.06	0.49
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.93	0.49
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.94	0.49
5:E:4:PHE:CG	5:E:5:ARG:N	2.80	0.49
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.94	0.49
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.28	0.49
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.42	0.49
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.13	0.49
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.93	0.49
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.28	0.49
8:V:175:VAL:HG12	8:V:176:CYS:N	2.27	0.49
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.60	0.49
10:X:-1:MET:CG	10:X:1:ASP:H	2.22	0.49
8:V:172:ASN:HB3	8:V:192:LEU:O	2.13	0.49
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.42	0.49
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.48	0.49
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.27	0.49
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.27	0.49
7:U:151:THR:HG22	7:U:157:TYR:CB	2.42	0.49
3:C:197:LEU:O	3:C:201:VAL:HG23	2.12	0.49
4:R:24:VAL:O	4:R:27:SER:HB3	2.13	0.49
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.93	0.49
5:E:77:SER:OG	5:E:137:LEU:HB2	2.11	0.49
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.94	0.49
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.21	0.49
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.61	0.49
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.93	0.49
6:T:18:ASP:N	6:T:18:ASP:OD2	2.39	0.49
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.78	0.49
11:Y:104:TYR:HE1	11:Y:180:GLU:OE2	1.94	0.49
2:B:163:ILE:HG13	2:B:164:SER:N	2.27	0.49
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.48	0.49
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.48	0.49
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:134:ILE:HD11	12:L:162:ALA:HB2	1.95	0.49
4:R:207:LEU:HD23	4:R:207:LEU:C	2.33	0.49
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.48	0.49
8:H:172:ASN:HB3	8:H:192:LEU:O	2.13	0.49
11:K:31:VAL:HG11	15:3:5:ABN:H3	1.95	0.49
13:1:35:ILE:HD12	13:1:35:ILE:N	2.28	0.49
13:M:35:ILE:N	13:M:35:ILE:HD12	2.28	0.49
9:I:114:ASP:HB2	17:I:851:HOH:O	2.13	0.49
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.42	0.49
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.13	0.49
11:Y:7:ARG:HH11	11:Y:108:PRO:HB2	1.77	0.49
13:1:104:VAL:CG2	13:1:178:ILE:HG22	2.40	0.48
5:S:123:ASN:ND2	5:S:123:ASN:N	2.61	0.48
13:1:113:VAL:HA	13:1:118:VAL:O	2.13	0.48
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.43	0.48
7:G:87:ASN:C	7:G:87:ASN:HD22	2.16	0.48
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.13	0.48
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.72	0.48
3:Q:57:LYS:NZ	17:Q:434:HOH:O	2.45	0.48
13:1:40:ASN:N	13:1:40:ASN:HD22	2.01	0.48
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.77	0.48
7:U:67:ILE:HD13	7:U:211:GLU:HG2	1.95	0.48
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.48	0.48
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.12	0.48
3:C:182:PRO:O	3:C:184:ALA:N	2.46	0.48
6:F:18:ASP:N	6:F:18:ASP:OD2	2.39	0.48
10:J:168:MET:CE	10:X:168:MET:HE3	2.41	0.48
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.49	0.48
7:U:225:SER:OG	7:U:228:ASN:ND2	2.46	0.48
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.95	0.48
10:J:2:ILE:HD13	10:J:170:PHE:CD2	2.48	0.48
9:I:9:LYS:HD3	9:I:145:ASN:HD22	1.78	0.48
11:K:44:THR:OG1	11:K:100:MET:HB2	2.13	0.48
8:H:196:VAL:HG23	17:H:520:HOH:O	2.14	0.48
12:Z:59:PHE:O	12:Z:62:SER:HB3	2.14	0.48
13:M:40:ASN:ND2	13:M:40:ASN:N	2.62	0.48
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.96	0.48
10:J:156:LYS:HE2	10:J:160:GLN:NE2	2.28	0.48
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.48	0.48
2:P:67:LEU:HD23	2:P:213:ALA:HB2	1.95	0.48
4:D:207:LEU:HD23	4:D:207:LEU:C	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:147:SER:OG	14:2:150:GLU:HG3	2.13	0.48
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.12	0.48
7:U:109:CYS:HB3	17:U:1330:HOH:O	2.14	0.48
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.94	0.48
3:Q:112:LEU:HD13	3:Q:112:LEU:O	2.14	0.48
6:T:35:THR:CG2	6:T:51:GLU:O	2.58	0.48
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.10	0.48
5:E:160:LEU:HD23	6:F:59:LEU:HA	1.94	0.48
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.95	0.48
13:M:113:VAL:HA	13:M:118:VAL:O	2.14	0.48
7:U:49:ILE:CD1	7:U:212:VAL:HG22	2.44	0.48
4:D:170:GLU:N	4:D:170:GLU:OE1	2.44	0.48
2:B:15:PHE:N	3:C:23:GLN:HE22	1.91	0.48
12:Z:146:LEU:HA	17:Z:757:HOH:O	2.13	0.48
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.62	0.48
6:F:173:LYS:O	6:F:177:GLU:HG3	2.14	0.48
5:S:4:PHE:CG	5:S:5:ARG:N	2.81	0.48
8:H:200:LYS:HE3	9:I:140:SER:O	2.14	0.48
13:1:104:VAL:HG23	13:1:178:ILE:CG2	2.42	0.47
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.15	0.47
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.13	0.47
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.14	0.47
7:U:107:MET:CE	7:U:112:LEU:HD13	2.44	0.47
5:S:201:LEU:O	5:S:202:ARG:HB2	2.15	0.47
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.27	0.47
7:G:225:SER:OG	7:G:228:ASN:ND2	2.47	0.47
8:H:126:SER:O	8:H:127:LEU:HD23	2.14	0.47
12:L:177:ILE:HD12	12:L:177:ILE:N	2.29	0.47
5:E:167:ALA:HB3	17:E:1131:HOH:O	2.13	0.47
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.49	0.47
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.02	0.47
10:J:168:MET:HG2	10:X:168:MET:CE	2.45	0.47
13:1:40:ASN:ND2	13:1:40:ASN:H	2.11	0.47
1:O:97:HIS:CD2	8:V:61:SER:OG	2.64	0.47
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.44	0.47
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.49	0.47
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.49	0.47
12:L:59:PHE:O	12:L:62:SER:HB3	2.14	0.47
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.96	0.47
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.95	0.47
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:134:VAL:O	5:E:153:PRO:HG3	2.14	0.47
10:J:36:GLN:HG3	10:J:184:ILE:HD12	1.96	0.47
7:G:158:VAL:HG22	7:G:159:GLY:N	2.30	0.47
7:G:82:ILE:N	7:G:83:PRO:HD2	2.30	0.47
5:E:179:THR:HG22	5:E:179:THR:O	2.15	0.47
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.76	0.47
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.11	0.47
1:O:26:TYR:CE1	7:U:17:PRO:HA	2.50	0.47
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.96	0.47
8:H:9:ASN:OD1	8:H:10:ASN:N	2.47	0.47
11:Y:105:THR:HB	11:Y:10(B):LYS:CD	2.45	0.47
5:S:150:GLU:O	5:S:157:VAL:HA	2.15	0.47
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.49	0.47
14:N:159:LEU:O	14:N:163:ILE:HD13	2.14	0.47
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.29	0.47
5:S:179:THR:O	5:S:179:THR:HG22	2.14	0.47
11:K:209:VAL:HG13	17:W:348:HOH:O	2.14	0.47
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.76	0.47
12:L:96:TYR:CE1	15:3:2:TY5:H49	2.49	0.47
12:Z:96:TYR:CE1	15:4:2:TY5:H49	2.50	0.47
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.14	0.47
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.15	0.47
6:T:127:ASN:HD22	6:T:128:SER:N	2.13	0.47
7:U:74:ILE:HD12	7:U:109:CYS:HA	1.96	0.47
10:X:76:PRO:HD2	17:X:275:HOH:O	2.15	0.47
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.79	0.47
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.15	0.47
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.41	0.47
5:E:12:THR:CG2	5:E:124:THR:HA	2.42	0.47
2:B:71:ASN:HD22	2:B:72:ASP:N	2.10	0.47
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.43	0.47
8:V:152:ILE:HD11	8:V:177:VAL:CG2	2.45	0.47
7:U:82:ILE:N	7:U:83:PRO:HD2	2.30	0.47
9:W:101:VAL:O	9:W:110:ILE:HA	2.14	0.47
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.44	0.47
13:M:83:LEU:O	13:M:87:MET:HG2	2.15	0.47
9:W:155:ILE:HG23	9:W:156:SER:N	2.30	0.47
5:E:123:ASN:ND2	5:E:123:ASN:N	2.62	0.47
11:Y:104:TYR:CD1	11:Y:180:GLU:HG3	2.49	0.47
12:L:90:LYS:HE3	12:L:93:PHE:O	2.14	0.47
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:VAL:O	9:I:110:ILE:HA	2.15	0.47
13:1:112:TYR:O	13:1:119:THR:HA	2.15	0.47
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.28	0.47
2:B:31:ILE:HD11	2:B:133:GLY:C	2.35	0.47
5:E:54:ASN:ND2	5:E:56:ASP:O	2.39	0.47
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.16	0.47
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.97	0.47
14:N:14:LEU:O	14:N:175:MET:HA	2.15	0.46
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.45	0.46
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.50	0.46
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.96	0.46
5:E:150:GLU:O	5:E:157:VAL:HA	2.14	0.46
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.97	0.46
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.97	0.46
14:2:107:LYS:CG	14:2:108:GLY:H	2.21	0.46
6:F:127:ASN:HD22	6:F:128:SER:N	2.13	0.46
2:P:31:ILE:HD11	2:P:133:GLY:C	2.35	0.46
12:Z:134:ILE:HD11	12:Z:162:ALA:HB2	1.97	0.46
12:Z:134:ILE:HD13	12:Z:158:SER:HB3	1.97	0.46
13:M:1:THR:HG22	17:M:214:HOH:O	2.16	0.46
14:2:159:LEU:O	14:2:163:ILE:HD13	2.14	0.46
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.97	0.46
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.46	0.46
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.44	0.46
8:V:196:VAL:HG23	17:V:652:HOH:O	2.15	0.46
7:G:74:ILE:HD12	7:G:109:CYS:HA	1.96	0.46
7:G:49:ILE:CD1	7:G:212:VAL:HG22	2.46	0.46
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.56	0.46
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.97	0.46
10:X:13:ILE:N	10:X:13:ILE:HD12	2.30	0.46
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.78	0.46
11:Y:135:TYR:CB	17:Y:593:HOH:O	2.63	0.46
6:T:192:GLN:NE2	6:T:195:LYS:HE2	2.30	0.46
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.51	0.46
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.97	0.46
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.45	0.46
