Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 01:38 AM EDT

PDB ID	:	3MG6
Title	:	Structure of yeast 20S open-gate proteasome with Compound 6
Authors	:	Sintchak, M.D.
Deposited on	:	2010-04-05
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The 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:

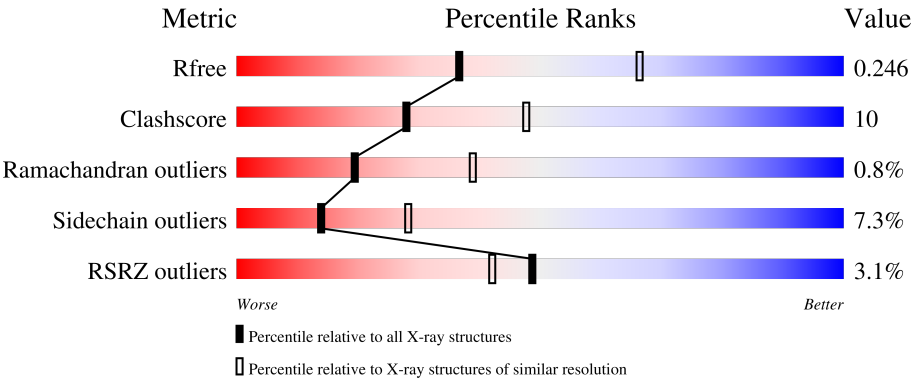
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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% 84% 15%
1	O	250	4% 79% 18%
2	B	245	4% 72% 21%
2	P	245	3% 72% 21%
3	C	243	9% 78% 18%

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Mol	Chain	Length	Quality of chain
3	Q	243	17% 71% 25%
4	D	250	5% 73% 21%
4	R	250	6% 69% 24%
5	E	234	5% 69% 27%
5	S	234	8% 71% 26%
6	F	248	3% 74% 17%
6	T	248	2% 76% 16%
7	G	252	2% 73% 20%
7	U	252	2% 77% 18%
8	H	222	82% 15%
8	V	222	77% 23%
9	I	205	86% 12%
9	W	205	78% 20%
10	J	198	3% 82% 17%
10	X	198	4% 76% 22%
11	K	212	79% 19%
11	Y	212	83% 14%
12	L	241	70% 20% 8%
12	Z	241	% 73% 15% 8%
13	1	266	74% 11% 12%
13	M	266	72% 13% 12%
14	2	196	% 83% 16%
14	N	196	86% 12%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 50276 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	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			
2	P	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	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
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	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
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	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	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			
6	T	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	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
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	F	2	Total	Mg	0	0
			2	2		
15	G	1	Total	Mg	0	0
			1	1		

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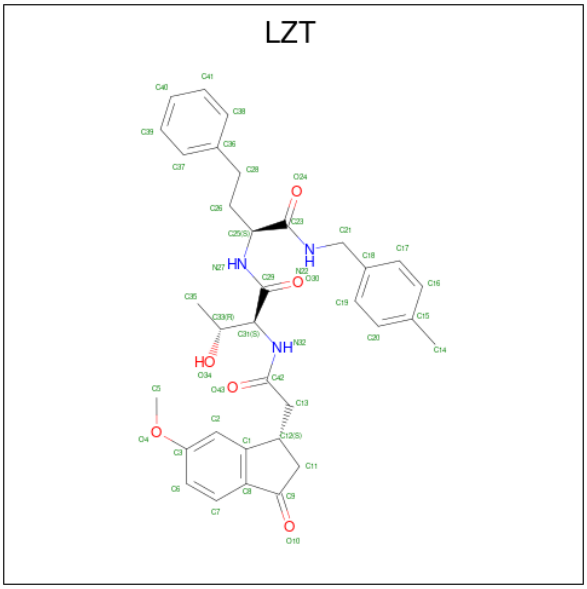
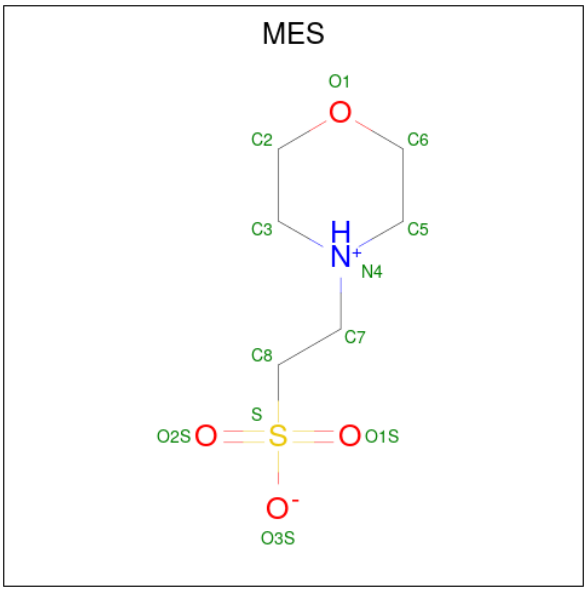
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	K	1	Total Mg 1 1	0	0
15	L	2	Total Mg 2 2	0	0
15	N	1	Total Mg 1 1	0	0

- Molecule 16 is N 2 -{[(1S)-6-methoxy-3-oxo-2,3-dihydro-1H-inden-1-yl]acetyl}-N-{(1S)-1 -[(4-methylbenzyl)carbamoyl]-3-phenylpropyl}-L-threoninamide (three-letter code: LZT) (formula: $C_{34}H_{39}N_3O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total C N O 43 34 3 6	0	0
16	Y	1	Total C N O 43 34 3 6	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	27	Total O 27 27	0	0
18	B	28	Total O 28 28	0	0
18	C	27	Total O 27 27	0	0
18	D	24	Total O 24 24	0	0
18	E	21	Total O 21 21	0	0
18	F	38	Total O 38 38	0	0
18	G	44	Total O 44 44	0	0
18	H	30	Total O 30 30	0	0
18	I	37	Total O 37 37	0	0
18	J	33	Total O 33 33	0	0

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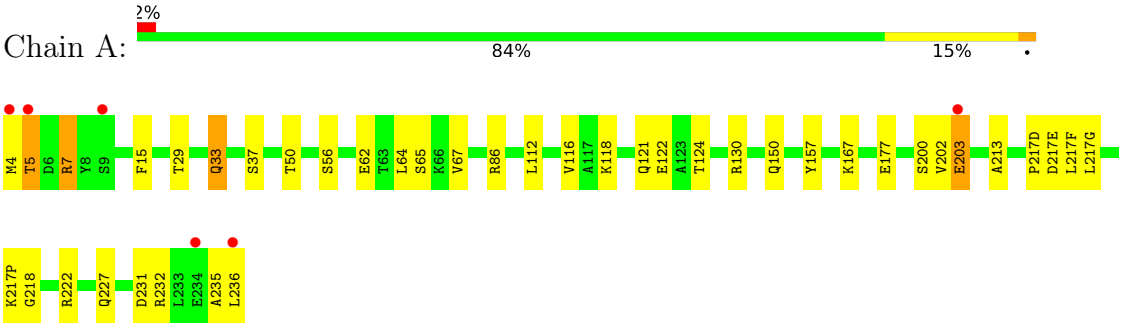
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	39	Total O 39 39	0	0
18	L	34	Total O 34 34	0	0
18	M	35	Total O 35 35	0	0
18	N	29	Total O 29 29	0	0
18	O	23	Total O 23 23	0	0
18	P	17	Total O 17 17	0	0
18	Q	32	Total O 32 32	0	0
18	R	21	Total O 21 21	0	0
18	S	23	Total O 23 23	0	0
18	T	24	Total O 24 24	0	0
18	U	34	Total O 34 34	0	0
18	V	27	Total O 27 27	0	0
18	W	32	Total O 32 32	0	0
18	X	38	Total O 38 38	0	0
18	Y	32	Total O 32 32	0	0
18	Z	31	Total O 31 31	0	0
18	1	46	Total O 46 46	0	0
18	2	32	Total O 32 32	0	0

3 Residue-property plots (i)

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.

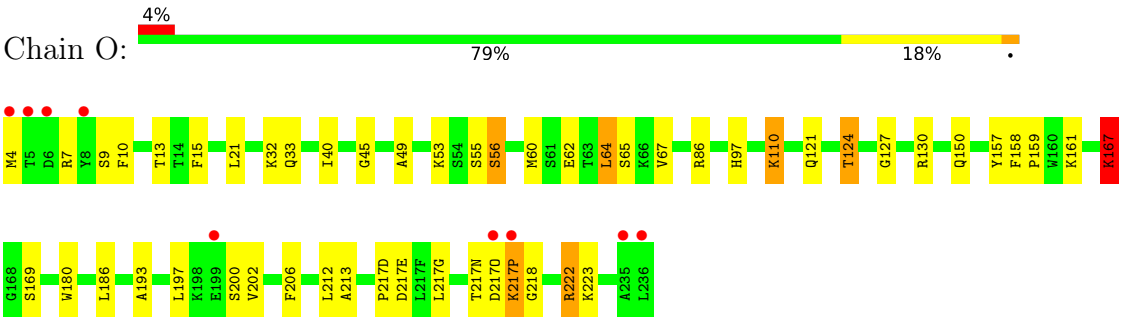
• Molecule 1: Proteasome component Y7

Chain A:



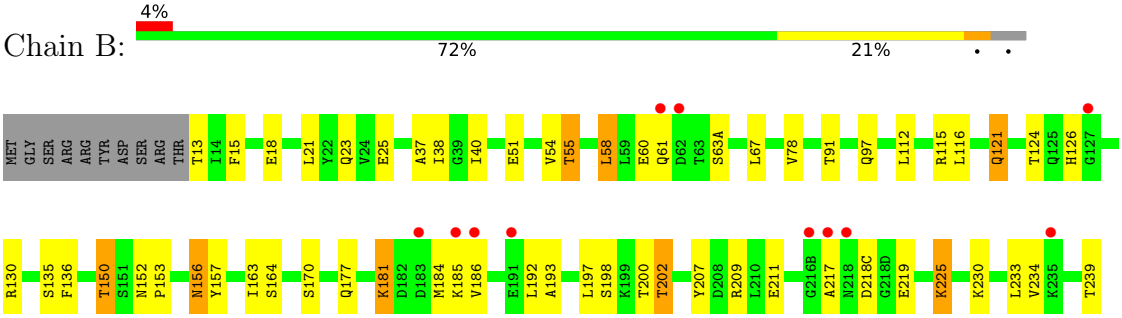
• Molecule 1: Proteasome component Y7

Chain O:



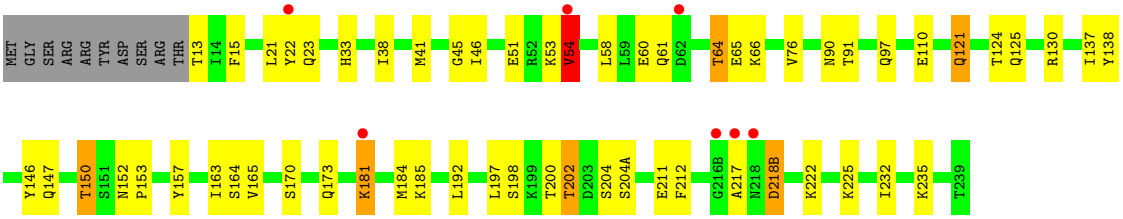
• Molecule 2: Proteasome component Y13

Chain B:



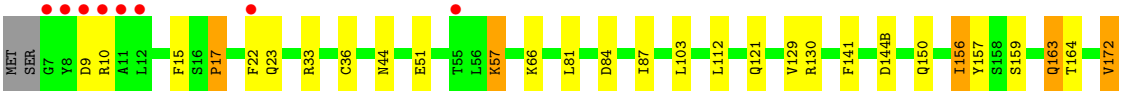
• Molecule 2: Proteasome component Y13

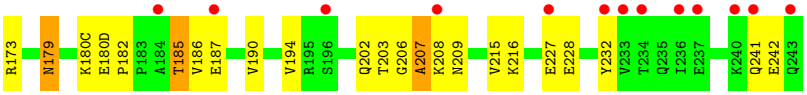
Chain P:



• Molecule 3: Proteasome component PRE6

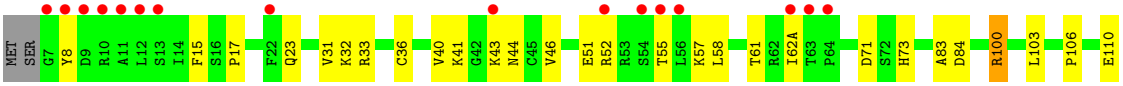
Chain C:

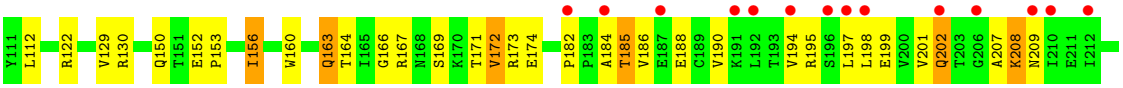


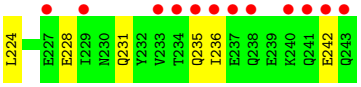


• Molecule 3: Proteasome component PRE6

Chain Q:

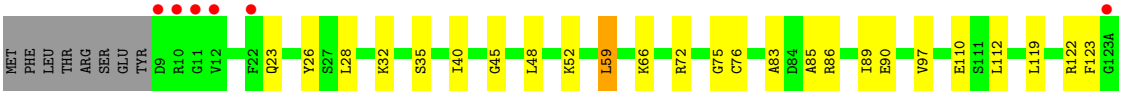


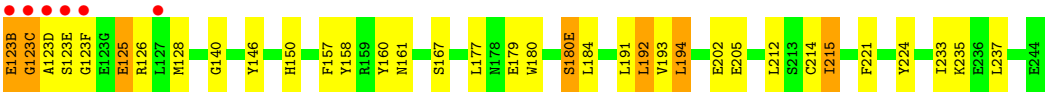




• Molecule 4: Proteasome component PUP2

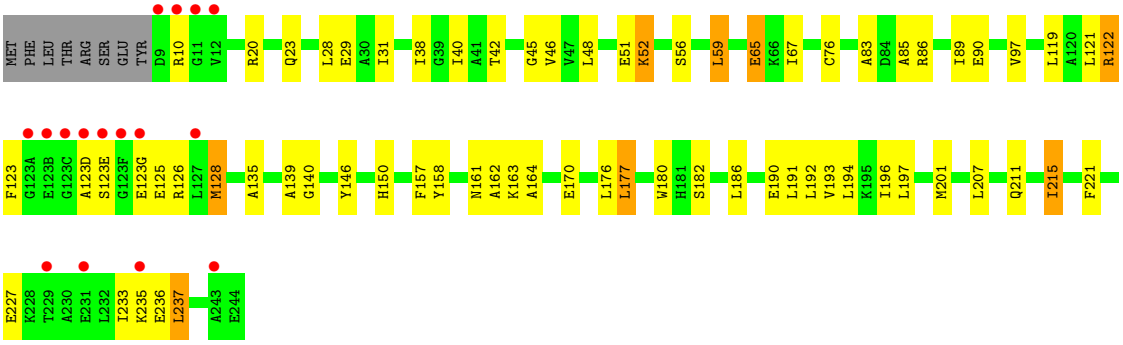
Chain D:



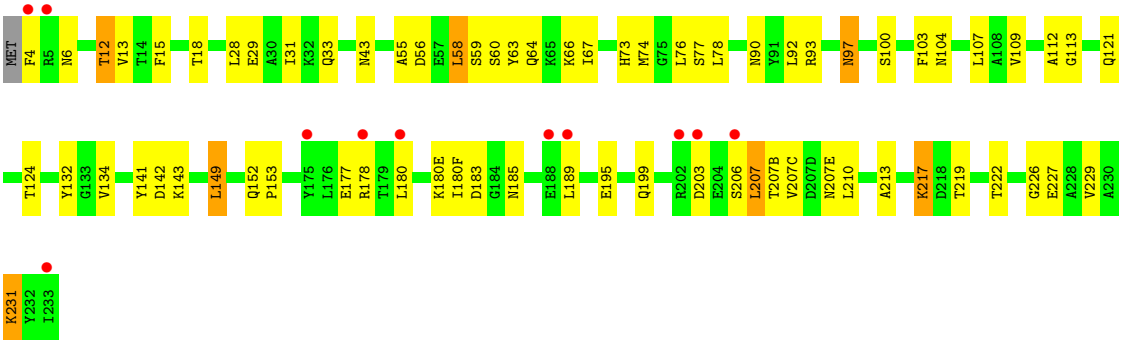


• Molecule 4: Proteasome component PUP2

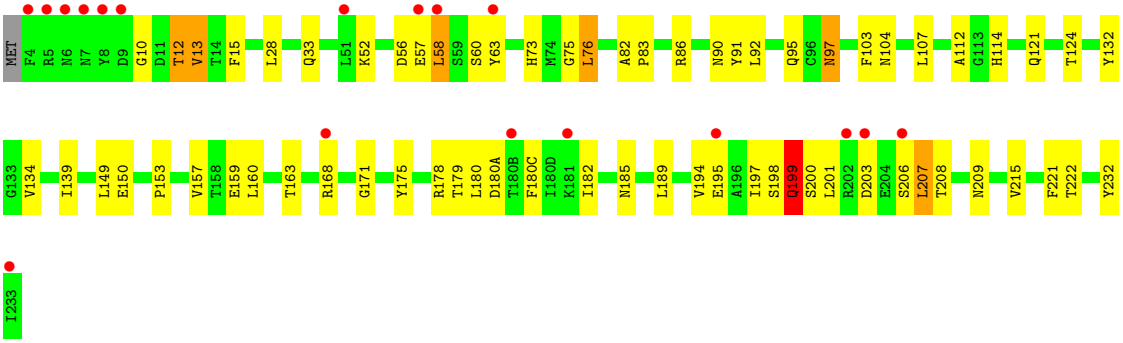
Chain R:



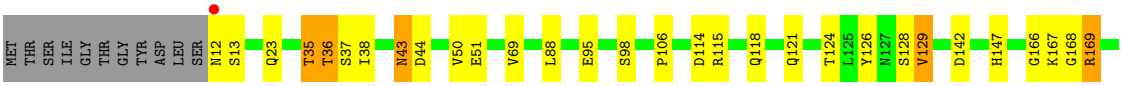
• Molecule 5: Proteasome component PRE5

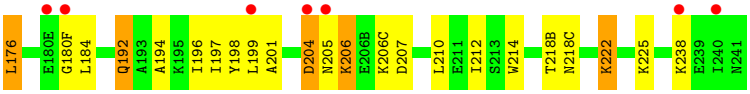


• Molecule 5: Proteasome component PRE5

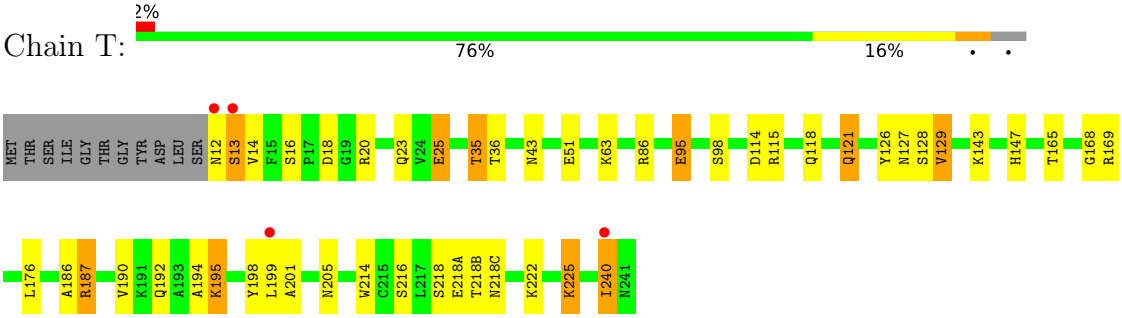


• Molecule 6: Proteasome component C1

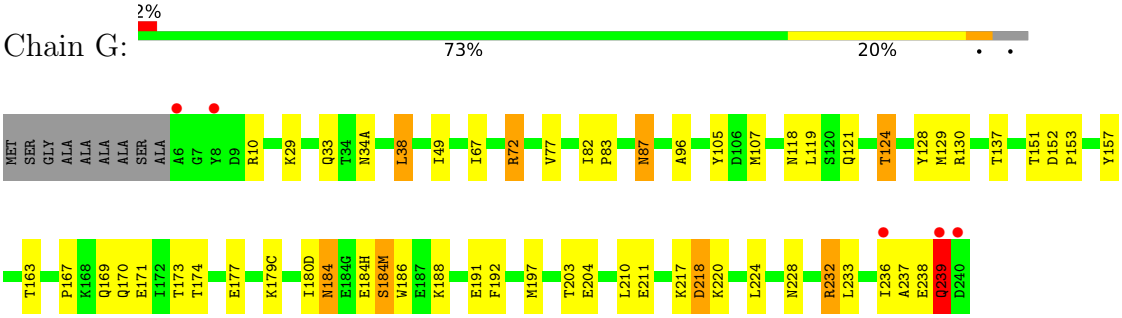




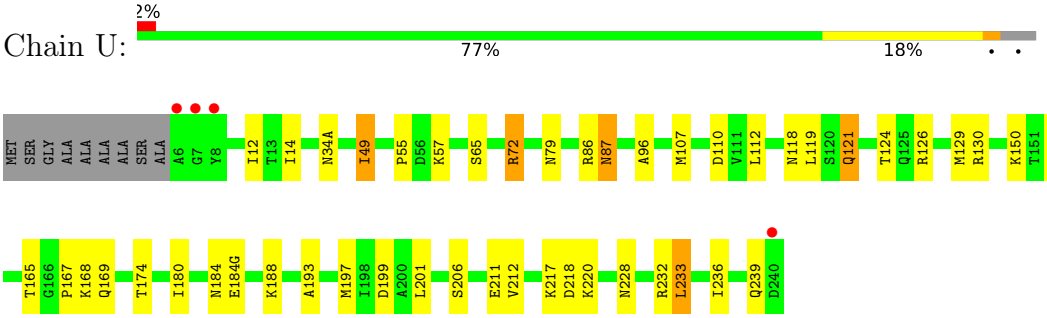
• Molecule 6: Proteasome component C1



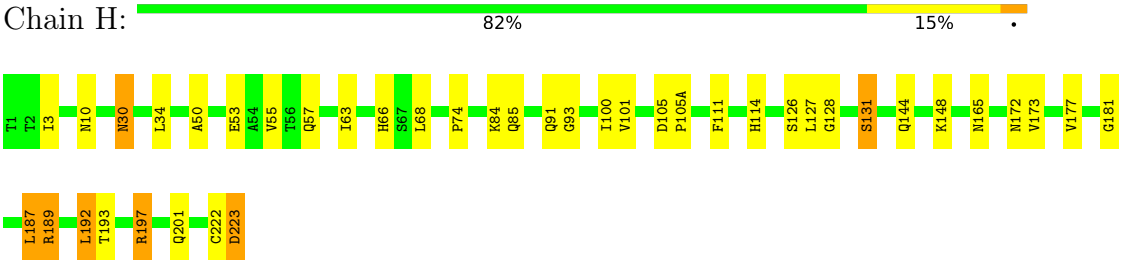
• Molecule 7: Proteasome component C7-alpha



• Molecule 7: Proteasome component C7-alpha

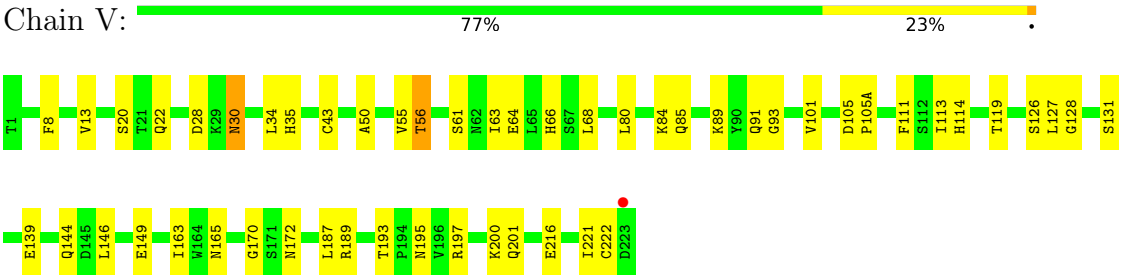


• Molecule 8: Proteasome component PUP1



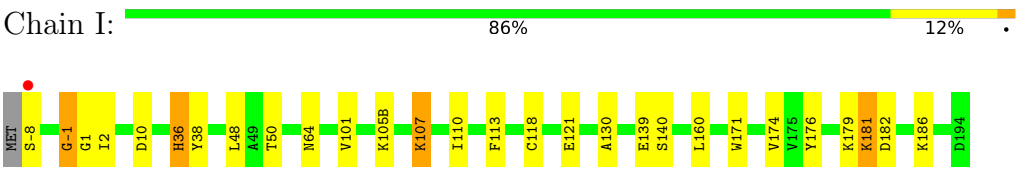
• Molecule 8: Proteasome component PUP1

Chain V:



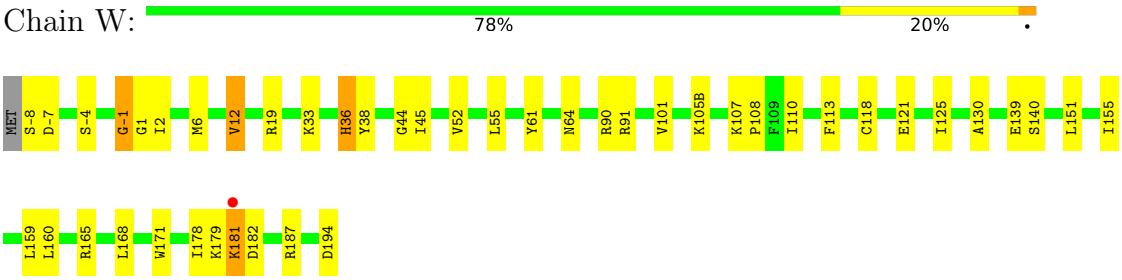
• Molecule 9: Proteasome component PUP3

Chain I:



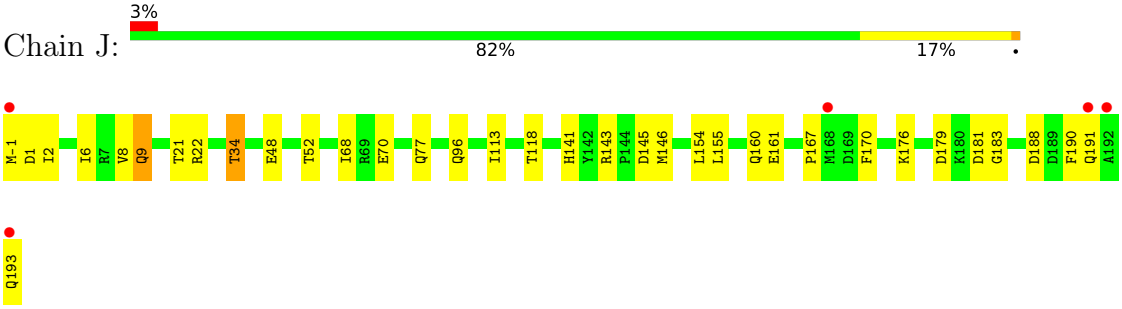
• Molecule 9: Proteasome component PUP3

Chain W:



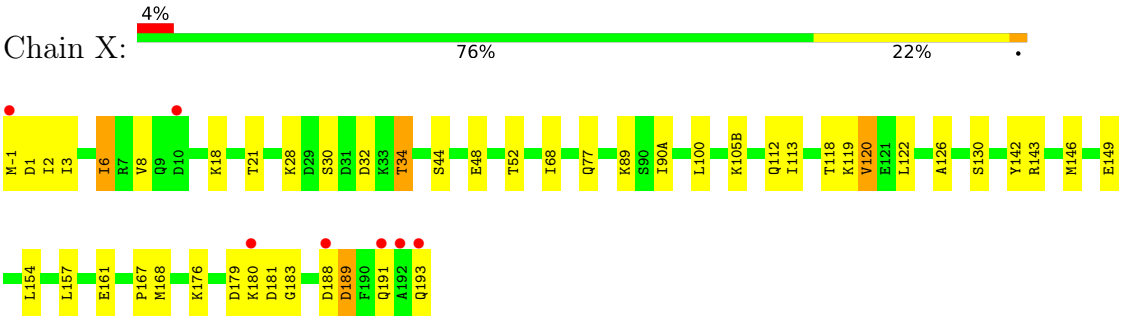
• Molecule 10: Proteasome component C11

Chain J:



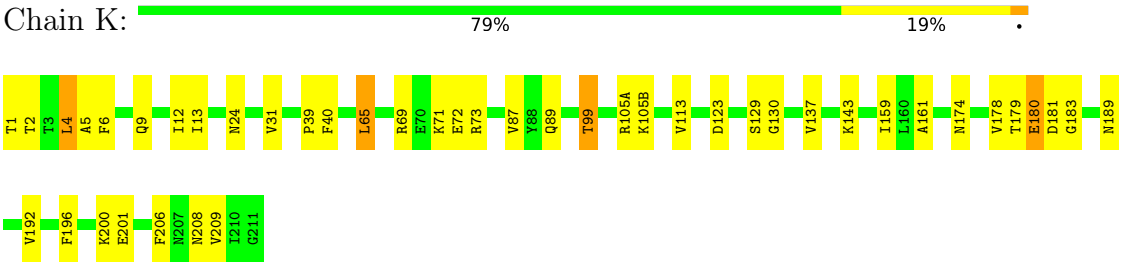
• Molecule 10: Proteasome component C11

Chain X:



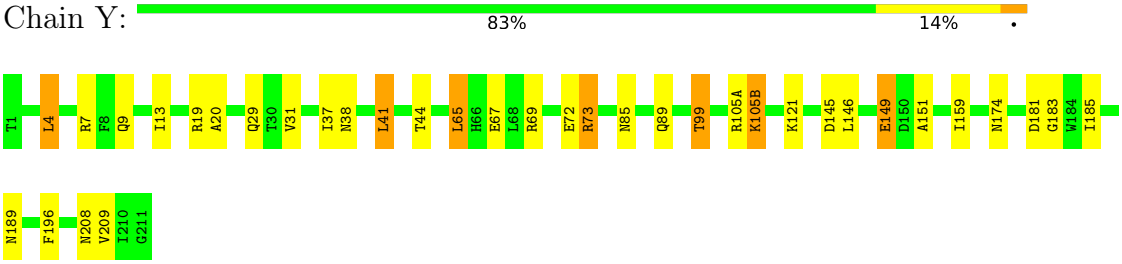
• Molecule 11: Proteasome component PRE2

Chain K:



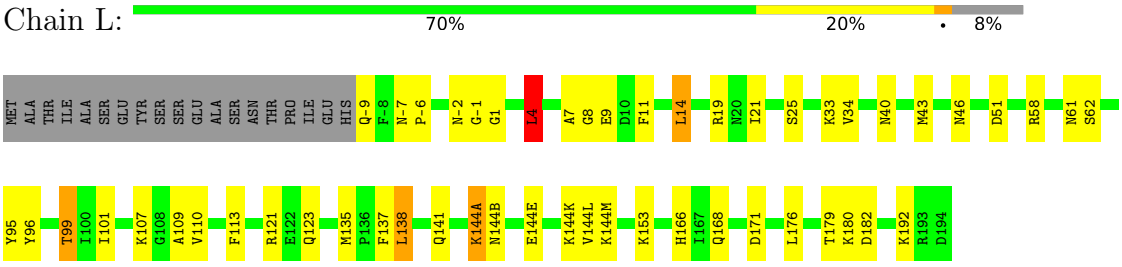
• Molecule 11: Proteasome component PRE2

Chain Y:



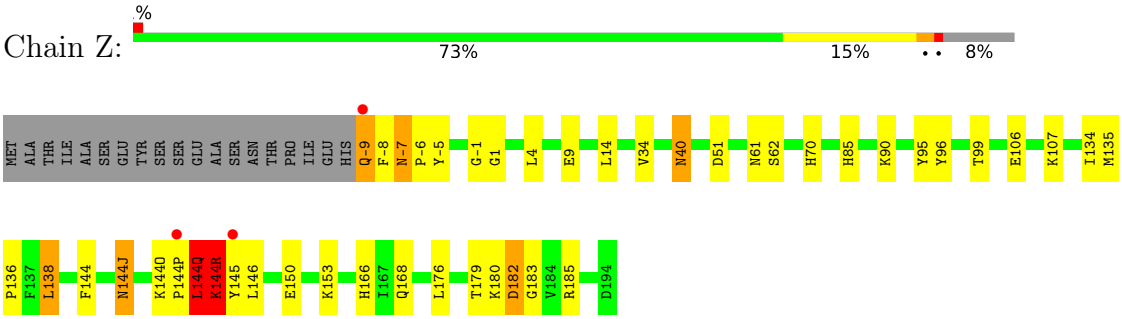
• Molecule 12: Proteasome component C5

Chain L:



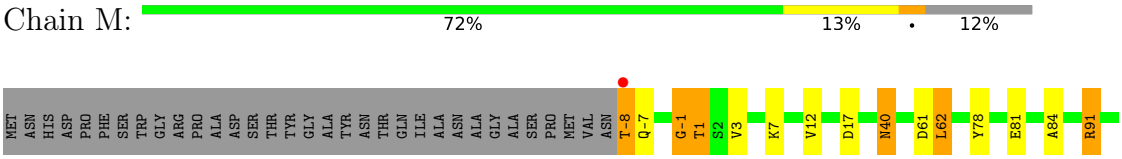
• Molecule 12: Proteasome component C5

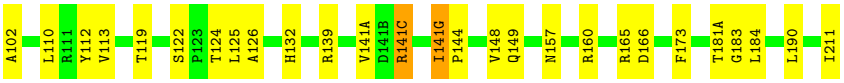
Chain Z:



• Molecule 13: Proteasome component PRE4

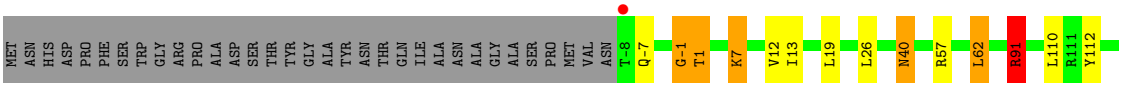
Chain M:

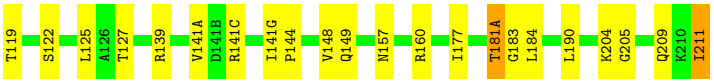




• Molecule 13: Proteasome component PRE4

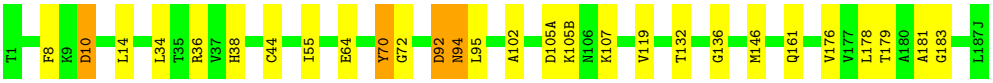
Chain 1:





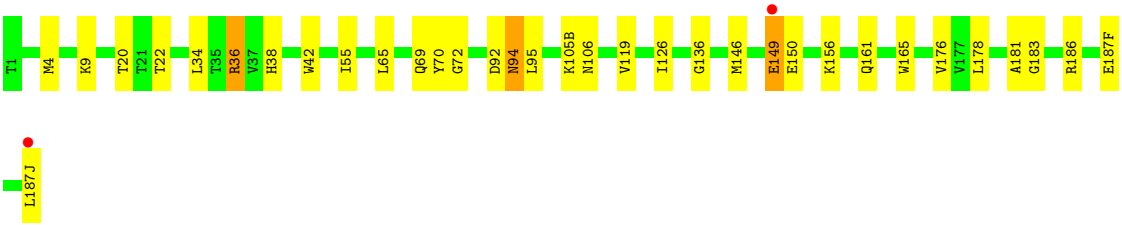
• Molecule 14: Proteasome component PRE3

Chain N:



• Molecule 14: Proteasome component PRE3

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.25Å 299.65Å 145.78Å 90.00° 113.67° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.60) 95.4 (49.94-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.249 0.213 , 0.246	Depositor DCC
R_{free} test set	3189 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	50276	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MES, LZT

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	0.51	0/1951	0.63	0/2639
1	O	0.54	0/1951	0.62	0/2639
2	B	0.48	0/1857	0.64	0/2513
2	P	0.50	0/1857	0.62	0/2513
3	C	0.47	0/1918	0.60	1/2591 (0.0%)
3	Q	0.51	0/1918	0.63	1/2591 (0.0%)
4	D	0.52	0/1883	0.67	1/2529 (0.0%)
4	R	0.53	0/1884	0.66	0/2532
5	E	0.48	0/1819	0.64	1/2451 (0.0%)
5	S	0.48	0/1821	0.63	1/2457 (0.0%)
6	F	0.51	0/1885	0.61	0/2540
6	T	0.54	0/1886	0.63	0/2543
7	G	0.81	1/1957 (0.1%)	0.67	2/2646 (0.1%)
7	U	0.55	0/1958	0.63	0/2649
8	H	0.84	1/1715 (0.1%)	0.78	1/2323 (0.0%)
8	V	0.55	1/1714 (0.1%)	0.65	0/2320
9	I	1.13	2/1610 (0.1%)	0.83	3/2171 (0.1%)
9	W	1.14	2/1610 (0.1%)	0.94	5/2171 (0.2%)
10	J	0.55	0/1611	0.67	0/2167
10	X	0.58	0/1611	0.68	0/2167
11	K	0.57	0/1680	0.69	0/2271
11	Y	0.53	0/1680	0.66	0/2271
12	L	0.56	0/1793	0.65	1/2414 (0.0%)
12	Z	0.55	0/1793	0.68	0/2414
13	1	0.76	1/1853 (0.1%)	0.85	3/2507 (0.1%)
13	M	1.06	2/1854 (0.1%)	0.85	5/2511 (0.2%)
14	2	0.58	0/1538	0.66	0/2078
14	N	1.17	2/1540 (0.1%)	0.82	5/2084 (0.2%)
All	All	0.67	12/50147 (0.0%)	0.69	30/67702 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
8	H	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	70	TYR	C-N	34.46	1.95	1.33
13	M	141(G)	ILE	C-N	31.31	1.93	1.34
9	I	-1	GLY	C-N	29.40	1.85	1.33
9	W	-1	GLY	C-N	28.22	1.83	1.33
9	W	36	HIS	C-N	27.17	1.96	1.34
8	H	187	LEU	C-N	26.78	1.95	1.34
9	I	36	HIS	C-N	24.98	1.91	1.34
7	G	218	ASP	C-N	24.96	1.91	1.34
13	M	-1	GLY	C-N	22.79	1.86	1.34
13	1	-1	GLY	C-N	21.41	1.83	1.34
14	N	92	ASP	C-N	18.41	1.76	1.34
8	V	43	CYS	CB-SG	-5.89	1.72	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	-1	GLY	O-C-N	-20.50	88.36	123.20
13	M	-1	GLY	O-C-N	-20.43	90.00	122.70
13	1	-1	GLY	O-C-N	-20.28	90.26	122.70
8	H	187	LEU	O-C-N	-19.97	90.75	122.70
9	I	36	HIS	O-C-N	-18.17	93.63	122.70
9	W	36	HIS	O-C-N	-14.68	99.21	122.70
9	W	36	HIS	CA-C-N	-14.13	86.11	117.20
14	N	92	ASP	O-C-N	-12.66	102.44	122.70
14	N	70	TYR	C-N-CA	-11.09	99.02	122.30
7	G	218	ASP	O-C-N	-9.88	106.90	122.70
9	I	-1	GLY	O-C-N	-9.43	107.17	123.20
9	I	36	HIS	CA-C-N	-9.42	96.48	117.20
14	N	92	ASP	CA-C-N	9.14	137.31	117.20
14	N	70	TYR	O-C-N	-8.59	108.60	123.20
9	W	-1	GLY	C-N-CA	7.27	137.57	122.30
13	1	-1	GLY	CA-C-N	-7.05	101.70	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	-1	GLY	CA-C-N	6.69	129.58	116.20
7	G	218	ASP	CA-C-N	6.66	131.84	117.20
13	M	91	ARG	NE-CZ-NH1	6.44	123.52	120.30
14	N	70	TYR	CA-C-N	6.35	128.90	116.20
13	M	166	ASP	CB-CG-OD2	6.31	123.97	118.30
4	D	59	LEU	CA-CB-CG	6.12	129.36	115.30
13	M	-1	GLY	CA-C-N	-5.84	104.35	117.20
3	Q	103	LEU	CA-CB-CG	5.70	128.41	115.30
13	1	91	ARG	NE-CZ-NH1	5.31	122.95	120.30
5	S	76	LEU	CA-CB-CG	5.20	127.26	115.30
12	L	4	LEU	CA-CB-CG	5.08	127.00	115.30
3	C	103	LEU	CA-CB-CG	5.03	126.87	115.30
13	M	91	ARG	NE-CZ-NH2	-5.03	117.79	120.30
5	E	93	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	181	GLY	Peptide
1	O	217(N)	THR	Peptide

