



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:55 AM UTC

PDB ID : 3NZW / pdb_00003nzw
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

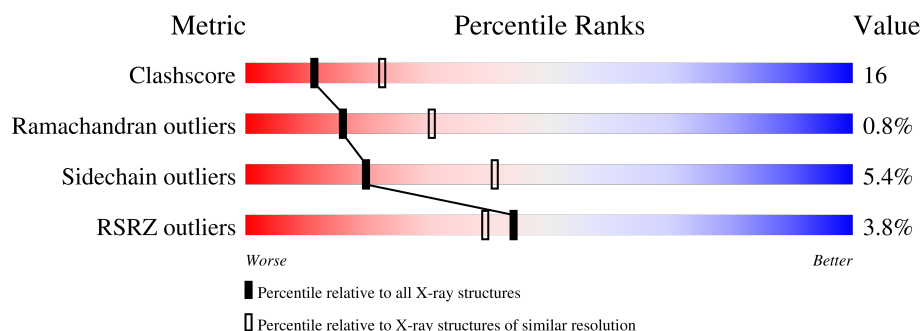
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	2% 76% 22% •
1	O	250	4% 76% 21% •
2	B	258	5% 57% 33% • 5%
2	P	258	8% 59% 32% • 5%
3	C	254	8% 55% 38% • 5%
3	Q	254	11% 56% 37% • 5%

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	261	
8	V	261	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	287	
11	Y	287	
12	L	241	
12	Z	241	
13	1	266	
13	M	266	
14	2	215	
14	N	215	
15	3	5	
15	4	5	

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			

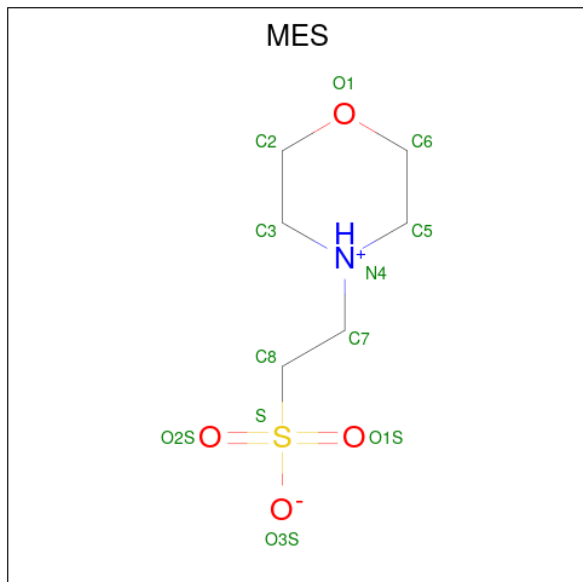
- Molecule 14 is a protein called Proteasome component PRE3.

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 (CCD ID: 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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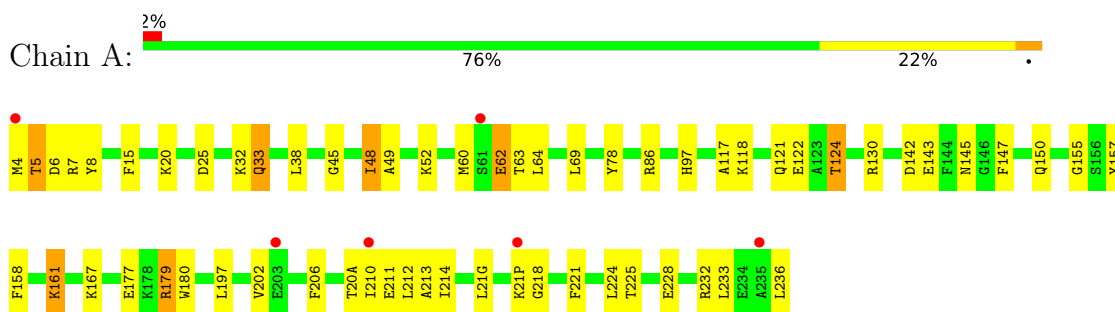
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	4	3	Total	O	0	0
			3	3		

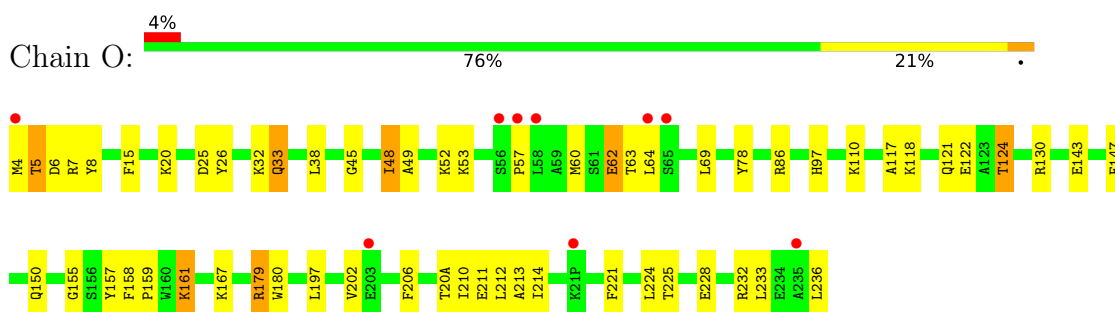
3 Residue-property plots

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

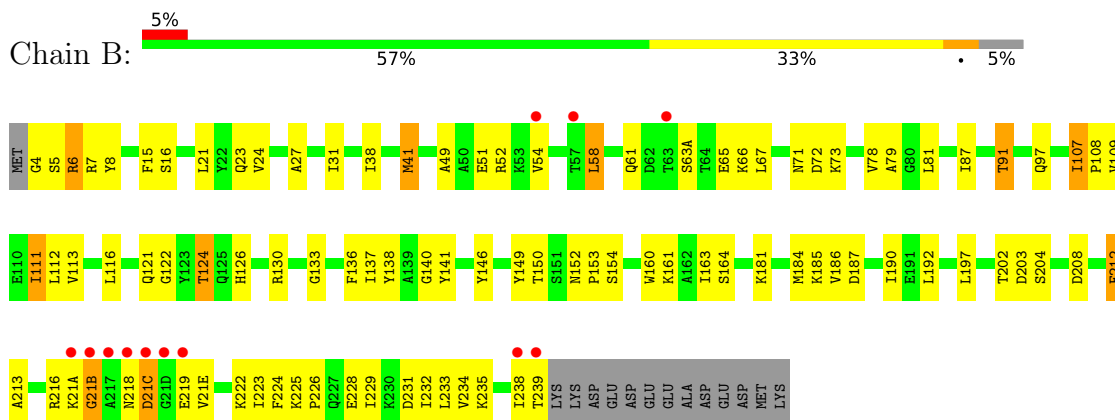
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

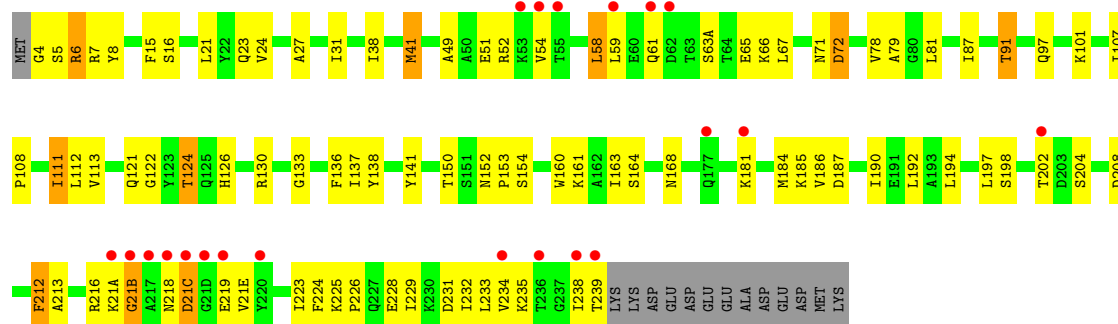


• Molecule 2: Proteasome component Y13



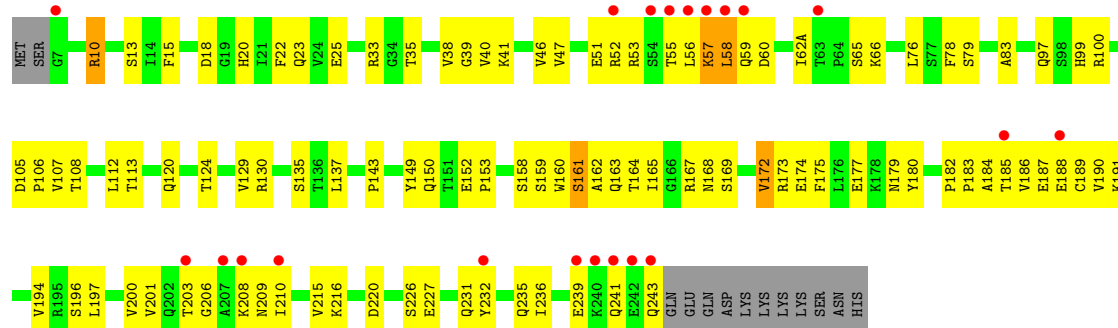
• Molecule 2: Proteasome component Y13

Chain P: 



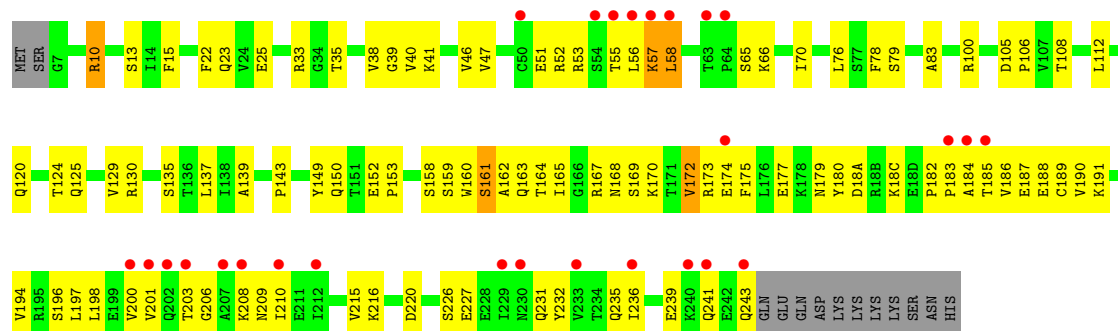
• Molecule 3: Proteasome component PRE6

Chain C: 



• Molecule 3: Proteasome component PRE6

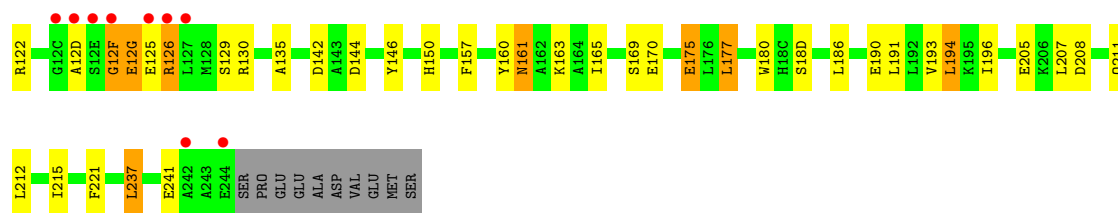
Chain Q: 



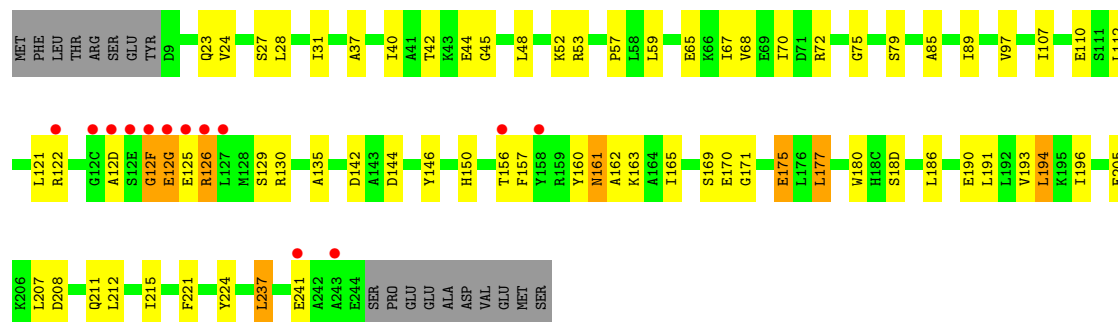
• Molecule 4: Proteasome component PUP2

Chain D: 

