Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 12:01 PM EDT

PDB ID	:	3MG4
Title	:	Structure of yeast 20S proteasome with Compound 1
Authors	:	Sintchak, M.D.
Deposited on	:	2010-04-05
Resolution	:	3.11 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 (i) 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 (i)) were used in the production of this report:

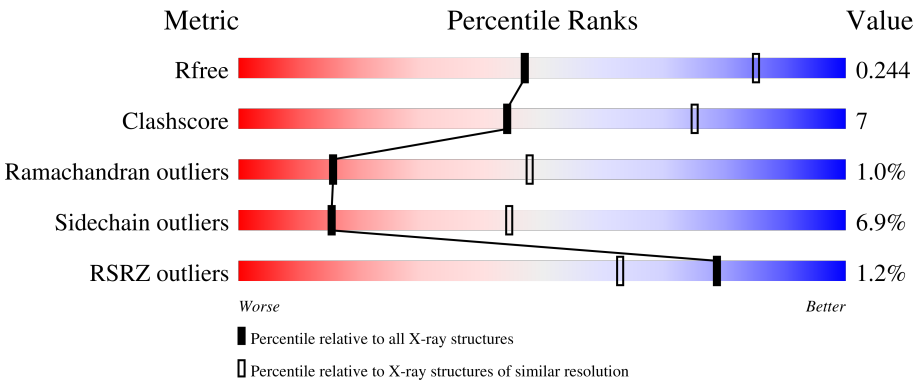
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	.% 84% 15% •
1	O	250	2% 84% 15% •
2	B	244	.% 73% 24% •
2	P	244	.% 76% 20% •
3	C	241	2% 80% 17% •

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Mol	Chain	Length	Quality of chain
3	Q	241	6% 74% 22%
4	D	242	4% 83% 15%
4	R	242	3% 82% 17%
5	E	233	3% 80% 19%
5	S	233	3% 76% 21%
6	F	244	77% 20%
6	T	244	% 81% 16%
7	G	243	77% 21%
7	U	243	75% 21%
8	H	222	86% 13%
8	V	222	80% 18%
9	I	204	86% 13%
9	W	204	83% 15%
10	J	198	% 81% 19%
10	X	198	2% 84% 14%
11	K	212	78% 19%
11	Y	212	79% 18%
12	L	222	77% 21%
12	Z	222	77% 18% 5%
13	1	233	80% 17%
13	M	233	83% 16%
14	2	196	% 80% 19%
14	N	196	80% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	F	242	-	-	-	X
15	MG	G	241	-	-	-	X

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49672 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
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	1862	1162	314	379	7	0	0	0
4	R	242	1862	1162	314	379	7	0	0	0

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	244	1897	1205	330	358	4	0	0	0
6	T	244	1897	1205	330	358	4	0	0	0

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	222	1685	1061	293	324	7	0	0	0
8	V	222	1685	1061	293	324	7	0	0	0

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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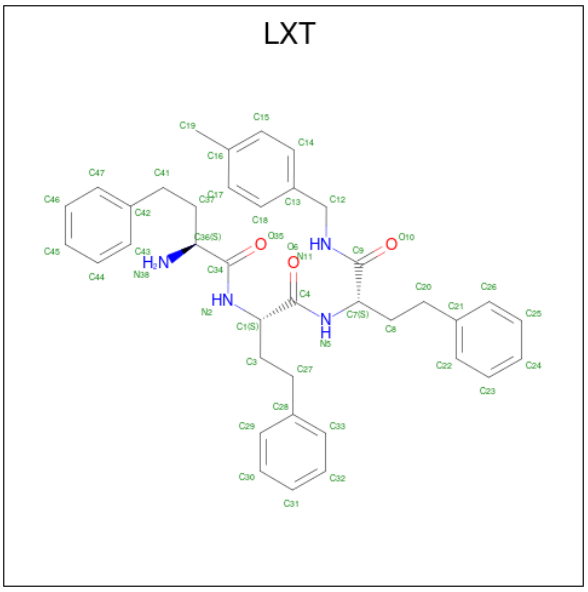
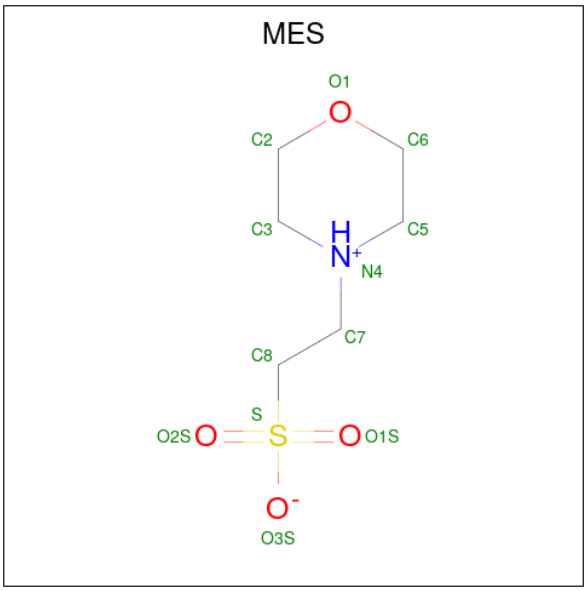
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	G	2	2	2	0	0
			Total	Mg		
15	H	1	1	1	0	0
			Total	Mg		
15	I	2	2	2	0	0
			Total	Mg		
15	K	1	1	1	0	0
			Total	Mg		
15	L	1	1	1	0	0
			Total	Mg		
15	N	1	1	1	0	0

- Molecule 16 is (2S)-2-amino-N-[(1S)-1-({(1S)-1-[(4-methylbenzyl)carbamoyl]-3-phenylpropyl}carbamoyl)-3-phenylpropyl]-4-phenylbutanamide (three-letter code: LXT) (formula: $C_{38}H_{44}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
16	K	1	45	38	4	3	0	0
			Total	C	N	O		
16	Y	1	45	38	4	3	0	0

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



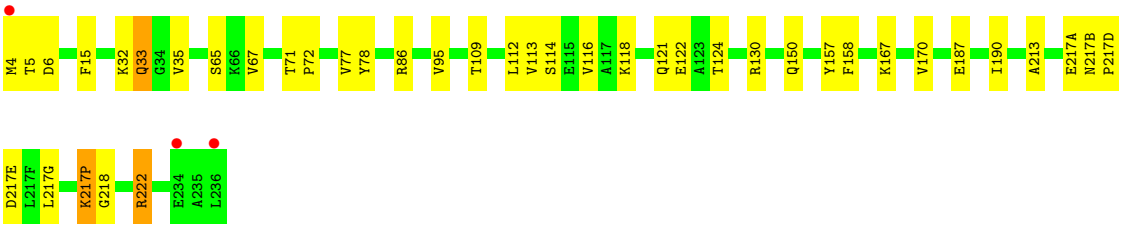
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
17	K	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
17	Y	1	12	6	1	4	1	0	0

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.

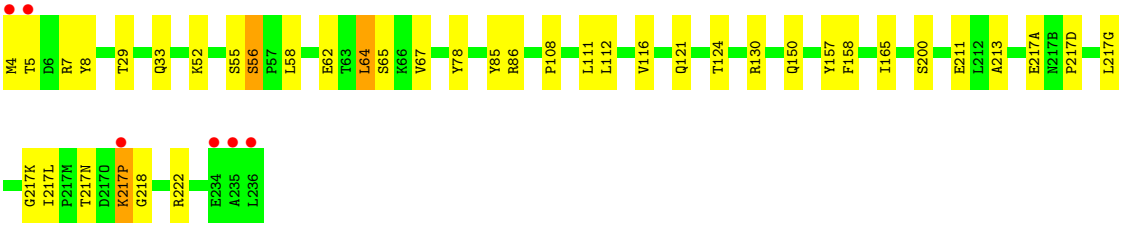
• Molecule 1: Proteasome component Y7

Chain A:



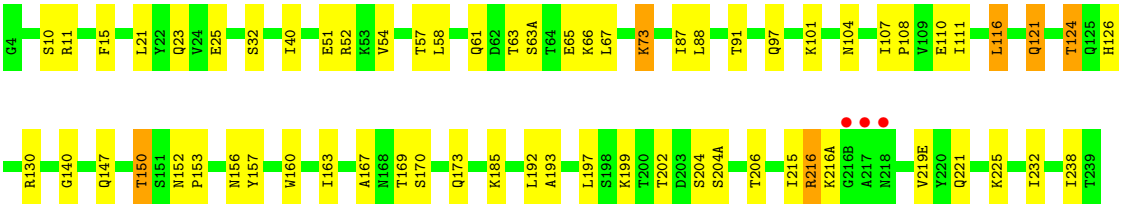
• Molecule 1: Proteasome component Y7

Chain O:



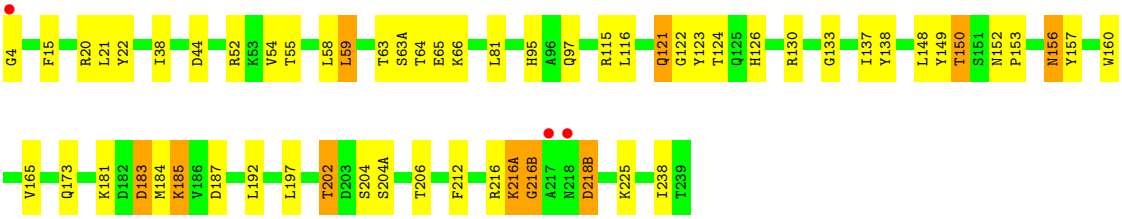
• Molecule 2: Proteasome component Y13

Chain B:



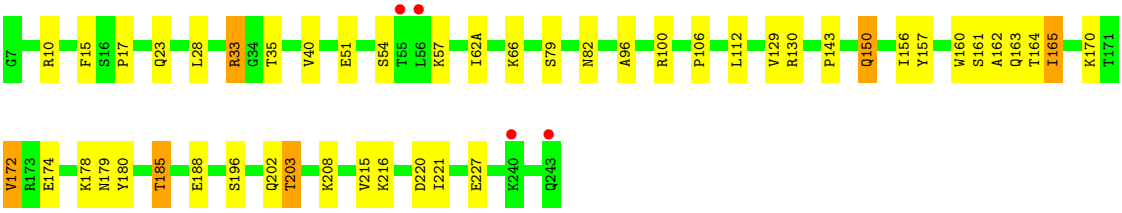
• Molecule 2: Proteasome component Y13

Chain P:



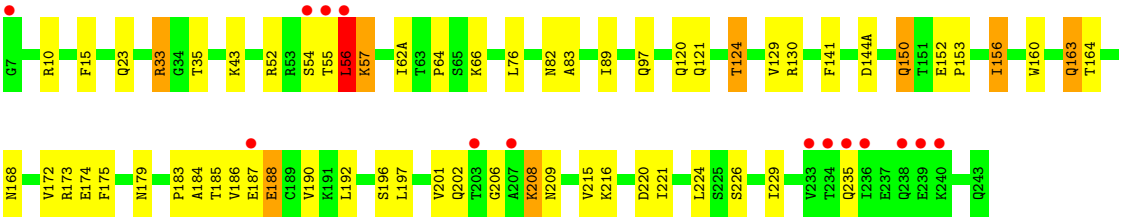
- Molecule 3: Proteasome component PRE6

Chain C:



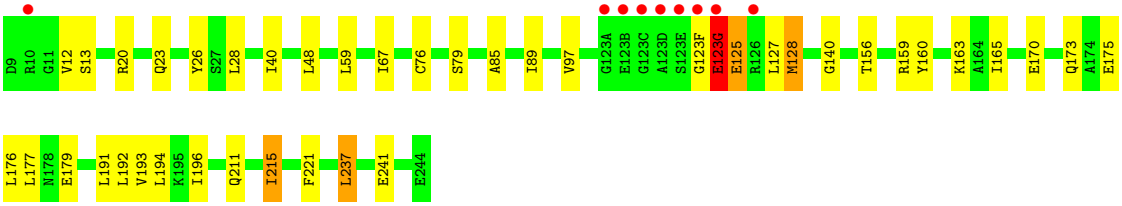
- Molecule 3: Proteasome component PRE6

Chain Q:



- Molecule 4: Proteasome component PUP2

Chain D:

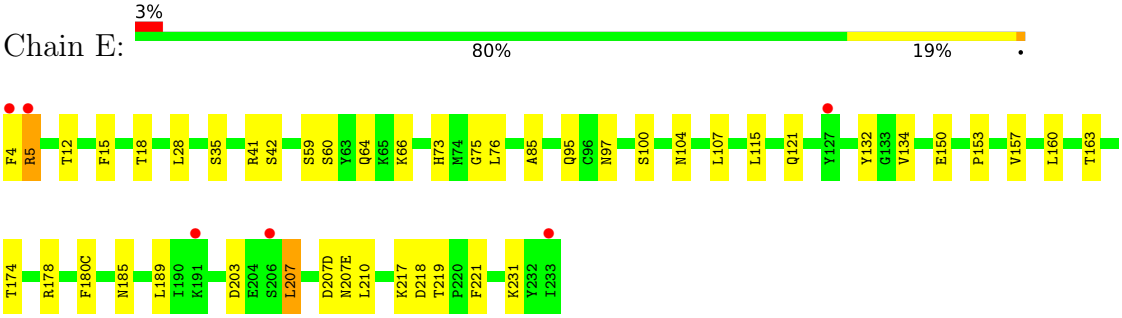


- Molecule 4: Proteasome component PUP2

Chain R:

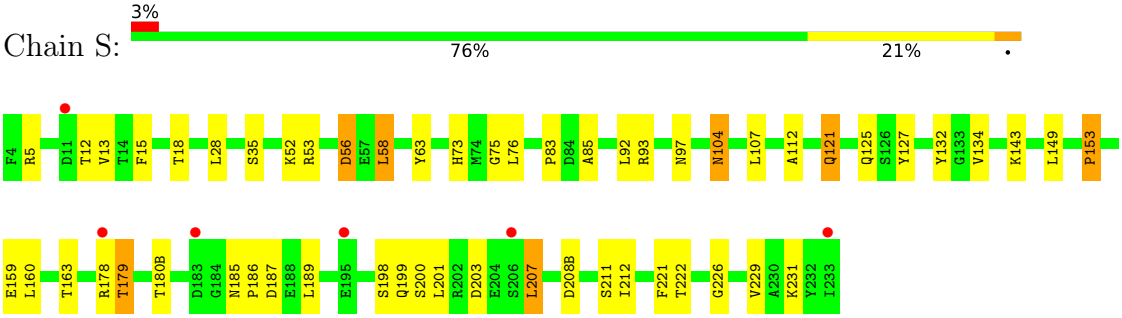
• Molecule 5: Proteasome component PRE5

Chain E:



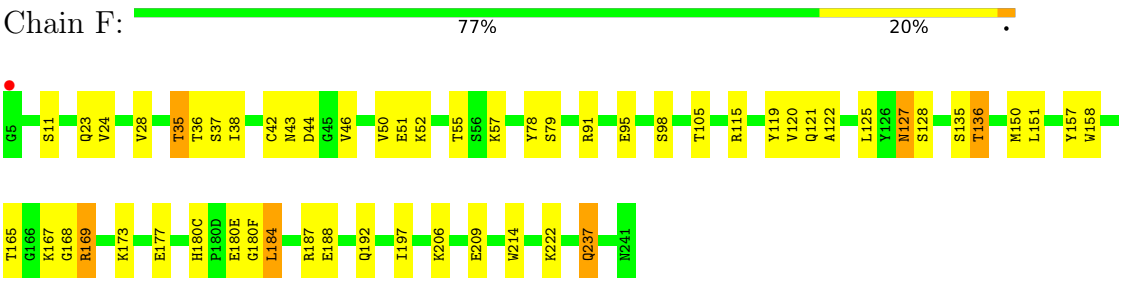
• Molecule 5: Proteasome component PRE5

Chain S:



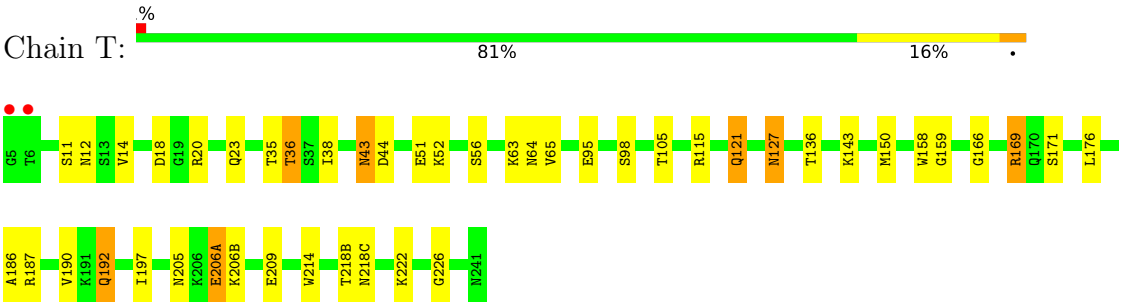
• Molecule 6: Proteasome component C1

Chain F:



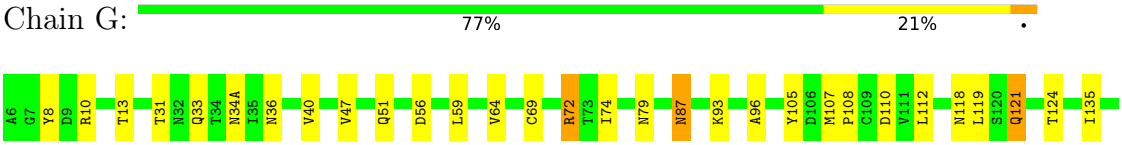
• Molecule 6: Proteasome component C1

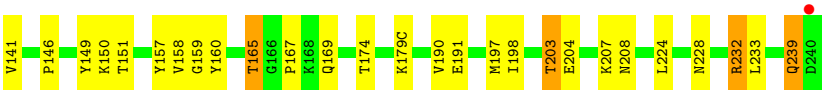
Chain T:



• Molecule 7: Proteasome component C7-alpha

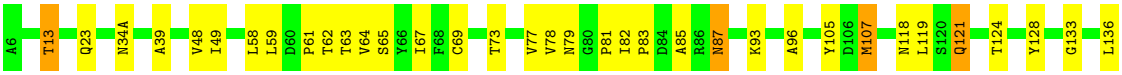
Chain G:





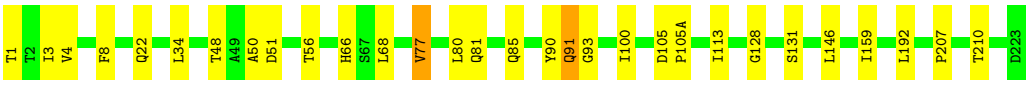
• Molecule 7: Proteasome component C7-alpha

Chain U:



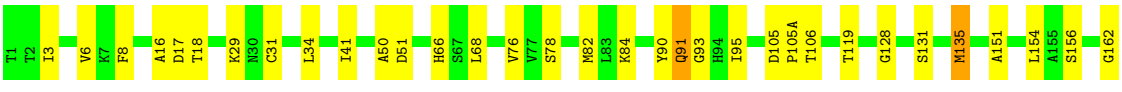
• Molecule 8: Proteasome component PUP1

Chain H:



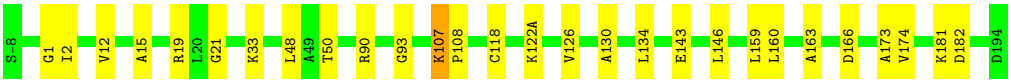
• Molecule 8: Proteasome component PUP1

Chain V:



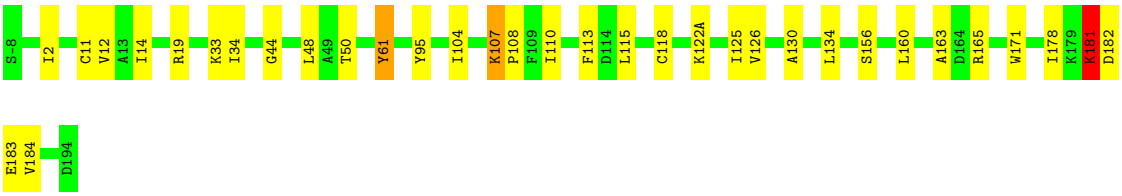
• Molecule 9: Proteasome component PUP3

Chain I:



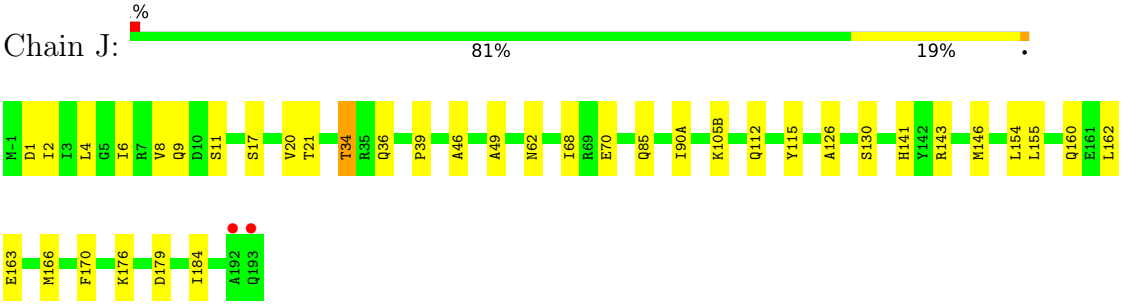
• Molecule 9: Proteasome component PUP3

Chain W:



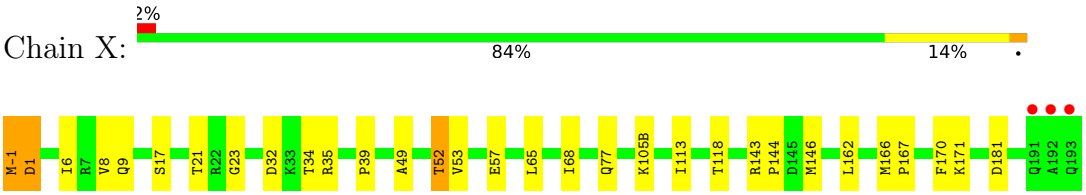
• Molecule 10: Proteasome component C11

Chain J:



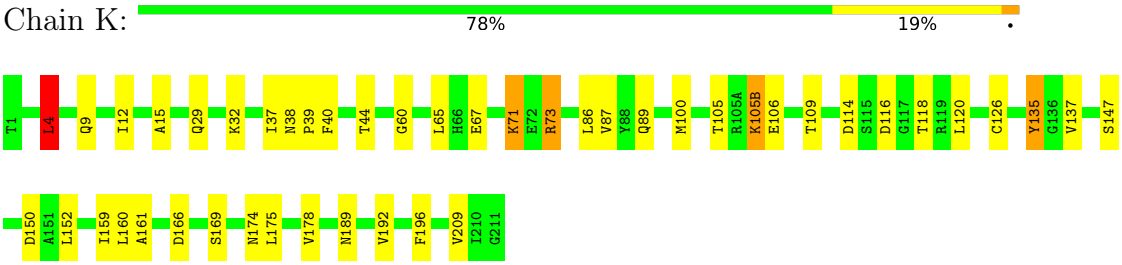
• Molecule 10: Proteasome component C11

Chain X:



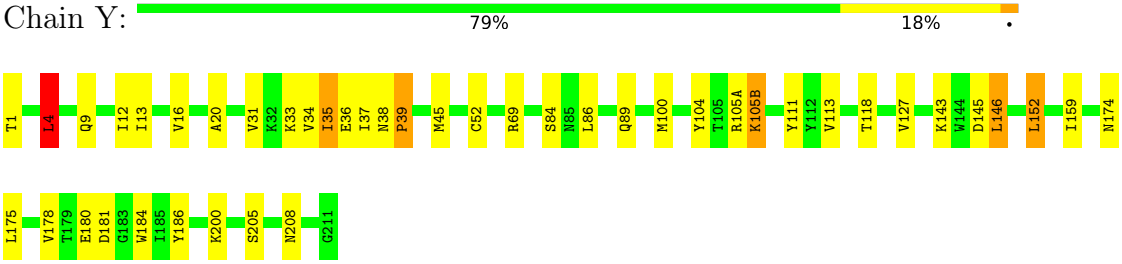
• Molecule 11: Proteasome component PRE2

Chain K:



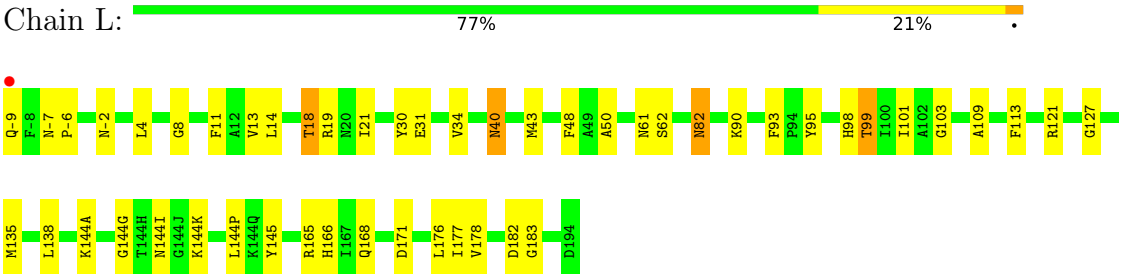
• Molecule 11: Proteasome component PRE2

Chain Y:



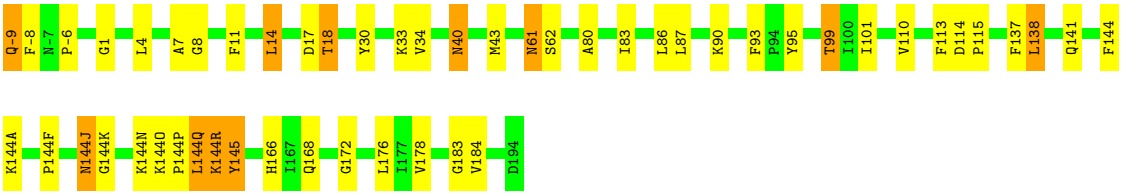
• Molecule 12: Proteasome component C5

Chain L:



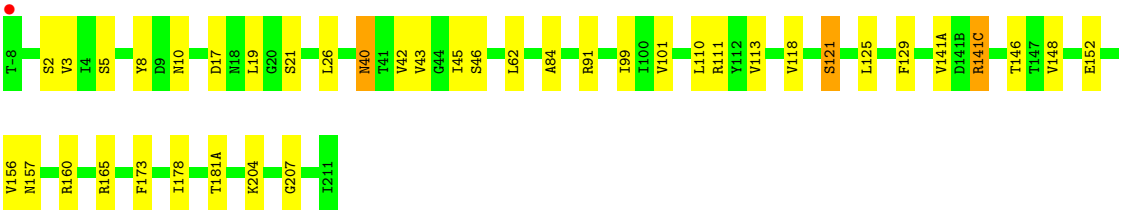
• Molecule 12: Proteasome component C5

Chain Z:



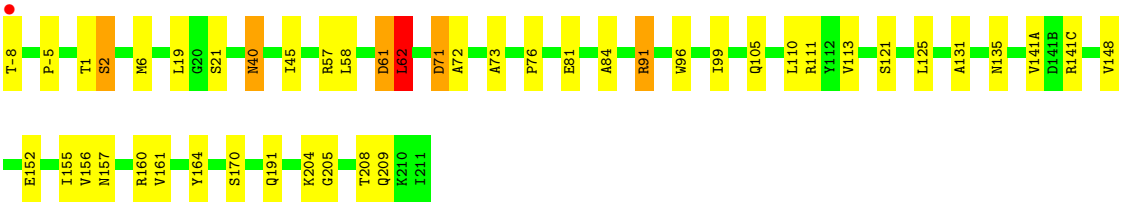
• Molecule 13: Proteasome component PRE4

Chain M:



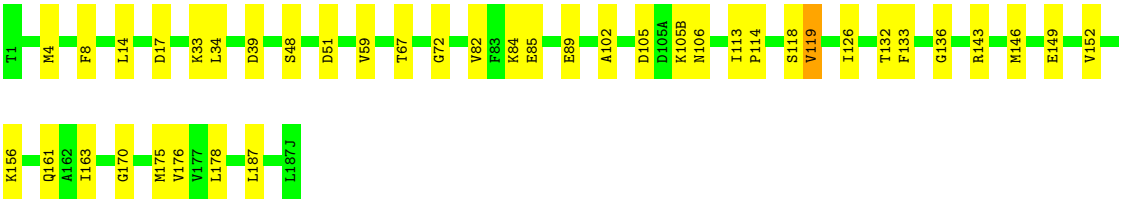
• Molecule 13: Proteasome component PRE4

Chain 1:



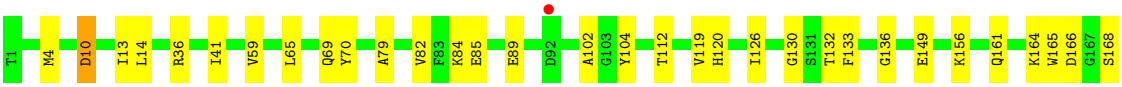
• Molecule 14: Proteasome component PRE3

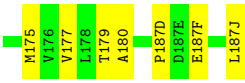
Chain N:



• Molecule 14: Proteasome component PRE3

Chain 2:




M175
V176
V177
L178
T179
A180
P187D
D187E
E187F
L187J

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.56Å 300.79Å 144.71Å 90.00° 112.73° 90.00°	Depositor
Resolution (Å)	50.00 – 3.11 47.61 – 3.11	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-3.11) 93.9 (47.61-3.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.250 0.200 , 0.244	Depositor DCC
R_{free} test set	3565 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	67.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 19.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49672	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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, LXT