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	1925	31	0
1	O	1915	0	1925	45	0
2	B	1829	0	1828	39	0
2	P	1829	0	1828	36	0
3	C	1891	0	1899	38	0
3	Q	1891	0	1899	62	0
4	D	1862	0	1832	42	0
4	R	1862	0	1833	45	0
5	E	1795	0	1793	43	0
5	S	1795	0	1795	43	0
6	F	1848	0	1842	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1848	0	1843	36	0
7	G	1921	0	1907	53	0
7	U	1921	0	1909	41	0
8	H	1685	0	1686	29	0
8	V	1685	0	1686	36	0
9	I	1581	0	1574	26	0
9	W	1581	0	1574	37	0
10	J	1585	0	1591	24	0
10	X	1585	0	1591	35	0
11	K	1644	0	1594	35	0
11	Y	1644	0	1594	30	0
12	L	1757	0	1712	44	0
12	Z	1757	0	1712	58	0
13	1	1824	0	1833	34	0
13	M	1824	0	1833	39	0
14	2	1512	0	1478	33	0
14	N	1512	0	1478	24	0
15	F	2	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
16	K	43	0	39	5	0
16	Y	43	0	39	4	0
17	K	12	0	13	2	0
17	Y	12	0	13	1	0
18	1	46	0	0	4	0
18	2	32	0	0	6	0
18	A	27	0	0	4	0
18	B	28	0	0	9	0
18	C	27	0	0	7	0
18	D	24	0	0	6	0
18	E	21	0	0	5	0
18	F	38	0	0	10	0
18	G	44	0	0	6	0
18	H	30	0	0	4	0
18	I	37	0	0	1	0
18	J	33	0	0	1	0
18	K	39	0	0	9	0
18	L	34	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	M	35	0	0	5	0
18	N	29	0	0	5	0
18	O	23	0	0	9	0
18	P	17	0	0	4	0
18	Q	32	0	0	19	0
18	R	21	0	0	10	0
18	S	23	0	0	4	0
18	T	24	0	0	7	0
18	U	34	0	0	7	0
18	V	27	0	0	4	0
18	W	32	0	0	3	0
18	X	38	0	0	5	0
18	Y	32	0	0	6	0
18	Z	31	0	0	6	0
All	All	50276	0	49098	979	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 10.