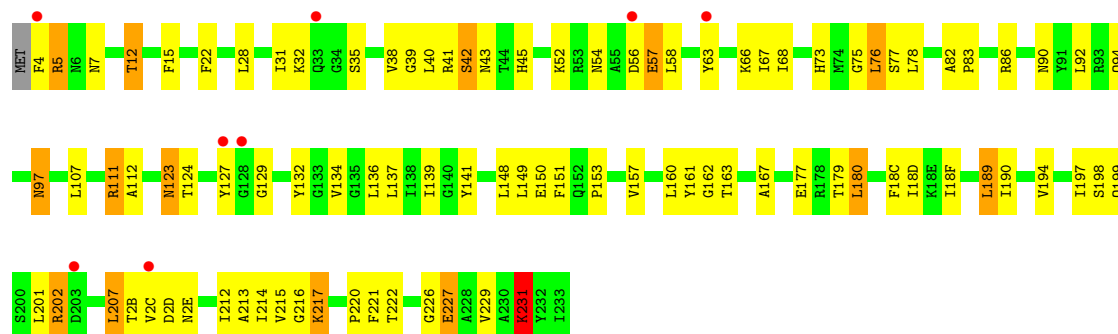




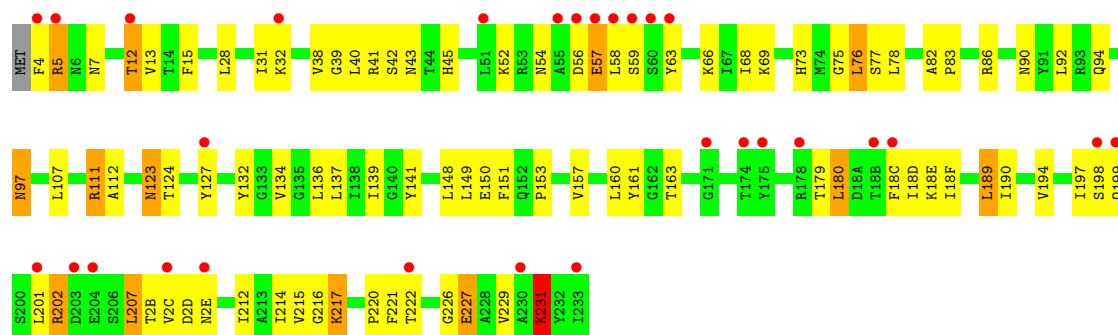
• Molecule 4: Proteasome component PUP2

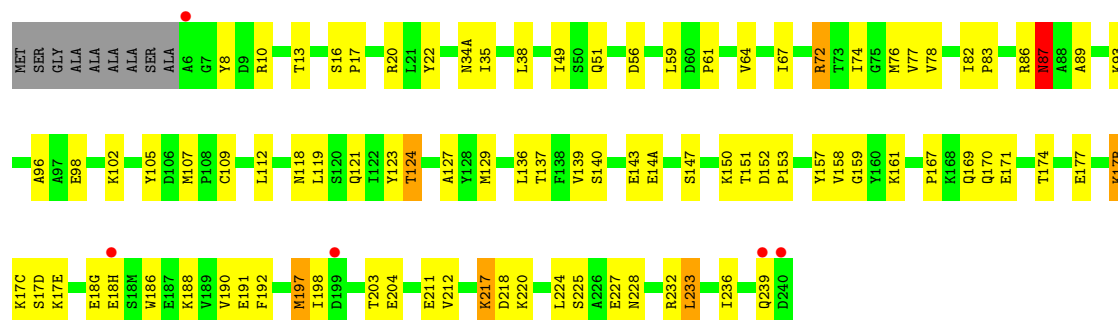


• Molecule 5: Proteasome component PRE5

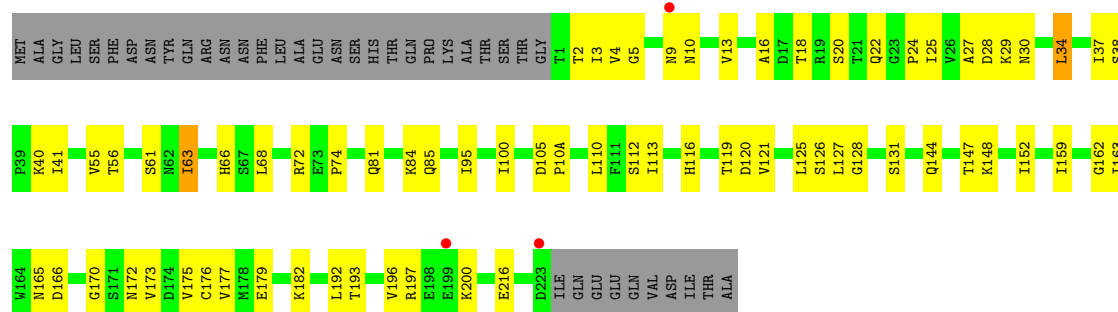


• Molecule 5: Proteasome component PRE5

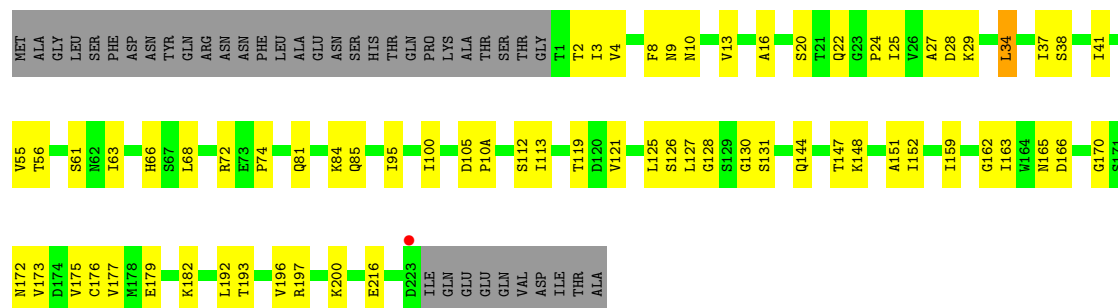




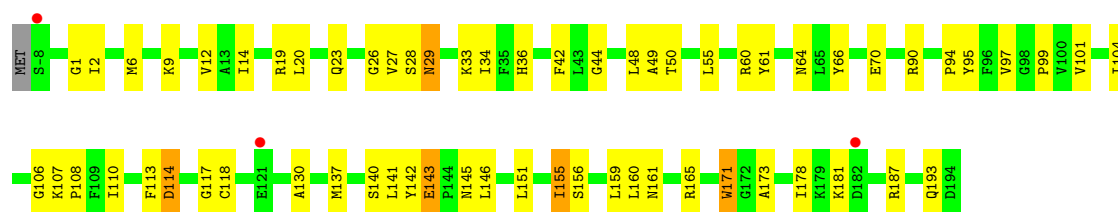
• Molecule 8: Proteasome component PUP1



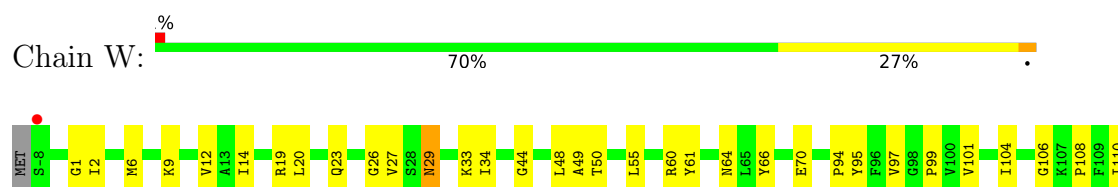
• Molecule 8: Proteasome component PUP1



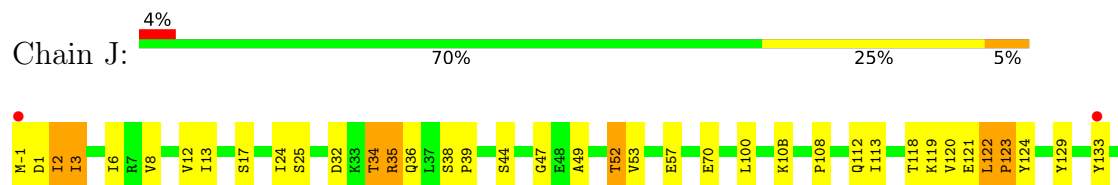
• Molecule 9: Proteasome component PUP3



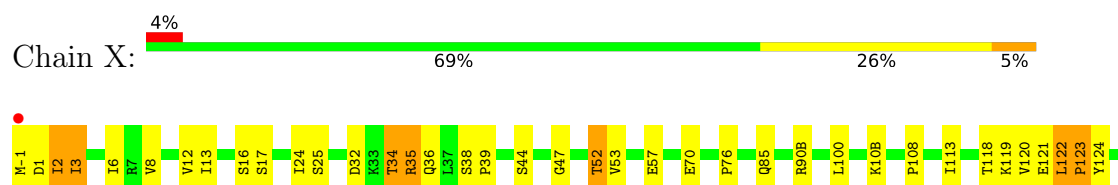
• Molecule 9: Proteasome component PUP3



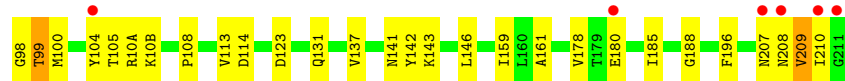
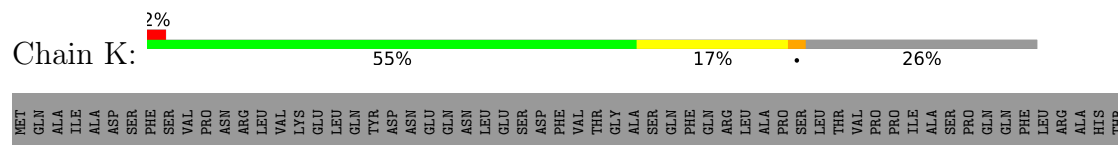
• Molecule 10: Proteasome component C11



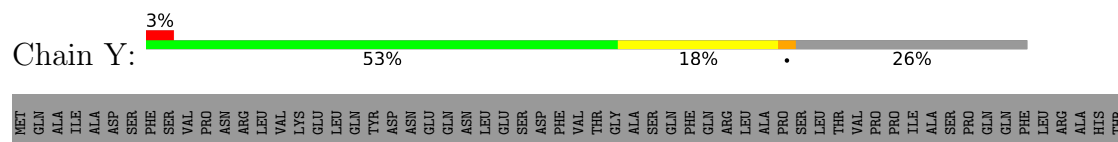
• Molecule 10: Proteasome component C11

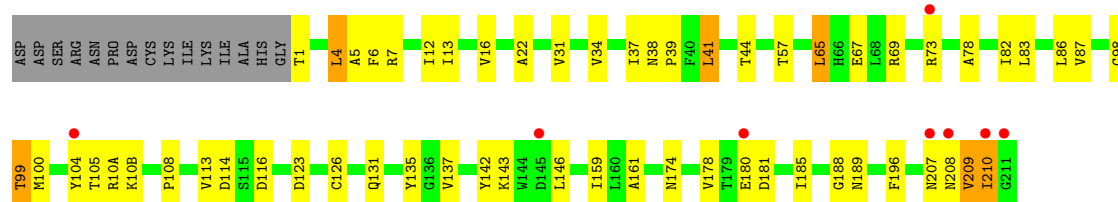


• Molecule 11: Proteasome component PRE2

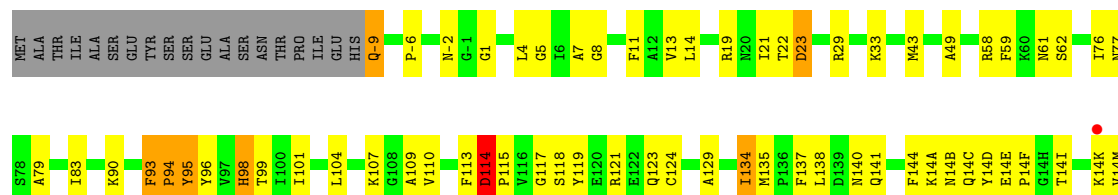


• Molecule 11: Proteasome component PRE2

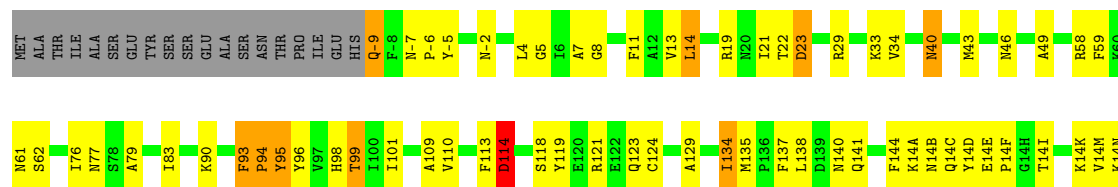




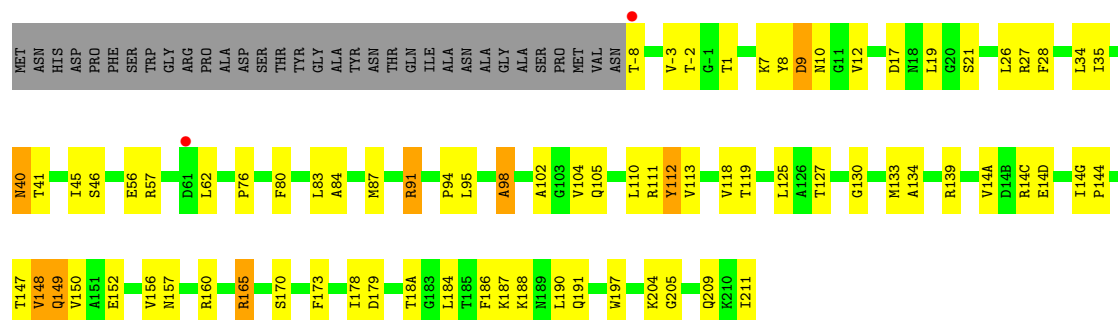
• Molecule 12: Proteasome component C5



• Molecule 12: Proteasome component C5

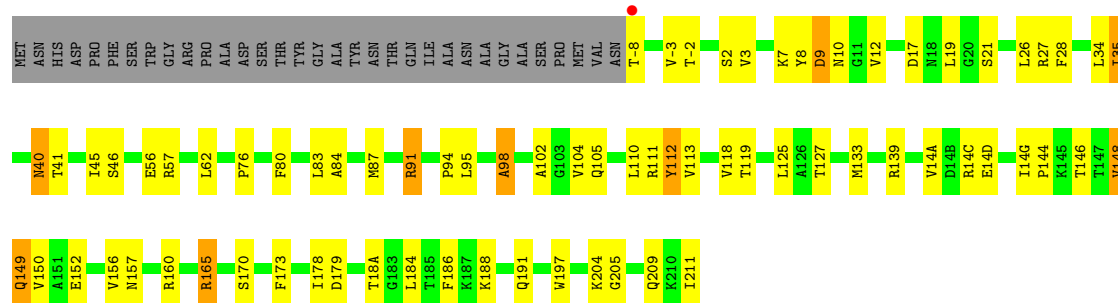


• Molecule 13: Proteasome component PRE4



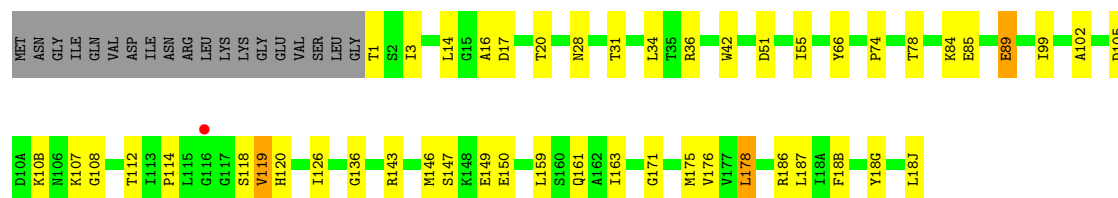
• Molecule 13: Proteasome component PRE4

Chain 1:  59% 25% 12%



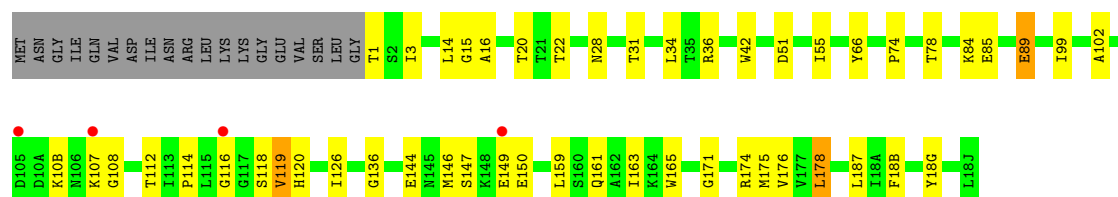
• Molecule 14: Proteasome component PRE3

Chain N:  68% 21% 9%

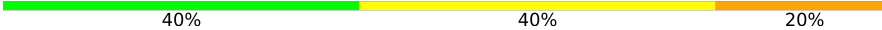


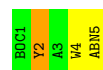
• Molecule 14: Proteasome component PRE3

Chain 2:  2% 68% 22% 9%

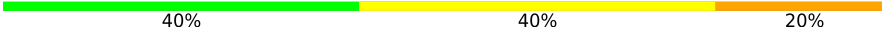


• Molecule 15: TMC-95A mimic ligand 2b

Chain 3:  40% 40% 20%



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

Chain 4:  40% 40% 20%



4 Data and refinement statistics

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 15.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.50) 97.7 (15.00-2.51)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.240 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
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 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ABN, MES, TY5, RE0, BOC

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	0.42	0/1952	0.92	3/2642 (0.1%)
1	O	0.40	0/1952	0.91	3/2642 (0.1%)
2	B	0.42	0/1934	0.89	7/2618 (0.3%)
2	P	0.43	0/1934	0.89	5/2618 (0.2%)
3	C	0.41	0/1919	0.91	4/2598 (0.2%)
3	Q	0.39	0/1919	0.91	5/2598 (0.2%)
4	D	0.40	0/1886	0.90	5/2541 (0.2%)
4	R	0.39	0/1886	0.90	5/2541 (0.2%)
5	E	0.37	0/1823	0.89	4/2463 (0.2%)
5	S	0.38	0/1823	0.89	2/2463 (0.1%)
6	F	0.39	0/1936	0.95	8/2614 (0.3%)
6	T	0.41	0/1936	0.95	9/2614 (0.3%)
7	G	0.48	1/1959 (0.1%)	0.94	8/2652 (0.3%)
7	U	0.45	0/1959	0.94	8/2652 (0.3%)
8	H	0.44	0/1715	0.93	1/2326 (0.0%)
8	V	0.43	0/1715	0.93	1/2326 (0.0%)
9	I	0.44	0/1611	1.00	11/2174 (0.5%)
9	W	0.45	0/1611	1.00	9/2174 (0.4%)
10	J	0.46	0/1613	0.97	6/2173 (0.3%)
10	X	0.47	0/1613	0.97	5/2173 (0.2%)
11	K	0.60	1/1681 (0.1%)	0.97	6/2274 (0.3%)
11	Y	0.44	0/1681	0.94	6/2274 (0.3%)
12	L	0.42	0/1795	1.05	12/2420 (0.5%)
12	Z	0.41	0/1795	1.03	12/2420 (0.5%)
13	1	0.45	0/1855	0.95	11/2514 (0.4%)
13	M	0.42	0/1855	0.94	8/2514 (0.3%)
14	2	0.45	0/1541	0.93	2/2087 (0.1%)
14	N	0.45	0/1541	0.93	2/2087 (0.1%)
15	3	0.81	0/4	0.73	0/4
15	4	0.81	0/4	0.76	0/4
All	All	0.43	2/50448 (0.0%)	0.94	168/68200 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	47	GLY	C-N	-14.08	1.21	1.33
7	G	107	MET	SD-CE	-5.29	1.66	1.79