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	0.41	0/1952	0.57	0/2642
1	O	0.44	0/1952	0.59	0/2642
2	B	0.42	0/1935	0.58	0/2618
2	P	0.43	0/1935	0.61	0/2618
3	C	0.45	2/1920 (0.1%)	0.59	0/2598
3	Q	0.45	0/1920	0.60	1/2598 (0.0%)
4	D	0.46	1/1887 (0.1%)	0.60	0/2541
4	R	0.44	0/1887	0.59	0/2541
5	E	0.40	0/1823	0.57	0/2463
5	S	0.42	0/1823	0.57	0/2463
6	F	0.41	0/1937	0.55	0/2614
6	T	0.44	0/1937	0.58	0/2614
7	G	0.43	0/1959	0.57	0/2652
7	U	0.45	0/1959	0.60	0/2652
8	H	0.43	0/1716	0.58	0/2326
8	V	0.42	0/1716	0.59	0/2326
9	I	0.42	0/1611	0.59	0/2174
9	W	0.44	0/1611	0.60	0/2174
10	J	0.42	0/1613	0.58	0/2173
10	X	0.42	0/1613	0.58	0/2173
11	K	0.43	0/1681	0.58	1/2274 (0.0%)
11	Y	0.43	0/1681	0.60	1/2274 (0.0%)
12	L	0.44	0/1795	0.57	0/2420
12	Z	0.47	0/1795	0.60	0/2420
13	1	0.44	0/1855	0.62	1/2514 (0.0%)
13	M	0.44	0/1855	0.61	0/2514
14	2	0.43	0/1541	0.59	0/2087
14	N	0.41	0/1541	0.55	0/2087
All	All	0.43	3/50450 (0.0%)	0.59	4/68192 (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
4	D	0	1
12	Z	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	123(G)	GLU	C-O	7.39	1.37	1.23
3	C	57	LYS	CE-NZ	6.06	1.64	1.49
3	C	203	THR	C-O	5.08	1.32	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	4	LEU	CA-CB-CG	5.38	127.68	115.30
11	K	4	LEU	CA-CB-CG	5.25	127.38	115.30
3	Q	56	LEU	CA-CB-CG	5.08	126.98	115.30
13	1	62	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	123(G)	GLU	Mainchain
1	O	217(N)	THR	Peptide
12	Z	145	TYR	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	1926	24	0
1	O	1915	0	1926	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1905	0	1901	32	0
2	P	1905	0	1901	36	0
3	C	1891	0	1900	30	0
3	Q	1891	0	1900	40	0
4	D	1862	0	1836	23	0
4	R	1862	0	1836	21	0
5	E	1795	0	1797	20	0
5	S	1795	0	1797	28	0
6	F	1897	0	1886	28	0
6	T	1897	0	1886	33	0
7	G	1921	0	1909	31	0
7	U	1921	0	1910	44	0
8	H	1685	0	1688	16	0
8	V	1685	0	1688	24	0
9	I	1581	0	1574	16	0
9	W	1581	0	1574	21	0
10	J	1585	0	1590	16	0
10	X	1585	0	1590	15	0
11	K	1644	0	1595	26	0
11	Y	1644	0	1595	29	0
12	L	1757	0	1711	31	0
12	Z	1757	0	1711	44	0
13	1	1824	0	1832	20	0
13	M	1824	0	1832	23	0
14	2	1512	0	1481	21	0
14	N	1512	0	1481	24	0
15	D	1	0	0	0	0
15	F	1	0	0	0	0
15	G	2	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	1	0	0	0	0
15	N	1	0	0	0	0
16	K	45	0	44	0	0
16	Y	45	0	44	4	0
17	K	12	0	13	0	0
17	Y	12	0	13	1	0
All	All	49672	0	49367	657	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (657) 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)
12:Z:144(O):LYS:HB3	12:Z:144(R):LYS:HZ3	1.01	1.13
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.06	0.96
12:Z:144(O):LYS:HB3	12:Z:144(R):LYS:NZ	1.81	0.95
3:C:163:GLN:HE21	3:C:164:THR:H	0.97	0.94
8:H:128:GLY:O	8:H:131:SER:HB2	1.69	0.93
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.34	0.92
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.33	0.92
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.33	0.90
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.35	0.89
11:Y:35:ILE:HG13	11:Y:45:MET:HE3	1.55	0.88
12:Z:144(O):LYS:CB	12:Z:144(R):LYS:HZ3	1.86	0.88
7:U:79:ASN:OD1	7:U:165:THR:HB	1.76	0.86
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.58	0.86
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.42	0.85
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.76	0.84
11:Y:35:ILE:HG13	11:Y:45:MET:CE	2.07	0.84
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.45	0.82
2:B:15:PHE:H	3:C:23:GLN:HE22	1.29	0.80
2:P:121:GLN:O	2:P:124:THR:HB	1.81	0.80
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.63	0.80
2:B:51:GLU:OE2	2:B:202:THR:HG23	1.82	0.80
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.27	0.79
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.64	0.79
3:C:163:GLN:HE21	3:C:164:THR:N	1.78	0.79
4:R:79:SER:HB3	4:R:165:ILE:HD12	1.64	0.79
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.48	0.78
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.64	0.78
8:H:90:TYR:O	8:H:93:GLY:N	2.18	0.76
2:B:202:THR:HG22	2:B:204:SER:H	1.49	0.76
12:L:18:THR:HG21	12:L:30:TYR:CD1	2.20	0.76
13:M:152:GLU:O	13:M:156:VAL:HG23	1.85	0.75
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.34	0.75
1:O:121:GLN:O	1:O:124:THR:HB	1.86	0.74
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.35	0.74
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.31	0.74
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.00	0.73
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.69	0.73
3:Q:185:THR:HB	3:Q:188:GLU:H	1.53	0.73
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.35	0.73
3:C:15:PHE:H	4:D:23:GLN:HE22	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.71	0.73
5:S:132:TYR:O	5:S:153:PRO:HB3	1.89	0.72
12:Z:144(P):PRO:O	12:Z:144(R):LYS:N	2.22	0.72
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.87	0.72
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.03	0.71
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.71	0.71
12:L:166:HIS:HD2	12:L:168:GLN:H	1.38	0.71
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.38	0.71
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.21	0.71
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.72	0.71
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.23	0.70
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.55	0.70
6:T:43:ASN:HD22	6:T:43:ASN:H	1.37	0.70
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.26	0.69
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.74	0.69
8:H:48:THR:HB	8:H:51:ASP:HB2	1.72	0.69
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.07	0.69
6:F:237:GLN:HE21	6:F:237:GLN:HA	1.57	0.69
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.75	0.68
6:T:192:GLN:HE21	6:T:192:GLN:HA	1.57	0.68
8:V:90:TYR:O	8:V:93:GLY:N	2.27	0.68
1:O:55:SER:O	1:O:56:SER:HB3	1.92	0.68
13:1:152:GLU:O	13:1:156:VAL:HG23	1.93	0.68
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.59	0.68
5:E:132:TYR:O	5:E:153:PRO:HB3	1.93	0.68
5:S:207:LEU:HD23	5:S:207:LEU:H	1.58	0.68
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.58	0.67
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.76	0.67
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.05	0.67
12:L:82:ASN:C	12:L:82:ASN:HD22	1.98	0.67
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.75	0.67
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.77	0.67
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.76	0.66
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.91	0.66
6:T:18:ASP:OD1	6:T:20:ARG:HD3	1.96	0.66
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.78	0.66
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.78	0.66
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.31	0.66
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.61	0.65
6:F:127:ASN:HD22	6:F:128:SER:N	1.94	0.65
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.78	0.65
11:K:105(B):LYS:H	11:K:105(B):LYS:HD2	1.60	0.65
10:J:112:GLN:HE22	10:J:126:ALA:H	1.46	0.64
6:F:78:TYR:HB3	6:F:136:THR:HG23	1.77	0.64
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.78	0.64
13:M:40:ASN:H	13:M:40:ASN:HD22	1.43	0.64
12:Z:144(O):LYS:HG2	12:Z:144(P):PRO:HD2	1.79	0.64
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.80	0.63
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.80	0.63
1:A:118:LYS:O	1:A:122:GLU:HG3	1.99	0.62
2:P:20:ARG:HE	3:Q:33:ARG:HH21	1.48	0.62
3:C:79:SER:HB2	3:C:165:ILE:HD12	1.81	0.62
6:F:36:THR:HB	6:F:168:GLY:H	1.64	0.62
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.64	0.62
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.63	0.62
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.29	0.62
10:X:143:ARG:O	10:X:146:MET:HG3	2.00	0.62
8:H:105:ASP:HB2	8:H:105(A):PRO:CD	2.29	0.62
6:F:127:ASN:HD22	6:F:127:ASN:C	2.03	0.62
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.30	0.61
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.81	0.61
5:S:56:ASP:HB3	5:S:58:LEU:H	1.65	0.61
12:Z:144(R):LYS:H	12:Z:144(R):LYS:CE	2.12	0.61
14:2:156:LYS:HE3	14:2:187(J):LEU:HD11	1.81	0.61
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.81	0.61
5:S:198:SER:HA	5:S:201:LEU:HD12	1.82	0.61
1:A:217(D):PRO:HA	1:A:217(P):LYS:O	2.00	0.61
1:A:217(B):ASN:C	1:A:217(E):ASP:H	2.04	0.61
2:P:181:LYS:O	2:P:184:MET:HG3	2.01	0.61
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.14	0.60
11:Y:35:ILE:HG22	11:Y:37:ILE:HG13	1.83	0.60
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.84	0.60
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.83	0.60
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.37	0.60
5:E:15:PHE:H	6:F:23:GLN:HE22	1.49	0.60
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.84	0.60
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.83	0.60
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.67	0.60
7:U:59:LEU:O	7:U:61:PRO:HD3	2.02	0.60
9:W:178:ILE:HA	9:W:184:VAL:HG22	1.84	0.60
10:J:11:SER:HB3	10:J:179:ASP:HB3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.83	0.60
11:Y:152:LEU:HD23	11:Y:175:LEU:HD22	1.83	0.60
3:C:185:THR:HB	3:C:188:GLU:H	1.67	0.59
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.83	0.59
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.84	0.59
2:P:55:THR:HG22	2:P:59:LEU:HD22	1.82	0.59
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.83	0.59
12:Z:-9:GLN:NE2	12:Z:-8:PHE:O	2.34	0.59
8:V:78:SER:O	8:V:82:MET:HG3	2.03	0.59
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.85	0.59
11:K:12:ILE:HB	11:K:178:VAL:HB	1.84	0.59
12:L:103:GLY:HA2	12:L:178:VAL:HG11	1.85	0.59
7:U:65:SER:HA	7:U:211:GLU:OE2	2.03	0.59
1:O:112:LEU:O	1:O:116:VAL:HG23	2.03	0.58
12:Z:18:THR:HG21	12:Z:30:TYR:CD1	2.37	0.58
1:O:86:ARG:HH21	7:U:118:ASN:ND2	1.99	0.58
11:Y:31:VAL:HG11	16:Y:212:LXT:H17	1.84	0.58
7:U:96:ALA:HA	7:U:107:MET:HE1	1.85	0.58
3:Q:76:LEU:HD22	3:Q:89:ILE:HG12	1.85	0.58
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.69	0.58
3:C:163:GLN:NE2	3:C:164:THR:H	1.82	0.58
3:C:185:THR:H	3:C:188:GLU:HG2	1.69	0.58
6:T:121:GLN:HE21	6:T:121:GLN:C	2.05	0.58
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.85	0.58
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.86	0.58
3:C:178:LYS:HB2	3:C:179:ASN:HD22	1.68	0.57
6:T:63:LYS:O	6:T:65:VAL:N	2.36	0.57
11:K:86:LEU:O	11:K:89:GLN:HB2	2.04	0.57
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.87	0.57
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	1.85	0.57
14:2:130:GLY:HA2	14:2:166:ASP:HB2	1.87	0.57
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.05	0.57
14:2:10:ASP:O	14:2:179:THR:HG22	2.04	0.57
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.39	0.56
7:U:147:SER:HB3	7:U:149:TYR:HE2	1.68	0.56
12:Z:83:ILE:HA	12:Z:86:LEU:HD12	1.87	0.56
14:2:14:LEU:O	14:2:175:MET:HA	2.05	0.56
9:I:130:ALA:HB2	9:I:166:ASP:CB	2.34	0.56
11:K:38:ASN:O	11:K:40:PHE:N	2.38	0.56
1:O:7:ARG:HH11	5:S:127:TYR:HD2	1.53	0.56
6:T:206(A):GLU:HG2	6:T:206(B):LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:121:GLN:O	7:U:124:THR:HB	2.05	0.56
6:F:35:THR:HG21	6:F:51:GLU:O	2.06	0.56
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.88	0.56
4:D:215:ILE:HG13	4:D:215:ILE:O	2.05	0.56
12:L:144(K):LYS:HD3	12:L:144(K):LYS:C	2.26	0.56
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.87	0.56
1:O:217(D):PRO:N	1:O:217(P):LYS:O	2.38	0.56
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.87	0.56
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.05	0.56
3:Q:215:VAL:HG12	3:Q:221:ILE:HG12	1.88	0.55
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	1.88	0.55
12:Z:144(J):ASN:CG	12:Z:144(K):GLY:N	2.60	0.55
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.53	0.55
9:W:181:LYS:NZ	9:W:181:LYS:HB3	2.21	0.55
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.53	0.55
4:R:175:GLU:O	4:R:179:GLU:HG2	2.07	0.55
8:V:18:THR:OG1	8:V:171:SER:HB2	2.06	0.55
1:O:108:PRO:HG2	1:O:111:LEU:HB2	1.88	0.55
11:Y:35:ILE:HG13	11:Y:45:MET:HE1	1.86	0.55
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.89	0.55
1:O:217(A):GLU:HB2	1:O:217(P):LYS:HB3	1.89	0.54
2:P:95:HIS:CE1	2:P:115:ARG:HD3	2.42	0.54
13:M:111:ARG:HH11	13:M:121:SER:HB2	1.72	0.54
11:Y:45:MET:CB	16:Y:212:LXT:H15	2.37	0.54
5:E:73:HIS:HE1	5:E:107:LEU:O	1.89	0.54
10:J:143:ARG:O	10:J:146:MET:HG3	2.07	0.54
11:K:67:GLU:HG2	11:K:73:ARG:HA	1.90	0.54
10:X:-1:MET:HG3	10:X:1:ASP:N	2.22	0.54
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.90	0.54
14:N:14:LEU:O	14:N:175:MET:HA	2.08	0.54
14:N:59:VAL:HG22	14:N:82:VAL:HG12	1.89	0.54
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.90	0.54
5:E:97:ASN:HD21	12:L:61:ASN:ND2	1.90	0.54
12:L:90:LYS:HE3	12:L:93:PHE:O	2.08	0.54
3:Q:156:ILE:HD11	4:R:82:THR:OG1	2.07	0.54
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.73	0.54
6:T:192:GLN:HA	6:T:192:GLN:NE2	2.23	0.54
10:X:162:LEU:O	10:X:166:MET:HB2	2.07	0.54
2:P:97:GLN:HB3	9:W:61:TYR:CD2	2.42	0.53
3:Q:163:GLN:HE21	3:Q:164:THR:N	2.05	0.53
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:45:ILE:HG12	13:1:99:ILE:HG12	1.90	0.53
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.90	0.53
7:G:34(A):ASN:ND2	7:G:167:PRO:HG2	2.24	0.53
9:W:126:VAL:HG11	9:W:134:LEU:HB3	1.89	0.53
4:D:159:ARG:HB3	5:E:60:SER:HB3	1.89	0.53
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.89	0.53
9:I:159:LEU:HD21	9:I:173:ALA:HB1	1.89	0.53
3:Q:57:LYS:HD3	3:Q:208:LYS:HZ3	1.73	0.53
12:Z:144:PHE:HB3	12:Z:144(R):LYS:HZ2	1.72	0.53
7:U:77:VAL:HG12	7:U:137:THR:HB	1.91	0.53
1:A:15:PHE:H	2:B:23:GLN:HE22	1.56	0.53
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.90	0.53
3:Q:52:ARG:HB2	3:Q:209:ASN:HD22	1.73	0.53
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.44	0.53
7:U:69:CYS:O	7:U:93:LYS:HE2	2.09	0.53
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.07	0.53
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.39	0.53
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.89	0.52
13:M:45:ILE:HG12	13:M:99:ILE:HG12	1.91	0.52
14:N:114:PRO:HD2	14:N:118:SER:O	2.09	0.52
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.92	0.52
1:O:67:VAL:HG11	1:O:213:ALA:HB2	1.91	0.52
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.92	0.52
2:B:87:ILE:O	2:B:91:THR:HG23	2.09	0.52
11:K:152:LEU:HD23	11:K:175:LEU:HD22	1.92	0.52
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.91	0.52
13:1:57:ARG:O	13:1:61:ASP:HB3	2.08	0.52
7:G:121:GLN:O	7:G:124:THR:HB	2.08	0.52
5:E:100:SER:O	5:E:104:ASN:HA	2.10	0.52
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.75	0.52
12:L:-2:ASN:HA	12:L:21:ILE:O	2.10	0.52
13:M:17:ASP:HA	13:M:173:PHE:CB	2.40	0.52
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.91	0.52
11:Y:1:THR:HB	17:Y:213:MES:O1S	2.09	0.52
11:Y:104:TYR:CD1	11:Y:180:GLU:HA	2.45	0.52
11:Y:45:MET:HB3	16:Y:212:LXT:H15	1.90	0.52
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.91	0.52
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.10	0.52
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.91	0.51
1:O:7:ARG:NH1	5:S:127:TYR:HD2	2.08	0.51
7:G:87:ASN:C	7:G:87:ASN:HD22	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:105:THR:OG1	11:K:106:GLU:HB2	2.11	0.51
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.93	0.51
7:G:47:VAL:HG11	7:G:190:VAL:HG22	1.92	0.51
12:L:135:MET:CE	9:W:165:ARG:NH2	2.74	0.51
7:U:96:ALA:HA	7:U:107:MET:CE	2.41	0.51
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.76	0.51
10:J:2:ILE:HD12	10:J:170:PHE:CD2	2.45	0.51
9:W:11:CYS:HA	9:W:104:ILE:HD11	1.91	0.51
14:N:176:VAL:HG12	14:N:178:LEU:CD1	2.41	0.51
2:P:122:GLY:C	2:P:124:THR:H	2.13	0.51
9:W:33:LYS:O	9:W:44:GLY:HA2	2.10	0.51
4:D:215:ILE:HG22	4:D:221:PHE:HD2	1.74	0.51
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.93	0.51
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.93	0.51
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.46	0.51
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.93	0.51
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.92	0.50
3:Q:206:GLY:HA2	3:Q:209:ASN:HB2	1.93	0.50
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.44	0.50
6:F:36:THR:HG22	6:F:51:GLU:OE2	2.11	0.50
2:P:181:LYS:HE2	2:P:183:ASP:OD1	2.12	0.50
4:R:79:SER:CB	4:R:165:ILE:HD12	2.40	0.50
7:G:79:ASN:OD1	7:G:165:THR:HB	2.11	0.50
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.93	0.50
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.15	0.50
6:T:35:THR:HG21	6:T:51:GLU:O	2.10	0.50
8:V:128:GLY:O	8:V:131:SER:HB2	2.10	0.50
12:Z:144(O):LYS:O	12:Z:144(R):LYS:HE2	2.11	0.50
9:I:15:ALA:HB1	9:I:159:LEU:HD22	1.93	0.50
11:K:44:THR:HG21	11:K:100:MET:HE3	1.93	0.50
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.46	0.50
5:S:73:HIS:HE1	5:S:107:LEU:O	1.95	0.50
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.93	0.50
4:R:85:ALA:O	4:R:89:ILE:HG12	2.12	0.50
7:U:87:ASN:C	7:U:87:ASN:HD22	2.15	0.50
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.60	0.50
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.77	0.50
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.93	0.50
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.94	0.50
1:O:217(K):GLY:HA3	8:V:186:TYR:HB3	1.94	0.50
11:Y:13:ILE:HD12	11:Y:152:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:ALA:O	3:C:100:ARG:HG3	2.12	0.49
5:E:41:ARG:NH1	5:E:42:SER:O	2.45	0.49
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.95	0.49
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.47	0.49
6:T:14:VAL:HG13	7:U:23:GLN:HE22	1.77	0.49
7:G:8:TYR:C	7:G:10:ARG:H	2.15	0.49
6:T:127:ASN:C	6:T:127:ASN:HD22	2.16	0.49
5:E:160:LEU:HD13	5:E:163:THR:HB	1.94	0.49
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.93	0.49
5:E:35:SER:O	5:E:66:LYS:NZ	2.43	0.49
13:M:26:LEU:HD12	14:2:164:LYS:O	2.12	0.49
8:V:84:LYS:NZ	8:V:119:THR:OG1	2.42	0.49
7:G:141:VAL:HA	7:G:146:PRO:HA	1.95	0.49
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.94	0.48
13:M:43:VAL:HG22	13:M:101:VAL:HG22	1.95	0.48
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.94	0.48
1:A:217(B):ASN:O	1:A:217(E):ASP:N	2.46	0.48
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.61	0.48
12:L:18:THR:HG22	12:L:31:GLU:H	1.78	0.48
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.95	0.48
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.13	0.48
6:T:43:ASN:HD22	6:T:43:ASN:N	2.10	0.48
7:U:87:ASN:C	7:U:87:ASN:ND2	2.66	0.48