All (979) 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)
13:1:-1:GLY:C	13:1:1:THR:H1	1.21	1.40
14:N:92:ASP:C	14:N:94:ASN:N	1.76	1.39
9:W:-1:GLY:C	9:W:1:GLY:H1	1.24	1.38
8:H:91:GLN:O	8:H:93:GLY:N	1.59	1.32
9:I:-1:GLY:C	9:I:1:GLY:N	1.86	1.28
13:M:-1:GLY:C	13:M:1:THR:N	1.86	1.28
9:W:-1:GLY:C	9:W:1:GLY:N	1.83	1.27
13:1:-1:GLY:C	13:1:1:THR:N	1.83	1.27
12:Z:145:TYR:HA	18:Z:670:HOH:O	1.32	1.27
13:M:-1:GLY:C	13:M:1:THR:H1	1.33	1.26
7:G:218:ASP:C	7:G:220:LYS:N	1.91	1.24
9:I:36:HIS:C	9:I:38:TYR:N	1.91	1.23
13:M:141(G):ILE:C	13:M:144:PRO:N	1.93	1.22
12:Z:144(P):PRO:O	12:Z:144(R):LYS:HG2	1.42	1.20
14:N:70:TYR:C	14:N:72:GLY:N	1.95	1.19
8:H:187:LEU:C	8:H:189:ARG:N	1.95	1.19
2:B:239:THR:HA	18:B:1122:HOH:O	1.44	1.17
9:W:36:HIS:C	9:W:38:TYR:N	1.96	1.17
11:K:181:ASP:C	11:K:183:GLY:HA2	1.65	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:70:TYR:C	14:2:72:GLY:N	2.00	1.14
7:G:96:ALA:HA	7:G:107:MET:HE2	1.30	1.12
13:1:141(G):ILE:C	13:1:144:PRO:N	2.01	1.12
2:P:200:THR:O	2:P:202:THR:N	1.81	1.11
9:I:-1:GLY:C	9:I:1:GLY:H3	1.44	1.10
5:E:90:ASN:HB3	18:E:285:HOH:O	1.52	1.08
8:V:187:LEU:C	8:V:189:ARG:N	2.07	1.08
2:B:234:VAL:HA	18:B:1122:HOH:O	1.52	1.06
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.16	1.06
7:U:96:ALA:HA	7:U:107:MET:HE2	1.33	1.06
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.21	1.05
11:Y:73:ARG:HD3	18:Y:220:HOH:O	1.58	1.04
4:R:59:LEU:HA	18:R:666:HOH:O	1.58	1.04
11:Y:89:GLN:HG3	18:Y:332:HOH:O	1.56	1.01
2:B:200:THR:C	2:B:202:THR:N	2.16	0.99
6:F:180(F):GLY:HA3	18:F:405:HOH:O	1.63	0.99
14:N:181:ALA:O	14:N:183:GLY:HA3	1.63	0.98
14:N:181:ALA:O	14:N:183:GLY:CA	2.11	0.98
4:D:180(E):SER:O	4:D:184:LEU:N	1.98	0.97
9:I:-1:GLY:C	9:I:1:GLY:H1	1.64	0.97
4:D:123(C):GLY:HA2	4:D:125:GLU:HA	1.44	0.97
11:K:181:ASP:C	11:K:183:GLY:CA	2.32	0.97
9:I:-8:SER:HA	18:I:197:HOH:O	1.65	0.97
10:X:-1:MET:HG3	10:X:1:ASP:H1	1.31	0.96
5:S:232:TYR:HE2	18:S:998:HOH:O	1.47	0.95
14:2:183:GLY:HA3	18:2:194:HOH:O	1.66	0.95
1:O:7:ARG:HG3	6:T:128:SER:HB3	1.48	0.94
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.14	0.94
14:2:92:ASP:O	14:2:94:ASN:N	2.00	0.93
11:K:181:ASP:O	11:K:183:GLY:HA2	1.69	0.93
12:Z:180:LYS:C	12:Z:182:ASP:N	2.22	0.93
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.31	0.93
8:H:10:ASN:HB3	18:H:938:HOH:O	1.68	0.92
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.34	0.92
7:U:199:ASP:HB3	18:U:281:HOH:O	1.68	0.92
12:Z:144(P):PRO:HD2	12:Z:144(R):LYS:NZ	1.85	0.90
5:E:15:PHE:H	6:F:23:GLN:HE22	1.20	0.90
16:K:213:LZT:H5	12:L:96:TYR:CE1	2.06	0.90
12:Z:-1:GLY:C	12:Z:1:GLY:N	2.26	0.89
7:G:184(M):SER:HA	7:G:186:TRP:N	1.88	0.89
12:Z:85:HIS:HD2	18:Z:199:HOH:O	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:181(A):THR:O	13:M:183:GLY:N	2.05	0.89
2:P:90:ASN:HB2	18:P:242:HOH:O	1.73	0.88
4:D:202:GLU:C	4:D:205:GLU:N	2.26	0.88
13:M:61:ASP:HB2	18:M:667:HOH:O	1.74	0.88
7:U:218:ASP:C	7:U:220:LYS:N	2.28	0.88
13:M:-1:GLY:C	13:M:1:THR:H2	1.74	0.88
3:Q:58:LEU:HA	18:Q:584:HOH:O	1.73	0.88
13:1:181(A):THR:C	13:1:183:GLY:N	2.27	0.88
6:F:207:ASP:HA	18:F:1076:HOH:O	1.73	0.87
10:X:-1:MET:HG3	10:X:1:ASP:N	1.91	0.86
3:C:15:PHE:H	4:D:23:GLN:HE22	1.21	0.86
7:G:96:ALA:HA	7:G:107:MET:CE	2.06	0.86
6:F:43:ASN:HB3	18:F:405:HOH:O	1.76	0.85
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.21	0.85
2:P:64:THR:HB	18:P:241:HOH:O	1.75	0.85
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.88	0.85
12:L:-1:GLY:O	12:L:1:GLY:HA3	1.74	0.85
3:Q:202:GLN:HB2	18:Q:937:HOH:O	1.74	0.85
12:Z:144(P):PRO:HD2	12:Z:144(R):LYS:HZ1	1.42	0.84
6:F:180(F):GLY:O	6:F:184:LEU:N	2.11	0.83
4:R:233:ILE:C	4:R:235:LYS:N	2.32	0.83
11:Y:181:ASP:C	11:Y:183:GLY:N	2.31	0.83
11:K:89:GLN:HG3	18:K:387:HOH:O	1.79	0.83
10:X:181:ASP:O	10:X:183:GLY:HA3	1.77	0.83
12:L:180:LYS:C	12:L:182:ASP:N	2.31	0.83
9:W:36:HIS:CA	9:W:38:TYR:N	2.41	0.83
11:K:208:ASN:HB3	18:K:215:HOH:O	1.78	0.83
3:Q:122:ARG:HD2	18:Q:248:HOH:O	1.77	0.83
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.60	0.82
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.91	0.82
4:R:123(D):ALA:HB3	4:R:126:ARG:HG3	1.59	0.82
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.28	0.82
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.62	0.82
13:1:-1:GLY:C	13:1:1:THR:H2	1.82	0.82
10:J:181:ASP:C	10:J:183:GLY:N	2.33	0.82
1:A:200:SER:O	1:A:202:VAL:HA	1.80	0.82
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.44	0.82
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	1.93	0.81
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.28	0.81
4:D:214:CYS:SG	18:D:869:HOH:O	2.38	0.81
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ASN:H	13:M:40:ASN:HD22	1.29	0.79
10:X:181:ASP:C	10:X:183:GLY:N	2.36	0.78
14:2:181:ALA:O	14:2:183:GLY:HA3	1.82	0.78
7:U:96:ALA:HA	7:U:107:MET:CE	2.12	0.78
9:I:179:LYS:O	9:I:181:LYS:N	2.16	0.78
8:V:91:GLN:C	8:V:93:GLY:N	2.36	0.78
12:Z:-1:GLY:O	12:Z:1:GLY:HA3	1.84	0.78
3:C:241:GLN:HB3	18:C:247:HOH:O	1.83	0.78
3:Q:185:THR:HB	18:Q:1281:HOH:O	1.83	0.77
18:R:412:HOH:O	12:Z:70:HIS:HE1	1.67	0.77
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.65	0.77
8:H:91:GLN:O	8:H:93:GLY:CA	2.33	0.77
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	1.81	0.77
1:O:15:PHE:H	2:P:23:GLN:HE22	1.31	0.77
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.31	0.77
6:F:206:LYS:HG2	18:F:425:HOH:O	1.85	0.77
9:W:-1:GLY:C	9:W:1:GLY:H3	1.84	0.76
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.83	0.76
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.34	0.76
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.00	0.76
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.51	0.76
1:A:15:PHE:H	2:B:23:GLN:HE22	1.34	0.76
12:Z:9:GLU:HB2	12:Z:145:TYR:HE2	1.49	0.76
14:2:149:GLU:HG3	18:2:192:HOH:O	1.84	0.76
3:C:159:SER:HB2	18:C:582:HOH:O	1.85	0.75
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.69	0.75
8:V:91:GLN:O	8:V:93:GLY:HA3	1.86	0.75
8:V:91:GLN:O	8:V:93:GLY:N	2.20	0.75
3:Q:185:THR:O	18:Q:1044:HOH:O	2.04	0.75
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.32	0.74
7:G:204:GLU:HG2	18:G:1211:HOH:O	1.88	0.74
11:K:24:ASN:HB2	18:K:364:HOH:O	1.88	0.74
18:O:391:HOH:O	9:W:105(B):LYS:HG2	1.87	0.74
1:O:65:SER:HA	18:O:237:HOH:O	1.86	0.74
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.70	0.73
6:T:199:LEU:C	6:T:201:ALA:N	2.41	0.73
6:T:35:THR:HG21	6:T:51:GLU:O	1.88	0.73
18:A:239:HOH:O	9:I:105(B):LYS:HG2	1.87	0.73
2:P:121:GLN:O	2:P:124:THR:HB	1.89	0.73
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.71	0.73
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:THR:O	3:C:130:ARG:HD3	1.89	0.73
3:C:209:ASN:HB2	18:C:244:HOH:O	1.89	0.73
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.04	0.73
2:B:225:LYS:HE2	18:B:1191:HOH:O	1.89	0.73
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.02	0.73
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.34	0.72
8:H:91:GLN:C	8:H:93:GLY:N	2.42	0.72
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.72	0.72
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.37	0.72
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.71	0.72
6:F:35:THR:HG21	6:F:51:GLU:O	1.89	0.72
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.88	0.71
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.38	0.71
1:A:7:ARG:CG	6:F:128:SER:HB3	2.21	0.71
9:W:-8:SER:HB3	18:W:199:HOH:O	1.90	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.03	0.71
13:M:-7:GLN:HB2	18:N:654:HOH:O	1.90	0.71
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.88	0.71
10:J:-1:MET:HG3	10:J:1:ASP:N	2.05	0.71
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.56	0.71
18:Q:845:HOH:O	4:R:29:GLU:CB	2.38	0.71
8:V:91:GLN:O	8:V:93:GLY:CA	2.38	0.71
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.05	0.71
3:Q:44:ASN:HB3	18:Q:249:HOH:O	1.90	0.70
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.06	0.70
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.39	0.70
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.56	0.70
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.57	0.70
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.39	0.70
14:N:181:ALA:O	14:N:183:GLY:N	2.24	0.70
14:N:70:TYR:C	14:N:72:GLY:CA	2.60	0.70
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.21	0.70
12:Z:179:THR:HG1	12:Z:182:ASP:N	1.88	0.70
5:E:60:SER:C	5:E:63:TYR:N	2.44	0.70
8:H:128:GLY:O	8:H:131:SER:HB3	1.90	0.70
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.39	0.70
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.55	0.70
9:W:36:HIS:HA	9:W:38:TYR:N	2.06	0.70
5:E:207(E):ASN:O	5:E:210:LEU:N	2.24	0.70
1:O:110:LYS:HG2	18:O:238:HOH:O	1.91	0.70
5:E:29:GLU:HG3	18:E:781:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:121:GLN:O	7:U:124:THR:HB	1.92	0.69
3:Q:188:GLU:HG3	18:Q:1044:HOH:O	1.92	0.69
13:1:57:ARG:CD	18:1:221:HOH:O	2.40	0.69
11:Y:149:GLU:HA	18:Y:377:HOH:O	1.91	0.69
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.73	0.69
6:F:168:GLY:HA3	6:F:201:ALA:HB1	1.74	0.69
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.40	0.69
8:V:187:LEU:O	8:V:189:ARG:N	2.25	0.69
2:B:181:LYS:O	2:B:184:MET:HG3	1.93	0.69
14:2:181:ALA:O	14:2:183:GLY:CA	2.40	0.69
3:C:242:GLU:HG3	18:C:247:HOH:O	1.92	0.69
5:S:134:VAL:O	5:S:153:PRO:HG3	1.92	0.69
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.74	0.69
12:Z:144(P):PRO:CD	12:Z:144(R):LYS:NZ	2.56	0.69
2:P:33:HIS:O	2:P:53:LYS:HE3	1.93	0.69
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.75	0.69
18:F:275:HOH:O	7:G:29:LYS:HE3	1.92	0.68
1:A:235:ALA:HA	18:A:318:HOH:O	1.93	0.68
11:K:72:GLU:HG3	18:K:1023:HOH:O	1.93	0.68
7:G:184(M):SER:CA	7:G:186:TRP:N	2.56	0.68
1:O:7:ARG:HG3	6:T:128:SER:CB	2.22	0.68
3:Q:160:TRP:CD2	18:R:666:HOH:O	2.45	0.68
10:X:28:LYS:HE3	11:Y:121:LYS:O	1.93	0.68
12:Z:144(P):PRO:O	12:Z:144(R):LYS:N	2.27	0.68
7:G:180(D):ILE:C	7:G:184:ASN:N	2.48	0.68
1:O:217(D):PRO:HA	1:O:217(P):LYS:O	1.92	0.67
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.59	0.67
9:I:36:HIS:CA	9:I:38:TYR:N	2.58	0.67
12:L:-1:GLY:C	12:L:1:GLY:N	2.47	0.67
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.41	0.67
4:R:59:LEU:HD22	18:R:666:HOH:O	1.94	0.67
7:G:72:ARG:HD2	18:G:302:HOH:O	1.94	0.67
3:Q:57:LYS:NZ	3:Q:208:LYS:HD3	2.09	0.67
5:S:12:THR:HG21	5:S:124:THR:HA	1.77	0.67
10:X:89:LYS:HB2	18:X:383:HOH:O	1.95	0.66
12:Z:-1:GLY:C	12:Z:1:GLY:H1	1.99	0.66
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.76	0.66
12:L:-1:GLY:O	12:L:1:GLY:CA	2.43	0.66
7:G:121:GLN:O	7:G:124:THR:HB	1.96	0.66
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.93	0.66
2:P:181:LYS:O	2:P:184:MET:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:GLN:NE2	3:C:164:THR:H	1.94	0.66
12:L:166:HIS:HE1	18:L:475:HOH:O	1.77	0.66
5:E:207:LEU:CA	5:E:207(E):ASN:HD22	2.03	0.66
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.60	0.66
1:A:5:THR:HB	18:A:630:HOH:O	1.96	0.66
7:U:228:ASN:HB3	18:U:241:HOH:O	1.94	0.66
10:X:6:ILE:HD11	10:X:142:TYR:CE1	2.30	0.65
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.79	0.65
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.78	0.65
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.77	0.65
3:Q:57:LYS:HZ3	3:Q:208:LYS:HD3	1.62	0.65
12:Z:144(O):LYS:HE2	12:Z:144(R):LYS:HD2	1.78	0.65
4:D:123(C):GLY:CA	4:D:125:GLU:HA	2.25	0.65
5:E:73:HIS:HE1	5:E:107:LEU:O	1.79	0.65
11:K:174:ASN:ND2	11:K:189:ASN:HD22	1.94	0.65
18:O:391:HOH:O	9:W:105(B):LYS:CG	2.41	0.65
13:1:-1:GLY:CA	13:1:1:THR:N	2.60	0.65
14:2:181:ALA:O	14:2:183:GLY:N	2.30	0.64
1:O:55:SER:O	1:O:56:SER:HB3	1.96	0.64
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.28	0.64
7:U:65:SER:HA	7:U:211:GLU:OE2	1.96	0.64
18:U:242:HOH:O	8:V:66:HIS:HD2	1.79	0.64
8:V:197:ARG:HD3	18:V:228:HOH:O	1.97	0.64
12:Z:144(P):PRO:CD	12:Z:144(R):LYS:HZ1	2.10	0.64
4:R:123(G):GLU:HB2	4:R:125:GLU:N	2.12	0.64
6:F:167:LYS:HD3	6:F:205:ASN:HD21	1.62	0.64
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.63	0.64
3:Q:171:THR:O	3:Q:174:GLU:HB3	1.98	0.63
2:P:202:THR:HG22	2:P:204:SER:H	1.64	0.63
10:X:-1:MET:HA	18:X:486:HOH:O	1.98	0.63
5:E:33:GLN:HB2	18:E:860:HOH:O	1.96	0.63
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.97	0.63
12:Z:-1:GLY:C	12:Z:1:GLY:CA	2.66	0.63
13:1:-7:GLN:HB2	18:2:182:HOH:O	1.97	0.63
5:E:12:THR:HG21	5:E:124:THR:HA	1.81	0.62
5:E:180(F):ILE:C	5:E:183:ASP:HA	2.19	0.62
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.64	0.62
4:R:237:LEU:HB3	18:R:740:HOH:O	1.98	0.62
6:T:192:GLN:HE22	6:T:195:LYS:HE3	1.62	0.62
7:U:96:ALA:CA	7:U:107:MET:HE2	2.20	0.62
4:R:192:LEU:O	4:R:196:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:52:LYS:HB2	5:S:63:TYR:CB	2.30	0.62
6:T:147:HIS:HD2	18:T:280:HOH:O	1.81	0.62
8:H:197:ARG:HD2	18:H:661:HOH:O	1.98	0.62
3:Q:57:LYS:HA	18:Q:409:HOH:O	1.99	0.62
6:T:225:LYS:HE2	18:T:994:HOH:O	1.99	0.62
18:B:1043:HOH:O	3:C:57:LYS:HB3	1.99	0.62
5:E:180(F):ILE:C	5:E:183:ASP:N	2.54	0.62
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.13	0.61
5:S:60:SER:HA	5:S:63:TYR:N	2.15	0.61
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.82	0.61
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.12	0.61
1:A:200:SER:O	1:A:202:VAL:CA	2.49	0.61
4:D:122:ARG:HD3	18:D:657:HOH:O	2.00	0.61
6:T:216:SER:HB3	6:T:218(A):GLU:HB2	1.82	0.61
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.80	0.61
18:Q:321:HOH:O	11:Y:105(B):LYS:HD3	1.99	0.61
7:U:126:ARG:HD2	18:U:662:HOH:O	1.99	0.61
6:T:12:ASN:C	6:T:14:VAL:H	2.04	0.61
7:G:238:GLU:O	7:G:239:GLN:HB3	2.00	0.61
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.32	0.61
18:Q:845:HOH:O	4:R:29:GLU:HG3	2.00	0.61
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.81	0.61
13:1:181(A):THR:HG21	18:1:358:HOH:O	2.01	0.61
11:K:181:ASP:C	11:K:183:GLY:HA3	2.21	0.61
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.83	0.60
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.84	0.60
2:P:200:THR:C	2:P:202:THR:N	2.54	0.60
6:T:187:ARG:HB2	18:T:458:HOH:O	1.99	0.60
12:Z:-1:GLY:C	12:Z:1:GLY:H3	2.03	0.60
7:G:228:ASN:HB3	18:G:422:HOH:O	2.01	0.60
11:K:24:ASN:CB	18:K:364:HOH:O	2.47	0.60
13:M:-1:GLY:CA	13:M:1:THR:H1	2.13	0.60
13:1:40:ASN:H	13:1:40:ASN:HD22	1.49	0.60
14:N:70:TYR:O	14:N:72:GLY:HA3	2.01	0.60
12:Z:9:GLU:HB2	12:Z:145:TYR:CE2	2.34	0.60
14:2:70:TYR:O	14:2:72:GLY:CA	2.49	0.60
7:U:87:ASN:C	7:U:87:ASN:HD22	2.04	0.60
8:H:187:LEU:O	8:H:189:ARG:N	2.32	0.60
1:A:7:ARG:HG3	6:F:128:SER:HB3	1.83	0.59
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.84	0.59
1:A:56:SER:HB2	18:A:1095:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:73:HIS:HE1	5:S:107:LEU:O	1.85	0.59
8:V:172:ASN:HD22	8:V:193:THR:HA	1.68	0.59
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.84	0.59
10:X:119:LYS:HE2	18:X:265:HOH:O	2.01	0.59
8:H:30:ASN:O	8:H:189:ARG:NH2	2.31	0.58
13:M:40:ASN:HD22	13:M:40:ASN:N	1.96	0.58
14:2:70:TYR:O	14:2:72:GLY:HA3	2.03	0.58
1:A:112:LEU:O	1:A:116:VAL:HG23	2.03	0.58
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.16	0.58
6:F:35:THR:CG2	6:F:51:GLU:O	2.51	0.58
10:J:143:ARG:O	10:J:146:MET:HG3	2.03	0.58
1:O:121:GLN:O	1:O:124:THR:HB	2.03	0.58
14:N:38:HIS:HD2	18:N:190:HOH:O	1.86	0.58
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.03	0.58
5:S:132:TYR:O	5:S:153:PRO:HB3	2.02	0.58
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.85	0.58
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.84	0.58
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.51	0.58
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.85	0.58
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.68	0.58
10:X:6:ILE:HD11	10:X:142:TYR:HE1	1.68	0.58
4:D:202:GLU:O	4:D:205:GLU:N	2.36	0.58
9:I:36:HIS:O	9:I:38:TYR:N	2.34	0.58
9:W:179:LYS:C	9:W:181:LYS:N	2.58	0.58
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.04	0.58
10:J:141:HIS:HB3	10:J:154:LEU:HD11	1.85	0.57
8:V:172:ASN:ND2	8:V:193:THR:HA	2.19	0.57
4:R:10:ARG:HD2	5:S:10:GLY:HA2	1.85	0.57
12:L:179:THR:HG1	12:L:182:ASP:N	2.03	0.57
1:O:222:ARG:HD2	18:O:956:HOH:O	2.04	0.57
16:Y:212:LZT:H5	12:Z:96:TYR:CE1	2.38	0.57
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.01	0.57
11:K:99:THR:HG22	11:K:113:VAL:HB	1.86	0.57
11:K:40:PHE:HA	11:K:183:GLY:N	2.20	0.57
14:N:92:ASP:O	14:N:94:ASN:N	2.34	0.57
6:T:35:THR:CG2	6:T:51:GLU:O	2.51	0.57
12:L:180:LYS:O	12:L:182:ASP:N	2.38	0.57
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.97	0.57
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.70	0.57
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.40	0.57
4:D:123(C):GLY:HA2	4:D:126:ARG:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:199:LEU:C	6:F:201:ALA:N	2.58	0.56
13:M:148:VAL:HG23	18:M:212:HOH:O	2.05	0.56
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.86	0.56
10:J:-1:MET:HG3	10:J:1:ASP:H3	1.69	0.56
13:M:-1:GLY:O	13:M:1:THR:N	2.23	0.56
1:O:200:SER:O	1:O:202:VAL:N	2.38	0.56
2:B:55:THR:HG23	18:B:241:HOH:O	2.06	0.56
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.69	0.56
11:K:129:SER:HB3	17:K:214:MES:H72	1.87	0.56
14:N:38:HIS:CD2	18:N:190:HOH:O	2.57	0.56
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.40	0.56
12:Z:185:ARG:HG2	18:Z:427:HOH:O	2.04	0.56
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.87	0.56
13:M:-8:THR:C	18:M:1072:HOH:O	2.44	0.56
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.87	0.56
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.87	0.56
4:D:32:LYS:O	4:D:167:SER:HA	2.05	0.56
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.87	0.56
4:D:224:TYR:HE2	18:D:869:HOH:O	1.89	0.56
7:G:184(M):SER:C	7:G:186:TRP:N	2.59	0.56
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.51	0.56
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.88	0.56
13:1:-1:GLY:CA	13:1:1:THR:H1	2.10	0.56
14:2:70:TYR:O	14:2:72:GLY:N	2.36	0.56
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.71	0.55
5:S:180:LEU:HA	5:S:180(C):PHE:CE2	2.41	0.55
5:E:132:TYR:O	5:E:153:PRO:HB3	2.07	0.55
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.37	0.55
6:F:126:TYR:HB2	6:F:129:VAL:HG22	1.88	0.55
18:N:189:HOH:O	13:1:211:ILE:HD11	2.06	0.55
3:Q:169:SER:HA	3:Q:172:VAL:HG13	1.88	0.55
10:X:120:VAL:HG13	10:X:122:LEU:HG	1.86	0.55
10:J:181:ASP:O	10:J:183:GLY:HA3	2.05	0.55
14:N:10:ASP:O	14:N:179:THR:HG22	2.06	0.55
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.87	0.55
6:F:192:GLN:HE21	6:F:192:GLN:HA	1.71	0.55
1:O:217(D):PRO:CA	1:O:217(P):LYS:O	2.54	0.55
11:Y:181:ASP:O	11:Y:183:GLY:HA3	2.06	0.55
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.19	0.55
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.89	0.55
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-1:GLY:O	12:Z:1:GLY:CA	2.54	0.55
13:M:132:HIS:HE1	18:M:705:HOH:O	1.88	0.55
5:S:149:LEU:HD12	5:S:159:GLU:HG3	1.88	0.55
6:T:126:TYR:HE1	7:U:129:MET:SD	2.29	0.55
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.89	0.55
9:W:19:ARG:HD3	9:W:168:LEU:O	2.06	0.55
4:D:122:ARG:CD	18:D:657:HOH:O	2.55	0.55
11:K:180:GLU:HB3	18:K:223:HOH:O	2.07	0.55
12:L:7:ALA:HB3	12:L:123:GLN:HE21	1.72	0.55
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.37	0.55
3:Q:208:LYS:HD2	3:Q:208:LYS:O	2.06	0.55
4:R:121:LEU:HD21	5:S:83:PRO:HB3	1.89	0.55
11:K:179:THR:O	11:K:183:GLY:HA3	2.06	0.55
1:O:97:HIS:HD2	8:V:61:SER:OG	1.90	0.55
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.20	0.55
2:B:163:ILE:HG13	2:B:164:SER:N	2.22	0.54
2:P:97:GLN:HE21	9:W:61:TYR:HA	1.72	0.54
12:Z:146:LEU:HD22	12:Z:150:GLU:HG2	1.88	0.54
3:Q:231:GLN:HB3	18:Q:771:HOH:O	2.06	0.54
12:Z:-9:GLN:HE21	12:Z:-8:PHE:H	1.55	0.54
2:P:163:ILE:HG13	2:P:164:SER:H	1.72	0.54
13:1:141(A):VAL:HG23	13:1:141(A):VAL:O	2.05	0.54
1:A:121:GLN:O	1:A:124:THR:HB	2.08	0.54
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.03	0.54
7:U:168:LYS:HD3	7:U:201:LEU:HD22	1.89	0.54
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.90	0.54
1:A:67:VAL:HG11	1:A:213:ALA:HB2	1.90	0.54
3:C:66:LYS:HG2	18:C:372:HOH:O	2.08	0.54
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.04	0.54
1:A:7:ARG:HG2	6:F:128:SER:HB3	1.88	0.54
3:Q:163:GLN:HE21	3:Q:164:THR:N	2.04	0.54
6:T:114:ASP:O	6:T:118:GLN:HG2	2.08	0.54
8:V:20:SER:OG	8:V:28:ASP:HB3	2.08	0.54
2:B:121:GLN:O	2:B:124:THR:HB	2.08	0.54
3:Q:160:TRP:CE2	18:R:666:HOH:O	2.61	0.54
10:X:143:ARG:O	10:X:146:MET:HG3	2.08	0.54
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.90	0.54
7:G:238:GLU:O	7:G:239:GLN:CB	2.56	0.53
8:H:126:SER:O	8:H:127:LEU:HD23	2.08	0.53
10:J:179:ASP:O	10:J:183:GLY:N	2.42	0.53
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:12:ASN:ND2	6:T:126:TYR:O	2.41	0.53
14:2:92:ASP:C	14:2:94:ASN:N	2.62	0.53
4:D:122:ARG:HA	4:D:126:ARG:HD3	1.90	0.53
10:J:113:ILE:HA	10:J:118:THR:O	2.08	0.53
2:P:222:LYS:HE2	18:P:1163:HOH:O	2.07	0.53
5:S:13:VAL:HG21	6:T:128:SER:O	2.09	0.53
5:E:180(F):ILE:C	5:E:183:ASP:CA	2.76	0.53
5:E:180(F):ILE:O	5:E:183:ASP:HA	2.09	0.53
13:M:-1:GLY:CA	13:M:1:THR:N	2.67	0.53
4:R:123:PHE:O	4:R:126:ARG:HD2	2.08	0.53
5:S:194:VAL:O	5:S:197:ILE:HG22	2.08	0.53
6:T:126:TYR:HB2	6:T:129:VAL:HG22	1.90	0.53
2:B:218(C):ASP:OD2	2:B:219:GLU:HB2	2.09	0.53
3:C:186:VAL:O	3:C:190:VAL:HG23	2.08	0.53
7:G:237:ALA:HB3	18:G:338:HOH:O	2.07	0.53
16:K:213:LZT:C5	12:L:96:TYR:CE1	2.86	0.53
10:X:181:ASP:C	10:X:183:GLY:CA	2.77	0.53
9:I:174:VAL:HG21	9:I:186:LYS:HE2	1.89	0.53
7:G:87:ASN:C	7:G:87:ASN:HD22	2.13	0.53
9:I:179:LYS:C	9:I:181:LYS:N	2.61	0.53
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.90	0.53
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.07	0.53
14:2:156:LYS:HG2	14:2:187(J):LEU:HD13	1.91	0.53
9:W:179:LYS:O	9:W:181:LYS:N	2.41	0.53
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.91	0.53
9:I:181:LYS:HG2	9:I:182:ASP:OD1	2.09	0.52
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.23	0.52
1:O:217(E):ASP:OD1	1:O:217(E):ASP:N	2.42	0.52
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.44	0.52
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.74	0.52
3:Q:156:ILE:HD12	4:R:83:ALA:HB2	1.91	0.52
11:Y:105(B):LYS:HD2	18:Y:222:HOH:O	2.09	0.52
4:D:233:ILE:C	4:D:235:LYS:N	2.63	0.52
2:P:163:ILE:HG13	2:P:164:SER:N	2.25	0.52
4:R:186:LEU:O	4:R:190:GLU:HG3	2.09	0.52
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.91	0.52
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.24	0.52
13:M:211:ILE:HD11	18:2:189:HOH:O	2.09	0.52
3:C:156:ILE:HD12	4:D:83:ALA:HB2	1.92	0.52
6:F:166:GLY:O	6:F:169:ARG:HB3	2.10	0.52
9:W:-1:GLY:O	9:W:1:GLY:N	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:181:ASP:C	11:Y:183:GLY:CA	2.77	0.52
1:A:227:GLN:NE2	1:A:231:ASP:OD1	2.43	0.52
18:Q:845:HOH:O	4:R:29:GLU:CG	2.56	0.52
6:T:218(B):THR:O	6:T:218(C):ASN:HB2	2.09	0.52
5:E:142:ASP:HB2	18:M:833:HOH:O	2.10	0.52
11:K:39:PRO:O	11:K:183:GLY:N	2.42	0.52
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.45	0.52
4:D:85:ALA:O	4:D:89:ILE:HG12	2.10	0.51
7:G:220:LYS:HE2	18:G:671:HOH:O	2.10	0.51
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.91	0.51
12:Z:-9:GLN:HE21	12:Z:-8:PHE:N	2.07	0.51
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.91	0.51
10:X:113:ILE:HA	10:X:118:THR:O	2.10	0.51
8:H:114:HIS:HB3	18:H:225:HOH:O	2.09	0.51
11:K:192:VAL:HG11	9:W:194:ASP:HB3	1.92	0.51
9:W:113:PHE:HA	9:W:118:CYS:O	2.10	0.51
13:1:-1:GLY:O	13:1:1:THR:N	2.21	0.51
7:G:173:THR:O	7:G:177:GLU:HG3	2.10	0.51
12:L:166:HIS:HD2	12:L:168:GLN:H	1.58	0.51
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.57	0.51
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.91	0.51
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.76	0.51
4:D:123:PHE:O	4:D:126:ARG:HD2	2.10	0.51
7:G:204:GLU:CG	18:G:1211:HOH:O	2.55	0.51
13:M:122:SER:HB3	13:M:124:THR:O	2.10	0.51
11:Y:20:ALA:HB1	16:Y:212:LZT:C35	2.40	0.51
6:T:126:TYR:CE1	7:U:129:MET:SD	3.04	0.51
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.08	0.51
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.26	0.51
10:X:18:LYS:HD2	10:X:30:SER:HA	1.93	0.51
5:E:231:LYS:HG2	18:E:636:HOH:O	2.11	0.50
12:L:135:MET:CE	9:W:165:ARG:NH2	2.74	0.50