10:X:35:ARG:NH1	10:X:57:GLU:OE2	2.44	0.46
6:F:103:TYR:O	6:F:104:LYS:HB3	2.16	0.46
9:I:14:ILE:HG12	9:I:34:ILE:HD12	1.98	0.46
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.45	0.46
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.51	0.46
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.31	0.46
10:X:34:THR:CG2	10:X:176:LYS:NZ	2.78	0.46
13:1:19:LEU:HD12	13:1:28:PHE:O	2.15	0.46
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.45	0.46
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.51	0.46
6:T:101:LYS:HE2	13:1:57:ARG:NH2	2.30	0.46
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.81	0.46
7:U:158:VAL:HG22	7:U:159:GLY:N	2.31	0.46
6:F:192:GLN:NE2	6:F:195:LYS:HE2	2.31	0.46
10:X:156:LYS:HE2	10:X:160:GLN:NE2	2.31	0.46
10:J:2:ILE:HD13	10:J:170:PHE:CG	2.50	0.46
10:X:113:ILE:HA	10:X:118:THR:O	2.16	0.46
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.46	0.46
8:V:126:SER:O	8:V:127:LEU:HD23	2.15	0.46
7:G:89:ALA:O	7:G:93:LYS:HG3	2.16	0.46
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.51	0.46
3:C:173:ARG:O	3:C:177:GLU:HG3	2.15	0.46
14:2:146:MET:HE1	17:2:774:HOH:O	2.14	0.46
2:B:71:ASN:ND2	2:B:72:ASP:N	2.61	0.46
7:U:203:THR:HG22	7:U:204:GLU:O	2.16	0.46
13:M:19:LEU:HD12	13:M:28:PHE:O	2.15	0.46
11:Y:31:VAL:HG11	15:4:5:ABN:H3	1.97	0.46
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.13	0.46
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.97	0.46
6:F:143:LYS:HB2	17:F:469:HOH:O	2.15	0.46
5:E:231:LYS:H	5:E:231:LYS:HD2	1.81	0.46
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.81	0.46
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.79	0.46
5:E:76:LEU:O	5:E:76:LEU:HD23	2.16	0.46
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.16	0.46
2:P:24:VAL:HG11	2:P:154:SER:HB3	1.98	0.46
10:J:168:MET:CE	10:X:168:MET:HG2	2.46	0.46
7:G:8:TYR:C	7:G:10:ARG:N	2.70	0.46
7:U:228:ASN:HD22	7:U:228:ASN:N	2.12	0.46
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.51	0.46
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.51	0.46
1:O:233:LEU:O	1:O:236:LEU:HB2	2.16	0.46
6:T:173:LYS:O	6:T:177:GLU:HG3	2.16	0.46
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.51	0.46
7:U:107:MET:HE1	7:U:112:LEU:HD13	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:201:LEU:O	5:E:202:ARG:HB2	2.15	0.45
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.51	0.45
1:O:110:LYS:HG2	17:O:376:HOH:O	2.16	0.45
1:A:233:LEU:O	1:A:236:LEU:HB2	2.16	0.45
3:C:97:GLN:NE2	17:C:255:HOH:O	2.47	0.45
13:M:104:VAL:HG23	13:M:178:ILE:CG2	2.43	0.45
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.97	0.45
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.27	0.45
3:C:159:SER:O	4:D:59:LEU:HD22	2.16	0.45
6:T:54:ILE:HG12	6:T:208:PHE:CA	2.46	0.45
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.98	0.45
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.79	0.45
7:U:87:ASN:ND2	7:U:87:ASN:C	2.68	0.45
6:F:214:TRP:CH2	6:F:21(A):GLU:HB3	2.50	0.45
2:B:24:VAL:HG11	2:B:154:SER:HB3	1.97	0.45
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.32	0.45
5:S:231:LYS:HD2	5:S:231:LYS:H	1.80	0.45
13:M:184:LEU:HD23	13:M:184:LEU:C	2.37	0.45
11:K:105:THR:HB	11:K:10(B):LYS:CD	2.45	0.45
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.82	0.45
2:P:71:ASN:ND2	2:P:72:ASP:N	2.63	0.45
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.51	0.45
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.98	0.45
2:P:186:VAL:O	2:P:190:ILE:HG13	2.16	0.45
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.51	0.45
8:V:3:ILE:HG13	8:V:100:ILE:HD12	1.99	0.45
5:E:38:VAL:HG12	5:E:39:GLY:N	2.32	0.45
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.52	0.45
14:2:116:GLY:HA3	17:2:192:HOH:O	2.16	0.45
5:S:38:VAL:HG12	5:S:39:GLY:N	2.31	0.45
14:2:85:GLU:O	14:2:89:GLU:HB2	2.17	0.45
4:D:237:LEU:O	4:D:241:GLU:HG3	2.16	0.45
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.37	0.45
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.98	0.45
9:I:113:PHE:HA	9:I:118:CYS:O	2.17	0.45
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.47	0.45
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.81	0.45
12:Z:160:THR:O	12:Z:164:GLU:HG2	2.17	0.45
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.98	0.45
9:I:155:ILE:HG23	9:I:156:SER:N	2.32	0.45
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:52:THR:CG2	10:X:53:VAL:H	2.30	0.45
1:O:161:LYS:N	2:P:58:LEU:O	2.45	0.45
12:L:134:ILE:HD13	12:L:158:SER:HB3	1.99	0.45
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.82	0.45
13:1:184:LEU:C	13:1:184:LEU:HD23	2.37	0.45
2:B:67:LEU:HD23	2:B:213:ALA:HB2	1.99	0.45
5:S:40:LEU:HD23	5:S:40:LEU:N	2.32	0.45
10:J:13:ILE:N	10:J:13:ILE:HD12	2.31	0.45
5:S:180:LEU:O	5:S:18(D):ILE:HG22	2.17	0.45
5:E:180:LEU:O	5:E:18(D):ILE:HG22	2.17	0.45
2:P:71:ASN:HD22	2:P:72:ASP:N	2.12	0.45
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.32	0.45
11:K:104:TYR:CD1	11:K:180:GLU:HG3	2.51	0.45
10:X:85:GLN:HB3	17:X:463:HOH:O	2.17	0.45
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.81	0.45
13:1:150:VAL:HG21	17:1:323:HOH:O	2.16	0.45
4:D:42:THR:C	4:D:44:GLU:H	2.19	0.45
10:J:35:ARG:NH1	10:J:57:GLU:OE2	2.43	0.45
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.51	0.45
8:V:9:ASN:ND2	8:V:147:THR:HA	2.32	0.45
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.45
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.97	0.45
6:F:69:VAL:HG12	17:F:319:HOH:O	2.16	0.45
13:M:9:ASP:OD1	13:M:10:ASN:N	2.50	0.45
6:T:103:TYR:O	6:T:104:LYS:HB3	2.16	0.45
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.11	0.45
4:R:160:TYR:HA	5:S:59:SER:HA	1.98	0.45
8:H:152:ILE:HD11	8:H:177:VAL:CG2	2.47	0.45
10:J:52:THR:CG2	10:J:53:VAL:H	2.29	0.45
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.31	0.45
9:W:33:LYS:O	9:W:44:GLY:HA2	2.16	0.45
5:S:52:LYS:O	5:S:63:TYR:HD2	2.00	0.45
4:R:42:THR:C	4:R:44:GLU:H	2.20	0.45
13:M:112:TYR:O	13:M:119:THR:HA	2.17	0.45
7:G:192:PHE:CD1	7:G:192:PHE:C	2.89	0.45
9:I:29:ASN:ND2	11:Y:208:ASN:HD22	1.92	0.45
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.98	0.45
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.99	0.45
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.98	0.45
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.17	0.45
2:P:223:ILE:HD12	2:P:223:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:237:LEU:O	4:R:241:GLU:HG3	2.17	0.45
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.52	0.45
6:F:83:PRO:HB2	17:F:1240:HOH:O	2.17	0.45
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.51	0.45
2:P:234:VAL:HA	2:P:239:THR:HA	1.98	0.45
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.99	0.45
6:F:12:ASN:ND2	6:F:131:PRO:HD3	2.32	0.45
5:E:40:LEU:HD23	5:E:40:LEU:N	2.32	0.45
10:J:129:TYR:HB3	10:X:24:ILE:HD11	1.98	0.45
11:K:208:ASN:HD22	9:W:29:ASN:ND2	1.92	0.45
5:S:12:THR:CG2	5:S:124:THR:HA	2.42	0.45
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.98	0.45
10:X:36:GLN:HG3	10:X:184:ILE:HD12	1.99	0.45
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.81	0.45
6:T:214:TRP:CH2	6:T:21(A):GLU:HB3	2.51	0.45
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.82	0.45
10:X:190:PHE:C	10:X:192:ALA:H	2.20	0.45
11:K:5:ALA:HA	11:K:13:ILE:O	2.16	0.45
7:U:192:PHE:CD1	7:U:192:PHE:C	2.89	0.45
7:G:67:ILE:HD13	7:G:211:GLU:CG	2.47	0.44
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.99	0.44
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.99	0.44
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.98	0.44
4:R:65:GLU:HA	17:R:750:HOH:O	2.17	0.44
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.82	0.44
10:X:135:PHE:CZ	17:X:622:HOH:O	2.57	0.44
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.53	0.44
1:O:4:MET:CG	1:O:5:THR:H	2.29	0.44
14:2:14:LEU:O	14:2:175:MET:HA	2.16	0.44
7:U:8:TYR:C	7:U:10:ARG:N	2.69	0.44
8:V:200:LYS:HE3	9:W:140:SER:O	2.17	0.44
12:Z:22:THR:O	12:Z:23:ASP:HB2	2.16	0.44
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.97	0.44
3:C:55:THR:C	3:C:56:LEU:HD22	2.38	0.44
8:H:9:ASN:ND2	8:H:147:THR:HA	2.33	0.44
2:B:229:ILE:O	2:B:233:LEU:HB2	2.17	0.44
2:B:234:VAL:HA	2:B:239:THR:HA	1.98	0.44
7:U:136:LEU:O	7:U:150:LYS:HA	2.17	0.44
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.53	0.44
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.82	0.44
4:D:12(F):GLY:HA3	17:E:965:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:190:PHE:C	10:J:192:ALA:H	2.20	0.44
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.53	0.44
12:L:5:GLY:O	12:L:124:CYS:HA	2.17	0.44
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.37	0.44
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.56	0.44
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.17	0.44
8:V:152:ILE:CD1	8:V:177:VAL:HG22	2.48	0.44
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.48	0.44
14:N:20:THR:HG23	14:N:31:THR:OG1	2.18	0.44
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.32	0.44
9:W:14:ILE:HG12	9:W:34:ILE:HD12	1.99	0.44
13:1:83:LEU:O	13:1:87:MET:HG2	2.17	0.44
14:2:15:GLY:HA2	14:2:174:ARG:O	2.17	0.44
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.52	0.44
7:G:136:LEU:O	7:G:150:LYS:HA	2.17	0.44
7:G:87:ASN:ND2	7:G:87:ASN:C	2.71	0.44
6:F:202:HIS:O	6:F:202:HIS:CG	2.71	0.44
13:1:40:ASN:N	13:1:40:ASN:ND2	2.64	0.44
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.47	0.44
8:V:9:ASN:OD1	8:V:10:ASN:N	2.50	0.44
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.17	0.44
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.98	0.44
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.18	0.44
5:E:90:ASN:O	5:E:94:GLN:HG3	2.18	0.44
5:S:194:VAL:HG13	5:S:207:LEU:CD1	2.48	0.44
6:F:54:ILE:HG12	6:F:208:PHE:CA	2.48	0.44
5:S:76:LEU:O	5:S:76:LEU:HD23	2.17	0.44
2:P:229:ILE:O	2:P:233:LEU:HB2	2.17	0.44
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.00	0.44