1:O:8:TYR:CD2	7:U:128:TYR:HB3	2.48	0.48
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.11	0.48
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.49	0.48
7:U:49:ILE:HD13	7:U:193:ALA:HB1	1.96	0.48
12:Z:-9:GLN:HE21	12:Z:-8:PHE:N	2.12	0.48
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	1.95	0.48
4:D:85:ALA:O	4:D:89:ILE:HG12	2.14	0.48
6:F:42:CYS:HB2	6:F:184:LEU:O	2.12	0.48
7:G:150:LYS:HB3	7:G:160:TYR:HE1	1.78	0.48
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.28	0.48
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.93	0.48
3:Q:179:ASN:HB3	3:Q:192:LEU:HD11	1.95	0.48
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.78	0.48
2:B:150:THR:O	2:B:157:TYR:HA	2.14	0.48
13:M:5:SER:OG	13:M:110:LEU:HD11	2.14	0.48
7:U:166:GLY:O	7:U:169:GLN:HB2	2.12	0.48
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.95	0.48
11:Y:105(B):LYS:H	11:Y:105(B):LYS:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.13	0.48
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.12	0.48
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.96	0.48
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.44	0.48
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.48	0.48
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.96	0.48
6:T:52:LYS:HB2	6:T:209:GLU:O	2.14	0.48
12:Z:144:PHE:HB3	12:Z:144(R):LYS:NZ	2.28	0.48
11:K:196:PHE:CZ	11:K:209:VAL:HG21	2.49	0.47
4:R:224:TYR:N	4:R:224:TYR:CD2	2.81	0.47
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.96	0.47
8:H:207:PRO:O	8:H:210:THR:OG1	2.31	0.47
8:V:41:ILE:HG12	8:V:76:VAL:HG22	1.96	0.47
2:B:40:ILE:HD12	2:B:193:ALA:HB2	1.96	0.47
6:F:122:ALA:HA	6:F:125:LEU:HD12	1.95	0.47
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.29	0.47
4:R:125:GLU:HG2	4:R:127:LEU:HD13	1.97	0.47
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.96	0.47
6:T:63:LYS:O	6:T:65:VAL:HG23	2.15	0.47
7:U:147:SER:HB3	7:U:149:TYR:CE2	2.48	0.47
6:F:180(F):GLY:O	6:F:184:LEU:CB	2.61	0.47
8:H:77:VAL:HG12	13:1:208:THR:HG22	1.96	0.47
10:X:52:THR:HG23	10:X:53:VAL:N	2.30	0.47
10:J:36:GLN:HG3	10:J:184:ILE:HD13	1.96	0.47
11:K:160:LEU:CD1	11:K:192:VAL:HG13	2.45	0.47
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.96	0.47
11:Y:1:THR:HG23	11:Y:33:LYS:NZ	2.30	0.47
2:B:97:GLN:NE2	2:B:97:GLN:HA	2.29	0.47
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.95	0.47
13:M:113:VAL:HA	13:M:118:VAL:O	2.15	0.47
4:R:224:TYR:N	4:R:224:TYR:HD2	2.13	0.47
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.45	0.47
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.96	0.47
1:A:121:GLN:O	1:A:124:THR:HB	2.14	0.47
13:M:165:ARG:CZ	8:V:135:MET:HE2	2.44	0.47
14:N:105:ASP:HB3	14:N:106:ASN:HB2	1.97	0.47
2:P:138:TYR:HB2	2:P:149:TYR:HB2	1.96	0.47
8:V:172:ASN:ND2	8:V:193:THR:HA	2.30	0.47
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.97	0.47
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.50	0.47
4:R:90:GLU:OE1	11:Y:69:ARG:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:THR:HG21	10:X:167:PRO:HB3	1.97	0.47
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.49	0.47
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.50	0.46
1:O:217(A):GLU:CB	1:O:217(P):LYS:HB3	2.45	0.46
2:P:150:THR:O	2:P:157:TYR:HA	2.15	0.46
12:Z:114:ASP:HB2	12:Z:115:PRO:HD2	1.96	0.46
3:C:227:GLU:H	3:C:227:GLU:CD	2.16	0.46
6:F:79:SER:HB2	6:F:165:THR:HG23	1.97	0.46
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.97	0.46
10:J:162:LEU:O	10:J:166:MET:HB2	2.15	0.46
4:R:70:ILE:HB	4:R:74:ILE:HG22	1.96	0.46
12:Z:80:ALA:HA	12:Z:113:PHE:HZ	1.79	0.46
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.60	0.46
3:C:150:GLN:O	3:C:157:TYR:HA	2.15	0.46
6:F:180(F):GLY:O	6:F:184:LEU:HB3	2.15	0.46
12:L:98:HIS:HD2	12:L:127:GLY:HA3	1.80	0.46
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.45	0.46
7:U:186:TRP:O	7:U:190:VAL:HG23	2.15	0.46
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.45	0.46
1:O:8:TYR:HD2	7:U:128:TYR:HB3	1.80	0.46
2:B:169:THR:O	2:B:173:GLN:HB2	2.15	0.46
3:Q:55:THR:HB	3:Q:56:LEU:HD22	1.98	0.46
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.97	0.46
5:S:52:LYS:O	5:S:63:TYR:HD2	1.99	0.46
8:V:162:GLY:O	8:V:166:ASP:HB3	2.16	0.46
9:W:2:ILE:HD11	9:W:163:ALA:HB2	1.97	0.46
5:E:85:ALA:HB2	5:E:134:VAL:HG21	1.97	0.46
7:G:74:ILE:HG21	7:G:112:LEU:HD23	1.98	0.46
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.98	0.46
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.97	0.46
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.83	0.46
5:E:207:LEU:HD23	5:E:207:LEU:H	1.81	0.46
10:J:1:ASP:HB2	10:J:46:ALA:HB1	1.97	0.46
11:K:166:ASP:OD1	11:K:169:SER:OG	2.27	0.46
12:L:165:ARG:HH21	8:V:29:LYS:HE2	1.81	0.46
4:R:215:ILE:HG13	4:R:215:ILE:O	2.15	0.46
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.97	0.46
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.98	0.46
14:N:8:PHE:HB2	14:N:146:MET:O	2.16	0.46
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.96	0.45
5:S:179:THR:HG22	5:S:180(B):THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.98	0.45
12:L:4:LEU:HD11	12:L:138:LEU:CD2	2.41	0.45
5:S:226:GLY:O	5:S:229:VAL:HG22	2.16	0.45
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.98	0.45
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.80	0.45
14:N:132:THR:O	14:2:133:PHE:HA	2.17	0.45
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.16	0.45
5:S:160:LEU:HD13	5:S:163:THR:HB	1.98	0.45
10:X:52:THR:CG2	10:X:53:VAL:H	2.29	0.45
10:X:113:ILE:HA	10:X:118:THR:O	2.16	0.45
2:P:137:ILE:HD11	2:P:165:VAL:HG22	1.98	0.45
12:Z:144:PHE:CB	12:Z:144(R):LYS:HZ2	2.29	0.45
2:P:216:ARG:HB3	2:P:216(A):LYS:H	1.48	0.45
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.97	0.45
1:A:112:LEU:O	1:A:116:VAL:HG23	2.17	0.45
10:J:163:GLU:O	10:X:171:LYS:NZ	2.49	0.45
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.47	0.45
2:P:173:GLN:HG2	3:Q:56:LEU:HD12	1.99	0.45
3:Q:57:LYS:HA	3:Q:57:LYS:HD2	1.72	0.45
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.99	0.45
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.17	0.45
14:N:67:THR:HA	14:N:72:GLY:O	2.17	0.45
3:Q:120:GLN:O	3:Q:124:THR:HG23	2.16	0.45
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.98	0.45
5:S:85:ALA:HB2	5:S:134:VAL:HG21	1.99	0.45
6:T:127:ASN:C	6:T:127:ASN:ND2	2.70	0.45
6:T:218(B):THR:O	6:T:218(C):ASN:HB2	2.16	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.98	0.45
12:Z:87:LEU:HD23	12:Z:95:TYR:HD1	1.82	0.45
3:C:35:THR:HB	3:C:51:GLU:HG3	1.99	0.45
6:T:12:ASN:HB3	6:T:127:ASN:HA	1.98	0.45
6:F:24:VAL:O	6:F:28:VAL:HG23	2.17	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.99	0.45
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.65	0.45
6:F:173:LYS:O	6:F:177:GLU:HG3	2.17	0.44
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.17	0.44
12:L:19:ARG:HG2	12:L:21:ILE:HG23	1.99	0.44
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	1.99	0.44
12:Z:40:ASN:ND2	12:Z:183:GLY:HA2	2.32	0.44
7:G:158:VAL:HG22	7:G:159:GLY:N	2.33	0.44
12:Z:7:ALA:O	12:Z:145:TYR:OH	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:17:ASP:O	12:Z:33:LYS:HE2	2.17	0.44
6:F:52:LYS:HB2	6:F:209:GLU:O	2.17	0.44
8:H:90:TYR:O	8:H:91:GLN:C	2.56	0.44
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.48	0.44
13:1:71:ASP:HA	13:1:73:ALA:HB2	2.00	0.44
13:M:165:ARG:NH1	8:V:135:MET:HE3	2.32	0.44
2:P:4:GLY:HA2	6:T:127:ASN:ND2	2.32	0.44
6:T:36:THR:HA	6:T:166:GLY:HA3	2.00	0.44
6:T:136:THR:O	6:T:150:MET:HA	2.18	0.44
11:Y:100:MET:HA	11:Y:111:TYR:O	2.18	0.44
1:A:217(B):ASN:C	1:A:217(E):ASP:N	2.68	0.44
7:G:36:ASN:HB2	7:G:51:GLN:OE1	2.17	0.44
7:G:69:CYS:O	7:G:93:LYS:HE2	2.18	0.44
7:G:107:MET:HA	7:G:108:PRO:HD3	1.89	0.44
12:L:82:ASN:C	12:L:82:ASN:ND2	2.70	0.44
6:T:169:ARG:HE	6:T:169:ARG:HB3	1.43	0.44
7:U:239:GLN:HE21	7:U:239:GLN:HB3	1.59	0.44
11:K:105(B):LYS:H	11:K:105(B):LYS:CD	2.29	0.44
2:P:21:LEU:O	2:P:22:TYR:C	2.55	0.44
12:Z:144(P):PRO:O	12:Z:144(R):LYS:HD3	2.18	0.44
6:F:35:THR:HG23	6:F:51:GLU:HB3	2.00	0.44
9:I:90:ARG:HH11	9:I:90:ARG:HA	1.82	0.44
7:U:82:ILE:N	7:U:83:PRO:HD2	2.32	0.44
13:1:40:ASN:H	13:1:40:ASN:HD22	1.66	0.44
3:C:160:TRP:CZ2	4:D:59:LEU:HD23	2.53	0.44
5:E:207:LEU:HD12	5:E:210:LEU:HD13	2.00	0.44
11:K:114:ASP:OD1	11:K:116:ASP:HB2	2.18	0.44
10:X:52:THR:CG2	10:X:53:VAL:N	2.81	0.44
2:P:44:ASP:OD1	2:P:185:LYS:HD3	2.18	0.43
8:V:6:VAL:HG11	8:V:154:LEU:HD23	2.00	0.43
3:C:178:LYS:HB2	3:C:179:ASN:ND2	2.32	0.43
9:I:1:GLY:HA3	9:I:33:LYS:HE2	2.00	0.43
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	2.00	0.43
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.52	0.43
6:F:57:LYS:HD3	6:F:57:LYS:HA	1.86	0.43
6:F:150:MET:O	6:F:157:TYR:HA	2.19	0.43
13:M:8:TYR:HE2	13:M:10:ASN:HB2	1.82	0.43
14:N:152:VAL:O	14:N:156:LYS:HB2	2.18	0.43
2:P:202:THR:HG22	2:P:204:SER:H	1.82	0.43
7:U:78:VAL:HG11	7:U:85:ALA:HB2	2.00	0.43
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:126:VAL:CG1	9:W:134:LEU:HB3	2.49	0.43
13:M:19:LEU:HD11	13:M:26:LEU:HB3	2.01	0.43
2:P:156:ASN:HD22	2:P:157:TYR:H	1.66	0.43
3:Q:152:GLU:HB2	3:Q:153:PRO:CD	2.49	0.43
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.99	0.43
2:B:73:LYS:O	2:B:140:GLY:HA2	2.19	0.43
5:E:4:PHE:CD2	5:E:5:ARG:HG3	2.54	0.43
2:P:81:LEU:HD23	2:P:133:GLY:HA3	2.01	0.43
3:Q:141:PHE:HE1	3:Q:144(A):ASP:O	2.02	0.43
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.81	0.43
1:A:71:THR:HB	1:A:72:PRO:HD2	1.99	0.43
2:B:160:TRP:CE3	2:B:163:ILE:HD13	2.54	0.43
9:I:2:ILE:HD11	9:I:163:ALA:HB2	2.01	0.43
1:O:150:GLN:O	1:O:157:TYR:HA	2.18	0.43
6:T:206(A):GLU:CD	6:T:206(A):GLU:H	2.21	0.43
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.83	0.43
9:I:143:GLU:HG3	9:I:146:LEU:HD21	2.00	0.43
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.99	0.43
9:W:61:TYR:CD1	9:W:61:TYR:C	2.92	0.43
12:Z:144(R):LYS:H	12:Z:144(R):LYS:HE3	1.82	0.43
2:B:32:SER:O	2:B:167:ALA:HA	2.19	0.43
4:R:156:THR:HG23	5:S:83:PRO:HD3	2.01	0.43
5:S:104:ASN:HB2	13:1:81:GLU:HG2	2.00	0.43
13:1:84:ALA:HA	13:1:113:VAL:HG21	2.01	0.43
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.83	0.43
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.83	0.43
14:N:113:ILE:HG12	14:N:119:VAL:HG13	2.00	0.43
7:U:13:THR:HB	7:U:124:THR:O	2.18	0.43
11:Y:174:ASN:ND2	11:Y:186:TYR:OH	2.52	0.43
12:Z:1:GLY:HA3	12:Z:33:LYS:HE3	2.01	0.43
13:M:165:ARG:NH1	8:V:135:MET:CE	2.82	0.43
5:S:15:PHE:H	6:T:23:GLN:HE22	1.67	0.43
8:V:51:ASP:HB3	8:V:95:ILE:HG23	2.01	0.43
12:Z:114:ASP:OD2	12:Z:114:ASP:C	2.58	0.43
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.49	0.42
4:D:123(G):GLU:HB3	4:D:125:GLU:H	1.41	0.42
2:P:216(B):GLY:O	2:P:218(B):ASP:HB2	2.19	0.42
4:D:127:LEU:O	4:D:128:MET:HB2	2.19	0.42
14:N:85:GLU:O	14:N:89:GLU:HB2	2.19	0.42
2:P:149:TYR:CZ	3:Q:62(A):ILE:HD12	2.54	0.42
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:121:GLN:C	6:T:121:GLN:NE2	2.72	0.42
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.48	0.42
1:A:217(A):GLU:HB2	1:A:217(P):LYS:HB3	2.01	0.42
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.49	0.42
9:I:48:LEU:HG	9:I:50:THR:HG22	2.01	0.42
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.54	0.42
11:Y:143:LYS:HB3	11:Y:146:LEU:HD13	2.00	0.42
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.54	0.42
14:N:133:PHE:HA	14:2:132:THR:O	2.19	0.42
5:S:198:SER:C	5:S:200:SER:H	2.22	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	2.01	0.42
12:Z:43:MET:HG3	12:Z:101:ILE:HG22	2.00	0.42
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.55	0.42
6:F:91:ARG:HG2	6:F:119:TYR:CD2	2.54	0.42
3:Q:175:PHE:O	3:Q:179:ASN:ND2	2.49	0.42
6:T:159:GLY:HA3	7:U:63:THR:HG21	2.00	0.42
7:G:96:ALA:HA	7:G:107:MET:CE	2.50	0.42
8:H:8:PHE:HB2	8:H:146:LEU:O	2.19	0.42
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.85	0.42
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.55	0.42
4:D:175:GLU:HG2	4:D:196:ILE:HG12	2.02	0.42
6:F:169:ARG:HE	6:F:169:ARG:HB3	1.55	0.42
2:B:121:GLN:O	2:B:124:THR:HB	2.20	0.42
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.54	0.42
13:1:58:LEU:O	13:1:62:LEU:HB2	2.20	0.42
10:J:17:SER:HB2	10:J:170:PHE:HB2	2.00	0.42
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.54	0.42
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.33	0.42
4:R:192:LEU:O	4:R:196:ILE:HG13	2.19	0.42
2:B:197:LEU:O	2:B:202:THR:OG1	2.37	0.42
7:G:207:LYS:HG3	7:G:208:ASN:OD1	2.20	0.42
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.85	0.42
5:S:35:SER:HB2	5:S:53:ARG:HB2	2.02	0.42
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.49	0.41
9:W:14:ILE:HG23	9:W:34:ILE:HD13	2.02	0.41
14:2:112:THR:HG22	14:2:120:HIS:HB2	2.01	0.41
1:A:124:THR:O	1:A:124:THR:CG2	2.68	0.41
3:C:170:LYS:O	3:C:174:GLU:HB2	2.20	0.41
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.81	0.41
12:L:144(G):GLY:C	12:L:144(I):ASN:H	2.24	0.41
13:M:3:VAL:HG23	13:M:46:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG22	1:A:78:TYR:H	1.86	0.41
1:A:109:THR:O	1:A:113:VAL:HG23	2.21	0.41
1:A:187:GLU:HA	1:A:190:ILE:HD12	2.02	0.41
1:O:52:LYS:HG3	1:O:211:GLU:HB2	2.01	0.41
10:X:166:MET:HA	10:X:167:PRO:HD3	1.94	0.41
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.55	0.41
9:I:2:ILE:HG21	9:I:130:ALA:HB3	2.02	0.41
5:S:104:ASN:HD22	5:S:104:ASN:HA	1.70	0.41
14:2:85:GLU:O	14:2:89:GLU:HB2	2.21	0.41
7:G:87:ASN:C	7:G:87:ASN:ND2	2.73	0.41
7:G:198:ILE:HG23	7:G:203:THR:O	2.21	0.41
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.50	0.41
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.02	0.41
11:Y:113:VAL:HA	11:Y:118:THR:O	2.20	0.41
12:Z:144(P):PRO:C	12:Z:144(R):LYS:HE2	2.41	0.41
6:F:180(C):HIS:C	6:F:180(E):GLU:H	2.23	0.41
7:U:67:ILE:HD12	7:U:211:GLU:HG2	2.02	0.41
11:Y:200:LYS:HG3	11:Y:205:SER:O	2.21	0.41
9:I:126:VAL:HG11	9:I:134:LEU:HB3	2.02	0.41
10:J:141:HIS:HB2	10:J:154:LEU:HD11	2.03	0.41
11:K:147:SER:OG	11:K:150:ASP:HB2	2.21	0.41
3:Q:150:GLN:HE21	3:Q:150:GLN:HB3	1.64	0.41
6:T:14:VAL:HG13	7:U:23:GLN:NE2	2.36	0.41
10:X:143:ARG:HA	10:X:144:PRO:HD3	1.96	0.41
12:Z:144(R):LYS:H	12:Z:144(R):LYS:CD	2.32	0.41
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	2.02	0.41
14:2:14:LEU:HD11	14:2:102:ALA:HB3	2.02	0.41
2:B:108:PRO:HB2	2:B:111:ILE:HD12	2.03	0.41
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.56	0.41
5:S:149:LEU:HD12	5:S:159:GLU:HG3	2.03	0.41
7:U:136:LEU:O	7:U:150:LYS:HA	2.21	0.41
8:V:211:THR:HG21	9:W:156:SER:HB3	2.03	0.41
1:A:150:GLN:O	1:A:157:TYR:HA	2.20	0.41
2:B:88:LEU:HB3	2:B:116:LEU:HD21	2.02	0.41
5:E:150:GLU:O	5:E:157:VAL:HA	2.21	0.41
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.56	0.41
8:H:1:THR:O	8:H:128:GLY:HA3	2.20	0.41
10:J:90(A):ILE:HD12	10:J:90(A):ILE:HA	1.97	0.41
2:P:148:LEU:HB3	2:P:160:TRP:O	2.21	0.41
5:S:121:GLN:OE1	5:S:125:GLN:NE2	2.54	0.41
7:U:39:ALA:HB2	7:U:48:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:158:VAL:HG22	7:U:159:GLY:N	2.36	0.41
9:W:48:LEU:HG	9:W:50:THR:HG22	2.03	0.41
11:Y:36:GLU:HG2	11:Y:184:TRP:CZ2	2.56	0.41
11:Y:45:MET:HB2	16:Y:212:LXT:H15	2.02	0.41
2:B:199:LYS:HB3	2:B:199:LYS:HE2	1.72	0.41
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.86	0.41
9:I:19:ARG:NH1	9:I:21:GLY:HA3	2.35	0.41
11:K:86:LEU:C	11:K:86:LEU:HD13	2.41	0.41
13:M:111:ARG:NH1	13:M:121:SER:HB2	2.36	0.41
13:1:161:VAL:O	13:1:164:TYR:HB2	2.21	0.41
4:D:173:GLN:HA	4:D:176:LEU:HD12	2.01	0.40
4:D:179:GLU:CB	4:D:192:LEU:HD21	2.50	0.40
5:E:95:GLN:HG3	5:E:115:LEU:HD13	2.02	0.40
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.57	0.40
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	2.04	0.40
6:T:186:ALA:O	6:T:190:VAL:HG23	2.22	0.40
12:Z:144(N):LYS:O	12:Z:144(O):LYS:C	2.58	0.40
2:B:216:ARG:HB3	2:B:216(A):LYS:H	1.58	0.40
3:C:215:VAL:HG12	3:C:221:ILE:HG12	2.02	0.40
8:H:81:GLN:HG3	8:H:85:GLN:NE2	2.37	0.40
13:1:1:THR:OG1	13:1:2:SER:N	2.54	0.40
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.87	0.40
1:A:222:ARG:HE	1:A:222:ARG:HB3	1.65	0.40
2:B:101:LYS:HG2	10:J:85:GLN:HE22	1.86	0.40
7:G:31:THR:HG21	7:G:135:ILE:HG13	2.02	0.40
7:G:72:ARG:NH2	14:N:39:ASP:OD2	2.54	0.40
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.02	0.40
14:N:17:ASP:CG	14:N:33:LYS:HZ2	2.24	0.40
4:D:194:LEU:HD12	4:D:194:LEU:HA	1.96	0.40
11:K:137:VAL:HG21	11:K:161:ALA:CB	2.52	0.40
14:N:143:ARG:O	14:N:146:MET:HG3	2.21	0.40
1:O:62:GLU:C	1:O:64:LEU:H	2.24	0.40
5:S:93:ARG:O	5:S:97:ASN:HB2	2.22	0.40
9:W:95:TYR:O	9:W:115:LEU:HB2	2.22	0.40
13:1:131:ALA:HA	13:1:135:ASN:HD22	1.86	0.40
14:2:41:ILE:HD13	14:2:79:ALA:HB2	2.03	0.40
2:B:21:LEU:O	2:B:25:GLU:HG2	2.22	0.40
6:F:120:VAL:HG21	6:F:151:LEU:HD21	2.03	0.40
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.04	0.40
7:U:81:PRO:HD2	7:U:133:GLY:O	2.22	0.40
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:144:PHE:CB	12:Z:144(R):LYS:NZ	2.85	0.40
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	233 (94%)	12 (5%)	3 (1%)	13	43
1	O	248/250 (99%)	230 (93%)	15 (6%)	3 (1%)	13	43
2	B	242/244 (99%)	218 (90%)	22 (9%)	2 (1%)	19	53
2	P	242/244 (99%)	217 (90%)	19 (8%)	6 (2%)	5	26
3	C	239/241 (99%)	232 (97%)	5 (2%)	2 (1%)	19	53
3	Q	239/241 (99%)	223 (93%)	11 (5%)	5 (2%)	7	29
4	D	240/242 (99%)	224 (93%)	13 (5%)	3 (1%)	12	41
4	R	240/242 (99%)	220 (92%)	19 (8%)	1 (0%)	34	68
5	E	231/233 (99%)	218 (94%)	10 (4%)	3 (1%)	12	41
5	S	231/233 (99%)	213 (92%)	13 (6%)	5 (2%)	6	28
6	F	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	34	68
6	T	242/244 (99%)	226 (93%)	14 (6%)	2 (1%)	19	53
7	G	241/243 (99%)	229 (95%)	11 (5%)	1 (0%)	34	68
7	U	241/243 (99%)	227 (94%)	13 (5%)	1 (0%)	34	68
8	H	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	29	63
8	V	220/222 (99%)	207 (94%)	11 (5%)	2 (1%)	17	51
9	I	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	29	63
9	W	202/204 (99%)	191 (95%)	10 (5%)	1 (0%)	29	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	196/198 (99%)	183 (93%)	10 (5%)	3 (2%)	10	38
10	X	196/198 (99%)	181 (92%)	10 (5%)	5 (3%)	5	25
11	K	210/212 (99%)	199 (95%)	9 (4%)	2 (1%)	15	48
11	Y	210/212 (99%)	199 (95%)	8 (4%)	3 (1%)	11	39
12	L	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	63
12	Z	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	17	51
13	1	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	34	68
13	M	231/233 (99%)	218 (94%)	12 (5%)	1 (0%)	34	68
14	2	194/196 (99%)	185 (95%)	8 (4%)	1 (0%)	29	63
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6312/6368 (99%)	5916 (94%)	334 (5%)	62 (1%)	15	48