1:O:13:THR:O	2:P:130:ARG:HD3	2.11	0.50
13:1:122:SER:HA	18:1:1247:HOH:O	2.11	0.50
3:C:17:PRO:HA	4:D:26:TYR:CE1	2.47	0.50
7:G:218:ASP:C	7:G:220:LYS:CA	2.78	0.50
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.91	0.50
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.41	0.50
8:V:101:VAL:HG13	8:V:111:PHE:HB2	1.93	0.50
8:V:114:HIS:HB3	18:V:224:HOH:O	2.11	0.50
2:P:76:VAL:HG12	2:P:138:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:91:TYR:O	5:S:95:GLN:HG2	2.12	0.50
14:2:70:TYR:C	14:2:72:GLY:CA	2.77	0.50
5:E:207:LEU:HD23	5:E:207:LEU:H	1.76	0.50
14:N:70:TYR:O	14:N:72:GLY:CA	2.58	0.50
3:Q:100:ARG:NH1	3:Q:106:PRO:HG3	2.25	0.50
3:Q:122:ARG:HD3	18:Q:806:HOH:O	2.12	0.50
12:Z:-1:GLY:C	12:Z:1:GLY:HA3	2.31	0.50
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.94	0.50
5:S:198:SER:C	5:S:200:SER:H	2.15	0.50
18:T:243:HOH:O	7:U:86:ARG:HD2	2.11	0.50
10:J:188:ASP:HB3	18:J:1104:HOH:O	2.11	0.50
3:Q:44:ASN:ND2	18:Q:878:HOH:O	2.45	0.50
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.94	0.50
4:R:59:LEU:CA	18:R:666:HOH:O	2.35	0.50
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.94	0.50
5:E:74:MET:HE2	5:E:109:VAL:HG22	1.92	0.50
14:N:105(A):ASP:HB3	18:N:438:HOH:O	2.10	0.50
8:V:126:SER:O	8:V:127:LEU:HD23	2.12	0.50
12:Z:166:HIS:HE1	18:Z:232:HOH:O	1.94	0.50
6:F:199:LEU:O	6:F:201:ALA:HA	2.11	0.49
12:L:-1:GLY:C	12:L:1:GLY:CA	2.80	0.49
8:V:89:LYS:HD3	18:V:376:HOH:O	2.12	0.49
2:P:54:VAL:HG12	18:P:456:HOH:O	2.12	0.49
4:R:90:GLU:OE1	11:Y:69:ARG:HD2	2.13	0.49
5:S:15:PHE:H	6:T:23:GLN:HE22	1.58	0.49
6:T:186:ALA:O	6:T:190:VAL:HG23	2.12	0.49
1:O:40:ILE:HD12	1:O:193:ALA:HB2	1.93	0.49
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.94	0.49
1:O:45:GLY:HA3	1:O:186:LEU:HD13	1.95	0.49
5:S:179:THR:O	5:S:179:THR:HG22	2.13	0.49
7:U:233:LEU:O	7:U:236:ILE:HG13	2.12	0.49
10:X:6:ILE:CD1	10:X:142:TYR:CE1	2.96	0.49
6:F:13:SER:HB2	7:G:130:ARG:HB3	1.94	0.49
6:F:199:LEU:O	6:F:201:ALA:CA	2.60	0.49
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.94	0.49
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.93	0.49
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.77	0.49
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.10	0.49
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.95	0.49
7:U:12:ILE:HG13	7:U:14:ILE:HG12	1.95	0.49
2:B:112:LEU:HD23	2:B:112:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:-1:MET:HG3	10:J:1:ASP:H1	1.74	0.49
12:L:-1:GLY:C	12:L:1:GLY:H3	2.16	0.49
6:T:168:GLY:HA3	6:T:201:ALA:HB1	1.94	0.49
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.94	0.49
11:Y:19:ARG:HH21	11:Y:29:GLN:HE22	1.60	0.49
12:Z:40:ASN:HA	18:Z:488:HOH:O	2.13	0.49
2:B:21:LEU:O	2:B:25:GLU:HG2	2.13	0.49
2:B:60:GLU:O	2:B:63(A):SER:HB2	2.13	0.49
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.24	0.49
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.95	0.49
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.95	0.49
2:P:137:ILE:HD11	2:P:165:VAL:HG22	1.94	0.49
4:R:140:GLY:HA2	4:R:215:ILE:HG12	1.95	0.49
12:Z:-5:TYR:CE2	12:Z:96:TYR:CD1	3.01	0.49
3:C:203:THR:HA	3:C:206:GLY:N	2.27	0.48
6:F:147:HIS:HD2	18:F:320:HOH:O	1.95	0.48
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.12	0.48
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.48	0.48
6:T:143:LYS:HB2	18:T:641:HOH:O	2.13	0.48
6:T:199:LEU:O	6:T:201:ALA:N	2.45	0.48
2:B:150:THR:O	2:B:157:TYR:HA	2.13	0.48
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.95	0.48
10:X:181:ASP:O	10:X:183:GLY:CA	2.57	0.48
10:X:181:ASP:C	10:X:183:GLY:HA3	2.31	0.48
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.96	0.48
3:C:190:VAL:O	3:C:194:VAL:HG23	2.14	0.48
7:G:77:VAL:CG1	7:G:137:THR:HB	2.44	0.48
8:H:223:ASP:N	8:H:223:ASP:OD2	2.46	0.48
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.49	0.48
7:U:87:ASN:C	7:U:87:ASN:ND2	2.66	0.48
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.94	0.48
2:B:115:ARG:HD3	18:B:243:HOH:O	2.13	0.48
3:C:163:GLN:HE21	3:C:164:THR:H	1.60	0.48
6:F:36:THR:HB	6:F:168:GLY:H	1.79	0.48
11:K:12:ILE:HB	11:K:178:VAL:HB	1.95	0.48
7:U:72:ARG:HD2	18:U:1017:HOH:O	2.14	0.48
4:D:123(B):GLU:N	4:D:126:ARG:HB2	2.29	0.48
4:D:158:TYR:CZ	5:E:55:ALA:HB2	2.49	0.48
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.95	0.48
12:Z:144(O):LYS:HG2	12:Z:144(R):LYS:NZ	2.29	0.48
14:2:181:ALA:C	14:2:183:GLY:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:O	1:A:122:GLU:HG3	2.13	0.48
2:B:209:ARG:CD	18:B:246:HOH:O	2.60	0.48
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.48	0.48
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.96	0.48
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.95	0.48
11:Y:185:ILE:HA	18:Y:221:HOH:O	2.13	0.48
13:1:181(A):THR:HB	18:1:357:HOH:O	2.13	0.48
4:D:180(E):SER:C	4:D:184:LEU:N	2.67	0.48
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.49	0.48
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.96	0.48
6:T:218:SER:HB3	18:T:506:HOH:O	2.13	0.48
2:P:147:GLN:HG2	3:Q:62(A):ILE:HG21	1.96	0.47
5:S:195:GLU:HB3	18:S:469:HOH:O	2.13	0.47
12:Z:180:LYS:O	12:Z:182:ASP:HA	2.14	0.47
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.49	0.47
5:S:208:THR:OG1	5:S:209:ASN:HB2	2.14	0.47
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.96	0.47
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.45	0.47
2:B:116:LEU:HD23	2:B:116:LEU:HA	1.73	0.47
11:K:6:PHE:HA	11:K:123:ASP:O	2.15	0.47
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.95	0.47
7:G:96:ALA:CA	7:G:107:MET:CE	2.87	0.47
10:X:149:GLU:HB2	18:X:578:HOH:O	2.15	0.47
10:J:167:PRO:HB3	10:X:21:THR:HG21	1.96	0.47
12:L:166:HIS:CE1	18:L:475:HOH:O	2.60	0.47
12:L:180:LYS:O	12:L:182:ASP:CA	2.63	0.47
1:A:177:GLU:HG3	2:B:58:LEU:HD22	1.95	0.47
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.96	0.47
1:O:217(O):ASP:CG	1:O:218:GLY:H	2.17	0.47
9:W:6:MET:HB2	9:W:151:LEU:HD11	1.97	0.47
10:X:189:ASP:O	10:X:193:GLN:HB2	2.14	0.47
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.96	0.47
3:C:22:PHE:HB2	18:C:751:HOH:O	2.14	0.47
4:D:112:LEU:C	4:D:112:LEU:HD13	2.35	0.47
6:F:36:THR:HG23	6:F:51:GLU:OE2	2.15	0.47
9:I:-1:GLY:C	9:I:1:GLY:CA	2.77	0.47
1:O:206:PHE:HB2	18:O:411:HOH:O	2.15	0.47
7:U:96:ALA:CA	7:U:107:MET:CE	2.88	0.47
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.97	0.47
9:W:33:LYS:O	9:W:44:GLY:HA2	2.14	0.47
12:Z:180:LYS:O	12:Z:182:ASP:CA	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:HB3	1:A:50:THR:HB	1.97	0.47
3:C:180(D):GLU:O	3:C:182:PRO:N	2.48	0.47
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.45	0.47
1:A:200:SER:O	1:A:202:VAL:N	2.48	0.47
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.79	0.47
6:F:206(C):LYS:HB2	18:F:244:HOH:O	2.14	0.47
7:G:184(M):SER:C	7:G:188:LYS:H	2.19	0.47
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.30	0.47
10:X:112:GLN:NE2	10:X:126:ALA:H	2.13	0.47
14:2:92:ASP:O	14:2:94:ASN:CA	2.62	0.47
13:M:165:ARG:HD3	8:V:139:GLU:OE1	2.15	0.46
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.98	0.46
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.50	0.46
9:W:6:MET:HG3	9:W:155:ILE:HD12	1.97	0.46
9:I:181:LYS:HG2	9:I:182:ASP:H	1.80	0.46
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.45	0.46
6:T:16:SER:OG	6:T:18:ASP:OD1	2.30	0.46
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.98	0.46
9:I:176:TYR:OH	9:I:186:LYS:HE3	2.16	0.46
11:K:1:THR:OG1	16:K:213:LZT:H21	2.16	0.46
18:Q:845:HOH:O	4:R:29:GLU:HB3	2.10	0.46
5:S:56:ASP:HB3	5:S:58:LEU:H	1.80	0.46
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.81	0.46
13:1:40:ASN:HD22	13:1:40:ASN:N	2.14	0.46
5:E:226:GLY:O	5:E:229:VAL:HG22	2.16	0.46
6:F:12:ASN:OD1	6:F:124:THR:HA	2.16	0.46
3:C:164:THR:HG21	3:C:172:VAL:HG22	1.98	0.46
7:G:82:ILE:N	7:G:83:PRO:CD	2.79	0.46
3:Q:17:PRO:O	18:Q:845:HOH:O	2.20	0.46
3:Q:41:LYS:HB2	3:Q:46:VAL:HG22	1.97	0.46
3:Q:57:LYS:HD3	3:Q:208:LYS:NZ	2.31	0.46
4:R:197:LEU:O	4:R:201:MET:HG3	2.16	0.46
9:W:181:LYS:N	9:W:181:LYS:HD2	2.31	0.46
4:D:123(C):GLY:HA2	4:D:126:ARG:N	2.31	0.46
3:Q:100:ARG:HH11	3:Q:106:PRO:HG3	1.81	0.46
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.46	0.46
10:X:44:SER:OG	10:X:100:LEU:HB2	2.16	0.46
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.98	0.46
8:H:172:ASN:ND2	8:H:193:THR:HG22	2.30	0.46
1:O:150:GLN:O	1:O:157:TYR:HA	2.16	0.46
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:242:GLU:HG3	18:Q:503:HOH:O	2.16	0.46
5:S:86:ARG:O	5:S:90:ASN:HB2	2.16	0.46
12:Z:144:PHE:CE2	12:Z:144(R):LYS:HG3	2.51	0.46
5:E:60:SER:CA	5:E:63:TYR:N	2.79	0.46
5:S:175:TYR:CZ	18:S:469:HOH:O	2.56	0.46
1:A:217(D):PRO:HA	1:A:217(P):LYS:O	2.15	0.46
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.46	0.46
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.97	0.46
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.80	0.46
3:C:185:THR:HG22	3:C:186:VAL:H	1.80	0.45
9:I:107:LYS:HE2	9:I:107:LYS:HB3	1.75	0.45
11:K:137:VAL:HG21	11:K:161:ALA:HB2	1.98	0.45
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.99	0.45
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.51	0.45
3:C:36:CYS:HB3	3:C:51:GLU:HG2	1.98	0.45
3:C:81:LEU:HB2	3:C:84:ASP:HB2	1.98	0.45
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.98	0.45
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.29	0.45
12:Z:144(J):ASN:OD1	12:Z:144(J):ASN:C	2.54	0.45
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.16	0.45
2:P:125:GLN:HG3	3:Q:130:ARG:HG3	1.98	0.45
3:Q:84:ASP:OD2	3:Q:130:ARG:NH2	2.48	0.45
1:A:217(E):ASP:OD1	1:A:217(E):ASP:N	2.46	0.45
6:F:69:VAL:HG12	18:F:246:HOH:O	2.15	0.45
10:J:21:THR:HG21	10:X:167:PRO:HB3	1.99	0.45
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.28	0.45
7:U:49:ILE:HD13	7:U:193:ALA:CB	2.46	0.45
3:C:207:ALA:N	18:C:244:HOH:O	2.48	0.45
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.52	0.45
5:E:180(E):LYS:O	5:E:183:ASP:N	2.49	0.45
13:M:17:ASP:HA	13:M:173:PHE:HA	1.99	0.45
16:K:213:LZT:H5	12:L:96:TYR:CD1	2.48	0.45
4:D:150:HIS:O	4:D:157:PHE:HA	2.16	0.45
10:J:181:ASP:O	10:J:183:GLY:N	2.48	0.45
11:K:180:GLU:HB2	18:K:312:HOH:O	2.16	0.45
7:U:180:ILE:CD1	7:U:184:ASN:HB2	2.47	0.45
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.98	0.45
5:E:207(B):THR:H	5:E:207(E):ASN:HB2	1.81	0.45
12:L:180:LYS:O	12:L:182:ASP:HA	2.17	0.45
1:O:64:LEU:HD23	1:O:65:SER:H	1.81	0.45
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:43:LYS:HB2	3:Q:184:ALA:HA	1.98	0.45
5:E:109:VAL:HG12	5:E:149:LEU:HD22	1.98	0.45
1:O:167:LYS:HD2	18:O:1233:HOH:O	2.17	0.45
3:Q:32:LYS:O	3:Q:167:ARG:HB3	2.16	0.45
10:X:2:ILE:HG12	10:X:130:SER:HB3	1.99	0.45
13:1:112:TYR:O	13:1:119:THR:HA	2.16	0.45
12:L:9:GLU:O	12:L:107:LYS:HA	2.17	0.44
2:P:150:THR:O	2:P:157:TYR:HA	2.16	0.44
4:R:215:ILE:HG13	4:R:215:ILE:O	2.16	0.44
5:S:232:TYR:CE2	18:S:998:HOH:O	2.38	0.44
7:U:206:SER:HB3	18:U:1006:HOH:O	2.17	0.44
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.47	0.44
1:A:150:GLN:O	1:A:157:TYR:HA	2.17	0.44
5:E:134:VAL:O	5:E:153:PRO:HG3	2.17	0.44
6:F:204:ASP:OD1	6:F:204:ASP:N	2.51	0.44
5:S:60:SER:CA	5:S:63:TYR:N	2.79	0.44
6:T:12:ASN:C	6:T:14:VAL:N	2.70	0.44
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	1.99	0.44
7:G:151:THR:HG22	7:G:157:TYR:CB	2.47	0.44
12:L:34:VAL:HG12	12:L:176:LEU:HD22	2.00	0.44
10:X:119:LYS:CE	18:X:265:HOH:O	2.63	0.44
11:Y:181:ASP:C	11:Y:183:GLY:HA3	2.38	0.44
16:Y:212:LZT:C5	12:Z:96:TYR:CE1	3.00	0.44
4:D:179:GLU:CB	4:D:192:LEU:HD21	2.46	0.44
13:M:141(C):ARG:HG3	13:M:141(C):ARG:NH1	2.23	0.44
14:N:176:VAL:HG12	14:N:178:LEU:CD1	2.47	0.44
10:J:21:THR:O	10:J:22:ARG:HD3	2.18	0.44
13:M:40:ASN:N	13:M:40:ASN:ND2	2.65	0.44
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.17	0.44
7:U:79:ASN:OD1	7:U:165:THR:HB	2.17	0.44
3:C:163:GLN:HE21	3:C:164:THR:N	2.16	0.44
4:D:123(C):GLY:CA	4:D:126:ARG:H	2.29	0.44
2:B:40:ILE:HD12	2:B:193:ALA:HB2	1.99	0.44
11:K:2:THR:OG1	11:K:130:GLY:HA3	2.17	0.44
3:Q:43:LYS:HG2	3:Q:182:PRO:HG2	1.98	0.44
3:C:179:ASN:HD22	3:C:179:ASN:N	2.16	0.44
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.99	0.44
11:Y:67:GLU:HG3	18:Y:301:HOH:O	2.18	0.44
7:G:191:GLU:HG3	7:G:232:ARG:HG3	1.99	0.44
8:H:101:VAL:HG13	8:H:111:PHE:HB2	1.99	0.44
9:I:181:LYS:HG2	9:I:182:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.48	0.44
14:2:38:HIS:HD2	18:2:191:HOH:O	2.00	0.44
2:B:78:VAL:HG22	2:B:136:PHE:HE2	1.82	0.43
6:F:43:ASN:CB	18:F:405:HOH:O	2.50	0.43
2:P:45:GLY:HA2	2:P:146:TYR:CE1	2.52	0.43
2:P:66:LYS:HB2	2:P:211:GLU:OE1	2.18	0.43
3:Q:84:ASP:CG	3:Q:130:ARG:HH22	2.21	0.43
3:Q:208:LYS:NZ	3:Q:209:ASN:HD21	2.15	0.43
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.53	0.43
7:U:150:LYS:O	7:U:157:TYR:HA	2.18	0.43
12:Z:144(P):PRO:CD	12:Z:144(R):LYS:HZ2	2.30	0.43
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.54	0.43
12:L:144(B):ASN:ND2	18:W:1195:HOH:O	2.51	0.43
4:R:163:LYS:HG3	4:R:164:ALA:N	2.32	0.43
4:R:233:ILE:O	4:R:236:GLU:N	2.48	0.43
5:S:150:GLU:O	5:S:157:VAL:HA	2.18	0.43
11:Y:13:ILE:HG13	11:Y:151:ALA:HB1	1.99	0.43
13:1:181(A):THR:O	13:1:183:GLY:N	2.49	0.43
14:2:65:LEU:HD12	14:2:65:LEU:HA	1.90	0.43
12:L:51:ASP:OD1	12:L:95:TYR:HA	2.17	0.43
6:T:240:ILE:HG23	18:T:444:HOH:O	2.18	0.43
8:V:30:ASN:O	8:V:189:ARG:NH2	2.46	0.43
12:Z:144(P):PRO:N	12:Z:144(R):LYS:HZ2	2.16	0.43
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.82	0.43
9:I:48:LEU:HG	9:I:50:THR:HG22	2.00	0.43
2:P:41:MET:HG2	2:P:46:ILE:HG12	2.00	0.43
9:W:55:LEU:HD23	9:W:55:LEU:HA	1.86	0.43
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.48	0.43
2:B:51:GLU:OE2	2:B:209:ARG:NH2	2.51	0.43
3:C:228:GLU:O	3:C:232:TYR:HD1	2.00	0.43
4:D:122:ARG:O	4:D:128:MET:HB3	2.19	0.43
7:G:77:VAL:HG12	7:G:137:THR:HB	2.00	0.43
8:H:105:ASP:HB2	8:H:105(A):PRO:CD	2.48	0.43
3:Q:36:CYS:HB3	3:Q:51:GLU:HG2	2.00	0.43
3:Q:110:GLU:HG3	18:Q:1030:HOH:O	2.18	0.43
3:Q:208:LYS:HD2	3:Q:208:LYS:C	2.39	0.43
8:V:128:GLY:O	8:V:131:SER:CB	2.66	0.43
9:W:36:HIS:C	9:W:38:TYR:CA	2.83	0.43
11:Y:208:ASN:H	11:Y:208:ASN:HD22	1.67	0.43
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.30	0.43
12:Z:144:PHE:CD2	12:Z:144(R):LYS:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:184(M):SER:O	7:G:186:TRP:CA	2.67	0.43
7:G:192:PHE:CD1	7:G:192:PHE:C	2.91	0.43
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.99	0.43
9:I:113:PHE:HA	9:I:118:CYS:O	2.19	0.43
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.59	0.43
4:R:51:GLU:HG3	4:R:201:MET:HG2	2.01	0.43
5:S:160:LEU:HD13	5:S:163:THR:HB	2.01	0.43
12:Z:85:HIS:CD2	18:Z:199:HOH:O	2.44	0.43
6:F:88:LEU:HD12	6:F:88:LEU:HA	1.83	0.43
10:J:181:ASP:O	10:J:183:GLY:CA	2.66	0.43
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.30	0.43
12:L:144(A):LYS:HA	12:L:144(A):LYS:HE3	2.01	0.43
4:D:90:GLU:OE1	11:K:69:ARG:HD2	2.19	0.43
7:G:151:THR:HG22	7:G:157:TYR:HB2	2.01	0.43
11:K:143:LYS:HD3	18:K:454:HOH:O	2.18	0.43
7:U:49:ILE:HG13	7:U:212:VAL:HG22	2.00	0.43
9:W:181:LYS:HG2	9:W:182:ASP:OD1	2.19	0.43
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.33	0.43
11:Y:208:ASN:H	11:Y:208:ASN:ND2	2.15	0.43
12:Z:51:ASP:OD1	12:Z:95:TYR:HA	2.19	0.43
8:H:50:ALA:HB2	9:I:118:CYS:HB2	2.00	0.43
10:J:2:ILE:HD12	10:J:170:PHE:CG	2.54	0.43
12:L:33:LYS:HE3	12:L:46:ASN:ND2	2.33	0.43
5:S:82:ALA:N	5:S:83:PRO:CD	2.82	0.43
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.66	0.43
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	2.01	0.43
2:B:15:PHE:H	3:C:23:GLN:HE22	1.65	0.43
2:B:209:ARG:NH1	18:B:245:HOH:O	2.50	0.43
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.49	0.43
6:F:169:ARG:HB3	6:F:169:ARG:HE	1.59	0.43
8:H:84:LYS:HG3	8:H:85:GLN:N	2.34	0.43
8:V:114:HIS:CD2	18:V:609:HOH:O	2.71	0.43
12:Z:144(Q):LEU:O	12:Z:144(R):LYS:O	2.36	0.43
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.22	0.42
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	2.01	0.42
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	2.00	0.42
2:B:37:ALA:O	2:B:164:SER:HA	2.20	0.42
6:F:126:TYR:CE1	7:G:129:MET:SD	3.12	0.42
1:O:32:LYS:NZ	1:O:169:SER:OG	2.52	0.42
5:S:103:PHE:HE2	13:1:62:LEU:HD21	1.85	0.42
16:Y:212:LZT:H37	17:Y:213:MES:H71	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:194:ALA:O	6:F:198:TYR:HD1	2.01	0.42
12:L:113:PHE:N	12:L:113:PHE:CD1	2.88	0.42
1:O:161:LYS:HB3	1:O:180:TRP:CZ2	2.55	0.42
4:R:122:ARG:CD	18:R:250:HOH:O	2.68	0.42
2:B:170:SER:HB3	18:B:354:HOH:O	2.19	0.42
7:G:203:THR:HG22	7:G:204:GLU:O	2.20	0.42
9:I:101:VAL:O	9:I:110:ILE:HA	2.19	0.42
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.34	0.42
7:U:49:ILE:HD13	7:U:193:ALA:HB3	2.01	0.42
5:E:60:SER:C	5:E:63:TYR:CA	2.88	0.42
12:L:180:LYS:HB3	18:L:204:HOH:O	2.19	0.42
1:O:9:SER:OG	3:Q:8:TYR:HD1	2.02	0.42
1:O:222:ARG:NH1	18:O:956:HOH:O	2.52	0.42
6:T:20:ARG:NE	6:T:25:GLU:OE1	2.53	0.42
9:W:110:ILE:HD12	9:W:125:ILE:HG12	2.01	0.42
14:2:156:LYS:HG2	14:2:187(J):LEU:CD1	2.48	0.42
7:G:191:GLU:HG2	7:G:236:ILE:HG23	2.02	0.42
8:H:53:GLU:OE2	8:H:57:GLN:NE2	2.52	0.42
1:O:197:LEU:O	1:O:202:VAL:HG23	2.20	0.42
7:U:110:ASP:OD2	7:U:110:ASP:N	2.49	0.42
10:X:179:ASP:O	10:X:183:GLY:N	2.53	0.42
5:E:58:LEU:HD12	5:E:58:LEU:HA	1.85	0.42
7:G:184(M):SER:O	7:G:186:TRP:N	2.53	0.42
12:L:99:THR:CG2	18:L:198:HOH:O	2.67	0.42
6:T:13:SER:O	7:U:130:ARG:HB3	2.20	0.42
12:Z:180:LYS:C	12:Z:182:ASP:CA	2.87	0.42
13:1:13:ILE:HG12	13:1:177:ILE:HG12	2.01	0.42
14:2:4:MET:HB3	14:2:126:ILE:HG22	2.01	0.42
7:G:38:LEU:HD23	7:G:197:MET:CE	2.50	0.42
12:L:43:MET:HG3	12:L:101:ILE:HG22	2.02	0.42
2:P:163:ILE:HA	2:P:173:GLN:HE22	1.84	0.42
5:E:15:PHE:H	6:F:23:GLN:NE2	2.01	0.42
5:E:100:SER:O	5:E:104:ASN:HA	2.20	0.42
12:L:-2:ASN:HA	12:L:21:ILE:O	2.20	0.42
3:Q:52:ARG:HB2	3:Q:209:ASN:HD22	1.85	0.42
4:R:227:GLU:H	4:R:227:GLU:CD	2.23	0.42
6:T:194:ALA:O	6:T:198:TYR:HD1	2.03	0.42
3:C:157:TYR:OH	4:D:86:ARG:NH2	2.53	0.41
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.67	0.41
7:G:87:ASN:C	7:G:87:ASN:ND2	2.74	0.41
16:K:213:LZT:H37	17:K:214:MES:H82	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:123(G):GLU:OE1	4:R:125:GLU:N	2.52	0.41
5:S:171:GLY:HA3	5:S:199:GLN:O	2.20	0.41
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.48	0.41
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	2.02	0.41
14:2:106:ASN:HA	18:2:834:HOH:O	2.19	0.41
5:E:113:GLY:HA3	18:E:981:HOH:O	2.20	0.41
8:V:8:PHE:HB2	8:V:146:LEU:O	2.20	0.41
4:D:97:VAL:HG11	11:K:65:LEU:HD22	2.02	0.41
5:E:66:LYS:O	5:E:77:SER:HA	2.20	0.41
5:E:67:ILE:HG21	5:E:213:ALA:HB2	2.02	0.41
7:G:210:LEU:HD23	7:G:210:LEU:HA	1.87	0.41
12:L:144(E):GLU:HB2	12:L:144(L):VAL:HB	2.03	0.41
7:U:107:MET:HE1	7:U:112:LEU:HD13	2.02	0.41
8:V:84:LYS:HG3	8:V:85:GLN:N	2.34	0.41
9:W:101:VAL:O	9:W:110:ILE:HA	2.20	0.41
10:X:180:LYS:HG3	10:X:181:ASP:OD1	2.20	0.41
2:B:207:TYR:CD1	2:B:230:LYS:HD3	2.55	0.41
10:J:9:GLN:HE21	10:J:9:GLN:HB3	1.61	0.41
11:K:71:LYS:HD3	18:K:360:HOH:O	2.21	0.41
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.20	0.41
8:V:35:HIS:CB	8:V:56:THR:HG21	2.50	0.41
10:X:154:LEU:HD12	10:X:154:LEU:HA	1.90	0.41
12:Z:180:LYS:O	12:Z:182:ASP:N	2.53	0.41
4:D:35:SER:HB2	18:D:183:HOH:O	2.21	0.41
11:K:5:ALA:HA	11:K:13:ILE:O	2.21	0.41
1:O:97:HIS:CE1	8:V:64:GLU:OE1	2.74	0.41
10:X:3:ILE:HD13	10:X:3:ILE:HA	1.86	0.41
1:A:29:THR:O	1:A:33:GLN:HG2	2.20	0.41
5:E:152:GLN:HA	5:E:153:PRO:HD3	1.96	0.41
13:M:141(A):VAL:HG23	13:M:141(A):VAL:O	2.20	0.41
1:O:13:THR:HG22	1:O:21:LEU:HD22	2.02	0.41
1:O:60:MET:HE1	18:U:247:HOH:O	2.19	0.41
2:P:13:THR:O	3:Q:130:ARG:HD3	2.21	0.41
4:R:162:ALA:HB1	4:R:176:LEU:HD22	2.03	0.41
2:B:156:ASN:HD22	2:B:156:ASN:HA	1.69	0.41
3:C:163:GLN:NE2	3:C:163:GLN:CA	2.83	0.41
5:E:143:LYS:HE3	13:M:78:TYR:OH	2.20	0.41
8:H:173:VAL:HB	8:H:192:LEU:HB2	2.01	0.41
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.86	0.41
5:S:180(C):PHE:HA	5:S:182:ILE:CD1	2.50	0.41
6:F:43:ASN:HD22	6:F:44:ASP:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:141:HIS:CB	10:J:154:LEU:HD11	2.48	0.41
13:M:139:ARG:NH1	8:V:165:ASN:HD22	2.12	0.41
14:N:8:PHE:HB2	14:N:146:MET:O	2.21	0.41
1:O:10:PHE:O	1:O:127:GLY:HA2	2.21	0.41
2:P:21:LEU:HD13	2:P:124:THR:HG23	2.03	0.41
3:Q:195:ARG:HA	3:Q:198:LEU:HD12	2.03	0.41
4:R:150:HIS:O	4:R:157:PHE:HA	2.21	0.41
5:S:52:LYS:HD2	5:S:63:TYR:O	2.20	0.41
9:W:90:ARG:CZ	18:W:590:HOH:O	2.69	0.41
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.51	0.41
3:C:141:PHE:HE1	3:C:144(B):ASP:O	2.04	0.41
4:D:66:LYS:HD3	18:D:183:HOH:O	2.20	0.41
6:F:114:ASP:O	6:F:118:GLN:HG2	2.20	0.41
6:F:176:LEU:HD13	6:F:196:ILE:CD1	2.50	0.41
6:F:218(B):THR:HB	6:F:222:LYS:HE3	2.03	0.41
8:H:197:ARG:CD	18:H:661:HOH:O	2.64	0.41
10:J:9:GLN:HG3	10:J:145:ASP:HA	2.02	0.41
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.83	0.41
18:O:391:HOH:O	9:W:105(B):LYS:HG3	2.14	0.41
4:R:20:ARG:HD2	18:R:245:HOH:O	2.21	0.41
5:S:198:SER:HA	5:S:201:LEU:HD12	2.02	0.41
9:W:45:ILE:HB	9:W:52:VAL:HG13	2.02	0.41
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.21	0.41
13:1:160:ARG:HH21	13:1:160:ARG:HD3	1.74	0.41
13:M:141(C):ARG:NH1	13:M:141(C):ARG:CG	2.83	0.41
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.69	0.41
4:R:85:ALA:O	4:R:89:ILE:HG12	2.21	0.41
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.59	0.41
14:2:146:MET:CE	14:2:150:GLU:HB3	2.50	0.41
6:F:176:LEU:HD13	6:F:196:ILE:HD13	2.03	0.40
6:F:210:LEU:HD21	6:F:212:ILE:HD11	2.03	0.40
10:J:190:PHE:HA	10:J:193:GLN:HB2	2.03	0.40
13:M:3:VAL:O	13:M:126:ALA:HA	2.21	0.40
13:M:112:TYR:O	13:M:119:THR:HA	2.22	0.40
6:T:121:GLN:HE21	6:T:121:GLN:HB3	1.74	0.40
2:B:21:LEU:HD13	2:B:124:THR:HG23	2.03	0.40
3:Q:71:ASP:HB3	3:Q:73:HIS:CE1	2.56	0.40
4:R:177:LEU:HD11	5:S:57:GLU:HB3	2.04	0.40
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.88	0.40
11:Y:85:ASN:HD22	11:Y:85:ASN:HA	1.70	0.40
10:J:48:GLU:HB3	10:J:96:GLN:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:99:THR:HG22	18:L:198:HOH:O	2.21	0.40
3:Q:224:LEU:HD12	3:Q:228:GLU:HB3	2.04	0.40
4:R:122:ARG:O	4:R:128:MET:HB3	2.21	0.40
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.03	0.40
11:Y:4:LEU:HD22	11:Y:4:LEU:C	2.42	0.40
11:Y:44:THR:O	11:Y:99:THR:HB	2.21	0.40
1:O:32:LYS:HA	1:O:32:LYS:CE	2.40	0.40
3:Q:31:VAL:O	3:Q:166:GLY:HA2	2.21	0.40
4:R:177:LEU:HD22	5:S:58:LEU:HD22	2.03	0.40
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.86	0.40
12:Z:135:MET:N	12:Z:136:PRO:CD	2.84	0.40
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.55	0.40
5:E:103:PHE:HE2	13:M:62:LEU:HD21	1.87	0.40
6:F:142:ASP:HB2	18:F:562:HOH:O	2.21	0.40
4:R:65:GLU:HA	18:R:510:HOH:O	2.22	0.40
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	2.03	0.40
13:1:7:LYS:HB3	13:1:12:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	246/250 (98%)	237 (96%)	5 (2%)	4 (2%)	9 19
1	O	246/250 (98%)	233 (95%)	10 (4%)	3 (1%)	13 27
2	B	231/245 (94%)	215 (93%)	14 (6%)	2 (1%)	17 35
2	P	231/245 (94%)	213 (92%)	13 (6%)	5 (2%)	6 12
3	C	235/243 (97%)	226 (96%)	7 (3%)	2 (1%)	17 35
3	Q	235/243 (97%)	223 (95%)	10 (4%)	2 (1%)	17 35
4	D	232/250 (93%)	215 (93%)	13 (6%)	4 (2%)	9 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	R	234/250 (94%)	220 (94%)	9 (4%)	5 (2%)	7 13
5	E	223/234 (95%)	211 (95%)	5 (2%)	7 (3%)	4 6
5	S	227/234 (97%)	213 (94%)	12 (5%)	2 (1%)	17 35
6	F	231/248 (93%)	219 (95%)	12 (5%)	0	100 100
6	T	233/248 (94%)	219 (94%)	12 (5%)	2 (1%)	17 35
7	G	237/252 (94%)	228 (96%)	8 (3%)	1 (0%)	34 57
7	U	239/252 (95%)	235 (98%)	2 (1%)	2 (1%)	19 39
8	H	218/222 (98%)	209 (96%)	8 (4%)	1 (0%)	29 52
8	V	216/222 (97%)	207 (96%)	9 (4%)	0	100 100
9	I	200/205 (98%)	194 (97%)	6 (3%)	0	100 100
9	W	200/205 (98%)	191 (96%)	8 (4%)	1 (0%)	29 52
10	J	193/198 (98%)	185 (96%)	7 (4%)	1 (0%)	29 52
10	X	193/198 (98%)	185 (96%)	6 (3%)	2 (1%)	15 32
11	K	208/212 (98%)	202 (97%)	5 (2%)	1 (0%)	29 52
11	Y	208/212 (98%)	201 (97%)	6 (3%)	1 (0%)	29 52
12	L	216/241 (90%)	206 (95%)	10 (5%)	0	100 100
12	Z	216/241 (90%)	206 (95%)	8 (4%)	2 (1%)	17 35
13	1	227/266 (85%)	219 (96%)	7 (3%)	1 (0%)	34 57
13	M	229/266 (86%)	218 (95%)	10 (4%)	1 (0%)	34 57
14	2	188/196 (96%)	182 (97%)	6 (3%)	0	100 100
14	N	192/196 (98%)	187 (97%)	5 (3%)	0	100 100
All	All	6184/6524 (95%)	5899 (95%)	233 (4%)	52 (1%)	19 39