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	114	ASP	O-C-N	-10.79	107.94	121.64
13	M	27	ARG	N-CA-C	10.67	122.67	111.14
13	1	27	ARG	N-CA-C	10.61	122.59	111.14
6	T	12	ASN	N-CA-C	8.88	121.86	111.02
6	F	12	ASN	N-CA-C	8.64	121.57	111.02
6	T	107	ILE	N-CA-C	8.53	118.25	108.96
6	F	107	ILE	N-CA-C	8.41	118.13	108.96
7	G	161	LYS	N-CA-C	-8.19	101.91	112.23
13	1	95	LEU	N-CA-C	-7.97	95.58	108.41
7	U	161	LYS	N-CA-C	-7.86	102.02	111.69
1	A	161	LYS	N-CA-C	-7.85	101.54	112.45
13	1	2	SER	N-CA-C	7.84	120.44	110.24
8	H	37	ILE	N-CA-C	-7.82	103.29	111.58
3	Q	161	SER	N-CA-C	-7.80	102.86	111.36
13	M	95	LEU	N-CA-C	-7.78	95.89	108.41
12	L	95	TYR	N-CA-C	-7.77	96.62	108.67
3	C	161	SER	N-CA-C	-7.76	102.90	111.36
1	O	161	LYS	N-CA-C	-7.68	101.78	112.45
2	B	161	LYS	N-CA-C	-7.60	104.14	113.41
12	Z	95	TYR	N-CA-C	-7.60	96.90	108.67
8	V	37	ILE	N-CA-C	-7.53	103.60	111.58
12	Z	134	ILE	N-CA-C	7.34	119.36	111.58
11	K	188	GLY	N-CA-C	7.32	124.31	112.61
12	L	134	ILE	N-CA-C	7.31	119.33	111.58
12	L	93	PHE	CA-C-N	7.27	127.27	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	93	PHE	C-N-CA	7.27	127.27	119.78
2	P	16	SER	N-CA-C	-7.22	101.83	110.13
4	D	70	ILE	N-CA-C	-7.18	105.63	111.81
6	T	135	SER	N-CA-C	-7.17	97.52	109.07
11	Y	188	GLY	N-CA-C	7.14	124.04	112.61
6	F	135	SER	N-CA-C	-7.12	97.61	109.07
12	Z	93	PHE	CA-C-N	7.09	127.08	119.78
12	Z	93	PHE	C-N-CA	7.09	127.08	119.78
3	Q	108	THR	N-CA-C	-6.95	101.56	110.53
2	B	16	SER	N-CA-C	-6.71	102.42	110.13
14	N	99	ILE	N-CA-C	6.67	117.45	108.11
5	S	57	GLU	N-CA-C	-6.67	105.01	113.02
1	O	143	GLU	N-CA-C	6.64	119.08	111.11
6	T	161	LYS	N-CA-C	-6.64	103.22	112.45
4	D	161	ASN	N-CA-C	-6.61	103.91	112.23
3	C	108	THR	N-CA-C	-6.60	102.01	110.53
4	R	161	ASN	N-CA-C	-6.59	103.93	112.23
14	2	99	ILE	N-CA-C	6.59	117.33	108.11
5	E	57	GLU	N-CA-C	-6.55	105.16	113.02
1	A	143	GLU	N-CA-C	6.51	118.92	111.11
10	J	123	PRO	N-CA-C	-6.49	104.70	113.40
5	E	161	TYR	N-CA-C	-6.45	104.10	112.23
7	G	239	GLN	N-CA-C	-6.41	107.32	114.62
6	F	161	LYS	N-CA-C	-6.40	103.55	112.45
7	U	239	GLN	N-CA-C	-6.34	107.40	114.62
9	W	60	ARG	N-CA-C	-6.33	104.30	111.14
9	I	26	GLY	N-CA-C	-6.30	102.97	111.54
10	X	123	PRO	N-CA-C	-6.29	104.97	113.40
12	Z	114	ASP	N-CA-C	-6.27	101.96	110.36
3	C	22	PHE	N-CA-C	6.24	118.88	111.33
4	R	70	ILE	N-CA-C	-6.22	105.76	111.67
13	1	98	ALA	N-CA-C	-6.21	98.27	108.76
5	S	161	TYR	N-CA-C	-6.14	104.49	112.23
9	I	60	ARG	N-CA-C	-6.14	104.51	111.14
7	G	16	SER	N-CA-C	-6.10	102.41	110.40
7	G	127	ALA	N-CA-C	6.06	118.85	111.82
6	F	14	VAL	N-CA-C	6.05	116.88	108.89
4	R	144	ASP	N-CA-C	6.04	117.94	111.36
4	R	169	SER	N-CA-C	6.02	117.64	111.14
13	M	98	ALA	N-CA-C	-5.99	98.51	108.34
6	T	14	VAL	N-CA-C	5.96	116.76	108.89
7	U	127	ALA	N-CA-C	5.92	118.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	144	ASP	N-CA-C	5.92	117.82	111.36
10	X	25	SER	N-CA-C	5.90	119.09	109.24
2	P	238	ILE	N-CA-C	-5.87	106.55	113.42
4	D	169	SER	N-CA-C	5.85	117.46	111.14
10	J	122	LEU	N-CA-C	5.84	117.66	108.55
9	I	142	TYR	N-CA-C	5.78	118.65	110.50
6	F	240	ILE	N-CA-C	-5.78	106.16	112.80
13	1	45	ILE	N-CA-C	5.76	116.78	108.48
9	W	26	GLY	N-CA-C	-5.75	102.99	111.03
12	L	146	LEU	N-CA-C	5.73	118.76	110.28
6	T	240	ILE	N-CA-C	-5.72	106.22	112.80
2	P	161	LYS	N-CA-C	-5.72	104.50	112.45
7	U	16	SER	N-CA-C	-5.71	102.92	110.40
9	I	95	TYR	N-CA-C	-5.71	99.98	109.46
12	Z	146	LEU	N-CA-C	5.70	118.71	110.28
9	W	95	TYR	N-CA-C	-5.69	100.02	109.46
13	1	-2	THR	N-CA-C	5.68	118.33	109.52
13	M	-2	THR	N-CA-C	5.68	118.47	109.50
3	Q	137	LEU	N-CA-C	-5.66	99.67	108.90
7	G	13	THR	N-CA-C	5.66	118.39	109.39
2	B	238	ILE	N-CA-C	-5.66	106.80	113.42
7	U	13	THR	N-CA-C	5.64	118.36	109.39
9	W	142	TYR	N-CA-C	5.64	118.45	110.50
11	Y	57	THR	N-CA-C	-5.62	105.23	111.36
9	W	94	PRO	N-CA-C	5.62	120.05	111.34
13	M	45	ILE	N-CA-C	5.62	116.57	108.48
10	X	122	LEU	N-CA-C	5.61	117.30	108.55
9	W	117	GLY	N-CA-C	5.61	122.49	114.64
9	I	94	PRO	N-CA-C	5.60	120.02	111.34
12	L	49	ALA	N-CA-C	5.54	118.03	111.33
12	Z	129	ALA	N-CA-C	5.53	117.75	111.11
10	J	25	SER	N-CA-C	5.53	118.47	109.24
9	I	117	GLY	N-CA-C	5.52	122.37	114.64
9	W	23	GLN	CB-CA-C	-5.52	110.23	116.63
10	J	122	LEU	CA-C-N	5.47	124.82	118.85
10	J	122	LEU	C-N-CA	5.47	124.82	118.85
3	Q	22	PHE	N-CA-C	5.47	118.75	111.75
13	1	9	ASP	N-CA-C	5.46	117.93	111.33
2	B	137	ILE	N-CA-C	-5.44	99.80	107.75
13	M	165	ARG	N-CA-C	5.43	120.18	113.50
10	X	122	LEU	CA-C-N	5.42	124.76	118.85
10	X	122	LEU	C-N-CA	5.42	124.76	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	94	PRO	N-CA-C	5.41	119.53	111.41
12	Z	183	GLY	N-CA-C	5.41	117.02	111.56
11	K	47	GLY	O-C-N	-5.41	115.67	122.70
2	P	72	ASP	N-CA-C	-5.38	106.71	113.28
12	L	129	ALA	N-CA-C	5.38	117.57	111.11
7	U	220	LYS	N-CA-C	5.37	116.58	108.46
11	Y	22	ALA	N-CA-C	-5.37	96.34	107.67
9	I	114	ASP	N-CA-C	-5.37	102.04	110.36
13	M	9	ASP	N-CA-C	5.36	117.81	111.33
12	Z	94	PRO	N-CA-C	5.33	119.68	111.21
3	C	137	LEU	N-CA-C	-5.33	99.61	108.34
7	G	220	LYS	N-CA-C	5.31	116.48	108.46
12	Z	49	ALA	N-CA-C	5.28	117.72	111.33
11	K	98	GLY	N-CA-C	-5.27	100.70	113.18
6	T	22	PHE	N-CA-C	5.27	118.49	111.75
1	A	78	TYR	N-CA-C	5.26	116.00	108.74
7	U	17(B)	LYS	N-CA-C	-5.26	105.55	111.28
11	K	57	THR	N-CA-C	-5.25	105.63	111.36
7	G	87	ASN	N-CA-C	-5.25	105.45	111.07
1	O	78	TYR	N-CA-C	5.25	115.98	108.74
4	R	129	SER	N-CA-C	5.24	117.73	111.71
11	K	22	ALA	N-CA-C	-5.22	96.65	107.67
11	K	131	GLN	N-CA-C	5.22	117.38	111.11
14	2	22	THR	N-CA-C	-5.21	96.80	107.70
12	L	23	ASP	CB-CA-C	-5.21	110.14	117.23
9	I	178	ILE	N-CA-C	5.21	115.47	108.17
7	G	17(B)	LYS	N-CA-C	-5.21	105.72	111.71
7	U	87	ASN	N-CA-C	-5.20	105.50	111.07
12	Z	145	TYR	N-CA-C	5.20	117.96	109.59
2	B	107	ILE	N-CA-C	5.19	114.04	108.95
12	L	183	GLY	N-CA-C	5.19	116.80	111.56
9	W	143	GLU	CA-C-N	5.19	125.47	119.92
9	W	143	GLU	C-N-CA	5.19	125.47	119.92
2	B	203	ASP	N-CA-C	-5.18	106.80	113.02
11	Y	98	GLY	N-CA-C	-5.18	100.90	113.18
12	Z	23	ASP	CB-CA-C	-5.18	110.18	117.23
5	E	42	SER	N-CA-C	-5.18	103.78	108.75
6	T	145	GLY	N-CA-C	5.17	119.15	111.76
9	I	143	GLU	CA-C-N	5.16	125.44	119.92
9	I	143	GLU	C-N-CA	5.16	125.44	119.92
9	I	23	GLN	CB-CA-C	-5.15	110.66	116.63
2	P	137	ILE	N-CA-C	-5.14	100.24	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	94	PRO	N-CA-C	5.14	119.12	111.41
2	B	109	VAL	N-CA-C	5.13	115.75	110.36
5	E	22	PHE	N-CA-C	5.13	116.87	111.28
3	Q	70	ILE	N-CA-C	-5.12	106.15	111.58
14	N	17	ASP	N-CA-C	-5.12	103.29	110.35
11	Y	131	GLN	N-CA-C	5.11	117.24	111.11
4	D	129	SER	N-CA-C	5.10	117.74	111.82
10	J	174	ILE	N-CA-C	-5.09	101.04	108.17
11	Y	116	ASP	N-CA-C	-5.08	107.03	113.18
12	L	94	PRO	N-CA-C	5.08	119.28	111.21
6	F	22	PHE	N-CA-C	5.07	118.24	111.75
6	T	63	LYS	N-CA-C	5.07	119.49	112.45
12	L	117	GLY	N-CA-C	5.05	121.49	114.92
13	1	3	VAL	N-CA-C	-5.05	100.25	107.78
13	1	35	ILE	N-CA-C	5.04	112.99	107.60
13	1	165	ARG	N-CA-C	5.04	119.70	113.50
6	F	63	LYS	N-CA-C	5.01	119.42	112.45

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	53	0
1	O	1915	0	1926	57	0
2	B	1904	0	1901	86	0
2	P	1904	0	1901	80	0
3	C	1890	0	1900	90	0
3	Q	1890	0	1900	86	0
4	D	1861	0	1836	48	0
4	R	1861	0	1836	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1795	0	1797	91	0
5	S	1795	0	1797	89	0
6	F	1896	0	1886	64	0
6	T	1896	0	1886	62	0
7	G	1921	0	1910	76	0
7	U	1921	0	1910	83	0
8	H	1684	0	1688	52	0
8	V	1684	0	1688	50	0
9	I	1581	0	1574	50	0
9	W	1581	0	1574	46	0
10	J	1585	0	1590	68	0
10	X	1585	0	1590	79	0
11	K	1644	0	1595	55	0
11	Y	1644	0	1595	58	0
12	L	1757	0	1711	51	0
12	Z	1757	0	1711	58	0
13	1	1824	0	1832	57	0
13	M	1824	0	1832	61	0
14	2	1512	0	1481	40	0
14	N	1512	0	1481	39	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	2	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
17	H	51	0	0	3	0
17	I	67	0	0	4	0
17	J	54	0	0	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	O	33	0	0	1	0
17	P	29	0	0	2	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	12	0
17	Y	50	0	0	6	0
17	Z	51	0	0	3	0
All	All	51030	0	49370	1604	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 16.