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
4	D	123(G)	GLU
5	E	5	ARG
5	E	203	ASP
5	E	217	LYS
6	F	184	LEU
7	G	239	GLN
8	H	91	GLN
10	J	8	VAL
10	J	49	ALA
11	K	39	PRO
2	P	216(B)	GLY
8	V	91	GLN
9	W	181	LYS
10	X	1	ASP
10	X	49	ALA
11	Y	208	ASN
12	Z	144(Q)	LEU
1	A	6	ASP
3	C	203	THR
4	D	128	MET
2	P	54	VAL
2	P	204(A)	SER

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Mol	Chain	Res	Type
3	Q	183	PRO
5	S	5	ARG
5	S	199	GLN
6	T	64	ASN
11	Y	39	PRO
1	A	5	THR
11	K	71	LYS
10	X	39	PRO
2	B	54	VAL
3	C	202	GLN
12	L	144(P)	LEU
1	O	5	THR
1	O	56	SER
2	P	123	TYR
3	Q	184	ALA
3	Q	226	SER
5	S	203	ASP
11	Y	146	LEU
2	B	11	ARG
4	D	123(F)	GLY
2	P	216(A)	LYS
2	P	218(B)	ASP
3	Q	202	GLN
4	R	128	MET
7	U	239	GLN
8	V	171	SER
10	X	23	GLY
13	1	72	ALA
5	S	153	PRO
1	O	217(L)	ILE
3	Q	64	PRO
13	M	207	GLY
10	X	8	VAL
5	S	186	PRO
12	Z	144(F)	PRO
10	J	39	PRO
6	T	226	GLY
14	2	187(D)	PRO
9	I	93	GLY