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
2	B	217	ALA
3	C	207	ALA
4	D	123(E)	SER
5	E	6	ASN
5	E	203	ASP
13	M	1	THR
2	P	54	VAL
2	P	217	ALA

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Mol	Chain	Res	Type
3	Q	207	ALA
5	S	199	GLN
5	S	203	ASP
12	Z	144(Q)	LEU
12	Z	144(R)	LYS
1	A	167	LYS
4	D	123(D)	ALA
5	E	199	GLN
5	E	217	LYS
7	G	239	GLN
8	H	189	ARG
1	O	53	LYS
2	P	218(B)	ASP
3	Q	202	GLN
4	R	128	MET
1	A	5	THR
1	A	217(F)	LEU
4	D	123(F)	GLY
5	E	180	LEU
11	K	180	GLU
1	O	167	LYS
4	R	123(E)	SER
7	U	55	PRO
7	U	239	GLN
9	W	91	ARG
10	X	8	VAL
10	X	188	ASP
11	Y	72	GLU
13	1	1	THR
1	A	203	GLU
5	E	56	ASP
5	E	231	LYS
2	P	22	TYR
4	R	182	SER
4	D	123(C)	GLY
2	P	204(A)	SER
4	R	56	SER
4	R	122	ARG
6	T	240	ILE
6	T	13	SER
10	J	8	VAL
1	O	56	SER

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Mol	Chain	Res	Type
3	C	17	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	199 (95%)	10 (5%)	25 49
1	O	209/209 (100%)	198 (95%)	11 (5%)	22 45
2	B	195/204 (96%)	177 (91%)	18 (9%)	9 17
2	P	195/204 (96%)	174 (89%)	21 (11%)	6 12
3	C	213/215 (99%)	193 (91%)	20 (9%)	8 17
3	Q	213/215 (99%)	199 (93%)	14 (7%)	16 33
4	D	198/206 (96%)	181 (91%)	17 (9%)	10 20
4	R	198/206 (96%)	181 (91%)	17 (9%)	10 20
5	E	192/193 (100%)	168 (88%)	24 (12%)	4 8
5	S	192/193 (100%)	174 (91%)	18 (9%)	8 17
6	F	196/205 (96%)	179 (91%)	17 (9%)	10 20
6	T	196/205 (96%)	177 (90%)	19 (10%)	8 15
7	G	207/210 (99%)	187 (90%)	20 (10%)	8 15
7	U	207/210 (99%)	195 (94%)	12 (6%)	20 40
8	H	181/181 (100%)	171 (94%)	10 (6%)	21 43
8	V	181/181 (100%)	168 (93%)	13 (7%)	14 29
9	I	172/173 (99%)	166 (96%)	6 (4%)	36 62
9	W	172/173 (99%)	162 (94%)	10 (6%)	20 40
10	J	175/175 (100%)	165 (94%)	10 (6%)	20 41
10	X	175/175 (100%)	163 (93%)	12 (7%)	15 31
11	K	169/169 (100%)	159 (94%)	10 (6%)	19 39
11	Y	169/169 (100%)	156 (92%)	13 (8%)	13 25
12	L	185/201 (92%)	173 (94%)	12 (6%)	17 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	Z	185/201 (92%)	173 (94%)	12 (6%)	17 34
13	1	199/224 (89%)	187 (94%)	12 (6%)	19 39
13	M	199/224 (89%)	190 (96%)	9 (4%)	27 52
14	2	162/162 (100%)	152 (94%)	10 (6%)	18 37
14	N	162/162 (100%)	154 (95%)	8 (5%)	25 48
All	All	5306/5454 (97%)	4921 (93%)	385 (7%)	14 28

All (385) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	7	ARG
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	65	SER
1	A	203	GLU
1	A	222	ARG
1	A	232	ARG
1	A	236	LEU
2	B	18	GLU
2	B	55	THR
2	B	58	LEU
2	B	61	GLN
2	B	91	THR
2	B	121	GLN
2	B	135	SER
2	B	150	THR
2	B	156	ASN
2	B	177	GLN
2	B	181	LYS
2	B	185	LYS
2	B	186	VAL
2	B	192	LEU
2	B	198	SER
2	B	202	THR
2	B	225	LYS
2	B	233	LEU
3	C	9	ASP
3	C	10	ARG