All (1604) 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:168:MET:HE3	10:X:168:MET:HE3	1.26	1.15
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.08	1.14
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.11	1.08
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.15	1.08
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.15	1.06
11:K:207:ASN:ND2	10:X:144:PRO:HG3	1.73	1.04
7:U:96:ALA:HA	7:U:107:MET:HE2	1.38	1.04
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	1.74	1.03
7:G:96:ALA:HA	7:G:107:MET:HE2	1.38	1.01
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.07	0.93
5:E:207:LEU:HD23	5:E:207:LEU:H	1.31	0.93
2:B:202:THR:HG22	2:B:204:SER:H	1.31	0.92
3:C:163:GLN:NE2	3:C:164:THR:H	1.67	0.92
9:I:29:ASN:HD21	11:Y:208:ASN:HD22	1.13	0.92
3:C:185:THR:HG22	3:C:187:GLU:H	1.33	0.92
11:K:208:ASN:HD22	9:W:29:ASN:HD21	1.12	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
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.36	0.88
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.74	0.88
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.54	0.88
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.84	0.88
3:Q:65:SER:HB2	17:Q:303:HOH:O	1.74	0.87
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.57	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:C:185:THR:HB	3:C:188:GLU:HG2	1.58	0.84
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.57	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:163:GLN:HE21	3:C:164:THR:H	0.87	0.81
10:J:133:TYR:HE1	17:X:876:HOH:O	1.63	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:HD2	11:K:10(B):LYS:N	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
10:J:168:MET:CE	10:X:168:MET:HE3	2.10	0.79
10:J:168:MET:HE3	10:X:168:MET:CE	2.12	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
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.31	0.77
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.81	0.77
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.65	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.68	0.74
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.35	0.74
10:X:-1:MET:HG2	10:X:1:ASP:H	1.51	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
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.88	0.73
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:219:GLU:HG2	2:B:21(E):VAL:H	1.53	0.73
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.97	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:97:ASN:HD21	12:Z:61:ASN:HD21	1.36	0.73
5:S:198:SER:HA	5:S:201:LEU:HG	1.70	0.73
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.38	0.72
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.90	0.72
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.19	0.72
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.02	0.72
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.72	0.72
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.71	0.72
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.70	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
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.73	0.71
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.72	0.71
14:2:107:LYS:HG2	14:2:108:GLY:H	1.55	0.71
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:166:HIS:HD2	12:L:168:GLN:H	1.37	0.71
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.20	0.70
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.70	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
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.56	0.70
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.55	0.70
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.36	0.70
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.06	0.70
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.74	0.70
14:N:51:ASP:O	14:N:55:ILE:HG12	1.90	0.70
4:R:121:LEU:HB2	17:R:853:HOH:O	1.90	0.70
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.56	0.70
1:A:179:ARG:HH11	1:A:179:ARG:HB3	1.55	0.70
7:U:86:ARG:HD2	17:U:248:HOH:O	1.90	0.70
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.26	0.70
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.55	0.70
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.72	0.70
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.03	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
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.56	0.70
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.21	0.70
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.56	0.69
13:M:40:ASN:H	13:M:40:ASN:HD22	1.39	0.69
2:P:121:GLN:O	2:P:124:THR:HB	1.91	0.69
13:1:14(A):VAL:HG23	13:1:14(A):VAL:O	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:C:33:ARG:NH1	3:C:33:ARG:HB2	2.08	0.69
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.75	0.69
4:D:186:LEU:O	4:D:190:GLU:HG3	1.94	0.68
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	1.91	0.68
3:C:232:TYR:O	3:C:236:ILE:HG12	1.94	0.68
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.76	0.68
2:P:71:ASN:ND2	2:P:72:ASP:H	1.91	0.68
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.06	0.68
14:N:107:LYS:HG2	14:N:108:GLY:H	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.76	0.68
5:S:123:ASN:HD22	5:S:123:ASN:N	1.92	0.68
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.76	0.68
13:1:40:ASN:H	13:1:40:ASN:HD22	1.39	0.68
3:C:185:THR:HG22	3:C:187:GLU:N	2.08	0.67
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.58	0.67
5:S:227:GLU:CD	5:S:227:GLU:H	2.01	0.67
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.75	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:HE21	1:A:33:GLN:HA	1.60	0.67
5:E:227:GLU:CD	5:E:227:GLU:H	2.01	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
1:A:4:MET:SD	1:A:5:THR:N	2.58	0.67
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.77	0.67
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.76	0.67
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.08	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
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.59	0.67
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.77	0.67
7:U:198:ILE:HG23	7:U:203:THR:O	1.95	0.67
10:X:-1:MET:HG2	10:X:1:ASP:N	2.10	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
2:B:6:ARG:HB2	5:E:127:TYR:OH	1.96	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
7:G:59:LEU:O	7:G:61:PRO:HD3	1.95	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
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.77	0.66
6:F:237:GLN:O	6:F:240:ILE:HG22	1.97	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
11:K:99:THR:HG22	11:K:113:VAL:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:207:LEU:HD23	5:S:207:LEU:N	2.08	0.65
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.77	0.65
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.32	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
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.61	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
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.10	0.65
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.79	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
1:A:97:HIS:HD2	8:H:61:SER:OG	1.81	0.64
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.08	0.64
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.80	0.64
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.44	0.64
7:U:96:ALA:HA	7:U:107:MET:CE	2.23	0.64
8:V:172:ASN:HD22	8:V:193:THR:HA	1.63	0.64
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.28	0.64
3:Q:170:LYS:HB2	17:Q:833:HOH:O	1.97	0.64
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.22	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
9:I:6:MET:HE3	9:I:155:ILE:HD12	1.80	0.64
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.23	0.64
5:E:123:ASN:N	5:E:123:ASN:HD22	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
17:B:565:HOH:O	3:C:33:ARG:HD2	1.98	0.63
5:E:207:LEU:HD23	5:E:207:LEU:N	2.08	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
6:F:203:GLU:O	6:F:206:LYS:HD2	1.99	0.63
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.33	0.63
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.97	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
7:U:8:TYR:C	7:U:10:ARG:H	2.07	0.63
4:R:53:ARG:O	4:R:53:ARG:HG2	1.99	0.63
5:S:227:GLU:CD	5:S:227:GLU:N	2.57	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
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.00	0.62
2:P:185:LYS:HD3	2:P:186:VAL:N	2.14	0.62
3:Q:241:GLN:C	3:Q:243:GLN:H	2.07	0.62
7:U:38:LEU:HD23	7:U:197:MET:HE3	1.81	0.62
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.80	0.62
1:O:121:GLN:O	1:O:124:THR:HB	1.99	0.62
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.00	0.62
2:B:41:MET:HE3	17:B:253:HOH:O	1.99	0.62
4:D:112:LEU:C	4:D:112:LEU:HD13	2.24	0.62
2:B:185:LYS:HD3	2:B:186:VAL:N	2.15	0.61
2:B:202:THR:HG22	2:B:204:SER:N	2.11	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
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.35	0.61
7:U:233:LEU:O	7:U:236:ILE:HG13	2.00	0.61
8:H:81:GLN:O	8:H:85:GLN:HG3	1.99	0.61
1:O:60:MET:HE3	1:O:63:THR:HG21	1.81	0.61
13:1:149:GLN:H	13:1:149:GLN:NE2	1.98	0.61
3:C:241:GLN:C	3:C:243:GLN:H	2.07	0.61
6:F:54:ILE:HG12	6:F:208:PHE:HA	1.82	0.61
13:M:149:GLN:NE2	13:M:149:GLN:H	1.99	0.61
6:T:186:ALA:O	6:T:190:VAL:HG23	2.00	0.61
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.82	0.61
9:W:137:MET:HE2	9:W:161:ASN:HB2	1.81	0.61
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.31	0.61
13:1:41:THR:OG1	13:1:76:PRO:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.01	0.61
5:E:227:GLU:CD	5:E:227:GLU:N	2.58	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
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.15	0.61
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.83	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
9:W:6:MET:HE3	9:W:155:ILE:HD12	1.82	0.61
1:A:60:MET:HE3	1:A:63:THR:HG21	1.83	0.61
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.30	0.61
4:R:112:LEU:HD13	4:R:112:LEU:C	2.26	0.60
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
9:I:137:MET:HE2	9:I:161:ASN:HB2	1.82	0.60
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.02	0.60
2:P:112:LEU:C	2:P:112:LEU:HD23	2.26	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
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.83	0.60
6:T:176:LEU:O	6:T:180:VAL:HG23	2.01	0.60
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	2.01	0.60
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.67	0.60
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.13	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
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.67	0.60
10:X:156:LYS:O	10:X:160:GLN:HG3	2.02	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
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.37	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
7:U:67:ILE:HD13	7:U:211:GLU:CD	2.27	0.60
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.17	0.60
11:Y:31:VAL:HG11	15:4:5:ABN:C3	2.32	0.60
7:G:186:TRP:O	7:G:190:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.37	0.59
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.83	0.59
7:G:8:TYR:C	7:G:10:ARG:H	2.08	0.59
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.83	0.59
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.85	0.59
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.02	0.59
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.31	0.59
10:X:3:ILE:HB	17:X:1164:HOH:O	2.02	0.59
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.37	0.59
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.82	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
2:B:15:PHE:H	3:C:23:GLN:NE2	1.89	0.59
10:J:133:TYR:HE2	10:J:166:MET:SD	2.26	0.59
10:J:144:PRO:CG	11:Y:207:ASN:HD21	1.99	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
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.03	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
7:G:77:VAL:CG1	7:G:137:THR:HB	2.33	0.59
5:S:194:VAL:O	5:S:197:ILE:HG22	2.03	0.59
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.02	0.59
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.03	0.59
7:G:67:ILE:HD13	7:G:211:GLU:CD	2.27	0.59
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.49	0.59
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.28	0.59
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.50	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
4:D:53:ARG:O	4:D:53:ARG:HG2	2.02	0.58
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.85	0.58
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.02	0.58
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.84	0.58
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.00	0.58
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.03	0.58
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.38	0.58
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.84	0.58
4:D:122:ARG:HH11	4:D:122:ARG:HG2	1.68	0.58
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.04	0.58
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.18	0.58
2:P:202:THR:HG22	2:P:204:SER:N	2.10	0.58
5:S:73:HIS:HE1	5:S:107:LEU:O	1.86	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
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.02	0.58
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.17	0.58
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.86	0.58
11:K:141:ASN:HD21	10:X:141:HIS:CE1	2.21	0.58
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.85	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
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.50	0.58
14:N:34:LEU:CD1	14:N:176:VAL:HG23	2.33	0.58
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.04	0.58
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.85	0.58
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.04	0.58
2:B:112:LEU:HD23	2:B:112:LEU:C	2.28	0.58
8:H:148:LYS:O	8:H:152:ILE:HG12	2.04	0.58
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.67	0.58
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.16	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
9:I:90:ARG:HD2	17:I:1159:HOH:O	2.04	0.57
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.34	0.57
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.86	0.57
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.29	0.57
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.86	0.57
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.86	0.57
12:L:21:ILE:C	12:L:21:ILE:HD12	2.28	0.57
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.04	0.57
8:V:148:LYS:O	8:V:152:ILE:HG12	2.03	0.57
9:W:192:ARG:HG3	17:W:201:HOH:O	2.03	0.57
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.04	0.57
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.19	0.57
10:J:52:THR:CG2	10:J:53:VAL:N	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:10(B):LYS:HZ2	10:J:10(B):LYS:HB2	1.69	0.57
3:C:191:LYS:HG3	3:C:236:ILE:HD11	1.85	0.57
6:F:176:LEU:O	6:F:180:VAL:HG23	2.04	0.57
12:Z:79:ALA:O	12:Z:83:ILE:HG12	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:136:SER:HB2	11:Y:161:ALA:HB1	1.87	0.57
12:L:145:TYR:CD1	12:L:146:LEU:N	2.72	0.57
3:Q:191:LYS:HG3	3:Q:236:ILE:HD11	1.87	0.57
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.40	0.57
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.70	0.57
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.73	0.57
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.85	0.57
10:X:52:THR:CG2	10:X:53:VAL:N	2.68	0.57
6:F:95:GLU:HG2	6:F:115:ARG:CB	2.32	0.57
2:P:41:MET:HE3	17:P:254:HOH:O	2.05	0.57
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.87	0.57
11:K:67:GLU:OE2	17:K:959:HOH:O	2.17	0.56
11:K:161:ALA:HB1	10:X:136:SER:HB2	1.86	0.56
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.05	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:X:133:TYR:HE2	10:X:166:MET:SD	2.27	0.56
3:C:46:VAL:O	3:C:215:VAL:HG12	2.04	0.56
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.70	0.56
10:J:136:SER:N	17:J:198:HOH:O	2.31	0.56
11:Y:104:TYR:CE1	11:Y:180:GLU:OE2	2.57	0.56
5:E:73:HIS:HE1	5:E:107:LEU:O	1.88	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
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.05	0.56
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.85	0.56
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.41	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
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.05	0.56
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.05	0.56
13:M:17:ASP:HA	13:M:173:PHE:CB	2.36	0.56
13:1:46:SER:OG	13:1:98:ALA:HB3	2.06	0.56
8:V:113:ILE:HG13	8:V:119:THR:HG22	1.88	0.56
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.04	0.56
13:1:152:GLU:O	13:1:156:VAL:HG23	2.06	0.56
1:A:48:ILE:HD12	1:A:48:ILE:O	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
7:U:87:ASN:C	7:U:87:ASN:HD22	2.14	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
9:I:27:VAL:O	17:I:510:HOH:O	2.18	0.55
1:A:69:LEU:C	1:A:69:LEU:HD23	2.31	0.55
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.87	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
2:P:231:ASP:O	2:P:235:LYS:HG2	2.07	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
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
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.21	0.55
12:L:135:MET:CE	9:W:165:ARG:NH2	2.69	0.55
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.89	0.55
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.07	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
3:C:235:GLN:O	3:C:239:GLU:HG2	2.07	0.55
10:J:44:SER:OG	10:J:100:LEU:HB2	2.07	0.55
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.41	0.55
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.32	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
14:2:34:LEU:CD1	14:2:176:VAL:HG23	2.34	0.55
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.88	0.55
6:F:127:ASN:C	6:F:127:ASN:HD22	2.14	0.55
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.88	0.55
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.22	0.55
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.89	0.55
10:X:52:THR:HG23	10:X:53:VAL:N	2.22	0.55
3:C:57:LYS:O	3:C:58:LEU:HB2	2.07	0.54
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:46:SER:OG	13:M:98:ALA:HB3	2.07	0.54
14:N:36:ARG:HD2	13:1:211:ILE:HD11	1.88	0.54
12:Z:96:TYR:CD1	15:4:2:TY5:H49	2.42	0.54
11:K:86:LEU:C	11:K:86:LEU:HD13	2.31	0.54
10:X:36:GLN:HG3	10:X:184:ILE:CD1	2.37	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
3:C:227:GLU:N	3:C:227:GLU:OE1	2.40	0.54
11:K:142:TYR:O	11:K:143:LYS:HD2	2.06	0.54
1:O:69:LEU:C	1:O:69:LEU:HD23	2.32	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
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
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.90	0.54
8:V:84:LYS:HG3	8:V:85:GLN:N	2.23	0.54
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.89	0.54
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.43	0.54
8:V:4:VAL:HG22	8:V:159:ILE:CD1	2.38	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
12:Z:114:ASP:CB	12:Z:118:SER:HB3	2.35	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
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.06	0.54
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.43	0.54
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.43	0.54
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.06	0.54
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.08	0.54
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.90	0.54
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.72	0.54
14:2:107:LYS:HG2	14:2:108:GLY:N	2.22	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
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
4:R:207:LEU:C	4:R:207:LEU:HD23	2.33	0.53
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.08	0.53
3:C:52:ARG:HD2	3:C:208:LYS:O	2.09	0.53
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:127:ASN:C	6:T:127:ASN:HD22	2.14	0.53
13:1:35:ILE:HG12	13:1:56:GLU:HG2	1.91	0.53
7:G:87:ASN:C	7:G:87:ASN:HD22	2.16	0.53
12:L:114:ASP:CB	12:L:118:SER:HB3	2.37	0.53
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.89	0.53
14:N:176:VAL:HG12	14:N:178:LEU:CD1	2.38	0.53
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.37	0.53
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.41	0.53
1:A:177:GLU:HG2	2:B:58:LEU:HD22	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
4:D:207:LEU:HD23	4:D:207:LEU:C	2.32	0.53
9:I:48:LEU:HG	9:I:50:THR:HG22	1.91	0.53
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.09	0.53
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.90	0.53
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.08	0.53
7:G:121:GLN:O	7:G:124:THR:HB	2.07	0.53
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.09	0.53
14:N:107:LYS:CG	14:N:108:GLY:H	2.21	0.53
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.08	0.53
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.09	0.53
4:R:79:SER:HB3	4:R:165:ILE:HD12	1.91	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
14:2:175:MET:HE3	14:2:18(B):PHE:CE2	2.44	0.53
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.24	0.53
13:M:40:ASN:HD22	13:M:40:ASN:N	1.99	0.53
14:N:175:MET:HE3	14:N:18(B):PHE:CE2	2.44	0.53
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.90	0.53
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.91	0.53
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.09	0.53
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.91	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
1:A:150:GLN:O	1:A:157:TYR:HA	2.09	0.52
14:N:107:LYS:HG2	14:N:108:GLY:N	2.23	0.52
4:R:85:ALA:O	4:R:89:ILE:HG12	2.09	0.52
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.09	0.52
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.75	0.52
5:E:41:ARG:NH1	5:E:42:SER:O	2.42	0.52
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.91	0.52
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.38	0.52
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.90	0.52
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.90	0.52
12:Z:99:THR:HG23	17:Z:231:HOH:O	2.09	0.52
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
1:O:150:GLN:O	1:O:157:TYR:HA	2.10	0.52
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.25	0.52
9:I:6:MET:CE	9:I:155:ILE:HA	2.40	0.52
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.74	0.52
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.42	0.52
5:S:69:LYS:HB3	17:S:528:HOH:O	2.09	0.52
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.23	0.52
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.24	0.52
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.09	0.52
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.40	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
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.44	0.52
14:2:176:VAL:HG12	14:2:178:LEU:CD1	2.39	0.52
11:K:73:ARG:NH2	11:K:104:TYR:O	2.43	0.52
5:S:77:SER:OG	5:S:137:LEU:HB2	2.10	0.52
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.90	0.52
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.91	0.52
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.09	0.52
13:M:57:ARG:HG2	13:M:57:ARG:HH11	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
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.92	0.52
11:K:10(A):ARG:HH11	11:K:10(A):ARG:HG2	1.75	0.52
4:R:175:GLU:HB3	4:R:196:ILE:HD13	1.92	0.52
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.92	0.52
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.92	0.52
2:B:78:VAL:HG22	2:B:136:PHE:CE2	2.45	0.51
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.93	0.51
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.44	0.51
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.93	0.51
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.75	0.51
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.40	0.51
9:W:143:GLU:CG	9:W:146:LEU:HD21	2.39	0.51
2:B:231:ASP:O	2:B:235:LYS:HG2	2.10	0.51
7:G:151:THR:HG22	7:G:157:TYR:CB	2.40	0.51
1:A:117:ALA:HB1	1:A:155:GLY:O	2.10	0.51
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
14:N:186:ARG:HD3	17:N:933:HOH:O	2.10	0.51
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.11	0.51
2:B:31:ILE:HD11	2:B:133:GLY:C	2.35	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:NH1	3:C:33:ARG:CB	2.73	0.51
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.93	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
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.92	0.51
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.51
2:P:31:ILE:HD11	2:P:133:GLY:C	2.35	0.51
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.10	0.51
7:U:77:VAL:HG12	7:U:137:THR:HB	1.91	0.51
3:C:66:LYS:HE2	3:C:78:PHE:CZ	2.46	0.51
8:H:116:HIS:HB2	17:H:324:HOH:O	2.11	0.51
13:M:35:ILE:HG12	13:M:56:GLU:HG2	1.92	0.51
5:S:86:ARG:HG3	5:S:86:ARG:HH11	1.76	0.51
9:W:6:MET:CE	9:W:155:ILE:HA	2.40	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
7:G:77:VAL:HG12	7:G:137:THR:HB	1.93	0.51
10:J:133:TYR:CE2	10:J:166:MET:SD	3.04	0.51
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.46	0.51
4:D:24:VAL:O	4:D:27:SER:HB3	2.11	0.51
10:J:-1:MET:CG	10:J:1:ASP:H	2.21	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
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.09	0.51
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.08	0.51
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.11	0.51
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.93	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
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
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.92	0.51
1:A:97:HIS:CD2	8:H:61:SER:OG	2.61	0.51
3:C:169:SER:HA	3:C:172:VAL:CG1	2.41	0.51
3:Q:66:LYS:HE2	3:Q:78:PHE:CZ	2.46	0.51
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.26	0.51
8:V:34:LEU:HB2	17:V:578:HOH:O	2.10	0.51
8:V:128:GLY:O	8:V:131:SER:HB2	2.11	0.51
10:X:2:ILE:HD13	10:X:170:PHE:CD2	2.46	0.51
2:B:27:ALA:O	2:B:31:ILE:HG12	2.11	0.50
3:C:168:ASN:O	3:C:172:VAL:HG12	2.11	0.50
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.41	0.50
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.93	0.50
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.11	0.50
11:K:7:ARG:HH11	11:K:108:PRO:HB2	1.76	0.50
5:S:18(D):ILE:HG12	5:S:18(D):ILE:O	2.11	0.50
13:1:57:ARG:HH11	13:1:57:ARG:HG2	1.76	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
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.41	0.50
7:U:228:ASN:HB3	17:U:242:HOH:O	2.10	0.50
4:D:85:ALA:O	4:D:89:ILE:HG12	2.12	0.50
7:G:8:TYR:C	7:G:10:ARG:N	2.70	0.50
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.12	0.50
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.42	0.50
4:R:42:THR:C	4:R:44:GLU:H	2.20	0.50
7:U:35:ILE:HD11	17:U:1201:HOH:O	2.12	0.50
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.47	0.50
3:C:175:PHE:O	3:C:179:ASN:HB2	2.12	0.50
7:G:67:ILE:HD13	7:G:211:GLU:HG2	1.93	0.50
8:H:72:ARG:HG3	8:H:72:ARG:HH11	1.76	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
13:1:146:THR:HA	17:1:323:HOH:O	2.12	0.50
3:C:158:SER:CB	4:D:59:LEU:HD21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:184:LEU:HD23	13:M:184:LEU:C	2.37	0.50
7:U:87:ASN:C	7:U:87:ASN:ND2	2.68	0.50
10:X:6:ILE:HD11	10:X:154:LEU:HD23	1.94	0.50
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.42	0.50
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.12	0.50
5:E:18(D):ILE:HG12	5:E:18(D):ILE:O	2.10	0.50
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.93	0.50
2:P:27:ALA:O	2:P:31:ILE:HG12	2.11	0.50
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.93	0.50
4:R:170:GLU:OE1	4:R:170:GLU:N	2.44	0.50
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.42	0.50
7:U:83:PRO:HG2	17:U:557:HOH:O	2.11	0.50
9:W:9:LYS:HD3	9:W:145:ASN:HD22	1.77	0.50
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.93	0.50
7:G:228:ASN:N	7:G:228:ASN:HD22	2.10	0.50
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.93	0.50
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.37	0.50
9:W:48:LEU:HG	9:W:50:THR:HG22	1.93	0.50
4:D:42:THR:C	4:D:44:GLU:H	2.19	0.50
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.46	0.50
5:E:86:ARG:HG3	5:E:86:ARG:HH11	1.76	0.50
5:E:160:LEU:CD2	6:F:59:LEU:HD12	2.42	0.50
10:J:6:ILE:HD11	10:J:154:LEU:HD23	1.94	0.50
12:L:113:PHE:N	12:L:113:PHE:CD1	2.80	0.50
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.47	0.50
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.47	0.50
13:1:184:LEU:C	13:1:184:LEU:HD23	2.37	0.50
5:E:139:ILE:HD12	5:E:215:VAL:HG12	1.93	0.50
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.39	0.50
12:L:-2:ASN:HA	12:L:21:ILE:O	2.12	0.50
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.10	0.50
3:Q:182:PRO:O	3:Q:184:ALA:N	2.45	0.50
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.47	0.50
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.93	0.50
5:S:134:VAL:O	5:S:153:PRO:HG3	2.11	0.50
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.94	0.50
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.94	0.50
6:F:35:THR:CG2	6:F:51:GLU:O	2.57	0.49
7:G:192:PHE:CD1	7:G:192:PHE:C	2.89	0.49
11:K:6:PHE:HA	11:K:123:ASP:O	2.12	0.49
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.47	0.49
3:C:185:THR:HG22	3:C:186:VAL:N	2.26	0.49
9:I:143:GLU:CG	9:I:146:LEU:HD21	2.41	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
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
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.27	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
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
1:A:48:ILE:HD11	1:A:213:ALA:HB3	1.94	0.49
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.77	0.49
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.47	0.49
7:U:192:PHE:CD1	7:U:192:PHE:C	2.89	0.49
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.94	0.49
10:X:190:PHE:C	10:X:192:ALA:H	2.20	0.49
5:E:4:PHE:CG	5:E:5:ARG:N	2.80	0.49
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.28	0.49
13:M:12:VAL:HG21	13:M:102:ALA:HB1	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
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.42	0.49
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.94	0.49
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.13	0.49
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.42	0.49
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.28	0.49
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.93	0.49
8:V:175:VAL:HG12	8:V:176:CYS:N	2.27	0.49
3:C:55:THR:C	3:C:56:LEU:HD22	2.38	0.49
3:C:197:LEU:O	3:C:201:VAL:HG23	2.12	0.49
5:E:77:SER:OG	5:E:137:LEU:HB2	2.11	0.49
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.94	0.49
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.60	0.49
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.27	0.49
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.42	0.49
4:R:24:VAL:O	4:R:27:SER:HB3	2.13	0.49
7:U:8:TYR:C	7:U:10:ARG:N	2.69	0.49
7:U:151:THR:HG22	7:U:157:TYR:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:172:ASN:HB3	8:V:192:LEU:O	2.13	0.49
10:X:-1:MET:CG	10:X:1:ASP:H	2.22	0.49
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.48	0.49
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.37	0.49
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.93	0.49
10:J:190:PHE:C	10:J:192:ALA:H	2.20	0.49
1:O:33:GLN:HE21	1:O:33:GLN:CA	2.21	0.49
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.56	0.49
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.93	0.49
6:T:18:ASP:OD2	6:T:18:ASP:N	2.39	0.49
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.61	0.49
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.94	0.49
2:B:163:ILE:HG13	2:B:164:SER:N	2.27	0.49
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.78	0.49
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.12	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
12:L:134:ILE:HD11	12:L:162:ALA:HB2	1.95	0.49
11:Y:104:TYR:HE1	11:Y:180:GLU:OE2	1.94	0.49
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.48	0.49
7:G:87:ASN:C	7:G:87:ASN:ND2	2.71	0.49
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.42	0.49
8:H:172:ASN:HB3	8:H:192:LEU:O	2.13	0.49
9:I:114:ASP:HB2	17:I:851:HOH:O	2.13	0.49
11:K:31:VAL:HG11	15:3:5:ABN:H3	1.95	0.49
13:M:35:ILE:HD12	13:M:35:ILE:N	2.28	0.49
11:Y:7:ARG:HH11	11:Y:108:PRO:HB2	1.77	0.49
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.13	0.49
13:1:35:ILE:N	13:1:35:ILE:HD12	2.28	0.49
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.43	0.48
5:S:123:ASN:N	5:S:123:ASN:ND2	2.61	0.48
13:1:104:VAL:CG2	13:1:178:ILE:HG22	2.40	0.48
13:1:113:VAL:HA	13:1:118:VAL:O	2.13	0.48
3:C:182:PRO:O	3:C:184:ALA:N	2.46	0.48
6:F:18:ASP:OD2	6:F:18:ASP:N	2.39	0.48
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.48	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
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.13	0.48
7:U:67:ILE:HD13	7:U:211:GLU:HG2	1.95	0.48
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.12	0.48
13:1:40:ASN:HD22	13:1:40:ASN:N	2.01	0.48
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.49	0.48
7:G:96:ALA:CA	7:G:107:MET:HE2	2.27	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
8:H:196:VAL:HG23	17:H:520:HOH:O	2.14	0.48
9:I:9:LYS:HD3	9:I:145:ASN:HD22	1.78	0.48
10:J:2:ILE:HD13	10:J:170:PHE:CD2	2.48	0.48
11:K:44:THR:OG1	11:K:100:MET:HB2	2.13	0.48
7:U:96:ALA:CA	7:U:107:MET:HE2	2.25	0.48
12:Z:59:PHE:O	12:Z:62:SER:HB3	2.14	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:40:ASN:N	13:M:40:ASN:ND2	2.62	0.48
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.48	0.48
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.95	0.48
2:P:67:LEU:HD23	2:P:213:ALA:HB2	1.95	0.48
3:C:76:LEU:HD23	3:C:76:LEU:C	2.39	0.48