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%)	198 (95%)	11 (5%)	22	53
1	O	209/209 (100%)	199 (95%)	10 (5%)	25	57
2	B	203/203 (100%)	179 (88%)	24 (12%)	5	21
2	P	203/203 (100%)	186 (92%)	17 (8%)	11	37
3	C	213/213 (100%)	200 (94%)	13 (6%)	18	49
3	Q	213/213 (100%)	193 (91%)	20 (9%)	8	32
4	D	198/198 (100%)	185 (93%)	13 (7%)	16	46
4	R	198/198 (100%)	179 (90%)	19 (10%)	8	30
5	E	192/192 (100%)	176 (92%)	16 (8%)	11	37
5	S	192/192 (100%)	171 (89%)	21 (11%)	6	25
6	F	201/201 (100%)	180 (90%)	21 (10%)	7	26
6	T	201/201 (100%)	183 (91%)	18 (9%)	9	33
7	G	207/207 (100%)	188 (91%)	19 (9%)	9	32
7	U	207/207 (100%)	193 (93%)	14 (7%)	16	45
8	H	181/181 (100%)	175 (97%)	6 (3%)	38	68
8	V	181/181 (100%)	170 (94%)	11 (6%)	18	49
9	I	172/172 (100%)	166 (96%)	6 (4%)	36	67
9	W	172/172 (100%)	164 (95%)	8 (5%)	26	58
10	J	175/175 (100%)	163 (93%)	12 (7%)	15	44
10	X	175/175 (100%)	166 (95%)	9 (5%)	24	55
11	K	169/169 (100%)	158 (94%)	11 (6%)	17	47
11	Y	169/169 (100%)	159 (94%)	10 (6%)	19	50
12	L	185/185 (100%)	175 (95%)	10 (5%)	22	53
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	47
13	1	199/199 (100%)	184 (92%)	15 (8%)	13	41
13	M	199/199 (100%)	187 (94%)	12 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2	162/162 (100%)	154 (95%)	8 (5%)	25	57
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	75
All	All	5332/5332 (100%)	4962 (93%)	370 (7%)	15	44