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Mol	Chain	Res	Type
3	C	33	ARG
3	C	44	ASN
3	C	57	LYS
3	C	87	ILE
3	C	112	LEU
3	C	121	GLN
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	179	ASN
3	C	180(C)	LYS
3	C	185	THR
3	C	187	GLU
3	C	202	GLN
3	C	208	LYS
3	C	215	VAL
3	C	227	GLU
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	59	LEU
4	D	72	ARG
4	D	76	CYS
4	D	110	GLU
4	D	119	LEU
4	D	123(B)	GLU
4	D	125	GLU
4	D	177	LEU
4	D	180(E)	SER
4	D	191	LEU
4	D	192	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
5	E	4	PHE
5	E	12	THR
5	E	13	VAL
5	E	18	THR
5	E	28	LEU
5	E	43	ASN
5	E	58	LEU

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Mol	Chain	Res	Type
5	E	64	GLN
5	E	76	LEU
5	E	78	LEU
5	E	97	ASN
5	E	121	GLN
5	E	149	LEU
5	E	177	GLU
5	E	178	ARG
5	E	185	ASN
5	E	189	LEU
5	E	195	GLU
5	E	206	SER
5	E	207	LEU
5	E	207(C)	VAL
5	E	219	THR
5	E	222	THR
5	E	227	GLU
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	98	SER
6	F	106	PRO
6	F	121	GLN
6	F	129	VAL
6	F	169	ARG
6	F	176	LEU
6	F	192	GLN
6	F	204	ASP
6	F	206	LYS
6	F	214	TRP
6	F	218(C)	ASN
6	F	222	LYS
6	F	225	LYS
6	F	238	LYS
7	G	10	ARG
7	G	33	GLN
7	G	38	LEU
7	G	49	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	124	THR

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Mol	Chain	Res	Type
7	G	128	TYR
7	G	163	THR
7	G	169	GLN
7	G	171	GLU
7	G	179(C)	LYS
7	G	184	ASN
7	G	184(H)	GLU
7	G	184(M)	SER
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
7	G	239	GLN
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	131	SER
8	H	144	GLN
8	H	192	LEU
8	H	197	ARG
8	H	222	CYS
8	H	223	ASP
9	I	107	LYS
9	I	121	GLU
9	I	140	SER
9	I	160	LEU
9	I	171	TRP
9	I	181	LYS
10	J	6	ILE
10	J	9	GLN
10	J	34	THR
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	77	GLN
10	J	155	LEU
10	J	160	GLN
10	J	191	GLN
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	65	LEU

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Mol	Chain	Res	Type
11	K	73	ARG
11	K	87	VAL
11	K	99	THR
11	K	105(A)	ARG
11	K	105(B)	LYS
11	K	201	GLU
12	L	-9	GLN
12	L	4	LEU
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	62	SER
12	L	99	THR
12	L	138	LEU
12	L	144(A)	LYS
12	L	144(K)	LYS
12	L	144(M)	LYS
13	M	-8	THR
13	M	7	LYS
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	141(C)	ARG
13	M	149	GLN
13	M	184	LEU
13	M	190	LEU
14	N	10	ASP
14	N	36	ARG
14	N	64	GLU
14	N	94	ASN
14	N	105(B)	LYS
14	N	107	LYS
14	N	119	VAL
14	N	132	THR
1	O	4	MET
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	110	LYS
1	O	124	THR
1	O	158	PHE

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Mol	Chain	Res	Type
1	O	167	LYS
1	O	217(P)	LYS
1	O	222	ARG
1	O	223	LYS
2	P	51	GLU
2	P	54	VAL
2	P	58	LEU
2	P	61	GLN
2	P	64	THR
2	P	65	GLU
2	P	91	THR
2	P	110	GLU
2	P	121	GLN
2	P	150	THR
2	P	170	SER
2	P	181	LYS
2	P	185	LYS
2	P	192	LEU
2	P	198	SER
2	P	202	THR
2	P	212	PHE
2	P	218(B)	ASP
2	P	225	LYS
2	P	232	ILE
2	P	235	LYS
3	Q	40	VAL
3	Q	55	THR
3	Q	61	THR
3	Q	100	ARG
3	Q	112	LEU
3	Q	129	VAL
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	185	THR
3	Q	199	GLU
3	Q	208	LYS
3	Q	235	GLN
4	R	28	LEU
4	R	42	THR
4	R	48	LEU

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Mol	Chain	Res	Type
4	R	52	LYS
4	R	59	LEU
4	R	65	GLU
4	R	76	CYS
4	R	86	ARG
4	R	119	LEU
4	R	158	TYR
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	207	LEU
4	R	215	ILE
4	R	237	LEU
5	S	12	THR
5	S	13	VAL
5	S	28	LEU
5	S	33	GLN
5	S	58	LEU
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	168	ARG
5	S	178	ARG
5	S	180(A)	ASP
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	206	SER
5	S	207	LEU
5	S	222	THR
6	T	25	GLU
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	63	LYS
6	T	95	GLU
6	T	98	SER
6	T	121	GLN
6	T	127	ASN
6	T	129	VAL

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Mol	Chain	Res	Type
6	T	165	THR
6	T	169	ARG
6	T	176	LEU
6	T	187	ARG
6	T	195	LYS
6	T	205	ASN
6	T	214	TRP
6	T	222	LYS
6	T	225	LYS
7	U	49	ILE
7	U	57	LYS
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	169	GLN
7	U	174	THR
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	22	GLN
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	63	ILE
8	V	68	LEU
8	V	144	GLN
8	V	149	GLU
8	V	200	LYS
8	V	221	ILE
8	V	222	CYS
9	W	-7	ASP
9	W	-4	SER
9	W	12	VAL
9	W	107	LYS
9	W	121	GLU
9	W	140	SER
9	W	159	LEU
9	W	160	LEU

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Mol	Chain	Res	Type
9	W	171	TRP
9	W	181	LYS
10	X	6	ILE
10	X	34	THR
10	X	48	GLU
10	X	52	THR
10	X	68	ILE
10	X	77	GLN
10	X	105(B)	LYS
10	X	120	VAL
10	X	157	LEU
10	X	168	MET
10	X	189	ASP
10	X	191	GLN
11	Y	4	LEU
11	Y	7	ARG
11	Y	9	GLN
11	Y	31	VAL
11	Y	41	LEU
11	Y	65	LEU
11	Y	73	ARG
11	Y	99	THR
11	Y	105(A)	ARG
11	Y	105(B)	LYS
11	Y	145	ASP
11	Y	146	LEU
11	Y	149	GLU
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	14	LEU
12	Z	40	ASN
12	Z	62	SER
12	Z	99	THR
12	Z	106	GLU
12	Z	138	LEU
12	Z	144(J)	ASN
12	Z	144(Q)	LEU
12	Z	144(R)	LYS
12	Z	182	ASP
13	1	7	LYS
13	1	40	ASN
13	1	62	LEU

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Mol	Chain	Res	Type
13	1	91	ARG
13	1	141(C)	ARG
13	1	148	VAL
13	1	149	GLN
13	1	181(A)	THR
13	1	184	LEU
13	1	190	LEU
13	1	204	LYS
13	1	211	ILE
14	2	9	LYS
14	2	20	THR
14	2	22	THR
14	2	36	ARG
14	2	94	ASN
14	2	105(B)	LYS
14	2	119	VAL
14	2	149	GLU
14	2	186	ARG
14	2	187(F)	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	227	GLN
2	B	23	GLN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
3	C	44	ASN
3	C	97	GLN
3	C	121	GLN
3	C	150	GLN
3	C	163	GLN
3	C	179	ASN
3	C	209	ASN
4	D	23	GLN
4	D	108	ASN
4	D	141	HIS
4	D	150	HIS

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Mol	Chain	Res	Type
4	D	161	ASN
4	D	226	ASN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	185	ASN
5	E	207(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	192	GLN
6	F	205	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	170	GLN
7	G	178	ASN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
10	J	9	GLN
10	J	54	GLN
10	J	85	GLN
10	J	112	GLN
10	J	186	GLN
11	K	85	ASN
11	K	141	ASN
11	K	174	ASN
11	K	208	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN

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Mol	Chain	Res	Type
12	L	67	HIS
12	L	70(A)	ASN
12	L	85	HIS
12	L	123	GLN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
14	N	38	HIS
14	N	145	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	61	GLN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	177	GLN
2	P	218	ASN
3	Q	82	ASN
3	Q	97	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	147	GLN
4	R	150	HIS
4	R	161	ASN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	97	ASN
5	S	104	ASN

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Mol	Chain	Res	Type
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	185	ASN
5	S	199	GLN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	147	HIS
6	T	180(C)	HIS
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	178	ASN
7	U	182	HIS
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
9	W	145	ASN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	96	GLN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN

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Mol	Chain	Res	Type
12	Z	40	ASN
12	Z	67	HIS
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	144(B)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	38	HIS
14	2	69	GLN
14	2	106	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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	LZT	Y	212	-	46,46,46	1.13	1 (2%)	62,63,63	1.57	7 (11%)
16	LZT	K	213	-	46,46,46	1.09	1 (2%)	62,63,63	1.79	7 (11%)
17	MES	Y	213	-	12,12,12	2.22	1 (8%)	14,16,16	1.68	2 (14%)
17	MES	K	214	-	12,12,12	1.96	1 (8%)	14,16,16	1.56	3 (21%)

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	LZT	Y	212	-	-	1/36/48/48	0/4/4/4
16	LZT	K	213	-	-	1/36/48/48	0/4/4/4
17	MES	Y	213	-	-	0/6/14/14	0/1/1/1
17	MES	K	214	-	-	5/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	213	MES	C8-S	-7.37	1.67	1.77
16	Y	212	LZT	C8-C9	-6.53	1.40	1.47
17	K	214	MES	C8-S	-6.37	1.68	1.77
16	K	213	LZT	C8-C9	-6.05	1.40	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	K	213	LZT	C12-C11-C9	-6.50	92.48	105.04
16	Y	212	LZT	C1-C8-C9	-6.12	105.49	109.64
16	K	213	LZT	C8-C1-C12	-5.44	105.88	111.60
16	Y	212	LZT	C12-C11-C9	-5.35	94.69	105.04
16	K	213	LZT	C1-C8-C9	-4.98	106.26	109.64
16	K	213	LZT	C5-O4-C3	-4.67	107.38	117.51
17	K	214	MES	O3S-S-C8	3.70	111.75	105.77
16	K	213	LZT	C7-C8-C9	3.60	134.66	128.38
16	Y	212	LZT	C5-O4-C3	-3.51	109.89	117.51
17	Y	213	MES	O2S-S-C8	3.51	111.14	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	212	LZT	C7-C8-C9	3.27	134.10	128.38
17	Y	213	MES	O3S-S-C8	3.22	110.97	105.77
16	Y	212	LZT	C11-C12-C1	-3.01	101.81	103.94
16	Y	212	LZT	C8-C1-C12	-2.81	108.64	111.60
17	K	214	MES	O2S-S-C8	2.76	110.23	106.92
16	K	213	LZT	O43-C42-C13	-2.19	118.29	121.50
17	K	214	MES	O1-C2-C3	-2.10	107.17	111.80
16	K	213	LZT	C18-C21-N22	-2.09	108.57	113.05
16	Y	212	LZT	C13-C12-C1	-2.03	108.84	113.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	214	MES	C7-C8-S-O2S
17	K	214	MES	C7-C8-S-O3S
17	K	214	MES	C8-C7-N4-C5
17	K	214	MES	C7-C8-S-O1S
17	K	214	MES	C8-C7-N4-C3
16	Y	212	LZT	C12-C13-C42-O43
16	K	213	LZT	C25-C26-C28-C36

There are no ring outliers.

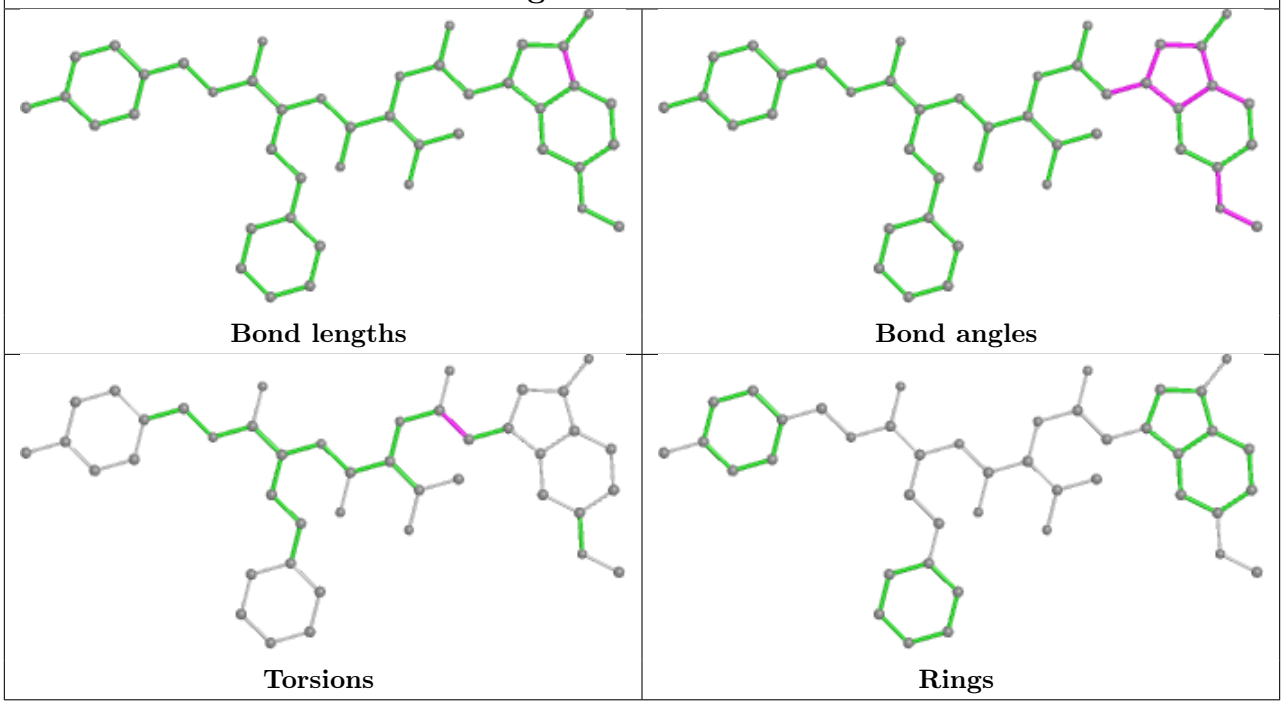
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	212	LZT	4	0
16	K	213	LZT	5	0
17	Y	213	MES	1	0
17	K	214	MES	2	0

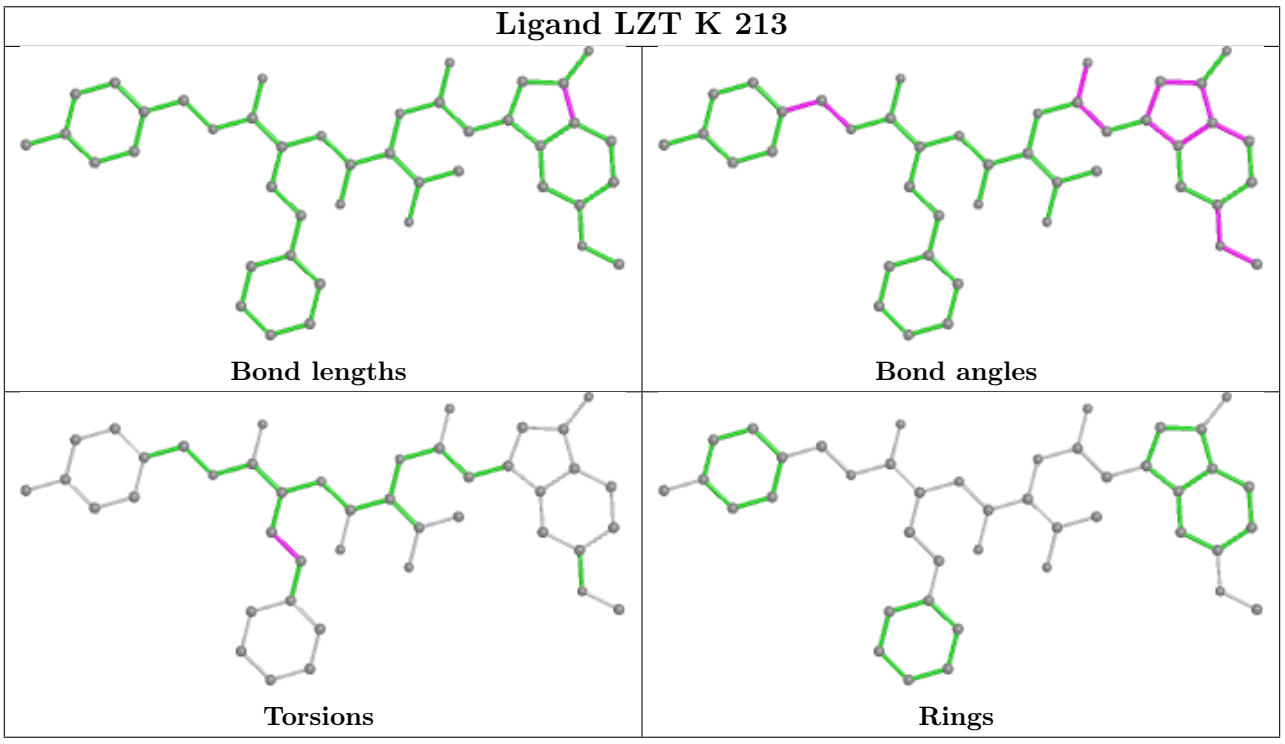
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand LZT Y 212



Ligand LZT K 213



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	4
5	E	4
4	R	3
13	M	3
14	N	3
14	2	3
9	I	3
7	G	3
9	W	3
13	1	3
3	C	2
10	X	2
10	J	2
3	Q	2
5	S	2
6	F	2
12	L	2
8	H	2
8	V	2
12	Z	2
11	K	1
1	A	1
1	O	1
2	P	1
6	T	1
11	Y	1
7	U	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	123(G):GLU	C	125:GLU	N	4.71
1	R	123(G):GLU	C	125:GLU	N	4.45
1	C	203:THR	C	206:GLY	N	3.60
1	X	-1:MET	C	1:ASP	N	3.56
1	J	-1:MET	C	1:ASP	N	3.41
1	K	181:ASP	C	183:GLY	N	3.23
1	Q	180(D):GLU	C	182:PRO	N	3.22
1	E	207(E):ASN	C	210:LEU	N	3.11