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	1.99	0.44
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.99	0.44
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.11	0.44
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.33	0.44
13:1:9:ASP:OD1	13:1:10:ASN:N	2.51	0.44
12:L:140:ASN:O	12:L:144:PHE:HA	2.18	0.44
2:B:41:MET:HE3	17:B:253:HOH:O	2.18	0.44
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.99	0.43
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.53	0.43
1:A:21(P):LYS:N	17:A:1147:HOH:O	2.37	0.43
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.99	0.43
6:T:35:THR:CG2	6:T:36:THR:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:18(C):PHE:CD1	5:S:18(D):ILE:N	2.86	0.43
8:V:152:ILE:HD11	8:V:177:VAL:HG22	2.00	0.43
2:B:160:TRP:CE2	2:B:163:ILE:HD13	2.53	0.43
9:I:49:ALA:HB3	10:J:118:THR:HG23	1.99	0.43
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.53	0.43
10:X:38:SER:HB2	10:X:39:PRO:HD2	2.01	0.43
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.48	0.43
12:L:-9:GLN:HG2	13:M:-8:THR:HG21	2.00	0.43
2:P:224:PHE:N	2:P:224:PHE:CD2	2.86	0.43
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.18	0.43
13:M:40:ASN:ND2	13:M:40:ASN:H	2.10	0.43
11:K:67:GLU:HG2	11:K:73:ARG:HA	1.99	0.43
2:P:6:ARG:HB2	5:S:127:TYR:OH	2.18	0.43
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.43
6:T:147:HIS:HD2	17:T:282:HOH:O	2.01	0.43
12:Z:-9:GLN:HG2	13:1:-8:THR:HG21	2.00	0.43
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.98	0.43
3:C:120:GLN:O	3:C:124:THR:HG23	2.18	0.43
12:L:1:GLY:HA3	12:L:33:LYS:HZ2	1.83	0.43
3:Q:18(A):ASP:OD1	3:Q:18(C):LYS:HB2	2.19	0.43
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.17	0.43
2:B:116:LEU:HD23	2:B:116:LEU:HA	1.88	0.43
7:G:107:MET:CE	7:G:112:LEU:HD13	2.48	0.43
5:E:18(C):PHE:CD1	5:E:18(D):ILE:N	2.86	0.43
5:E:214:ILE:HG12	5:E:215:VAL:N	2.34	0.43
3:C:76:LEU:HD23	3:C:76:LEU:C	2.39	0.43
7:G:203:THR:HG22	7:G:204:GLU:O	2.18	0.43
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.17	0.43
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.40	0.43
3:C:167:ARG:O	3:C:168:ASN:HB2	2.17	0.43
11:Y:67:GLU:HG2	11:Y:73:ARG:HA	2.00	0.43
7:U:67:ILE:HD13	7:U:211:GLU:CG	2.48	0.43
12:Z:148:VAL:O	12:Z:152:ILE:HG12	2.18	0.43
6:T:12:ASN:ND2	6:T:131:PRO:HD3	2.33	0.43
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.00	0.43
6:T:202:HIS:CG	6:T:202:HIS:O	2.72	0.43
5:E:194:VAL:HG13	5:E:207:LEU:CD1	2.48	0.43
7:G:188:LYS:HA	7:G:188:LYS:HD3	1.84	0.43
9:W:113:PHE:HA	9:W:118:CYS:O	2.17	0.43
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.48	0.43
12:L:22:THR:O	12:L:23:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:137:MET:HE3	9:I:141:LEU:HD11	2.00	0.43
2:P:38:ILE:HD12	2:P:197:LEU:HG	2.00	0.43
7:G:171:GLU:OE1	7:G:171:GLU:N	2.49	0.43
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.82	0.43
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.84	0.43
2:B:160:TRP:HA	3:C:59:GLN:HA	2.00	0.43
5:S:214:ILE:HG12	5:S:215:VAL:N	2.34	0.43
5:S:190:ILE:HG23	5:S:212:ILE:HD13	2.00	0.43
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.00	0.43
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.82	0.43
5:S:90:ASN:O	5:S:94:GLN:HG3	2.18	0.43
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.54	0.43
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.56	0.43
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.00	0.43
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.19	0.43
11:K:4:LEU:HD13	11:K:159:ILE:HD11	2.01	0.43
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.00	0.43
12:L:148:VAL:O	12:L:152:ILE:HG12	2.18	0.43
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	2.01	0.43
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.01	0.43
3:C:38:VAL:HG22	3:C:39:GLY:N	2.33	0.43
3:C:185:THR:CG2	3:C:186:VAL:N	2.81	0.43
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.19	0.43
12:L:114:ASP:O	12:L:115:PRO:C	2.57	0.43
13:M:14(A):VAL:O	13:M:14(A):VAL:CG2	2.62	0.43
10:J:113:ILE:HA	10:J:118:THR:O	2.19	0.43
2:P:194:LEU:O	2:P:198:SER:HB2	2.18	0.43
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.34	0.43
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	2.00	0.43
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.33	0.43
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.84	0.43
7:U:171:GLU:N	7:U:171:GLU:OE1	2.49	0.43
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.45	0.43
9:W:104:ILE:HG21	9:W:181:LYS:HG2	2.00	0.43
9:I:104:ILE:HG21	9:I:181:LYS:HG2	2.00	0.43
9:W:55:LEU:HA	9:W:55:LEU:HD23	1.91	0.43
4:D:37:ALA:HB3	4:D:165:ILE:HG13	2.00	0.43
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.00	0.43
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.49	0.43
12:L:160:THR:O	12:L:164:GLU:HG2	2.18	0.43
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:212:ILE:HG22	6:F:213:SER:N	2.34	0.43
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.33	0.43
3:Q:76:LEU:HD23	3:Q:76:LEU:C	2.39	0.43
2:P:122:GLY:C	2:P:124:THR:H	2.22	0.42
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.34	0.42
12:L:93:PHE:N	12:L:94:PRO:HD3	2.33	0.42
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.01	0.42
7:U:109:CYS:HB2	7:U:140:SER:OG	2.18	0.42
5:E:76:LEU:C	5:E:76:LEU:HD23	2.39	0.42
11:K:16:VAL:HG21	11:K:34:VAL:HG23	2.01	0.42
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.54	0.42
13:1:-3:VAL:HA	13:1:21:SER:O	2.19	0.42
2:B:21:LEU:HD13	2:B:124:THR:HG23	2.00	0.42
3:Q:159:SER:O	4:R:59:LEU:HD22	2.19	0.42
4:D:122:ARG:NH1	4:D:122:ARG:HG2	2.33	0.42
13:1:57:ARG:NH1	13:1:57:ARG:HG2	2.34	0.42
12:Z:109:ALA:HA	17:Z:375:HOH:O	2.18	0.42
6:T:212:ILE:HG22	6:T:213:SER:N	2.34	0.42
12:Z:151:VAL:O	12:Z:155:VAL:HG23	2.19	0.42
2:P:113:VAL:HG22	2:P:138:TYR:CG	2.54	0.42
3:Q:120:GLN:O	3:Q:124:THR:HG23	2.19	0.42
11:K:78:ALA:O	11:K:82:ILE:HG12	2.19	0.42
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.02	0.42
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.19	0.42
10:X:3:ILE:HG22	10:X:3:ILE:O	2.18	0.42
8:H:152:ILE:HD11	8:H:177:VAL:HG22	2.02	0.42
3:C:227:GLU:O	3:C:231:GLN:HG3	2.19	0.42
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.49	0.42
4:R:37:ALA:HB3	4:R:165:ILE:HG13	2.01	0.42
8:V:128:GLY:O	8:V:131:SER:CB	2.68	0.42
1:O:210:ILE:N	1:O:210:ILE:HD12	2.34	0.42
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.42
1:A:62:GLU:H	1:A:62:GLU:CD	2.23	0.42
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.84	0.42
2:B:141:TYR:C	2:B:141:TYR:CD1	2.93	0.42
3:Q:227:GLU:O	3:Q:231:GLN:HG3	2.19	0.42
11:Y:10(A):ARG:NH1	11:Y:10(A):ARG:HG2	2.33	0.42
1:O:49:ALA:HB2	1:O:212:LEU:HG	2.02	0.42
1:A:212:LEU:HD23	1:A:212:LEU:C	2.40	0.42
12:L:33:LYS:HB3	12:L:33:LYS:HE2	1.83	0.42
1:O:159:PRO:O	2:P:59:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:LYS:O	2:B:226:PRO:C	2.58	0.42
4:D:150:HIS:O	4:D:157:PHE:HA	2.20	0.42
3:C:47:VAL:HG23	3:C:189:CYS:SG	2.60	0.42
2:B:224:PHE:CD2	2:B:224:PHE:N	2.87	0.42
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.55	0.42
3:Q:185:THR:CG2	3:Q:186:VAL:N	2.82	0.42
5:S:15:PHE:H	6:T:23:GLN:NE2	2.00	0.42
7:U:188:LYS:HA	7:U:188:LYS:HD3	1.84	0.42
1:A:5:THR:O	1:A:7:ARG:HG3	2.19	0.42
11:K:137:VAL:HG21	11:K:161:ALA:HB2	2.02	0.42
2:B:31:ILE:HD12	2:B:79:ALA:O	2.20	0.42
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.49	0.42
5:S:76:LEU:C	5:S:76:LEU:HD23	2.40	0.42
2:B:113:VAL:HG22	2:B:138:TYR:CG	2.55	0.42
14:2:3:ILE:HG22	14:2:16:ALA:HB2	2.02	0.42
10:J:120:VAL:HG13	10:J:122:LEU:HG	2.01	0.42
12:Z:33:LYS:HE2	12:Z:33:LYS:HB3	1.83	0.42
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.22	0.42
13:M:57:ARG:HG2	13:M:57:ARG:NH1	2.33	0.42
8:V:25:ILE:HD12	8:V:25:ILE:N	2.35	0.42
2:P:224:PHE:N	2:P:224:PHE:HD2	2.18	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.42
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.01	0.42
13:M:187:LYS:HB3	13:M:190:LEU:HD11	2.02	0.42
4:R:72:ARG:HG3	17:R:1302:HOH:O	2.19	0.42
2:B:121:GLN:HG3	3:C:83:ALA:HB1	2.00	0.42
2:P:141:TYR:C	2:P:141:TYR:CD1	2.92	0.42
1:O:5:THR:O	1:O:7:ARG:HG3	2.20	0.42
7:U:67:ILE:HD13	7:U:211:GLU:OE1	2.20	0.42
5:S:35:SER:HB3	5:S:66:LYS:HZ3	1.85	0.42
1:A:210:ILE:HD12	1:A:210:ILE:N	2.35	0.42
4:R:194:LEU:HA	4:R:194:LEU:HD12	1.88	0.42
7:U:49:ILE:HD13	7:U:212:VAL:HG22	2.01	0.42
2:B:7:ARG:HD2	2:B:8:TYR:CZ	2.54	0.42
6:F:120:VAL:HG21	6:F:151:LEU:HD21	2.01	0.42
9:W:159:LEU:HD21	9:W:173:ALA:HB1	2.01	0.42
1:O:62:GLU:CD	1:O:62:GLU:H	2.22	0.42
1:O:45:GLY:HA2	1:O:147:PHE:CE2	2.54	0.42
1:A:4:MET:CG	1:A:5:THR:H	2.29	0.42
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.19	0.42
10:J:143:ARG:HB2	10:J:146:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	2.01	0.42
11:K:4:LEU:C	11:K:4:LEU:HD22	2.40	0.42
14:N:85:GLU:O	14:N:89:GLU:HB2	2.19	0.42
12:Z:19:ARG:HB2	12:Z:171:ASP:OD2	2.20	0.42
2:B:38:ILE:HD12	2:B:197:LEU:HG	2.02	0.42
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.55	0.42
13:M:14(C):ARG:CG	13:M:14(C):ARG:HH11	2.29	0.42
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.54	0.42
2:B:186:VAL:O	2:B:190:ILE:HG13	2.20	0.42
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	2.02	0.42
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	2.02	0.42
13:M:147:THR:OG1	13:M:150:VAL:HG23	2.19	0.42
8:V:175:VAL:CG1	8:V:176:CYS:N	2.83	0.42
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.49	0.42
7:U:14(A):GLU:OE2	8:V:72:ARG:HD3	2.19	0.42
8:V:2:THR:O	8:V:16:ALA:HA	2.20	0.42
12:L:104:LEU:HA	12:L:107:LYS:O	2.20	0.42
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.55	0.42
8:V:162:GLY:O	8:V:166:ASP:HB3	2.19	0.42
2:B:223:ILE:N	2:B:223:ILE:HD12	2.34	0.42
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.67	0.42
10:X:-1:MET:CG	10:X:1:ASP:N	2.79	0.42
6:T:194:ALA:O	6:T:198:TYR:HD1	2.02	0.42
10:J:34:THR:CG2	10:J:176:LYS:NZ	2.81	0.42
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.55	0.42