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.12	0.48
3:Q:112:LEU:O	3:Q:112:LEU:HD13	2.14	0.48
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.94	0.48
7:U:109:CYS:HB3	17:U:1330:HOH:O	2.14	0.48
14:2:147:SER:OG	14:2:150:GLU:HG3	2.13	0.48
4:D:170:GLU:OE1	4:D:170:GLU:N	2.44	0.48
5:E:160:LEU:HD23	6:F:59:LEU:HA	1.94	0.48
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.10	0.48
13:M:113:VAL:HA	13:M:118:VAL:O	2.14	0.48
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.95	0.48
6:T:35:THR:CG2	6:T:51:GLU:O	2.58	0.48
7:U:49:ILE:CD1	7:U:212:VAL:HG22	2.44	0.48
2:B:15:PHE:N	3:C:23:GLN:HE22	1.91	0.48
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.56	0.48
6:F:173:LYS:O	6:F:177:GLU:HG3	2.14	0.48
8:H:200:LYS:HE3	9:I:140:SER:O	2.14	0.48
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.62	0.48
5:S:4:PHE:CG	5:S:5:ARG:N	2.81	0.48
12:Z:146:LEU:HA	17:Z:757:HOH:O	2.13	0.48
5:E:76:LEU:HD23	5:E:76:LEU:C	2.39	0.47
10:J:168:MET:CE	10:X:168:MET:CE	2.85	0.47
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:1:104:VAL:HG23	13:1:178:ILE:CG2	2.42	0.47
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.49	0.47
5:E:167:ALA:HB3	17:E:1131:HOH:O	2.13	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:N	12:L:177:ILE:HD12	2.29	0.47
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.27	0.47
5:S:201:LEU:O	5:S:202:ARG:HB2	2.15	0.47
7:U:107:MET:CE	7:U:112:LEU:HD13	2.44	0.47
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.44	0.47
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.78	0.47
10:J:168:MET:HG2	10:X:168:MET:CE	2.45	0.47
11:K:4:LEU:HD22	11:K:4:LEU:C	2.40	0.47
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.02	0.47
12:L:59:PHE:O	12:L:62:SER:HB3	2.14	0.47
1:O:97:HIS:CD2	8:V:61:SER:OG	2.64	0.47
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.49	0.47
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.96	0.47
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.49	0.47
13:1:40:ASN:H	13:1:40:ASN:ND2	2.11	0.47
5:E:134:VAL:O	5:E:153:PRO:HG3	2.14	0.47
5:E:179:THR:HG22	5:E:179:THR:O	2.15	0.47
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.95	0.47
7:G:82:ILE:N	7:G:83:PRO:HD2	2.30	0.47
7:G:158:VAL:HG22	7:G:159:GLY:N	2.30	0.47
10:J:36:GLN:HG3	10:J:184:ILE:HD12	1.96	0.47
10:J:146:MET:HE1	10:J:154:LEU:HD22	1.95	0.47
2:P:122:GLY:C	2:P:124:THR:H	2.22	0.47
3:Q:76:LEU:C	3:Q:76:LEU:HD23	2.39	0.47
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.50	0.47
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.11	0.47
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.76	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
1:O:26:TYR:CE1	7:U:17:PRO:HA	2.50	0.47
14:N:159:LEU:O	14:N:163:ILE:HD13	2.14	0.47
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.49	0.47
5:S:150:GLU:O	5:S:157:VAL:HA	2.15	0.47
5:S:179:THR:O	5:S:179:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:10(B):LYS:HB2	10:X:10(B):LYS:NZ	2.29	0.47
11:Y:105:THR:HB	11:Y:10(B):LYS:CD	2.45	0.47
1:A:212:LEU:C	1:A:212:LEU:HD23	2.40	0.47
2:B:141:TYR:CD1	2:B:141:TYR:C	2.93	0.47
2:B:225:LYS:O	2:B:226:PRO:C	2.58	0.47
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.14	0.47
11:K:209:VAL:HG13	17:W:348:HOH:O	2.14	0.47
12:L:96:TYR:CE1	15:3:2:TY5:H49	2.49	0.47
12:L:114:ASP:O	12:L:115:PRO:C	2.57	0.47
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.15	0.47
5:S:76:LEU:C	5:S:76:LEU:HD23	2.40	0.47
6:T:127:ASN:HD22	6:T:128:SER:N	2.13	0.47
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.76	0.47
7:U:74:ILE:HD12	7:U:109:CYS:HA	1.96	0.47
8:V:72:ARG:HG3	8:V:72:ARG:HH11	1.79	0.47
10:X:76:PRO:HD2	17:X:275:HOH:O	2.15	0.47
10:X:146:MET:HE1	10:X:154:LEU:HD22	1.96	0.47
12:Z:96:TYR:CE1	15:4:2:TY5:H49	2.50	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
5:E:12:THR:CG2	5:E:124:THR:HA	2.42	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
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.41	0.47
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.15	0.47
7:U:82:ILE:N	7:U:83:PRO:HD2	2.30	0.47
8:V:152:ILE:HD11	8:V:177:VAL:CG2	2.45	0.47
9:W:101:VAL:O	9:W:110:ILE:HA	2.14	0.47
5:E:123:ASN:N	5:E:123:ASN:ND2	2.62	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.15	0.47
12:L:90:LYS:HE3	12:L:93:PHE:O	2.14	0.47
1:O:62:GLU:H	1:O:62:GLU:CD	2.22	0.47
2:P:141:TYR:CD1	2:P:141:TYR:C	2.92	0.47
9:W:155:ILE:HG23	9:W:156:SER:N	2.30	0.47
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.14	0.47
11:Y:104:TYR:CD1	11:Y:180:GLU:HG3	2.49	0.47
13:1:112:TYR:O	13:1:119:THR:HA	2.15	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
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:150:GLU:O	5:E:157:VAL:HA	2.14	0.46
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.96	0.46
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.97	0.46
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.45	0.46
14:N:14:LEU:O	14:N:175:MET:HA	2.15	0.46
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.50	0.46
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.97	0.46
6:F:127:ASN:HD22	6:F:128:SER:N	2.13	0.46
13:M:1:THR:HG22	17:M:214:HOH:O	2.16	0.46
12:Z:134:ILE:HD13	12:Z:158:SER:HB3	1.97	0.46
12:Z:134:ILE:HD11	12:Z:162:ALA:HB2	1.97	0.46
14:2:107:LYS:CG	14:2:108:GLY:H	2.21	0.46
14:2:159:LEU:O	14:2:163:ILE:HD13	2.14	0.46
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.44	0.46
7:G:49:ILE:CD1	7:G:212:VAL:HG22	2.46	0.46
7:G:74:ILE:HD12	7:G:109:CYS:HA	1.96	0.46
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.97	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
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.46	0.46
7:U:17(C):LYS:HB2	7:U:17(C):LYS:HE3	1.78	0.46
8:V:196:VAL:HG23	17:V:652:HOH:O	2.15	0.46
10:X:13:ILE:HD12	10:X:13:ILE:N	2.30	0.46
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.51	0.46
6:F:103:TYR:O	6:F:104:LYS:HB3	2.16	0.46
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.45	0.46
9:I:14:ILE:HG12	9:I:34:ILE:HD12	1.98	0.46
6:T:192:GLN:NE2	6:T:195:LYS:HE2	2.30	0.46
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.97	0.46
10:X:35:ARG:NH1	10:X:57:GLU:OE2	2.44	0.46
11:Y:135:TYR:CB	17:Y:593:HOH:O	2.63	0.46
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.45	0.46
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.51	0.46
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.82	0.46
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.31	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
7:U:158:VAL:HG22	7:U:159:GLY:N	2.31	0.46
10:X:34:THR:CG2	10:X:176:LYS:NZ	2.78	0.46
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.81	0.46
13:1:19:LEU:HD12	13:1:28:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.45	0.46
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.51	0.46
5:E:35:SER:HB3	5:E:66:LYS:HZ3	1.79	0.46
6:F:192:GLN:NE2	6:F:195:LYS:HE2	2.31	0.46
7:G:89:ALA:O	7:G:93:LYS:HG3	2.16	0.46
10:J:2:ILE:HD13	10:J:170:PHE:CG	2.50	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
10:X:113:ILE:HA	10:X:118:THR:O	2.16	0.46
10:X:156:LYS:HE2	10:X:160:GLN:NE2	2.31	0.46
2:B:71:ASN:ND2	2:B:72:ASP:N	2.61	0.46
3:C:173:ARG:O	3:C:177:GLU:HG3	2.15	0.46
5:E:231:LYS:H	5:E:231:LYS:HD2	1.81	0.46
6:F:143:LYS:HB2	17:F:469:HOH:O	2.15	0.46
13:M:19:LEU:HD12	13:M:28:PHE:O	2.15	0.46
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.97	0.46
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.13	0.46
3:Q:241:GLN:C	3:Q:243:GLN:N	2.73	0.46
7:U:203:THR:HG22	7:U:204:GLU:O	2.16	0.46
11:Y:31:VAL:HG11	15:4:5:ABN:H3	1.97	0.46
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.81	0.46
5:E:76:LEU:HD23	5:E:76:LEU:O	2.16	0.46
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.16	0.46
13:M:112:TYR:C	13:M:112:TYR:CD2	2.94	0.46
2:P:24:VAL:HG11	2:P:154:SER:HB3	1.98	0.46
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.79	0.46
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.51	0.46
5:E:78:LEU:HD12	5:E:78:LEU:C	2.41	0.46
10:J:168:MET:CE	10:X:168:MET:HG2	2.46	0.46
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.51	0.46
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.51	0.46
1:O:233:LEU:O	1:O:236:LEU:HB2	2.16	0.46
6:T:157:TYR:CD1	6:T:157:TYR:C	2.94	0.46
6:T:173:LYS:O	6:T:177:GLU:HG3	2.16	0.46
7:U:228:ASN:N	7:U:228:ASN:HD22	2.12	0.46
1:A:62:GLU:CD	1:A:62:GLU:H	2.23	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
4:D:59:LEU:HD13	4:D:59:LEU:C	2.41	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:208:ASN:O	11:K:209:VAL:C	2.59	0.45
1:O:110:LYS:HG2	17:O:376:HOH:O	2.16	0.45
2:B:24:VAL:HG11	2:B:154:SER:HB3	1.97	0.45
3:C:159:SER:O	4:D:59:LEU:HD22	2.16	0.45
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.79	0.45
6:F:214:TRP:CH2	6:F:21(A):GLU:HB3	2.50	0.45
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.97	0.45
13:M:34:LEU:C	13:M:35:ILE:HD12	2.41	0.45
13:M:104:VAL:HG23	13:M:178:ILE:CG2	2.43	0.45
5:S:231:LYS:H	5:S:231:LYS:HD2	1.80	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
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.25	0.45
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.32	0.45
13:1:14(C):ARG:HH11	13:1:14(C):ARG:CG	2.27	0.45
1:A:20(A):THR:C	1:A:210:ILE:HD12	2.41	0.45
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.51	0.45
4:D:237:LEU:O	4:D:241:GLU:HG3	2.16	0.45
11:K:105:THR:HB	11:K:10(B):LYS:CD	2.45	0.45
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.98	0.45
2:P:71:ASN:ND2	2:P:72:ASP:N	2.63	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
5:S:38:VAL:HG12	5:S:39:GLY:N	2.31	0.45
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.82	0.45
8:V:3:ILE:HG13	8:V:100:ILE:HD12	1.99	0.45
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.52	0.45
14:2:85:GLU:O	14:2:89:GLU:HB2	2.17	0.45
14:2:116:GLY:HA3	17:2:192:HOH:O	2.16	0.45
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.98	0.45
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.98	0.45
9:I:113:PHE:HA	9:I:118:CYS:O	2.17	0.45
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.81	0.45
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.47	0.45
12:Z:160:THR:O	12:Z:164:GLU:HG2	2.17	0.45
13:1:34:LEU:C	13:1:35:ILE:HD12	2.41	0.45
2:B:67:LEU:HD23	2:B:213:ALA:HB2	1.99	0.45
5:E:38:VAL:HG12	5:E:39:GLY:N	2.32	0.45
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.82	0.45
9:I:155:ILE:HG23	9:I:156:SER:N	2.32	0.45
10:J:13:ILE:HD12	10:J:13:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:134:ILE:HD13	12:L:158:SER:HB3	1.99	0.45
1:O:161:LYS:N	2:P:58:LEU:O	2.45	0.45
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.99	0.45
5:S:40:LEU:N	5:S:40:LEU:HD23	2.32	0.45
5:S:78:LEU:C	5:S:78:LEU:HD12	2.41	0.45
10:X:52:THR:CG2	10:X:53:VAL:H	2.30	0.45
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.81	0.45
5:E:180:LEU:O	5:E:18(D):ILE:HG22	2.17	0.45
6:F:69:VAL:HG12	17:F:319:HOH:O	2.16	0.45
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.97	0.45
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.32	0.45
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.45
10:J:35:ARG:NH1	10:J:57:GLU:OE2	2.43	0.45
11:K:104:TYR:CD1	11:K:180:GLU:HG3	2.51	0.45
13:M:9:ASP:OD1	13:M:10:ASN:N	2.50	0.45
2:P:71:ASN:HD22	2:P:72:ASP:N	2.12	0.45
5:S:4:PHE:O	5:S:5:ARG:C	2.60	0.45
5:S:180:LEU:O	5:S:18(D):ILE:HG22	2.17	0.45
6:T:103:TYR:O	6:T:104:LYS:HB3	2.16	0.45
8:V:9:ASN:ND2	8:V:147:THR:HA	2.32	0.45
10:X:85:GLN:HB3	17:X:463:HOH:O	2.17	0.45
11:Y:114:ASP:OD1	11:Y:114:ASP:C	2.59	0.45
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.51	0.45
13:1:150:VAL:HG21	17:1:323:HOH:O	2.16	0.45
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.11	0.45
6:F:127:ASN:C	6:F:127:ASN:ND2	2.74	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
11:K:114:ASP:OD1	11:K:114:ASP:C	2.59	0.45
13:M:112:TYR:O	13:M:119:THR:HA	2.17	0.45
4:R:160:TYR:HA	5:S:59:SER:HA	1.98	0.45
5:S:52:LYS:O	5:S:63:TYR:HD2	2.00	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
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.98	0.45
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.98	0.45
9:I:29:ASN:ND2	11:Y:208:ASN:HD22	1.92	0.45
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.99	0.45
2:P:223:ILE:HD12	2:P:223:ILE:N	2.31	0.45
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.17	0.45
4:R:237:LEU:O	4:R:241:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD12	1:A:38:LEU:C	2.42	0.45
5:E:40:LEU:N	5:E:40:LEU:HD23	2.32	0.45
6:F:12:ASN:ND2	6:F:131:PRO:HD3	2.32	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
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.52	0.45
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.99	0.45
9:W:61:TYR:CD1	9:W:61:TYR:C	2.94	0.45
5:E:4:PHE:O	5:E:5:ARG:C	2.60	0.45
6:F:157:TYR:C	6:F:157:TYR:CD1	2.94	0.45
10:J:129:TYR:HB3	10:X:24:ILE:HD11	1.98	0.45
11:K:5:ALA:HA	11:K:13:ILE:O	2.16	0.45
11:K:208:ASN:HD22	9:W:29:ASN:ND2	1.92	0.45
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.98	0.45
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.81	0.45
5:S:12:THR:CG2	5:S:124:THR:HA	2.42	0.45
6:T:203:GLU:C	6:T:205:ASN:H	2.25	0.45
6:T:214:TRP:CH2	6:T:21(A):GLU:HB3	2.51	0.45
7:U:38:LEU:C	7:U:38:LEU:HD12	2.42	0.45
10:X:36:GLN:HG3	10:X:184:ILE:HD12	1.99	0.45
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.82	0.45
7:G:67:ILE:HD13	7:G:211:GLU:CG	2.47	0.44
9:I:6:MET:HE1	9:I:155:ILE:HA	1.99	0.44
1:O:38:LEU:HD12	1:O:38:LEU:C	2.42	0.44
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.99	0.44
4:R:65:GLU:HA	17:R:750:HOH:O	2.17	0.44
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.82	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
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.89	0.44
1:O:4:MET:CG	1:O:5:THR:H	2.29	0.44
1:O:20(A):THR:C	1:O:210:ILE:HD12	2.42	0.44
1:O:212:LEU:HD23	1:O:212:LEU:C	2.42	0.44
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.53	0.44
8:V:200:LYS:HE3	9:W:140:SER:O	2.17	0.44
10:X:135:PHE:CZ	17:X:622:HOH:O	2.57	0.44
11:Y:208:ASN:O	11:Y:209:VAL:C	2.60	0.44
12:Z:22:THR:O	12:Z:23:ASP:HB2	2.16	0.44
14:2:14:LEU:O	14:2:175:MET:HA	2.16	0.44
2:B:41:MET:HE1	3:C:60:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:9:ASN:ND2	8:H:147:THR:HA	2.33	0.44
4:R:59:LEU:C	4:R:59:LEU:HD13	2.43	0.44
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.53	0.44
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.48	0.44
7:U:136:LEU:O	7:U:150:LYS:HA	2.17	0.44
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.97	0.44
4:D:12(F):GLY:HA3	17:E:965:HOH:O	2.16	0.44
6:F:203:GLU:C	6:F:205:ASN:H	2.25	0.44
12:L:5:GLY:O	12:L:124:CYS:HA	2.17	0.44
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.82	0.44
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.17	0.44
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.53	0.44
2:B:122:GLY:C	2:B:124:THR:H	2.24	0.44
3:C:112:LEU:HD13	3:C:112:LEU:C	2.42	0.44
9:I:20:LEU:C	9:I:20:LEU:HD13	2.43	0.44
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.48	0.44
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.32	0.44
14:N:20:THR:HG23	14:N:31:THR:OG1	2.18	0.44
2:P:225:LYS:O	2:P:226:PRO:C	2.59	0.44
8:V:152:ILE:CD1	8:V:177:VAL:HG22	2.48	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
6:F:202:HIS:O	6:F:202:HIS:CG	2.71	0.44
7:G:136:LEU:O	7:G:150:LYS:HA	2.17	0.44
10:J:133:TYR:C	17:J:198:HOH:O	2.61	0.44
7:U:18(H):GLU:N	7:U:18(H):GLU:CD	2.76	0.44
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.18	0.44
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.47	0.44
5:E:90:ASN:O	5:E:94:GLN:HG3	2.18	0.44
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.98	0.44
8:V:9:ASN:OD1	8:V:10:ASN:N	2.50	0.44
10:X:133:TYR:C	17:X:203:HOH:O	2.61	0.44
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.17	0.44
13:1:40:ASN:N	13:1:40:ASN:ND2	2.64	0.44
6:F:54:ILE:HG12	6:F:208:PHE:CA	2.48	0.44
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.00	0.44
2:P:229:ILE:O	2:P:233:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	1.99	0.44
5:S:13:VAL:CG2	6:T:129:VAL:C	2.90	0.44
5:S:76:LEU:HD23	5:S:76:LEU:O	2.17	0.44
5:S:194:VAL:HG13	5:S:207:LEU:CD1	2.48	0.44
12:L:140:ASN:O	12:L:144:PHE:HA	2.18	0.44
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.11	0.44
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.99	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
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.99	0.43
1:A:21(P):LYS:N	17:A:1147:HOH:O	2.37	0.43
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.53	0.43
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.99	0.43
9:I:61:TYR:CD1	9:I:61:TYR:C	2.95	0.43
13:1:112:TYR:CD2	13:1:112:TYR:C	2.95	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
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
5:S:18(C):PHE:CD1	5:S:18(D):ILE:N	2.86	0.43
6:T:35:THR:CG2	6:T:36:THR:N	2.81	0.43
8:V:152:ILE:HD11	8:V:177:VAL:HG22	2.00	0.43
10:X:38:SER:HB2	10:X:39:PRO:HD2	2.01	0.43
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.18	0.43
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.53	0.43
14:2:146:MET:HE3	14:2:150:GLU:HB3	2.01	0.43
2:B:116:LEU:HD23	2:B:116:LEU:HA	1.88	0.43
3:C:120:GLN:O	3:C:124:THR:HG23	2.18	0.43
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.43
11:K:67:GLU:HG2	11:K:73:ARG:HA	1.99	0.43
13:M:40:ASN:H	13:M:40:ASN:ND2	2.10	0.43
2:P:6:ARG:HB2	5:S:127:TYR:OH	2.18	0.43
3:Q:18(A):ASP:OD1	3:Q:18(C):LYS:HB2	2.19	0.43
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.98	0.43
6:T:147:HIS:HD2	17:T:282:HOH:O	2.01	0.43
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.17	0.43
12:Z:-9:GLN:HG2	13:1:-8:THR:HG21	2.00	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:167:ARG:O	3:C:168:ASN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.17	0.43
7:G:203:THR:HG22	7:G:204:GLU:O	2.18	0.43
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.00	0.43
6:T:12:ASN:ND2	6:T:131:PRO:HD3	2.33	0.43
6:T:202:HIS:CG	6:T:202:HIS:O	2.72	0.43
7:U:67:ILE:HD13	7:U:211:GLU:CG	2.48	0.43
11:Y:67:GLU:HG2	11:Y:73:ARG:HA	2.00	0.43
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.40	0.43
12:Z:148:VAL:O	12:Z:152:ILE:HG12	2.18	0.43
3:C:241:GLN:C	3:C:243:GLN:N	2.73	0.43
5:E:194:VAL:HG13	5:E:207:LEU:CD1	2.48	0.43
7:G:171:GLU:OE1	7:G:171:GLU:N	2.49	0.43
7:G:188:LYS:HD3	7:G:188:LYS:HA	1.84	0.43
12:L:22:THR:O	12:L:23:ASP:HB2	2.18	0.43
2:P:38:ILE:HD12	2:P:197:LEU:HG	2.00	0.43
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.48	0.43
9:W:113:PHE:HA	9:W:118:CYS:O	2.17	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
7:G:107:MET:CE	7:G:112:LEU:HD13	2.48	0.43
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.00	0.43
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.54	0.43
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.00	0.43
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.82	0.43
5:S:90:ASN:O	5:S:94:GLN:HG3	2.18	0.43
5:S:190:ILE:HG23	5:S:212:ILE:HD13	2.00	0.43
5:S:214:ILE:HG12	5:S:215:VAL:N	2.34	0.43
6:T:127:ASN:C	6:T:127:ASN:ND2	2.74	0.43
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.82	0.43
10:X:44:SER:HG	10:X:100:LEU:HB2	1.82	0.43
3:C:38:VAL:HG22	3:C:39:GLY:N	2.33	0.43
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.01	0.43
7:G:18(H):GLU:CD	7:G:18(H):GLU:N	2.77	0.43
11:K:4:LEU:HD13	11:K:159:ILE:HD11	2.01	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
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.19	0.43
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.00	0.43
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.19	0.43
3:C:185:THR:CG2	3:C:186:VAL:N	2.81	0.43
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:-1:MET:HE2	10:J:47:GLY:HA2	2.00	0.43
10:J:113:ILE:HA	10:J:118:THR:O	2.19	0.43
13:M:14(A):VAL:O	13:M:14(A):VAL:CG2	2.62	0.43
2:P:194:LEU:O	2:P:198:SER:HB2	2.18	0.43
7:U:171:GLU:OE1	7:U:171:GLU:N	2.49	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
2:B:122:GLY:C	2:B:124:THR:N	2.77	0.43
4:D:37:ALA:HB3	4:D:165:ILE:HG13	2.00	0.43
6:F:212:ILE:HG22	6:F:213:SER:N	2.34	0.43
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.00	0.43
9:I:104:ILE:HG21	9:I:181:LYS:HG2	2.00	0.43
12:L:160:THR:O	12:L:164:GLU:HG2	2.18	0.43
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.45	0.43
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.49	0.43
9:W:55:LEU:HD23	9:W:55:LEU:HA	1.91	0.43
9:W:104:ILE:HG21	9:W:181:LYS:HG2	2.00	0.43
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.33	0.43
4:D:208:ASP:OD1	4:D:208:ASP:C	2.60	0.42
5:E:136:LEU:HD12	5:E:151:PHE:CD2	2.54	0.42
11:K:16:VAL:HG21	11:K:34:VAL:HG23	2.01	0.42
12:L:93:PHE:N	12:L:94:PRO:HD3	2.33	0.42
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.34	0.42
7:U:109:CYS:HB2	7:U:140:SER:OG	2.18	0.42
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.01	0.42
10:X:190:PHE:C	10:X:192:ALA:N	2.76	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
4:D:122:ARG:HG2	4:D:122:ARG:NH1	2.33	0.42
7:G:38:LEU:C	7:G:38:LEU:HD12	2.45	0.42
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.02	0.42
11:K:78:ALA:O	11:K:82:ILE:HG12	2.19	0.42
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.19	0.42
2:P:113:VAL:HG22	2:P:138:TYR:CG	2.54	0.42
2:P:122:GLY:C	2:P:124:THR:N	2.76	0.42
3:Q:120:GLN:O	3:Q:124:THR:HG23	2.19	0.42
3:Q:159:SER:O	4:R:59:LEU:HD22	2.19	0.42
12:Z:109:ALA:HA	17:Z:375:HOH:O	2.18	0.42
12:Z:151:VAL:O	12:Z:155:VAL:HG23	2.19	0.42
13:1:57:ARG:HG2	13:1:57:ARG:NH1	2.34	0.42
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:GLU:O	3:C:231:GLN:HG3	2.19	0.42
5:E:18(C):PHE:CD1	5:E:18(C):PHE:C	2.98	0.42
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.00	0.42
8:H:152:ILE:HD11	8:H:177:VAL:HG22	2.02	0.42
14:N:146:MET:HE3	14:N:150:GLU:HB3	2.02	0.42
1:O:210:ILE:HD12	1:O:210:ILE:N	2.34	0.42
4:R:37:ALA:HB3	4:R:165:ILE:HG13	2.01	0.42
4:R:142:ASP:OD2	4:R:142:ASP:C	2.62	0.42
8:V:128:GLY:O	8:V:131:SER:CB	2.68	0.42
10:X:3:ILE:HG22	10:X:3:ILE:O	2.18	0.42
1:A:221:PHE:CD2	1:A:221:PHE:C	2.97	0.42
2:B:224:PHE:N	2:B:224:PHE:CD2	2.87	0.42
3:C:47:VAL:HG23	3:C:189:CYS:SG	2.60	0.42
4:D:150:HIS:O	4:D:157:PHE:HA	2.20	0.42
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.84	0.42
12:L:33:LYS:HB3	12:L:33:LYS:HE2	1.83	0.42
1:O:49:ALA:HB2	1:O:212:LEU:HG	2.02	0.42
1:O:159:PRO:O	2:P:59:LEU:HD12	2.19	0.42
3:Q:227:GLU:O	3:Q:231:GLN:HG3	2.19	0.42
5:S:18(C):PHE:CD1	5:S:18(C):PHE:C	2.98	0.42
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.33	0.42
1:A:5:THR:O	1:A:7:ARG:HG3	2.19	0.42
2:B:31:ILE:HD12	2:B:79:ALA:O	2.20	0.42
2:B:113:VAL:HG22	2:B:138:TYR:CG	2.55	0.42
10:J:120:VAL:HG13	10:J:122:LEU:HG	2.01	0.42
10:J:190:PHE:C	10:J:192:ALA:N	2.76	0.42
11:K:137:VAL:HG21	11:K:161:ALA:HB2	2.02	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:82:ILE:CG2	7:U:83:PRO:HD3	2.49	0.42
7:U:188:LYS:HD3	7:U:188:LYS:HA	1.84	0.42
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.55	0.42
14:2:3:ILE:HG22	14:2:16:ALA:HB2	2.02	0.42
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.22	0.42
4:D:142:ASP:OD2	4:D:142:ASP:C	2.62	0.42
13:M:57:ARG:HG2	13:M:57:ARG:NH1	2.33	0.42
13:M:187:LYS:HB3	13:M:190:LEU:HD11	2.02	0.42
2:P:224:PHE:N	2:P:224:PHE:HD2	2.18	0.42
4:R:72:ARG:HG3	17:R:1302:HOH:O	2.19	0.42
6:T:212:ILE:HG22	6:T:213:SER:N	2.34	0.42
8:V:25:ILE:HD12	8:V:25:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.01	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.42
12:Z:33:LYS:HB3	12:Z:33:LYS:HE2	1.83	0.42
1:A:210:ILE:HD12	1:A:210:ILE:N	2.35	0.42
2:B:7:ARG:HD2	2:B:8:TYR:CZ	2.54	0.42
2:B:121:GLN:HG3	3:C:83:ALA:HB1	2.00	0.42
6:F:120:VAL:HG21	6:F:151:LEU:HD21	2.01	0.42
8:H:147:THR:O	8:H:148:LYS:C	2.63	0.42
1:O:5:THR:O	1:O:7:ARG:HG3	2.20	0.42
1:O:45:GLY:HA2	1:O:147:PHE:CE2	2.54	0.42
1:O:122:GLU:C	1:O:124:THR:H	2.26	0.42
4:R:194:LEU:HD12	4:R:194:LEU:HA	1.88	0.42
5:S:216:GLY:O	5:S:217:LYS:C	2.62	0.42
7:U:49:ILE:HD13	7:U:212:VAL:HG22	2.01	0.42
7:U:67:ILE:HD13	7:U:211:GLU:OE1	2.20	0.42
9:W:159:LEU:HD21	9:W:173:ALA:HB1	2.01	0.42
10:X:146:MET:HE3	10:X:150:GLU:HB3	2.02	0.42
1:A:4:MET:CG	1:A:5:THR:H	2.29	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
10:J:143:ARG:HB2	10:J:146:MET:HG3	2.02	0.42
14:N:85:GLU:O	14:N:89:GLU:HB2	2.19	0.42
9:W:20:LEU:HD13	9:W:20:LEU:C	2.45	0.42
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	2.01	0.42
12:Z:19:ARG:HB2	12:Z:171:ASP:OD2	2.20	0.42
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.19	0.42
2:B:186:VAL:O	2:B:190:ILE:HG13	2.20	0.42
2:B:223:ILE:N	2:B:223:ILE:HD12	2.34	0.42
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.54	0.42
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.49	0.42
12:L:104:LEU:HA	12:L:107:LYS:O	2.20	0.42
13:M:14(C):ARG:HH11	13:M:14(C):ARG:CG	2.29	0.42
13:M:147:THR:OG1	13:M:150:VAL:HG23	2.19	0.42
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	2.02	0.42
6:T:205:ASN:C	6:T:20(B):GLU:H	2.28	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
8:V:162:GLY:O	8:V:166:ASP:HB3	2.19	0.42
8:V:175:VAL:CG1	8:V:176:CYS:N	2.83	0.42
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.55	0.42
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:18(G):TYR:CD1	14:2:18(G):TYR:C	2.98	0.42
3:C:13:SER:O	4:D:130:ARG:HD3	2.20	0.42
4:D:205:GLU:OE2	4:D:205:GLU:HA	2.20	0.42
5:E:216:GLY:O	5:E:217:LYS:C	2.62	0.42
8:H:162:GLY:O	8:H:166:ASP:HB3	2.20	0.42
9:I:19:ARG:HB2	9:I:171:TRP:HB2	2.02	0.42
9:I:34:ILE:HB	17:I:955:HOH:O	2.19	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
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.34	0.42
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.55	0.42
6:T:194:ALA:O	6:T:198:TYR:HD1	2.02	0.42
10:X:-1:MET:HE2	10:X:47:GLY:HA2	2.00	0.42
12:Z:5:GLY:HA2	12:Z:13:VAL:O	2.20	0.42
14:2:146:MET:CE	14:2:150:GLU:HB3	2.50	0.42
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.67	0.42
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
11:K:4:LEU:C	11:K:4:LEU:CD2	2.93	0.41
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.02	0.41
5:S:45:HIS:HB2	5:S:189:LEU:HD12	2.02	0.41
6:T:172:ALA:O	6:T:176:LEU:CD2	2.68	0.41
7:U:20:ARG:NH2	7:U:22:TYR:CE1	2.88	0.41
1:A:48:ILE:HD12	1:A:48:ILE:H	1.85	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
12:L:5:GLY:HA2	12:L:13:VAL:O	2.20	0.41
14:N:10(B):LYS:HD3	14:N:10(B):LYS:O	2.20	0.41
3:Q:57:LYS:HD2	3:Q:57:LYS:C	2.46	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
2:B:41:MET:HE2	2:B:146:TYR:O	2.19	0.41
3:C:227:GLU:H	3:C:227:GLU:CD	2.29	0.41
5:E:45:HIS:HB2	5:E:189:LEU:HD12	2.03	0.41
8:H:2:THR:O	8:H:16:ALA:HA	2.19	0.41
8:H:128:GLY:O	8:H:131:SER:CB	2.68	0.41
10:J:38:SER:HB2	10:J:39:PRO:HD2	2.02	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
7:U:35:ILE:HG23	7:U:51:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.77	0.41
2:B:224:PHE:N	2:B:224:PHE:HD2	2.18	0.41
3:C:57:LYS:HD2	3:C:58:LEU:N	2.35	0.41
7:G:67:ILE:HD13	7:G:211:GLU:OE1	2.19	0.41
8:H:5:GLY:HA3	8:H:110:LEU:HD11	2.01	0.41
8:H:172:ASN:ND2	8:H:193:THR:HA	2.33	0.41
11:K:40:PHE:CD2	11:K:40:PHE:N	2.88	0.41
12:L:19:ARG:HB2	12:L:171:ASP:OD2	2.20	0.41
1:O:130:ARG:HH21	7:U:124:THR:HG23	1.80	0.41
2:P:51:GLU:CD	2:P:202:THR:HG23	2.46	0.41
4:R:208:ASP:OD1	4:R:208:ASP:C	2.62	0.41
7:U:217:LYS:O	7:U:218:ASP:HB2	2.19	0.41
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.55	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
8:H:25:ILE:HD12	8:H:25:ILE:N	2.35	0.41
8:H:152:ILE:CD1	8:H:177:VAL:HG22	2.50	0.41
13:M:-3:VAL:HA	13:M:21:SER:O	2.21	0.41
14:N:18(G):TYR:CD1	14:N:18(G):TYR:C	2.98	0.41
3:Q:194:VAL:O	3:Q:198:LEU:HG	2.20	0.41
9:W:6:MET:HE1	9:W:155:ILE:HA	2.01	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	2.01	0.41
5:E:42:SER:OG	5:E:43:ASN:N	2.54	0.41
5:E:189:LEU:HD23	5:E:189:LEU:HA	1.90	0.41
7:G:150:LYS:O	7:G:157:TYR:HA	2.20	0.41
7:G:172:ILE:HD13	7:G:197:MET:HE1	2.03	0.41
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.50	0.41
12:L:1:GLY:N	17:L:755:HOH:O	2.51	0.41
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.35	0.41
1:O:48:ILE:O	1:O:48:ILE:CD1	2.68	0.41
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.56	0.41
2:P:228:GLU:O	2:P:232:ILE:HG22	2.21	0.41
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.20	0.41
6:T:38:ILE:HG22	6:T:164:ALA:HB2	2.02	0.41
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.01	0.41
3:C:113:THR:HG21	3:C:149:TYR:HB3	2.03	0.41
6:F:136:THR:O	6:F:150:MET:HA	2.21	0.41
8:H:18:THR:HB	8:H:30:ASN:HD22	1.86	0.41
12:L:83:ILE:HB	12:L:113:PHE:CE2	2.56	0.41
1:O:221:PHE:CD2	1:O:221:PHE:C	2.98	0.41
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:220:PRO:O	5:S:222:THR:HG23	2.21	0.41
11:Y:83:LEU:HD23	11:Y:99:THR:HG21	2.03	0.41
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.36	0.41
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.36	0.41
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.60	0.41
5:E:52:LYS:O	5:E:63:TYR:HD2	2.03	0.41
7:G:173:THR:HG22	7:G:177:GLU:OE2	2.21	0.41
12:L:14(Q):LEU:O	12:L:14(W):LYS:C	2.63	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
10:X:90(B):ARG:NH1	17:X:266:HOH:O	2.41	0.41
14:2:114:PRO:HD2	14:2:118:SER:O	2.21	0.41
1:A:52:LYS:HG3	1:A:211:GLU:HB2	2.03	0.41
2:B:51:GLU:CD	2:B:202:THR:HG23	2.46	0.41
5:E:148:LEU:HD23	5:E:162:GLY:HA2	2.03	0.41
5:E:220:PRO:O	5:E:222:THR:HG23	2.20	0.41
6:F:175:GLU:HA	6:F:175:GLU:OE2	2.21	0.41
6:F:205:ASN:C	6:F:20(B):GLU:H	2.29	0.41
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.56	0.41
4:R:68:VAL:HG21	4:R:89:ILE:HD12	2.03	0.41
6:T:37:SER:HB3	6:T:50:VAL:HG23	2.03	0.41
8:V:113:ILE:HD12	8:V:113:ILE:N	2.36	0.41
9:W:49:ALA:HB3	10:X:118:THR:HG23	2.02	0.41
9:W:147:GLU:O	9:W:148:PRO:C	2.64	0.41
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.21	0.41
1:A:45:GLY:HA2	1:A:147:PHE:CE2	2.56	0.41
1:A:49:ALA:HB2	1:A:212:LEU:HG	2.02	0.41
2:B:73:LYS:O	2:B:140:GLY:HA2	2.21	0.41
7:G:98:GLU:HG2	7:G:102:LYS:HD3	2.03	0.41
7:G:109:CYS:HB2	7:G:140:SER:OG	2.21	0.41
14:N:143:ARG:NH2	14:N:146:MET:HE3	2.36	0.41
4:R:170:GLU:HG2	4:R:171:GLY:N	2.36	0.41
10:X:34:THR:CG2	10:X:176:LYS:HZ2	2.32	0.41
3:C:18:ASP:OD2	3:C:20:HIS:ND1	2.53	0.40
6:F:12:ASN:OD1	6:F:12:ASN:C	2.64	0.40
7:G:43:LYS:HB2	7:G:18(G):GLU:O	2.21	0.40
7:G:49:ILE:HD13	7:G:212:VAL:HG22	2.03	0.40
8:H:112:SER:OG	8:H:120:ASP:HB2	2.21	0.40
11:K:1:THR:HB	16:K:212:MES:O2S	2.21	0.40
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.02	0.40
13:M:130:GLY:O	13:M:134:ALA:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:236:LEU:C	1:O:236:LEU:HD13	2.46	0.40
4:R:224:TYR:N	4:R:224:TYR:CD2	2.89	0.40
5:S:18(C):PHE:C	5:S:18(E):LYS:N	2.80	0.40
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.21	0.40
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.57	0.40
5:E:18(C):PHE:CA	5:E:18(F):ILE:HG12	2.45	0.40
5:E:190:ILE:HG23	5:E:212:ILE:HD13	2.02	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
11:K:104:TYR:CE2	11:K:108:PRO:HG3	2.57	0.40
13:M:14(G):ILE:HB	13:M:144:PRO:HD3	2.03	0.40
1:O:48:ILE:HD12	1:O:48:ILE:H	1.86	0.40
1:O:52:LYS:HG3	1:O:211:GLU:HB2	2.02	0.40
5:S:42:SER:OG	5:S:43:ASN:N	2.53	0.40
5:S:66:LYS:O	5:S:77:SER:HA	2.21	0.40
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.22	0.40
6:T:68:GLN:OE1	6:T:89:VAL:HG21	2.21	0.40
7:U:123:TYR:CE1	7:U:129:MET:HE3	2.56	0.40
7:U:139:VAL:HA	7:U:147:SER:O	2.21	0.40
1:A:197:LEU:O	1:A:202:VAL:HG23	2.22	0.40
2:B:213:ALA:HA	2:B:222:LYS:O	2.21	0.40
2:B:228:GLU:O	2:B:232:ILE:HG22	2.22	0.40
4:D:17:PRO:HD2	17:D:1171:HOH:O	2.20	0.40
7:G:48:VAL:CG1	7:G:139:VAL:HG11	2.52	0.40
7:G:139:VAL:HA	7:G:147:SER:O	2.21	0.40
8:H:40:LYS:C	8:H:41:ILE:HD12	2.47	0.40
9:I:28:SER:HB2	10:J:120:VAL:HG21	2.03	0.40
2:P:7:ARG:HD2	2:P:8:TYR:CZ	2.55	0.40
2:P:168:ASN:HA	17:P:943:HOH:O	2.21	0.40
3:Q:13:SER:O	4:R:130:ARG:HD3	2.22	0.40
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.22	0.40
6:T:114:ASP:O	6:T:118:GLN:HG2	2.21	0.40
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.21	0.40
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.51	0.40
13:1:14(G):ILE:HB	13:1:144:PRO:HD3	2.03	0.40
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.21	0.40
5:E:67:ILE:HG21	5:E:213:ALA:HB2	2.03	0.40
5:E:177:GLU:OE1	6:F:56:SER:HB2	2.21	0.40
6:F:114:ASP:O	6:F:118:GLN:HG2	2.21	0.40
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.85	0.40
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:5:SER:O	2:P:6:ARG:C	2.63	0.40
2:P:31:ILE:HD12	2:P:79:ALA:O	2.21	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
4:R:150:HIS:O	4:R:157:PHE:HA	2.21	0.40
10:X:16:SER:HB2	17:X:1152:HOH:O	2.20	0.40
10:X:53:VAL:HB	17:X:726:HOH:O	2.21	0.40
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	2.04	0.40
2:B:5:SER:O	2:B:6:ARG:C	2.64	0.40
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.57	0.40
2:B:202:THR:CG2	2:B:204:SER:HB2	2.51	0.40
6:F:43:ASN:N	6:F:43:ASN:ND2	2.69	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
6:F:101:LYS:HE2	13:M:57:ARG:NH2	2.36	0.40
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.78	0.40
8:H:34:LEU:HB2	17:H:540:HOH:O	2.22	0.40
9:I:28:SER:CB	10:J:120:VAL:HG21	2.52	0.40
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.56	0.40
1:O:197:LEU:O	1:O:202:VAL:HG23	2.21	0.40
6:T:192:GLN:O	6:T:196:ILE:HG13	2.22	0.40
7:U:89:ALA:O	7:U:93:LYS:HG3	2.21	0.40
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.05	0.40
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.04	0.40
14:2:20:THR:HG23	14:2:31:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	16 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	248/250 (99%)	236 (95%)	9 (4%)	3 (1%)	10	20
2	B	242/258 (94%)	221 (91%)	17 (7%)	4 (2%)	7	13
2	P	242/258 (94%)	222 (92%)	16 (7%)	4 (2%)	7	13
3	C	239/254 (94%)	223 (93%)	12 (5%)	4 (2%)	7	13
3	Q	239/254 (94%)	224 (94%)	11 (5%)	4 (2%)	7	13
4	D	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	9	18
4	R	240/260 (92%)	225 (94%)	12 (5%)	3 (1%)	9	18
5	E	231/234 (99%)	210 (91%)	16 (7%)	5 (2%)	5	9
5	S	231/234 (99%)	208 (90%)	18 (8%)	5 (2%)	5	9
6	F	242/288 (84%)	231 (96%)	8 (3%)	3 (1%)	10	20
6	T	242/288 (84%)	230 (95%)	9 (4%)	3 (1%)	10	20
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%)	8	16
10	X	196/198 (99%)	186 (95%)	8 (4%)	2 (1%)	12	24
11	K	210/287 (73%)	203 (97%)	6 (3%)	1 (0%)	24	43
11	Y	210/287 (73%)	202 (96%)	7 (3%)	1 (0%)	24	43
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
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%)	16	31