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	203:THR	C	206:GLY	N	3.00
1	E	204:GLU	C	206:SER	N	2.97
1	A	200:SER	C	202:VAL	N	2.92
1	O	200:SER	C	202:VAL	N	2.84
1	C	180(D):GLU	C	182:PRO	N	2.83
1	S	60:SER	C	63:TYR	N	2.82
1	M	181(A):THR	C	183:GLY	N	2.80
1	R	202:GLU	C	205:GLU	N	2.78
1	S	204:GLU	C	206:SER	N	2.77
1	F	180(F):GLY	C	184:LEU	N	2.76
1	N	181:ALA	C	183:GLY	N	2.76
1	D	180(E):SER	C	184:LEU	N	2.67
1	2	181:ALA	C	183:GLY	N	2.66
1	D	233:ILE	C	235:LYS	N	2.63
1	2	92:ASP	C	94:ASN	N	2.62
1	I	179:LYS	C	181:LYS	N	2.61
1	G	184(M):SER	C	186:TRP	N	2.59
1	F	199:LEU	C	201:ALA	N	2.58
1	W	179:LYS	C	181:LYS	N	2.58
1	E	180(F):ILE	C	183:ASP	N	2.54
1	P	200:THR	C	202:THR	N	2.54
1	G	180(D):ILE	C	184:ASN	N	2.48
1	L	-1:GLY	C	1:GLY	N	2.47
1	E	60:SER	C	63:TYR	N	2.44
1	H	91:GLN	C	93:GLY	N	2.42
1	T	199:LEU	C	201:ALA	N	2.41
1	V	91:GLN	C	93:GLY	N	2.36
1	X	181:ASP	C	183:GLY	N	2.36
1	J	181:ASP	C	183:GLY	N	2.33
1	R	233:ILE	C	235:LYS	N	2.32
1	L	180:LYS	C	182:ASP	N	2.31
1	Y	181:ASP	C	183:GLY	N	2.31
1	U	218:ASP	C	220:LYS	N	2.28
1	1	181(A):THR	C	183:GLY	N	2.27
1	D	202:GLU	C	205:GLU	N	2.26
1	Z	-1:GLY	C	1:GLY	N	2.26
1	Z	180:LYS	C	182:ASP	N	2.22
1	B	200:THR	C	202:THR	N	2.16
1	V	187:LEU	C	189:ARG	N	2.07
1	1	141(G):ILE	C	144:PRO	N	2.01
1	2	70:TYR	C	72:GLY	N	2.00
1	W	36:HIS	C	38:TYR	N	1.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	187:LEU	C	189:ARG	N	1.95
1	N	70:TYR	C	72:GLY	N	1.95
1	M	141(G):ILE	C	144:PRO	N	1.93
1	G	218:ASP	C	220:LYS	N	1.91
1	I	36:HIS	C	38:TYR	N	1.91
1	I	-1:GLY	C	1:GLY	N	1.86
1	M	-1:GLY	C	1:THR	N	1.86
1	W	-1:GLY	C	1:GLY	N	1.83
1	1	-1:GLY	C	1:THR	N	1.83
1	N	92:ASP	C	94:ASN	N	1.76

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.04	6 (2%) 59 53	38, 56, 80, 104	0
1	O	250/250 (100%)	-0.03	9 (3%) 42 35	38, 57, 80, 104	0
2	B	235/245 (95%)	0.10	11 (4%) 31 25	36, 60, 90, 96	0
2	P	235/245 (95%)	0.07	7 (2%) 50 43	36, 60, 90, 96	0
3	C	241/243 (99%)	0.40	21 (8%) 10 7	43, 71, 111, 126	0
3	Q	241/243 (99%)	0.76	42 (17%) 1 0	44, 71, 111, 126	0
4	D	242/250 (96%)	0.19	12 (4%) 28 23	35, 62, 96, 103	0
4	R	242/250 (96%)	0.28	16 (6%) 18 13	36, 62, 96, 102	0
5	E	233/234 (99%)	0.15	11 (4%) 31 25	42, 62, 93, 105	0
5	S	233/234 (99%)	0.33	18 (7%) 13 10	42, 62, 92, 105	0
6	F	237/248 (95%)	-0.05	8 (3%) 45 38	35, 54, 85, 96	0
6	T	237/248 (95%)	-0.10	4 (1%) 70 66	34, 54, 82, 96	0
7	G	243/252 (96%)	-0.24	5 (2%) 63 58	33, 49, 73, 94	0
7	U	243/252 (96%)	-0.23	4 (1%) 72 68	32, 49, 72, 94	0
8	H	222/222 (100%)	-0.25	0 100 100	36, 46, 62, 89	0
8	V	222/222 (100%)	-0.32	1 (0%) 91 89	36, 47, 63, 90	0
9	I	204/205 (99%)	-0.21	1 (0%) 91 89	34, 45, 61, 77	0
9	W	204/205 (99%)	-0.15	1 (0%) 91 89	34, 45, 62, 77	0
10	J	198/198 (100%)	-0.14	5 (2%) 57 51	37, 48, 63, 120	0
10	X	198/198 (100%)	-0.14	7 (3%) 44 36	36, 49, 63, 120	0
11	K	212/212 (100%)	-0.33	0 100 100	34, 45, 63, 72	0
11	Y	212/212 (100%)	-0.30	0 100 100	34, 45, 63, 72	0
12	L	222/241 (92%)	-0.30	0 100 100	33, 46, 68, 73	0
12	Z	222/241 (92%)	-0.24	3 (1%) 75 71	32, 46, 68, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/266 (87%)	-0.36	1 (0%) 92 91	33, 44, 57, 63	0
13	M	233/266 (87%)	-0.32	1 (0%) 92 91	34, 44, 58, 63	0
14	2	196/196 (100%)	-0.31	2 (1%) 82 80	33, 41, 58, 68	0
14	N	196/196 (100%)	-0.36	0 100 100	33, 41, 58, 69	0
All	All	6336/6524 (97%)	-0.07	196 (3%) 49 42	32, 51, 89, 126	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	123(F)	GLY	16.1
4	D	123(E)	SER	11.7
4	D	123(B)	GLU	11.0
4	R	123(E)	SER	10.9
3	C	7	GLY	10.7
2	P	217	ALA	9.2
2	B	218	ASN	9.0
13	M	-8	THR	8.7
6	F	12	ASN	8.7
4	D	123(D)	ALA	8.4
5	S	4	PHE	8.4
7	G	240	ASP	8.2
4	R	123(D)	ALA	8.1
4	R	10	ARG	7.7
2	B	217	ALA	7.6
2	P	218	ASN	7.1
5	S	206	SER	6.9
10	J	192	ALA	6.8
7	U	240	ASP	6.8
4	R	123(C)	GLY	6.7
3	C	11	ALA	6.6
4	D	123(C)	GLY	6.5
3	C	9	ASP	6.3
4	D	10	ARG	6.3
7	U	6	ALA	6.1
10	X	191	GLN	6.1
3	Q	56	LEU	6.1
3	C	8	TYR	5.9
13	1	-8	THR	5.7
4	D	9	ASP	5.4
10	J	193	GLN	5.3
3	C	240	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
10	X	193	GLN	5.2
4	D	123(F)	GLY	5.1
1	A	5	THR	5.1
4	R	123(B)	GLU	5.1
5	E	206	SER	5.1
3	Q	238	GLN	5.0
4	R	9	ASP	5.0
3	Q	233	VAL	5.0
4	D	123(A)	GLY	4.9
3	C	243	GLN	4.9
1	O	4	MET	4.9
3	C	208	LYS	4.8
4	D	127	LEU	4.8
7	G	6	ALA	4.7
2	P	216(B)	GLY	4.7
3	Q	241	GLN	4.6
10	X	188	ASP	4.6
3	C	55	THR	4.5
3	Q	236	ILE	4.5
10	J	191	GLN	4.4
5	E	4	PHE	4.4
3	Q	229	ILE	4.4
4	D	11	GLY	4.3
3	Q	8	TYR	4.3
3	Q	62(A)	ILE	4.3
4	R	123(A)	GLY	4.3
1	O	217(P)	LYS	4.3
2	B	216(B)	GLY	4.3
3	Q	234	THR	4.3
3	Q	7	GLY	4.2
3	Q	55	THR	4.2
6	T	13	SER	4.2
5	S	233	ILE	4.1
1	A	4	MET	4.1
5	S	5	ARG	4.0
7	U	7	GLY	3.9
10	X	192	ALA	3.9
3	Q	240	LYS	3.9
6	T	12	ASN	3.9
4	R	235	LYS	3.8
4	R	11	GLY	3.8
3	Q	63	THR	3.7

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Mol	Chain	Res	Type	RSRZ
5	S	57	GLU	3.7
3	Q	187	GLU	3.7
5	S	58	LEU	3.7
10	J	-1	MET	3.7
5	S	8	TYR	3.6
7	G	239	GLN	3.6
3	Q	64	PRO	3.5
7	G	8	TYR	3.4
10	X	-1	MET	3.4
2	B	62	ASP	3.4
14	2	187(J)	LEU	3.4
3	Q	54	SER	3.4
5	S	51	LEU	3.4
1	A	203	GLU	3.4
5	E	5	ARG	3.4
3	Q	237	GLU	3.4
9	I	-8	SER	3.3
3	Q	198	LEU	3.3
3	C	184	ALA	3.3
5	S	6	ASN	3.3
5	S	181	LYS	3.2
8	V	223	ASP	3.2
6	F	205	ASN	3.2
3	C	233	VAL	3.2
12	Z	145	TYR	3.2
3	Q	194	VAL	3.2
6	F	180(F)	GLY	3.2
3	Q	192	LEU	3.1
6	F	199	LEU	3.1
5	E	233	ILE	3.1
5	S	202	ARG	3.1
6	T	199	LEU	3.0
1	O	236	LEU	3.0
3	C	236	ILE	3.0
1	A	236	LEU	2.9
4	D	12	VAL	2.9
3	C	187	GLU	2.9
4	R	123(G)	GLU	2.9
9	W	181	LYS	2.9
4	R	12	VAL	2.9
1	O	8	TYR	2.9
3	Q	184	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
7	U	8	TYR	2.8
3	C	234	THR	2.8
6	F	240	ILE	2.7
5	S	168	ARG	2.7
2	B	127	GLY	2.7
3	C	241	GLN	2.7
1	O	5	THR	2.7
5	E	203	ASP	2.7
3	C	237	GLU	2.7
4	R	231	GLU	2.7
2	P	62	ASP	2.7
3	Q	191	LYS	2.7
5	S	7	ASN	2.6
3	Q	12	LEU	2.6
1	A	234	GLU	2.6
5	S	63	TYR	2.6
12	Z	144(P)	PRO	2.6
3	Q	243	GLN	2.6
3	Q	197	LEU	2.6
2	P	54	VAL	2.6
3	Q	10	ARG	2.6
3	Q	9	ASP	2.6
6	T	240	ILE	2.5
1	A	9	SER	2.5
3	Q	182	PRO	2.5
6	F	238	LYS	2.5
4	D	22	PHE	2.5
3	Q	235	GLN	2.5
2	P	181	LYS	2.5
6	F	204	ASP	2.5
5	S	9	ASP	2.4
4	R	243	ALA	2.4
2	B	186	VAL	2.4
3	C	10	ARG	2.4
3	Q	43	LYS	2.4
5	E	178	ARG	2.4
3	Q	52	ARG	2.3
3	Q	11	ALA	2.3
1	O	6	ASP	2.3
1	O	217(O)	ASP	2.3
12	Z	-9	GLN	2.3
3	Q	227	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
10	X	10	ASP	2.3
5	E	188	GLU	2.3
5	E	202	ARG	2.3
3	C	12	LEU	2.3
3	Q	196	SER	2.3
3	Q	209	ASN	2.3
3	Q	22	PHE	2.3
3	C	196	SER	2.2
1	O	235	ALA	2.2
3	C	232	TYR	2.2
2	B	61	GLN	2.2
3	Q	212	ILE	2.2
1	O	199	GLU	2.2
3	C	227	GLU	2.2
3	Q	210	ILE	2.2
5	E	180	LEU	2.2
14	2	149	GLU	2.2
4	R	229	THR	2.2
5	S	180(B)	THR	2.2
3	Q	13	SER	2.1
5	E	189	LEU	2.1
5	S	195	GLU	2.1
5	E	175	TYR	2.1
2	B	185	LYS	2.1
4	R	127	LEU	2.1
3	Q	242	GLU	2.1
2	B	235	LYS	2.1
10	X	180	LYS	2.1
2	B	191	GLU	2.1
7	G	236	ILE	2.1
2	B	183	ASP	2.1
3	C	22	PHE	2.1
5	S	203	ASP	2.0
2	P	22	TYR	2.0
3	Q	206	GLY	2.0
3	Q	202	GLN	2.0
10	J	168	MET	2.0
6	F	180(E)	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

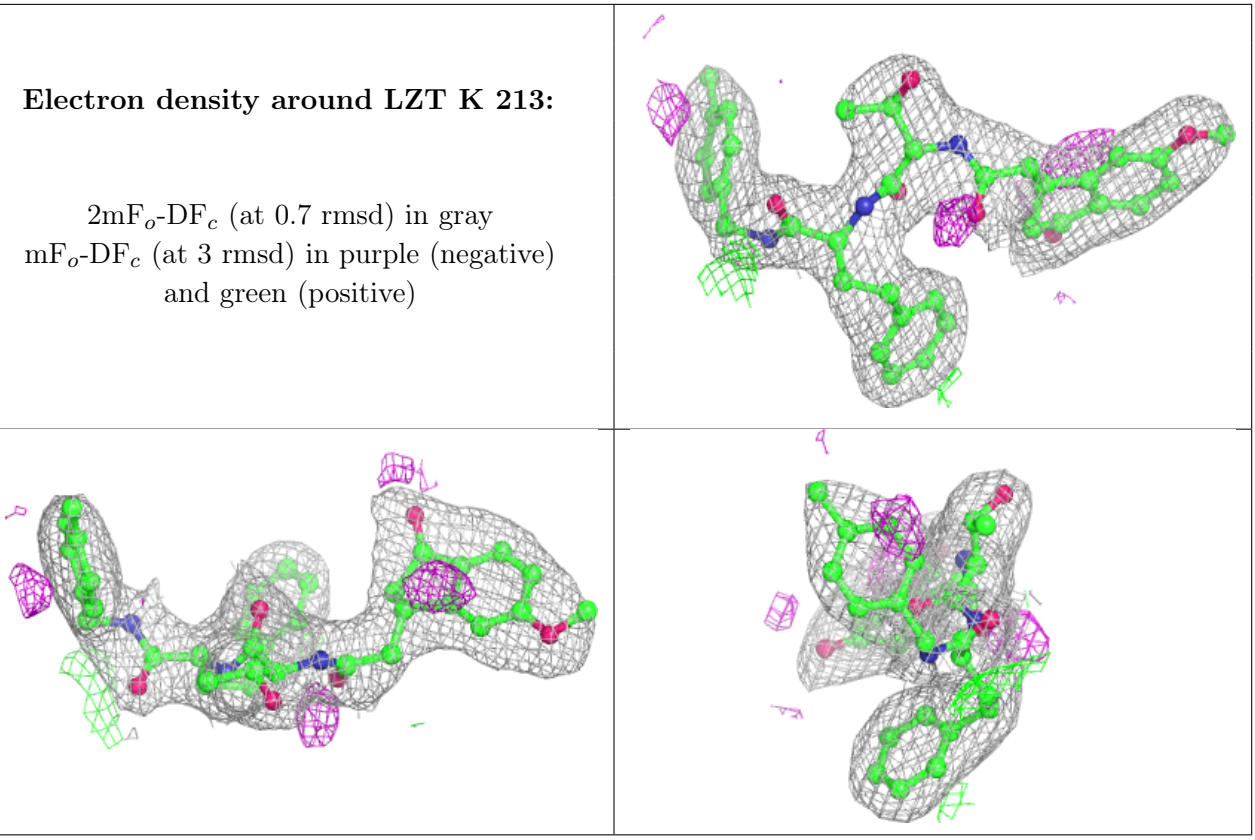
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	I	195	1/1	0.69	0.36	78,78,78,78	0
15	MG	I	196	1/1	0.71	0.28	65,65,65,65	0
15	MG	L	195	1/1	0.77	0.19	58,58,58,58	0
15	MG	F	243	1/1	0.81	0.80	116,116,116,116	0
15	MG	K	212	1/1	0.84	0.15	53,53,53,53	0
15	MG	L	196	1/1	0.85	0.19	57,57,57,57	0
15	MG	F	242	1/1	0.86	0.20	67,67,67,67	0
15	MG	G	241	1/1	0.88	0.08	66,66,66,66	0
17	MES	K	214	12/12	0.93	0.20	78,83,85,85	0
15	MG	N	188	1/1	0.94	0.15	40,40,40,40	0
17	MES	Y	213	12/12	0.94	0.17	79,83,85,85	0
16	LZT	K	213	43/43	0.95	0.17	32,38,45,49	0
15	MG	H	224	1/1	0.97	0.06	50,50,50,50	0
16	LZT	Y	212	43/43	0.97	0.15	34,39,45,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

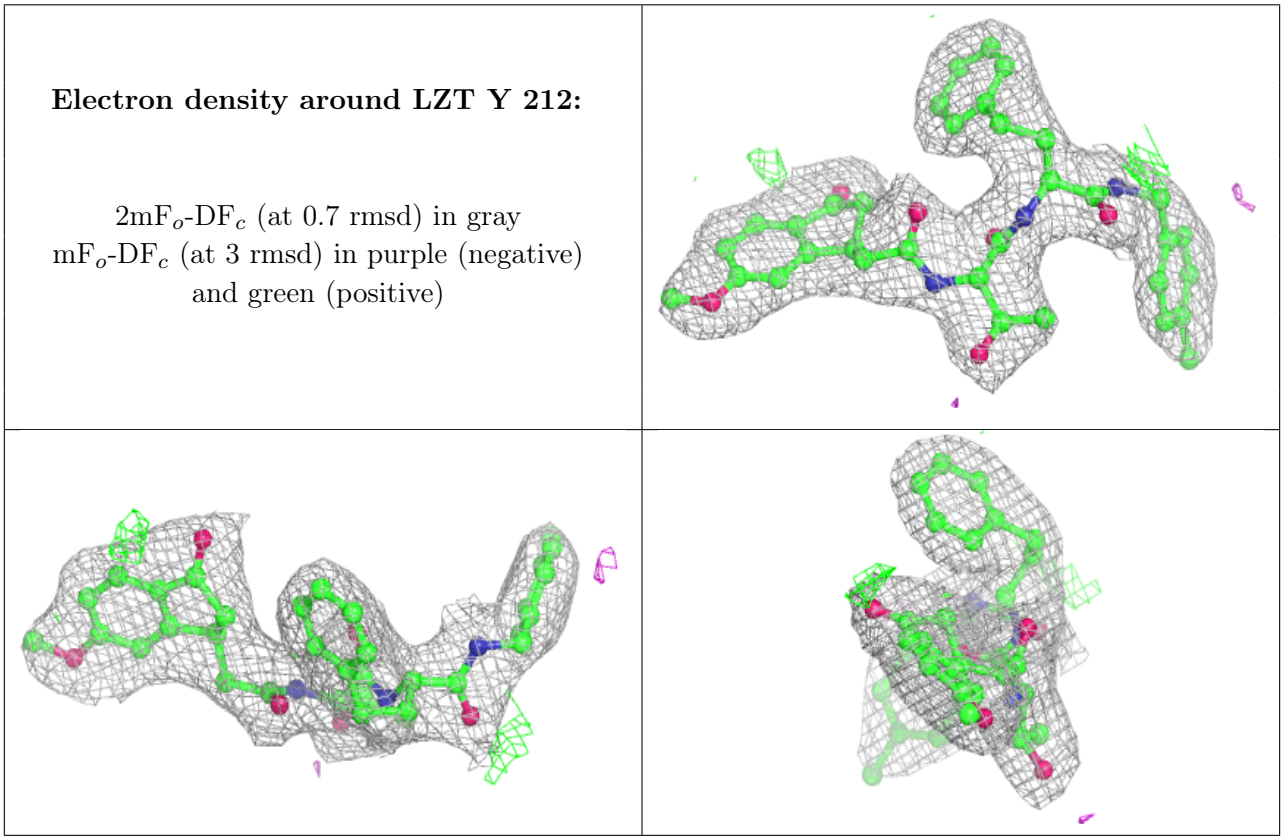
Electron density around LZT K 213:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LZT Y 212:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.