9:I:34:ILE:HB	17:I:955:HOH:O	2.19	0.42
12:Z:5:GLY:HA2	12:Z:13:VAL:O	2.20	0.42
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.55	0.42
8:H:162:GLY:O	8:H:166:ASP:HB3	2.20	0.42
3:C:13:SER:O	4:D:130:ARG:HD3	2.20	0.42
9:I:19:ARG:HB2	9:I:171:TRP:HB2	2.02	0.42
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.20	0.42
10:J:168:MET:CE	10:X:168:MET:HE2	2.49	0.41
6:T:172:ALA:O	6:T:176:LEU:CD2	2.68	0.41
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.87	0.41
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.55	0.41
5:S:45:HIS:HB2	5:S:189:LEU:HD12	2.02	0.41
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.02	0.41
7:U:20:ARG:NH2	7:U:22:TYR:CE1	2.88	0.41
14:N:10(B):LYS:HD3	14:N:10(B):LYS:O	2.20	0.41
1:A:48:ILE:H	1:A:48:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:5:GLY:HA2	12:L:13:VAL:O	2.20	0.41
7:U:98:GLU:HG2	7:U:102:LYS:HD3	2.02	0.41
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.01	0.41
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	2.02	0.41
3:C:79:SER:OG	3:C:165:ILE:HG13	2.21	0.41
7:G:29:LYS:HA	7:G:29:LYS:HD2	1.81	0.41
7:U:35:ILE:HG23	7:U:51:GLN:HB2	2.02	0.41
8:H:128:GLY:O	8:H:131:SER:CB	2.68	0.41
5:E:45:HIS:HB2	5:E:189:LEU:HD12	2.03	0.41
12:L:76:ILE:HG23	12:L:77:ASN:N	2.35	0.41
14:N:114:PRO:HD2	14:N:118:SER:O	2.20	0.41
8:H:2:THR:O	8:H:16:ALA:HA	2.19	0.41
10:J:38:SER:HB2	10:J:39:PRO:HD2	2.02	0.41
7:U:217:LYS:O	7:U:218:ASP:HB2	2.19	0.41
1:O:130:ARG:HH21	7:U:124:THR:HG23	1.80	0.41
3:C:57:LYS:HD2	3:C:58:LEU:N	2.35	0.41
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.55	0.41
8:H:172:ASN:ND2	8:H:193:THR:HA	2.33	0.41
7:G:67:ILE:HD13	7:G:211:GLU:OE1	2.19	0.41
2:B:224:PHE:HD2	2:B:224:PHE:N	2.18	0.41
12:L:19:ARG:HB2	12:L:171:ASP:OD2	2.20	0.41
8:H:5:GLY:HA3	8:H:110:LEU:HD11	2.01	0.41
11:K:40:PHE:CD2	11:K:40:PHE:N	2.88	0.41
3:Q:194:VAL:O	3:Q:198:LEU:HG	2.20	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	2.01	0.41
8:H:152:ILE:CD1	8:H:177:VAL:HG22	2.50	0.41
3:Q:241:GLN:C	3:Q:243:GLN:N	2.73	0.41
8:H:25:ILE:N	8:H:25:ILE:HD12	2.35	0.41
3:C:201:VAL:HG21	3:C:210:ILE:HD11	2.01	0.41
7:G:131:PRO:HB3	17:G:243:HOH:O	2.19	0.41
13:M:-3:VAL:HA	13:M:21:SER:O	2.21	0.41
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.56	0.41
1:O:48:ILE:CD1	1:O:48:ILE:O	2.68	0.41
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.50	0.41
7:G:150:LYS:O	7:G:157:TYR:HA	2.20	0.41
5:E:42:SER:OG	5:E:43:ASN:N	2.54	0.41
6:T:38:ILE:HG22	6:T:164:ALA:HB2	2.02	0.41
12:L:1:GLY:N	17:L:755:HOH:O	2.51	0.41
5:E:189:LEU:HA	5:E:189:LEU:HD23	1.90	0.41
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.35	0.41
2:P:228:GLU:O	2:P:232:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.01	0.41
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.20	0.41
11:Y:83:LEU:HD23	11:Y:99:THR:HG21	2.03	0.41
12:L:83:ILE:HB	12:L:113:PHE:CE2	2.56	0.41
13:M:112:TYR:C	13:M:112:TYR:CD2	2.94	0.41
3:C:113:THR:HG21	3:C:149:TYR:HB3	2.03	0.41
8:H:18:THR:HB	8:H:30:ASN:HD22	1.86	0.41
5:S:220:PRO:O	5:S:222:THR:HG23	2.21	0.41
6:F:136:THR:O	6:F:150:MET:HA	2.21	0.41
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.36	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.55	0.41
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.51	0.41
5:E:52:LYS:O	5:E:63:TYR:HD2	2.03	0.41
1:A:232:ARG:NH1	1:A:232:ARG:HG3	2.36	0.41
7:G:173:THR:HG22	7:G:177:GLU:OE2	2.21	0.41
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.60	0.41
14:2:114:PRO:HD2	14:2:118:SER:O	2.21	0.41
10:X:90(B):ARG:NH1	17:X:266:HOH:O	2.41	0.41
6:T:157:TYR:CD1	6:T:157:TYR:C	2.94	0.41
5:E:78:LEU:HD12	5:E:78:LEU:C	2.41	0.41
11:K:208:ASN:O	11:K:209:VAL:C	2.59	0.41
4:D:59:LEU:C	4:D:59:LEU:HD13	2.41	0.41
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.56	0.41
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.25	0.41
9:W:49:ALA:HB3	10:X:118:THR:HG23	2.02	0.41
3:C:241:GLN:C	3:C:243:GLN:N	2.73	0.41
6:F:175:GLU:OE2	6:F:175:GLU:HA	2.21	0.41
8:V:113:ILE:HD12	8:V:113:ILE:N	2.36	0.41
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.21	0.41
4:R:68:VAL:HG21	4:R:89:ILE:HD12	2.03	0.41
5:E:148:LEU:HD23	5:E:162:GLY:HA2	2.03	0.41
13:M:34:LEU:C	13:M:35:ILE:HD12	2.41	0.41
6:T:37:SER:HB3	6:T:50:VAL:HG23	2.03	0.41
1:A:52:LYS:HG3	1:A:211:GLU:HB2	2.03	0.41
5:E:220:PRO:O	5:E:222:THR:HG23	2.20	0.41
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.59	0.41
10:X:34:THR:CG2	10:X:176:LYS:HZ2	2.32	0.41
1:A:20(A):THR:C	1:A:210:ILE:HD12	2.41	0.41
4:R:170:GLU:HG2	4:R:171:GLY:N	2.36	0.41
7:G:109:CYS:HB2	7:G:140:SER:OG	2.21	0.41
1:A:49:ALA:HB2	1:A:212:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LYS:O	2:B:140:GLY:HA2	2.21	0.41
1:A:45:GLY:HA2	1:A:147:PHE:CE2	2.56	0.41
7:G:98:GLU:HG2	7:G:102:LYS:HD3	2.03	0.41
9:W:61:TYR:C	9:W:61:TYR:CD1	2.94	0.41
7:G:43:LYS:HB2	7:G:18(G):GLU:O	2.21	0.40
5:S:42:SER:OG	5:S:43:ASN:N	2.53	0.40
13:1:34:LEU:C	13:1:35:ILE:HD12	2.41	0.40
6:T:127:ASN:C	6:T:127:ASN:ND2	2.74	0.40
8:H:112:SER:OG	8:H:120:ASP:HB2	2.21	0.40
7:G:49:ILE:HD13	7:G:212:VAL:HG22	2.03	0.40
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.21	0.40
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.02	0.40
11:K:1:THR:HB	16:K:212:MES:O2S	2.21	0.40
3:C:18:ASP:OD2	3:C:20:HIS:ND1	2.53	0.40
4:R:224:TYR:N	4:R:224:TYR:CD2	2.89	0.40
13:M:130:GLY:O	13:M:134:ALA:HB3	2.20	0.40
5:S:78:LEU:HD12	5:S:78:LEU:C	2.41	0.40
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.22	0.40
5:E:18(C):PHE:CA	5:E:18(F):ILE:HG12	2.45	0.40
13:M:14(G):ILE:HB	13:M:144:PRO:HD3	2.03	0.40
11:K:104:TYR:CE2	11:K:108:PRO:HG3	2.57	0.40
1:O:48:ILE:H	1:O:48:ILE:HD12	1.86	0.40
5:S:66:LYS:O	5:S:77:SER:HA	2.21	0.40
5:E:190:ILE:HG23	5:E:212:ILE:HD13	2.02	0.40
6:T:68:GLN:OE1	6:T:89:VAL:HG21	2.21	0.40
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.57	0.40
7:U:139:VAL:HA	7:U:147:SER:O	2.21	0.40
6:F:162:GLY:O	7:G:58:LEU:HB3	2.21	0.40
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.57	0.40
1:O:52:LYS:HG3	1:O:211:GLU:HB2	2.02	0.40
13:1:14(G):ILE:HB	13:1:144:PRO:HD3	2.03	0.40
6:F:127:ASN:ND2	6:F:127:ASN:C	2.74	0.40
5:S:4:PHE:O	5:S:5:ARG:C	2.60	0.40
2:B:213:ALA:HA	2:B:222:LYS:O	2.21	0.40
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.51	0.40
9:I:28:SER:HB2	10:J:120:VAL:HG21	2.03	0.40
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.21	0.40
7:G:139:VAL:HA	7:G:147:SER:O	2.21	0.40
7:G:48:VAL:CG1	7:G:139:VAL:HG11	2.52	0.40
2:P:7:ARG:HD2	2:P:8:TYR:CZ	2.55	0.40
2:B:228:GLU:O	2:B:232:ILE:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:13:SER:O	4:R:130:ARG:HD3	2.22	0.40
1:A:197:LEU:O	1:A:202:VAL:HG23	2.22	0.40
6:T:114:ASP:O	6:T:118:GLN:HG2	2.21	0.40
2:P:168:ASN:HA	17:P:943:HOH:O	2.21	0.40
4:D:17:PRO:HD2	17:D:1171:HOH:O	2.20	0.40
11:K:114:ASP:OD1	11:K:114:ASP:C	2.59	0.40
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.22	0.40
3:Q:57:LYS:HG2	3:Q:208:LYS:NZ	2.37	0.40
3:Q:167:ARG:O	3:Q:168:ASN:HB2	2.21	0.40
10:X:53:VAL:HB	17:X:726:HOH:O	2.21	0.40
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.40
2:P:31:ILE:HD12	2:P:79:ALA:O	2.21	0.40
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.85	0.40
10:X:16:SER:HB2	17:X:1152:HOH:O	2.20	0.40
5:E:177:GLU:OE1	6:F:56:SER:HB2	2.21	0.40
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.21	0.40
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	2.04	0.40
5:E:67:ILE:HG21	5:E:213:ALA:HB2	2.03	0.40
6:F:114:ASP:O	6:F:118:GLN:HG2	2.21	0.40
4:R:150:HIS:O	4:R:157:PHE:HA	2.21	0.40
2:B:202:THR:CG2	2:B:204:SER:HB2	2.51	0.40
6:T:192:GLN:O	6:T:196:ILE:HG13	2.22	0.40
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.57	0.40
10:X:44:SER:HG	10:X:100:LEU:HB2	1.85	0.40
14:2:20:THR:HG23	14:2:31:THR:OG1	2.21	0.40
6:F:101:LYS:HE2	13:M:57:ARG:NH2	2.36	0.40
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.56	0.40
9:I:28:SER:CB	10:J:120:VAL:HG21	2.52	0.40
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.04	0.40
7:U:89:ALA:O	7:U:93:LYS:HG3	2.21	0.40
8:H:34:LEU:HB2	17:H:540:HOH:O	2.22	0.40
1:O:197:LEU:O	1:O:202:VAL:HG23	2.21	0.40
6:F:49:ALA:HA	6:F:211:GLU:O	2.20	0.40
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.39	0.40
7:G:17(C):LYS:HE3	7:G:17(C):LYS:HB2	1.78	0.40
6:F:43:ASN:N	6:F:43:ASN:ND2	2.69	0.40
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.05	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	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	24	41
1	O	248/250 (99%)	236 (95%)	9 (4%)	3 (1%)	16	29
2	B	242/258 (94%)	221 (91%)	17 (7%)	4 (2%)	11	19
2	P	242/258 (94%)	222 (92%)	16 (7%)	4 (2%)	11	19
3	C	239/254 (94%)	223 (93%)	12 (5%)	4 (2%)	11	19
3	Q	239/254 (94%)	224 (94%)	11 (5%)	4 (2%)	11	19
4	D	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	15	26
4	R	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	15	26
5	E	231/234 (99%)	210 (91%)	16 (7%)	5 (2%)	8	13
5	S	231/234 (99%)	208 (90%)	18 (8%)	5 (2%)	8	13
6	F	242/288 (84%)	231 (96%)	8 (3%)	3 (1%)	16	29
6	T	242/288 (84%)	230 (95%)	9 (4%)	3 (1%)	16	29
7	G	241/252 (96%)	228 (95%)	13 (5%)	0	100	100
7	U	241/252 (96%)	227 (94%)	14 (6%)	0	100	100
8	H	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
8	V	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	196/198 (99%)	185 (94%)	8 (4%)	3 (2%)	13	22
10	X	196/198 (99%)	186 (95%)	8 (4%)	2 (1%)	19	34
11	K	210/287 (73%)	203 (97%)	6 (3%)	1 (0%)	34	55
11	Y	210/287 (73%)	202 (96%)	7 (3%)	1 (0%)	34	55
12	L	220/241 (91%)	208 (94%)	12 (6%)	0	100	100
12	Z	220/241 (91%)	208 (94%)	12 (6%)	0	100	100
13	1	231/266 (87%)	221 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/266 (87%)	221 (96%)	10 (4%)	0	100	100
14	2	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
14	N	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
15	3	1/5 (20%)	1 (100%)	0	0	100	100
15	4	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6314/6948 (91%)	5962 (94%)	302 (5%)	50 (1%)	24	41