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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	26	51
1	O	209/209 (100%)	200 (96%)	9 (4%)	26	51
2	B	203/216 (94%)	195 (96%)	8 (4%)	28	55
2	P	203/216 (94%)	195 (96%)	8 (4%)	28	55
3	C	213/226 (94%)	206 (97%)	7 (3%)	33	61
3	Q	213/226 (94%)	206 (97%)	7 (3%)	33	61
4	D	198/215 (92%)	186 (94%)	12 (6%)	17	35
4	R	198/215 (92%)	186 (94%)	12 (6%)	17	35
5	E	192/193 (100%)	177 (92%)	15 (8%)	11	24
5	S	192/193 (100%)	177 (92%)	15 (8%)	11	24
6	F	201/239 (84%)	183 (91%)	18 (9%)	9	19
6	T	201/239 (84%)	182 (90%)	19 (10%)	8	17
7	G	207/210 (99%)	198 (96%)	9 (4%)	26	51
7	U	207/210 (99%)	198 (96%)	9 (4%)	26	51
8	H	181/214 (85%)	171 (94%)	10 (6%)	19	40
8	V	181/214 (85%)	172 (95%)	9 (5%)	22	44
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	72
9	W	172/173 (99%)	168 (98%)	4 (2%)	44	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	175/175 (100%)	167 (95%)	8 (5%)	24	48
10	X	175/175 (100%)	167 (95%)	8 (5%)	24	48
11	K	169/235 (72%)	161 (95%)	8 (5%)	23	47
11	Y	169/235 (72%)	161 (95%)	8 (5%)	23	47
12	L	185/201 (92%)	165 (89%)	20 (11%)	6	13
12	Z	185/201 (92%)	164 (89%)	21 (11%)	5	12
13	1	199/224 (89%)	191 (96%)	8 (4%)	28	54
13	M	199/224 (89%)	191 (96%)	8 (4%)	28	54
14	2	162/178 (91%)	155 (96%)	7 (4%)	26	51
14	N	162/178 (91%)	155 (96%)	7 (4%)	26	51
All	All	5332/5816 (92%)	5045 (95%)	287 (5%)	20	41