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21(C)	ASP
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
5	E	5	ARG
2	P	21(C)	ASP
3	Q	58	LEU
3	Q	203	THR
4	R	12(G)	GLU
5	S	5	ARG
2	B	54	VAL
2	B	21(B)	GLY
5	E	202	ARG
10	J	192	ALA
2	P	54	VAL
2	P	21(B)	GLY
5	S	202	ARG
5	S	217	LYS
10	X	192	ALA
1	A	5	THR
1	A	167	LYS
3	C	183	PRO
4	D	12(F)	GLY
4	D	18(D)	SER
5	E	217	LYS
6	F	205	ASN
6	F	206	LYS
1	O	5	THR
1	O	167	LYS
2	P	6	ARG

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Mol	Chain	Res	Type
3	Q	183	PRO
4	R	12(F)	GLY
4	R	18(D)	SER
6	T	143	LYS
6	T	205	ASN
6	T	206	LYS
2	B	6	ARG
5	E	180	LEU
6	F	143	LYS
11	K	209	VAL
1	O	53	LYS
5	S	180	LEU
5	E	231	LYS
10	J	8	VAL
10	J	49	ALA
3	Q	53	ARG
5	S	231	LYS
10	X	8	VAL
11	Y	209	VAL
3	C	53	ARG

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	209/209 (100%)	200 (96%)	9 (4%)	35	61
1	O	209/209 (100%)	201 (96%)	8 (4%)	40	67
2	B	203/216 (94%)	192 (95%)	11 (5%)	27	49
2	P	203/216 (94%)	192 (95%)	11 (5%)	27	49
3	C	213/226 (94%)	203 (95%)	10 (5%)	32	56
3	Q	213/226 (94%)	203 (95%)	10 (5%)	32	56
4	D	198/215 (92%)	186 (94%)	12 (6%)	23	42
4	R	198/215 (92%)	186 (94%)	12 (6%)	23	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	192/193 (100%)	175 (91%)	17 (9%)	12	23
5	S	192/193 (100%)	175 (91%)	17 (9%)	12	23
6	F	201/239 (84%)	188 (94%)	13 (6%)	21	39
6	T	201/239 (84%)	188 (94%)	13 (6%)	21	39
7	G	207/210 (99%)	197 (95%)	10 (5%)	31	55
7	U	207/210 (99%)	197 (95%)	10 (5%)	31	55
8	H	181/214 (85%)	175 (97%)	6 (3%)	45	73
8	V	181/214 (85%)	174 (96%)	7 (4%)	39	66
9	I	172/173 (99%)	167 (97%)	5 (3%)	50	77
9	W	172/173 (99%)	167 (97%)	5 (3%)	50	77
10	J	175/175 (100%)	169 (97%)	6 (3%)	44	72
10	X	175/175 (100%)	169 (97%)	6 (3%)	44	72
11	K	169/235 (72%)	160 (95%)	9 (5%)	28	50
11	Y	169/235 (72%)	159 (94%)	10 (6%)	24	44
12	L	185/201 (92%)	177 (96%)	8 (4%)	35	61
12	Z	185/201 (92%)	173 (94%)	12 (6%)	21	39
13	1	199/224 (89%)	191 (96%)	8 (4%)	38	64
13	M	199/224 (89%)	191 (96%)	8 (4%)	38	64
14	2	162/178 (91%)	154 (95%)	8 (5%)	31	55
14	N	162/178 (91%)	154 (95%)	8 (5%)	31	55
All	All	5332/5816 (92%)	5063 (95%)	269 (5%)	30	53

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	33	GLN
1	A	48	ILE
1	A	62	GLU
1	A	64	LEU
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
1	A	214	ILE
2	B	58	LEU

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Mol	Chain	Res	Type
2	B	71	ASN
2	B	91	THR
2	B	121	GLN
2	B	124	THR
2	B	150	THR
2	B	156	ASN
2	B	185	LYS
2	B	192	LEU
2	B	212	PHE
2	B	218	ASN
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	172	VAL
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	28	LEU
4	D	48	LEU
4	D	72	ARG
4	D	107	ILE
4	D	110	GLU
4	D	126	ARG
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
4	D	244	GLU
5	E	12	THR
5	E	32	LYS
5	E	56	ASP
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	117	CYS
5	E	121	GLN

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Mol	Chain	Res	Type
5	E	123	ASN
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	227	GLU
5	E	231	LYS
6	F	18	ASP
6	F	43	ASN
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	167	LYS
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	184	ASN
7	G	197	MET
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	121	VAL
8	H	144	GLN
9	I	29	ASN
9	I	61	TYR
9	I	155	ILE
9	I	160	LEU
9	I	171	TRP
10	J	3	ILE

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Mol	Chain	Res	Type
10	J	34	THR
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
11	K	4	LEU
11	K	41	LEU
11	K	65	LEU
11	K	87	VAL
11	K	99	THR
11	K	104	TYR
11	K	10(B)	LYS
11	K	185	ILE
11	K	210	ILE
12	L	-9	GLN
12	L	14	LEU
12	L	40	ASN
12	L	58	ARG
12	L	98	HIS
12	L	99	THR
12	L	114	ASP
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
14	N	36	ARG
14	N	84	LYS
14	N	89	GLU
14	N	10(B)	LYS
14	N	119	VAL
14	N	126	ILE
14	N	186	ARG
14	N	18(I)	GLN
1	O	33	GLN
1	O	48	ILE
1	O	62	GLU
1	O	64	LEU

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Mol	Chain	Res	Type
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
1	O	214	ILE
2	P	58	LEU
2	P	71	ASN
2	P	91	THR
2	P	121	GLN
2	P	124	THR
2	P	150	THR
2	P	156	ASN
2	P	185	LYS
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	28	LEU
4	R	48	LEU
4	R	72	ARG
4	R	107	ILE
4	R	110	GLU
4	R	126	ARG
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
4	R	244	GLU
5	S	12	THR
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	76	LEU

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Mol	Chain	Res	Type
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	117	CYS
5	S	121	GLN
5	S	123	ASN
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	227	GLU
5	S	231	LYS
6	T	18	ASP
6	T	43	ASN
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	167	LYS
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	197	ARG

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Mol	Chain	Res	Type
9	W	29	ASN
9	W	61	TYR
9	W	155	ILE
9	W	160	LEU
9	W	171	TRP
10	X	3	ILE
10	X	34	THR
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
11	Y	4	LEU
11	Y	9	GLN
11	Y	41	LEU
11	Y	65	LEU
11	Y	87	VAL
11	Y	99	THR
11	Y	104	TYR
11	Y	10(B)	LYS
11	Y	185	ILE
11	Y	210	ILE
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	14	LEU
12	Z	40	ASN
12	Z	58	ARG
12	Z	82	ASN
12	Z	96	TYR
12	Z	98	HIS
12	Z	99	THR
12	Z	114	ASP
12	Z	1(I)	ASN
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
14	2	36	ARG