All (287) 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	41	MET
2	B	58	LEU
2	B	91	THR
2	B	111	ILE
2	B	124	THR
2	B	150	THR
2	B	192	LEU
2	B	212	PHE
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	135	SER
3	C	150	GLN
3	C	172	VAL

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Mol	Chain	Res	Type
3	C	174	GLU
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	107	ILE
4	D	110	GLU
4	D	126	ARG
4	D	175	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
5	E	7	ASN
5	E	12	THR
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	111	ARG
5	E	123	ASN
5	E	149	LEU
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	35	THR
6	F	43	ASN
6	F	72	ARG
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	169	ARG
6	F	176	LEU
6	F	18(A)	ASP
6	F	18(B)	HIS
6	F	18(C)	HIS
6	F	18(D)	PRO
6	F	18(E)	GLU

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Mol	Chain	Res	Type
6	F	187	ARG
6	F	192	GLN
6	F	203	GLU
6	F	205	ASN
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	169	GLN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	13	VAL
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	63	ILE
8	H	68	LEU
8	H	95	ILE
8	H	121	VAL
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	155	ILE
9	I	160	LEU
9	I	171	TRP
10	J	2	ILE
10	J	3	ILE
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	121	GLU
10	J	168	MET
11	K	4	LEU
11	K	41	LEU
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	99	THR
11	K	185	ILE

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Mol	Chain	Res	Type
11	K	210	ILE
12	L	-9	GLN
12	L	14	LEU
12	L	58	ARG
12	L	98	HIS
12	L	99	THR
12	L	114	ASP
12	L	14(A)	LYS
12	L	14(B)	ASN
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	148	VAL
13	M	149	GLN
13	M	191	GLN
13	M	204	LYS
14	N	1	THR
14	N	78	THR
14	N	89	GLU
14	N	119	VAL
14	N	126	ILE
14	N	149	GLU
14	N	178	LEU
1	O	32	LYS
1	O	33	GLN
1	O	48	ILE
1	O	62	GLU
1	O	64	LEU
1	O	124	THR

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Mol	Chain	Res	Type
1	O	158	PHE
1	O	179	ARG
1	O	214	ILE
2	P	41	MET
2	P	58	LEU
2	P	91	THR
2	P	111	ILE
2	P	124	THR
2	P	150	THR
2	P	192	LEU
2	P	212	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	135	SER
3	Q	150	GLN
3	Q	172	VAL
3	Q	174	GLU
4	R	28	LEU
4	R	48	LEU
4	R	52	LYS
4	R	107	ILE
4	R	110	GLU
4	R	126	ARG
4	R	175	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	7	ASN
5	S	12	THR
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	111	ARG
5	S	123	ASN
5	S	149	LEU
5	S	189	LEU
5	S	199	GLN

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Mol	Chain	Res	Type
5	S	207	LEU
5	S	227	GLU
5	S	231	LYS
6	T	18	ASP
6	T	35	THR
6	T	43	ASN
6	T	72	ARG
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	167	LYS
6	T	169	ARG
6	T	176	LEU
6	T	18(A)	ASP
6	T	18(B)	HIS
6	T	18(C)	HIS
6	T	18(D)	PRO
6	T	18(E)	GLU
6	T	187	ARG
6	T	192	GLN
6	T	203	GLU
6	T	205	ASN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	169	GLN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	95	ILE
8	V	121	VAL
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	155	ILE

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Mol	Chain	Res	Type
9	W	160	LEU
9	W	171	TRP
10	X	2	ILE
10	X	3	ILE
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	121	GLU
10	X	168	MET
11	Y	4	LEU
11	Y	41	LEU
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	99	THR
11	Y	185	ILE
11	Y	210	ILE
12	Z	-9	GLN
12	Z	14	LEU
12	Z	40	ASN
12	Z	58	ARG
12	Z	98	HIS
12	Z	99	THR
12	Z	114	ASP
12	Z	14(A)	LYS
12	Z	14(B)	ASN
12	Z	14(C)	GLN
12	Z	14(D)	TYR
12	Z	14(E)	GLU
12	Z	14(F)	PRO
12	Z	14(I)	THR
12	Z	14(K)	LYS
12	Z	14(M)	VAL
12	Z	14(N)	LYS
12	Z	14(O)	LYS
12	Z	14(P)	PRO
12	Z	14(Q)	LEU
12	Z	14(W)	LYS
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG

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Mol	Chain	Res	Type
13	1	112	TYR
13	1	148	VAL
13	1	149	GLN
13	1	191	GLN
13	1	204	LYS
14	2	1	THR
14	2	78	THR
14	2	89	GLU
14	2	119	VAL
14	2	126	ILE
14	2	149	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (220) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	150	GLN
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	173	GLN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	59	GLN
3	C	82	ASN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	179	ASN
3	C	209	ASN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN

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Mol	Chain	Res	Type
4	D	147	GLN
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	94	GLN
5	E	95	GLN
5	E	104	ASN
5	E	114	HIS
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	156	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
6	F	237	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	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN

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Mol	Chain	Res	Type
9	I	29	ASN
9	I	56	ASN
9	I	81	GLN
9	I	145	ASN
9	I	157	GLN
9	I	193	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	131	GLN
11	K	189	ASN
11	K	207	ASN
11	K	208	ASN
12	L	61	ASN
12	L	141	GLN
12	L	143	ASN
12	L	14(B)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	40	ASN
13	M	54	HIS
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	189	ASN
13	M	191	GLN
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	150	GLN
2	P	23	GLN
2	P	71	ASN

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Mol	Chain	Res	Type
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	59	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	179	ASN
3	Q	209	ASN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	95	GLN
5	S	104	ASN
5	S	114	HIS
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	87	HIS
6	T	90	ASN
6	T	121	GLN

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Mol	Chain	Res	Type
6	T	127	ASN
6	T	192	GLN
6	T	237	GLN
6	T	241	ASN
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	29	ASN
9	W	56	ASN
9	W	81	GLN
9	W	145	ASN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	85	GLN
10	X	106	ASN
10	X	112	GLN
10	X	141	HIS
10	X	160	GLN
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	141	ASN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN

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Mol	Chain	Res	Type
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	141	GLN
12	Z	143	ASN
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	1	-7	GLN
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	189	ASN
13	1	191	GLN
14	2	141	ASN
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	RE0	4	4	15	15,17,18	1.52	4 (26%)	19,25,27	2.27	7 (36%)
15	RE0	3	4	15	15,17,18	1.43	2 (13%)	19,25,27	2.44	7 (36%)
15	TY5	4	2	15	19,20,21	1.86	8 (42%)	20,25,27	0.92	1 (5%)
15	TY5	3	2	15	19,20,21	1.89	9 (47%)	20,25,27	0.93	1 (5%)

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	RE0	4	4	15	-	0/6/23/25	0/2/2/2
15	RE0	3	4	15	-	0/6/23/25	0/2/2/2
15	TY5	4	2	15	-	0/10/11/13	0/2/2/2
15	TY5	3	2	15	-	0/10/11/13	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	2	TY5	CE2-CZ	3.00	1.44	1.38
15	4	2	TY5	CE2-CZ	2.78	1.43	1.38
15	3	4	RE0	CZ3-CH2	2.52	1.43	1.38
15	4	2	TY5	C49-C50	2.46	1.56	1.50
15	4	4	RE0	CB-CA	2.46	1.57	1.54
15	4	4	RE0	CZ3-CH2	2.37	1.43	1.38
15	4	2	TY5	C55-C50	2.37	1.43	1.38
15	3	2	TY5	C53-C52	2.27	1.43	1.38
15	3	2	TY5	C55-C50	2.25	1.43	1.38
15	4	2	TY5	C54-C53	2.21	1.43	1.38
15	4	4	RE0	CZ3-CE3	2.18	1.42	1.38
15	3	4	RE0	CZ3-CE3	2.16	1.42	1.38
15	3	2	TY5	C54-C53	2.13	1.42	1.38
15	3	2	TY5	C52-C51	2.12	1.42	1.38
15	4	2	TY5	CE1-CZ	2.12	1.42	1.38
15	4	2	TY5	C51-C50	2.11	1.43	1.38
15	3	2	TY5	C54-C55	2.10	1.42	1.38
15	3	2	TY5	CD2-CG	2.06	1.43	1.38
15	3	2	TY5	C49-C50	2.06	1.55	1.50
15	4	2	TY5	CD2-CG	2.05	1.43	1.38
15	4	2	TY5	OH-CZ	2.05	1.42	1.37
15	3	2	TY5	CD1-CE1	2.04	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	4	RE0	CG-CD2	2.04	1.53	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	4	RE0	CG-CD2-CE2	-7.08	105.97	108.86
15	4	4	RE0	CG-CD2-CE2	-6.39	106.25	108.86
15	4	4	RE0	CD2-CE2-NE1	3.67	112.06	109.60
15	3	4	RE0	CD2-CE2-NE1	3.48	111.93	109.60
15	3	4	RE0	OG-CG-CD1	-3.03	102.42	108.65
15	4	2	TY5	C49-OH-CZ	3.01	124.79	117.62
15	3	2	TY5	C49-OH-CZ	2.99	124.75	117.62
15	3	4	RE0	CZ2-CE2-NE1	-2.90	124.96	130.83
15	4	4	RE0	CE2-NE1-CD1	-2.83	109.98	111.85
15	4	4	RE0	OG-CG-CD1	-2.76	102.97	108.65
15	3	4	RE0	CE2-NE1-CD1	-2.69	110.07	111.85
15	4	4	RE0	CZ2-CE2-NE1	-2.66	125.45	130.83
15	4	4	RE0	CG-CD1-NE1	2.40	109.86	108.43
15	3	4	RE0	CG-CD1-NE1	2.22	109.75	108.43
15	3	4	RE0	CD2-CG-CD1	2.15	102.27	101.51
15	4	4	RE0	CB-CG-CD2	2.07	117.70	112.74

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	4	2	TY5	2	0
15	3	2	TY5	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	Y	212	-	12,12,12	2.47	5 (41%)	15,16,16	1.99	5 (33%)
16	MES	K	212	-	12,12,12	1.07	0	15,16,16	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MES	Y	212	-	-	1/6/14/14	0/1/1/1
16	MES	K	212	-	-	4/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	212	MES	O2S-S	4.70	1.58	1.45
16	Y	212	MES	C7-N4	3.72	1.55	1.47
16	Y	212	MES	C8-S	3.49	1.82	1.77
16	Y	212	MES	C3-N4	3.02	1.55	1.46
16	Y	212	MES	C5-N4	2.97	1.54	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	212	MES	O3S-S-O1S	4.53	122.72	111.40
16	Y	212	MES	C6-C5-N4	-3.82	104.32	110.12
16	Y	212	MES	O3S-S-O2S	-2.78	104.46	111.40
16	Y	212	MES	C2-C3-N4	2.55	113.99	110.12
16	Y	212	MES	C6-O1-C2	2.02	116.42	109.88

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	212	MES	C8-C7-N4-C3
16	Y	212	MES	C8-C7-N4-C3
16	K	212	MES	C7-C8-S-O3S
16	K	212	MES	C7-C8-S-O1S
16	K	212	MES	C7-C8-S-O2S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	212	MES	1	0
16	K	212	MES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.11	6 (2%) 59 55	33, 46, 75, 104	0
1	O	250/250 (100%)	0.05	9 (3%) 46 41	37, 53, 81, 104	0
2	B	244/258 (94%)	0.23	12 (4%) 35 31	32, 52, 89, 116	0
2	P	244/258 (94%)	0.36	21 (8%) 16 14	34, 53, 90, 116	0
3	C	241/254 (94%)	0.31	21 (8%) 16 14	33, 55, 107, 120	0
3	Q	241/254 (94%)	0.61	27 (11%) 10 8	38, 60, 111, 122	0
4	D	242/260 (93%)	0.22	9 (3%) 45 40	34, 54, 89, 120	0
4	R	242/260 (93%)	0.39	13 (5%) 31 27	37, 58, 90, 122	0
5	E	233/234 (99%)	0.35	8 (3%) 48 43	43, 59, 85, 110	0
5	S	233/234 (99%)	0.84	29 (12%) 8 6	41, 64, 90, 108	0
6	F	244/288 (84%)	0.17	5 (2%) 65 61	36, 53, 88, 103	0
6	T	244/288 (84%)	0.49	15 (6%) 27 23	32, 55, 92, 106	0
7	G	243/252 (96%)	-0.04	6 (2%) 58 54	33, 46, 76, 113	0
7	U	243/252 (96%)	0.10	5 (2%) 63 59	32, 50, 74, 113	0
8	H	222/261 (85%)	-0.16	3 (1%) 73 70	28, 45, 65, 90	0
8	V	222/261 (85%)	-0.14	1 (0%) 87 85	30, 49, 67, 93	0
9	I	204/205 (99%)	-0.36	3 (1%) 72 68	28, 43, 62, 76	0
9	W	204/205 (99%)	-0.31	2 (0%) 79 76	31, 44, 64, 78	0
10	J	198/198 (100%)	-0.14	8 (4%) 42 38	29, 43, 64, 120	0
10	X	198/198 (100%)	-0.16	7 (3%) 47 42	29, 45, 62, 120	0
11	K	212/287 (73%)	-0.19	7 (3%) 49 45	26, 42, 65, 78	0
11	Y	212/287 (73%)	-0.10	8 (3%) 44 39	33, 46, 68, 79	0
12	L	222/241 (92%)	-0.15	5 (2%) 61 57	29, 46, 66, 91	0
12	Z	222/241 (92%)	-0.11	4 (1%) 67 64	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%)	-0.22	1 (0%) 88 86	31, 45, 59, 64	0
13	M	233/266 (87%)	-0.20	2 (0%) 81 78	30, 47, 61, 65	0
14	2	196/215 (91%)	-0.19	4 (2%) 65 61	27, 44, 66, 80	0
14	N	196/215 (91%)	-0.26	1 (0%) 87 85	32, 43, 64, 76	0
15	3	1/5 (20%)	-0.86	0 100 100	33, 33, 33, 33	0
15	4	1/5 (20%)	0.45	0 100 100	43, 43, 43, 43	0
All	All	6370/6948 (91%)	0.06	242 (3%) 44 39	26, 49, 82, 122	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	Z	145	TYR	8.4
12	L	145	TYR	8.1
3	Q	56	LEU	8.0
4	D	12(E)	SER	7.7
11	Y	208	ASN	7.7
4	D	12(D)	ALA	7.6
11	K	208	ASN	7.4
4	D	12(C)	GLY	7.3
4	R	12(D)	ALA	7.1
2	B	21(B)	GLY	6.7
7	U	240	ASP	6.4
10	J	193	GLN	6.3
2	P	217	ALA	6.3
10	J	192	ALA	6.0
3	C	56	LEU	5.8
3	C	55	THR	5.8
5	S	4	PHE	5.7
10	X	193	GLN	5.5
4	R	12(E)	SER	5.5
3	Q	58	LEU	5.4
2	B	217	ALA	5.0
10	J	-1	MET	5.0
4	R	12(C)	GLY	4.9
10	X	-1	MET	4.8
10	X	192	ALA	4.8
7	G	6	ALA	4.8
2	B	218	ASN	4.7
11	Y	104	TYR	4.6
2	P	239	THR	4.4

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Mol	Chain	Res	Type	RSRZ
5	E	4	PHE	4.4
2	B	239	THR	4.3
3	C	54	SER	4.2
2	B	21(D)	GLY	4.2
2	P	54	VAL	4.2
4	R	126	ARG	4.2
3	C	203	THR	4.1
2	P	21(B)	GLY	4.1
4	D	126	ARG	4.0
11	K	207	ASN	4.0
11	Y	207	ASN	4.0
7	U	6	ALA	3.9
11	K	210	ILE	3.9
12	L	14(P)	PRO	3.9
5	S	2(E)	ASN	3.9
11	K	104	TYR	3.8
11	Y	180	GLU	3.8
3	Q	55	THR	3.8
3	Q	63	THR	3.7
4	D	242	ALA	3.6
10	J	191	GLN	3.6
1	O	4	MET	3.6
1	O	56	SER	3.6
4	R	12(F)	GLY	3.6
6	F	5	GLY	3.6
5	S	63	TYR	3.5
4	D	127	LEU	3.5
9	W	-8	SER	3.5
5	S	55	ALA	3.5
8	H	223	ASP	3.5
13	M	-8	THR	3.5
11	K	180	GLU	3.4
11	K	211	GLY	3.4
10	X	133	TYR	3.4
10	X	191	GLN	3.4
8	V	223	ASP	3.4
4	R	127	LEU	3.4
3	Q	236	ILE	3.4
5	S	5	ARG	3.3
3	Q	54	SER	3.2
3	C	59	GLN	3.2
11	Y	210	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	208	LYS	3.2
9	I	121	GLU	3.2
5	E	128	GLY	3.2
3	Q	233	VAL	3.1
2	P	219	GLU	3.1
2	P	21(D)	GLY	3.1
2	B	21(A)	LYS	3.1
4	D	12(F)	GLY	3.1
3	C	243	GLN	3.0
3	C	207	ALA	3.0
13	M	61	ASP	3.0
5	S	18(C)	PHE	3.0
7	G	236	ILE	3.0
7	U	18(H)	GLU	3.0
10	J	168	MET	3.0
10	X	168	MET	3.0
13	1	-8	THR	3.0
5	E	203	ASP	3.0
7	G	7	GLY	3.0
11	Y	211	GLY	3.0
6	T	199	LEU	2.9
2	P	218	ASN	2.9
12	L	14(W)	LYS	2.9
3	C	58	LEU	2.9
12	Z	14(Q)	LEU	2.9
3	Q	201	VAL	2.9
12	Z	14(W)	LYS	2.9
1	O	64	LEU	2.9
3	Q	57	LYS	2.9
2	P	220	TYR	2.9
5	E	127	TYR	2.9
2	B	54	VAL	2.8
6	T	18(A)	ASP	2.8
10	J	190	PHE	2.8
5	S	32	LYS	2.8
2	P	61	GLN	2.8
6	T	223	PHE	2.8
3	Q	230	ASN	2.8
14	2	107	LYS	2.8
8	H	199	GLU	2.8
3	Q	64	PRO	2.7
2	B	219	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	Q	200	VAL	2.7
14	2	116	GLY	2.7
3	Q	203	THR	2.7
4	D	244	GLU	2.7
11	K	73	ARG	2.7
6	T	20(C)	LYS	2.6
1	A	4	MET	2.6
5	S	59	SER	2.6
3	Q	241	GLN	2.6
3	Q	229	ILE	2.6
5	S	204	GLU	2.6
3	Q	202	GLN	2.6
3	Q	210	ILE	2.6
2	B	238	ILE	2.6
14	2	149	GLU	2.6
5	E	63	TYR	2.6
4	D	125	GLU	2.5
5	S	18(B)	THR	2.5
9	I	-8	SER	2.5
2	P	62	ASP	2.5
6	F	204	ASP	2.5
7	G	239	GLN	2.5
1	O	21(P)	LYS	2.5
6	T	241	ASN	2.5
5	S	57	GLU	2.5
6	T	240	ILE	2.5
3	Q	183	PRO	2.5
4	R	125	GLU	2.5
2	P	21(C)	ASP	2.5
2	P	21(A)	LYS	2.5
6	T	18(B)	HIS	2.5
1	A	235	ALA	2.5
3	Q	212	ILE	2.4
6	T	207	ASP	2.4
7	U	239	GLN	2.4
5	S	174	THR	2.4
4	R	12(G)	GLU	2.4
5	S	56	ASP	2.4
3	C	232	TYR	2.4
3	Q	174	GLU	2.4
5	S	203	ASP	2.4
11	Y	73	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
4	R	158	TYR	2.4
3	C	242	GLU	2.4
3	Q	243	GLN	2.4
5	S	175	TYR	2.4
10	J	133	TYR	2.4
5	S	230	ALA	2.4
14	N	116	GLY	2.3
3	C	57	LYS	2.3
5	S	2(C)	VAL	2.3
4	R	241	GLU	2.3
5	S	222	THR	2.3
6	T	18(F)	GLY	2.3
3	C	241	GLN	2.3
6	F	240	ILE	2.3
6	T	206	LYS	2.3
10	J	189	ASP	2.3
1	O	235	ALA	2.3
8	H	9	ASN	2.3
3	C	52	ARG	2.3
5	S	178	ARG	2.3
12	L	14(Q)	LEU	2.3
3	Q	208	LYS	2.2
1	A	61	SER	2.2
2	B	21(C)	ASP	2.2
2	P	53	LYS	2.2
12	L	14(K)	LYS	2.2
11	Y	145	ASP	2.2
14	2	105	ASP	2.2
3	C	188	GLU	2.2
3	C	239	GLU	2.2
10	X	190	PHE	2.2
3	Q	50	CYS	2.2
6	T	184	LEU	2.2
1	O	65	SER	2.2
5	S	60	SER	2.2
1	O	203	GLU	2.2
5	E	2(C)	VAL	2.1
2	P	202	THR	2.1
4	R	156	THR	2.1
5	S	51	LEU	2.1
3	C	210	ILE	2.1
6	T	54	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	204	ASP	2.1
1	O	57	PRO	2.1
2	P	181	LYS	2.1
12	Z	14(P)	PRO	2.1
2	P	177	GLN	2.1
5	S	199	GLN	2.1
4	R	243	ALA	2.1
7	G	237	ALA	2.1
3	Q	185	THR	2.1
5	S	171	GLY	2.1
5	S	201	LEU	2.1
6	T	5	GLY	2.1
5	S	198	SER	2.1
6	F	63	LYS	2.1
2	B	57	THR	2.1
3	C	7	GLY	2.1
1	A	203	GLU	2.1
1	A	210	ILE	2.1
1	A	21(P)	LYS	2.1
7	U	199	ASP	2.1
6	T	174	ALA	2.1
2	B	63	THR	2.1
2	P	55	THR	2.1
5	S	12	THR	2.1
3	Q	240	LYS	2.1
5	E	56	ASP	2.1
9	I	182	ASP	2.1
2	P	234	VAL	2.0
3	Q	184	ALA	2.0
3	Q	207	ALA	2.0
4	R	122	ARG	2.0
1	O	58	LEU	2.0
2	P	59	LEU	2.0
5	S	58	LEU	2.0
6	F	205	ASN	2.0
2	P	238	ILE	2.0
3	C	185	THR	2.0
3	C	240	LYS	2.0
5	S	233	ILE	2.0
5	E	33	GLN	2.0
9	W	122	ALA	2.0
7	G	171	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	P	236	THR	2.0
3	C	63	THR	2.0
5	S	127	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	RE0	3	4	16/17	0.91	0.10	34,36,39,46	0
15	RE0	4	4	16/17	0.92	0.08	41,43,44,49	0
15	TY5	4	2	19/20	0.94	0.07	33,41,44,44	0
15	TY5	3	2	19/20	0.96	0.06	37,40,47,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	MES	Y	212	12/12	0.94	0.14	59,62,64,64	0
16	MES	K	212	12/12	0.96	0.10	48,54,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.