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Mol	Chain	Res	Type
14	2	84	LYS
14	2	89	GLU
14	2	10(B)	LYS
14	2	119	VAL
14	2	126	ILE
14	2	186	ARG
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	161	ASN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN

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Mol	Chain	Res	Type
5	E	123	ASN
5	E	125	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	87	HIS
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	91	GLN
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	81	GLN
9	I	145	ASN
10	J	54	GLN
10	J	62	ASN
10	J	85	GLN
10	J	112	GLN
10	J	141	HIS
10	J	186	GLN
10	J	193	GLN
11	K	207	ASN
11	K	208	ASN
12	L	61	ASN
12	L	85	HIS

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Mol	Chain	Res	Type
12	L	14(B)	ASN
12	L	166	HIS
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	161	ASN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN

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Mol	Chain	Res	Type
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	170	GLN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	81	GLN
9	W	145	ASN
10	X	54	GLN
10	X	62	ASN
10	X	85	GLN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	85	ASN

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Mol	Chain	Res	Type
11	Y	141	ASN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	69	GLN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	TY5	3	2	15	19,20,21	1.75	4 (21%)	22,25,27	1.08	2 (9%)
15	RE0	3	4	15	15,17,18	1.26	1 (6%)	21,25,27	2.39	7 (33%)
15	TY5	4	2	15	19,20,21	1.74	5 (26%)	22,25,27	1.03	2 (9%)
15	RE0	4	4	15	15,17,18	1.36	2 (13%)	21,25,27	2.27	7 (33%)

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	TY5	3	2	15	-	0/9/11/13	0/2/2/2
15	RE0	3	4	15	-	0/5/23/25	0/2/2/2
15	TY5	4	2	15	-	0/9/11/13	0/2/2/2
15	RE0	4	4	15	-	0/5/23/25	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	2	TY5	C51-C50	2.01	1.43	1.38
15	4	2	TY5	CE1-CZ	2.02	1.42	1.38
15	3	2	TY5	C53-C52	2.03	1.43	1.38
15	3	2	TY5	C49-C50	2.07	1.55	1.50
15	4	4	RE0	CH2-CZ3	2.12	1.43	1.38
15	3	2	TY5	C55-C50	2.14	1.43	1.38
15	3	4	RE0	CH2-CZ3	2.24	1.43	1.38
15	4	2	TY5	C55-C50	2.25	1.43	1.38
15	4	4	RE0	CB-CA	2.47	1.57	1.54
15	4	2	TY5	C49-C50	2.48	1.56	1.50
15	4	2	TY5	CE2-CZ	2.63	1.43	1.38
15	3	2	TY5	CE2-CZ	2.83	1.44	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	4	RE0	CG-CD2-CE2	-6.39	105.97	108.80
15	4	4	RE0	CG-CD2-CE2	-5.75	106.25	108.80
15	4	4	RE0	CE2-NE1-CD1	-3.52	109.98	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3	4	RE0	OG-CG-CD1	-3.47	102.42	108.30
15	3	4	RE0	CE2-NE1-CD1	-3.36	110.07	111.88
15	4	4	RE0	O-C-CA	-3.33	116.81	125.49
15	3	4	RE0	O-C-CA	-3.23	117.07	125.49
15	4	4	RE0	OG-CG-CD1	-3.15	102.97	108.30
15	3	4	RE0	CZ2-CE2-NE1	-2.96	124.96	131.02
15	3	2	TY5	O-C-CA	-2.88	117.98	125.49
15	4	4	RE0	CZ2-CE2-NE1	-2.72	125.45	131.02
15	4	2	TY5	O-C-CA	-2.66	118.57	125.49
15	3	4	RE0	CG-CD1-NE1	2.15	109.75	108.39
15	4	4	RE0	CG-CD1-NE1	2.32	109.86	108.39
15	3	2	TY5	C49-OH-CZ	2.63	124.75	117.70
15	4	2	TY5	C49-OH-CZ	2.64	124.79	117.70
15	3	4	RE0	CD2-CE2-NE1	3.53	111.93	109.61
15	4	4	RE0	CD2-CE2-NE1	3.72	112.06	109.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	2	TY5	2	0
15	4	2	TY5	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\|>2$
16	MES	K	212	-	11,12,12	0.98	0	14,16,16	0.82	0
16	MES	Y	212	-	11,12,12	2.24	4 (36%)	14,16,16	2.11	4 (28%)

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
16	MES	K	212	-	-	0/6/14/14	0/1/1/1
16	MES	Y	212	-	-	0/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	212	MES	C5-N4	2.92	1.54	1.46
16	Y	212	MES	C3-N4	2.97	1.55	1.46
16	Y	212	MES	C7-N4	3.60	1.55	1.47
16	Y	212	MES	O2S-S	4.21	1.58	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	212	MES	C6-C5-N4	-3.83	104.32	110.12
16	Y	212	MES	O3S-S-O2S	-3.07	104.46	111.61
16	Y	212	MES	C2-C3-N4	2.55	113.99	110.12
16	Y	212	MES	O3S-S-O1S	4.78	122.72	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	212	MES	1	0
16	Y	212	MES	1	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	250/250 (100%)	-0.08	3 (1%) 81 83	33, 46, 75, 104	0
1	O	250/250 (100%)	0.08	9 (3%) 46 51	37, 53, 81, 104	0
2	B	244/258 (94%)	0.15	8 (3%) 50 55	32, 52, 89, 116	0
2	P	244/258 (94%)	0.24	17 (6%) 19 22	34, 53, 90, 116	0
3	C	241/254 (94%)	0.26	17 (7%) 19 21	33, 55, 107, 120	0
3	Q	241/254 (94%)	0.79	52 (21%) 1 1	38, 60, 111, 122	0
4	D	242/260 (93%)	0.19	11 (4%) 37 42	34, 54, 89, 120	0
4	R	242/260 (93%)	0.33	15 (6%) 24 27	37, 58, 90, 122	0
5	E	233/234 (99%)	0.40	25 (10%) 8 8	43, 59, 85, 110	0
5	S	233/234 (99%)	0.73	35 (15%) 3 3	41, 64, 90, 108	0
6	F	244/288 (84%)	0.07	7 (2%) 55 60	36, 53, 88, 103	0
6	T	244/288 (84%)	0.26	18 (7%) 17 19	32, 55, 92, 106	0
7	G	243/252 (96%)	-0.02	8 (3%) 50 55	33, 46, 76, 113	0
7	U	243/252 (96%)	0.02	5 (2%) 67 71	32, 50, 74, 113	0
8	H	222/261 (85%)	-0.16	2 (0%) 85 88	28, 45, 65, 90	0
8	V	222/261 (85%)	-0.19	1 (0%) 91 92	30, 49, 67, 93	0
9	I	204/205 (99%)	-0.14	2 (0%) 84 86	28, 43, 62, 76	0
9	W	204/205 (99%)	-0.03	3 (1%) 76 79	31, 44, 64, 78	0
10	J	198/198 (100%)	-0.08	6 (3%) 54 59	29, 43, 64, 120	0
10	X	198/198 (100%)	-0.07	9 (4%) 37 42	29, 45, 62, 120	0
11	K	212/287 (73%)	-0.16	5 (2%) 62 66	26, 42, 65, 78	0
11	Y	212/287 (73%)	-0.05	7 (3%) 50 55	33, 46, 68, 79	0
12	L	222/241 (92%)	-0.08	4 (1%) 71 75	29, 46, 66, 91	0
12	Z	222/241 (92%)	-0.05	4 (1%) 71 75	31, 46, 67, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/266 (87%)	-0.26	1 (0%) 93 93	31, 45, 59, 64	0
13	M	233/266 (87%)	-0.22	1 (0%) 93 93	30, 47, 61, 65	0
14	2	196/215 (91%)	-0.15	1 (0%) 91 92	27, 44, 66, 80	0
14	N	196/215 (91%)	-0.30	0 100 100	32, 43, 64, 76	0
15	3	1/5 (20%)	-0.78	0 100 100	33, 33, 33, 33	0
15	4	1/5 (20%)	0.26	0 100 100	43, 43, 43, 43	0
All	All	6370/6948 (91%)	0.06	276 (4%) 39 44	26, 49, 82, 122	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(C)	GLY	13.0
3	C	55	THR	11.5
4	R	12(D)	ALA	11.4
4	D	12(D)	ALA	11.2
7	U	6	ALA	10.6
4	R	12(F)	GLY	10.5
2	B	218	ASN	10.1
10	X	193	GLN	9.8
4	D	12(E)	SER	9.5
10	J	193	GLN	8.7
3	C	56	LEU	8.7
7	U	240	ASP	8.6
3	Q	236	ILE	8.0
4	D	12(F)	GLY	8.0
2	P	217	ALA	7.9
3	Q	56	LEU	7.9
4	R	12(C)	GLY	7.7
10	J	192	ALA	7.6
4	R	12(E)	SER	7.6
2	B	217	ALA	7.3
12	Z	145	TYR	7.3
2	P	218	ASN	7.2
12	L	145	TYR	7.2
10	X	192	ALA	6.9
5	S	5	ARG	6.8
4	R	126	ARG	6.3
3	Q	55	THR	6.1
5	E	4	PHE	6.1
7	G	6	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	4	MET	5.8
3	Q	63	THR	5.7
1	O	235	ALA	5.6
3	Q	233	VAL	5.6
11	Y	208	ASN	5.5
1	O	236	LEU	5.5
5	E	233	ILE	5.5
5	S	4	PHE	5.4
3	Q	54	SER	5.3
3	Q	241	GLN	5.3
1	O	4	MET	5.2
6	F	5	GLY	5.2
3	Q	243	GLN	5.0
3	C	203	THR	5.0
7	G	236	ILE	5.0
1	A	236	LEU	4.9
5	E	127	TYR	4.9
5	E	5	ARG	4.9
3	Q	242	GLU	4.9
12	Z	14(W)	LYS	4.8
7	G	240	ASP	4.7
3	Q	203	THR	4.7
5	S	18(C)	PHE	4.7
5	E	203	ASP	4.6
3	Q	201	VAL	4.6
5	S	203	ASP	4.6
5	S	51	LEU	4.4
5	S	178	ARG	4.4
13	M	-8	THR	4.4
5	S	233	ILE	4.4
2	B	21(B)	GLY	4.4
6	F	240	ILE	4.4
11	K	208	ASN	4.3
5	S	206	SER	4.3
3	Q	202	GLN	4.2
10	X	-1	MET	4.2
2	P	21(B)	GLY	4.1
3	Q	237	GLU	4.0
3	Q	240	LYS	3.9
4	D	126	ARG	3.9
3	Q	232	TYR	3.9
11	Y	104	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
4	R	9	ASP	3.8
6	T	240	ILE	3.8
2	P	219	GLU	3.8
11	K	104	TYR	3.8
4	D	12(G)	GLU	3.8
11	K	210	ILE	3.7
12	L	14(P)	PRO	3.7
3	Q	239	GLU	3.7
3	C	240	LYS	3.6
3	Q	184	ALA	3.6
5	S	127	TYR	3.6
3	C	236	ILE	3.5
3	Q	197	LEU	3.5
10	J	-1	MET	3.5
3	Q	235	GLN	3.4
6	T	199	LEU	3.4
6	T	232	ALA	3.4
10	X	189	ASP	3.4
2	P	21(A)	LYS	3.4
7	G	239	GLN	3.4
8	V	223	ASP	3.3
5	E	197	ILE	3.3
13	1	-8	THR	3.3
3	Q	189	CYS	3.3
5	S	191	LYS	3.3
12	L	14(W)	LYS	3.2
3	Q	18(D)	GLU	3.2
3	Q	230	ASN	3.2
5	S	180	LEU	3.2
5	E	178	ARG	3.2
3	Q	206	GLY	3.2
5	S	189	LEU	3.2
4	R	12(B)	GLU	3.2
4	D	127	LEU	3.2
6	T	184	LEU	3.1
5	S	18(B)	THR	3.1
3	Q	183	PRO	3.1
3	Q	234	THR	3.1
3	Q	53	ARG	3.1
3	Q	40	VAL	3.1
5	S	195	GLU	3.1
3	Q	175	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	P	22	TYR	3.0
3	Q	210	ILE	3.0
3	Q	229	ILE	3.0
5	S	232	TYR	3.0
4	R	10	ARG	3.0
3	Q	58	LEU	3.0
3	Q	198	LEU	3.0
3	Q	179	ASN	3.0
3	C	237	GLU	3.0
2	B	21(A)	LYS	3.0
5	S	229	VAL	3.0
3	Q	196	SER	3.0
4	R	12(G)	GLU	3.0
12	L	-9	GLN	2.9
6	T	18(B)	HIS	2.9
5	S	2(C)	VAL	2.9
3	Q	238	GLN	2.9
5	S	210	LEU	2.9
5	S	192	ALA	2.9
5	E	189	LEU	2.9
5	S	197	ILE	2.9
2	P	220	TYR	2.9
5	E	175	TYR	2.8
3	Q	200	VAL	2.8
10	X	191	GLN	2.8
1	O	229	ILE	2.8
4	R	127	LEU	2.8
3	Q	207	ALA	2.8
3	C	188	GLU	2.8
3	C	54	SER	2.8
3	C	243	GLN	2.8
3	Q	187	GLU	2.7
5	S	201	LEU	2.7
6	F	43	ASN	2.7
3	C	232	TYR	2.7
3	Q	194	VAL	2.7
5	S	18(E)	LYS	2.7
5	S	168	ARG	2.7
6	T	198	TYR	2.7
5	E	18(C)	PHE	2.7
4	R	121	LEU	2.7
12	Z	14(M)	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	P	21(C)	ASP	2.7
6	T	18(D)	PRO	2.7
3	C	208	LYS	2.7
5	E	18(E)	LYS	2.6
1	O	175	PHE	2.6
6	F	201	ALA	2.6
4	R	241	GLU	2.6
3	C	210	ILE	2.6
1	A	235	ALA	2.6
2	P	186	VAL	2.6
6	F	18(E)	GLU	2.6
7	U	8	TYR	2.6
1	O	234	GLU	2.6
11	K	211	GLY	2.6
3	Q	178	LYS	2.6
3	Q	172	VAL	2.6
5	E	195	GLU	2.6
5	E	206	SER	2.6
4	R	11	GLY	2.6
3	Q	191	LYS	2.6
10	J	191	GLN	2.6
2	P	185	LYS	2.6
7	G	8	TYR	2.6
5	E	180	LEU	2.6
3	Q	62(A)	ILE	2.6
2	B	219	GLU	2.6
10	X	168	MET	2.6
3	C	202	GLN	2.6
5	E	193	GLY	2.5
6	T	217	LEU	2.5
3	Q	171	THR	2.5
6	T	223	PHE	2.5
6	T	228	LEU	2.5
2	P	181	LYS	2.5
6	F	18(D)	PRO	2.5
14	2	107	LYS	2.5
4	D	9	ASP	2.5
9	I	182	ASP	2.5
4	R	243	ALA	2.5
3	C	191	LYS	2.5
8	H	223	ASP	2.5
11	Y	211	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	125	GLU	2.5
6	T	18(A)	ASP	2.5
3	Q	43	LYS	2.5
5	S	198	SER	2.5
9	W	181	LYS	2.4
5	S	212	ILE	2.4
2	P	54	VAL	2.4
6	T	18(E)	GLU	2.4
3	Q	64	PRO	2.4
3	C	241	GLN	2.4
2	B	54	VAL	2.4
5	E	6	ASN	2.4
5	S	32	LYS	2.4
5	E	186	PRO	2.4
1	O	21(P)	LYS	2.4
3	Q	195	ARG	2.4
5	E	2(C)	VAL	2.4
5	E	212	ILE	2.4
5	S	188	GLU	2.4
5	E	202	ARG	2.3
8	H	199	GLU	2.3
5	E	128	GLY	2.3
3	Q	182	PRO	2.3
5	E	204	GLU	2.3
6	T	57	LYS	2.3
3	C	209	ASN	2.3
6	T	6	THR	2.3
4	D	10	ARG	2.3
3	C	187	GLU	2.3
5	S	174	THR	2.3
2	B	239	THR	2.3
2	P	236	THR	2.3
5	S	176	LEU	2.2
6	T	179	LEU	2.2
2	P	239	THR	2.2
5	S	202	ARG	2.2
2	P	63	THR	2.2
9	I	181	LYS	2.2
10	X	133	TYR	2.2
5	E	192	ALA	2.2
9	W	-8	SER	2.2
6	T	238	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	49	VAL	2.2
7	U	7	GLY	2.2
7	U	239	GLN	2.2
12	Z	14(P)	PRO	2.2
2	P	6	ARG	2.2
1	O	233	LEU	2.2
6	T	191	LYS	2.2
7	G	234	VAL	2.1
2	B	227	GLN	2.1
4	R	229	THR	2.1
7	G	237	ALA	2.1
10	X	190	PHE	2.1
3	Q	18(C)	LYS	2.1
3	Q	212	ILE	2.1
5	S	12	THR	2.1
5	S	184	GLY	2.1
3	Q	44	ASN	2.1
11	Y	207	ASN	2.1
1	O	210	ILE	2.1
11	Y	10(A)	ARG	2.1
11	Y	180	GLU	2.1
6	F	204	ASP	2.1
5	S	175	TYR	2.1
6	T	43	ASN	2.0
2	P	184	MET	2.0
3	Q	231	GLN	2.0
5	S	199	GLN	2.0
10	X	92	ARG	2.0
11	K	10(A)	ARG	2.0
9	W	163	ALA	2.0
5	S	63	TYR	2.0
4	D	22	PHE	2.0
10	J	92	ARG	2.0
11	Y	73	ARG	2.0
10	J	168	MET	2.0
7	G	18(A)	ILE	2.0
5	E	232	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	RE0	4	4	16/17	0.95	0.14	-	41,43,44,49	0
15	RE0	3	4	16/17	0.95	0.18	-	34,36,39,46	0
15	TY5	3	2	19/20	0.94	0.15	-	37,40,47,47	0
15	TY5	4	2	19/20	0.94	0.13	-	33,41,44,44	0

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
16	MES	Y	212	12/12	0.96	0.23	3.94	59,62,64,64	0
16	MES	K	212	12/12	0.98	0.18	2.09	48,54,56,57	0

6.5 Other polymers (i)

There are no such residues in this entry.