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	32	LYS
1	A	33	GLN
1	A	35	VAL
1	A	65	SER
1	A	95	VAL
1	A	114	SER
1	A	158	PHE
1	A	170	VAL
1	A	217(P)	LYS
1	A	222	ARG
2	B	10	SER
2	B	57	THR
2	B	58	LEU
2	B	61	GLN
2	B	63	THR
2	B	67	LEU
2	B	73	LYS
2	B	104	ASN
2	B	110	GLU
2	B	116	LEU
2	B	121	GLN
2	B	124	THR
2	B	150	THR
2	B	156	ASN
2	B	170	SER
2	B	185	LYS
2	B	192	LEU
2	B	204(A)	SER
2	B	206	THR
2	B	216	ARG
2	B	219(E)	VAL
2	B	225	LYS
2	B	232	ILE

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Mol	Chain	Res	Type
2	B	238	ILE
3	C	10	ARG
3	C	28	LEU
3	C	33	ARG
3	C	54	SER
3	C	66	LYS
3	C	82	ASN
3	C	112	LEU
3	C	150	GLN
3	C	156	ILE
3	C	165	ILE
3	C	172	VAL
3	C	185	THR
3	C	208	LYS
4	D	12	VAL
4	D	13	SER
4	D	20	ARG
4	D	28	LEU
4	D	48	LEU
4	D	76	CYS
4	D	125	GLU
4	D	156	THR
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	18	THR
5	E	28	LEU
5	E	64	GLN
5	E	76	LEU
5	E	121	GLN
5	E	174	THR
5	E	178	ARG
5	E	180(C)	PHE
5	E	185	ASN
5	E	189	LEU
5	E	207	LEU
5	E	207(D)	ASP
5	E	218	ASP
5	E	219	THR

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Mol	Chain	Res	Type
5	E	231	LYS
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	44	ASP
6	F	46	VAL
6	F	55	THR
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	135	SER
6	F	136	THR
6	F	167	LYS
6	F	169	ARG
6	F	187	ARG
6	F	188	GLU
6	F	192	GLN
6	F	206	LYS
6	F	214	TRP
6	F	222	LYS
6	F	237	GLN
7	G	13	THR
7	G	33	GLN
7	G	40	VAL
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	151	THR
7	G	157	TYR
7	G	165	THR
7	G	169	GLN
7	G	174	THR
7	G	179(C)	LYS
7	G	197	MET
7	G	203	THR
7	G	204	GLU
7	G	232	ARG
7	G	233	LEU
7	G	239	GLN
8	H	22	GLN

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Mol	Chain	Res	Type
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	77	VAL
8	H	192	LEU
9	I	107	LYS
9	I	122(A)	LYS
9	I	160	LEU
9	I	174	VAL
9	I	181	LYS
9	I	182	ASP
10	J	4	LEU
10	J	6	ILE
10	J	9	GLN
10	J	34	THR
10	J	62	ASN
10	J	68	ILE
10	J	70	GLU
10	J	105(B)	LYS
10	J	115	TYR
10	J	130	SER
10	J	155	LEU
10	J	160	GLN
11	K	4	LEU
11	K	9	GLN
11	K	29	GLN
11	K	32	LYS
11	K	71	LYS
11	K	73	ARG
11	K	87	VAL
11	K	105(B)	LYS
11	K	109	THR
11	K	118	THR
11	K	135	TYR
12	L	-9	GLN
12	L	14	LEU
12	L	18	THR
12	L	40	ASN
12	L	62	SER
12	L	82	ASN
12	L	99	THR
12	L	144(A)	LYS

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Mol	Chain	Res	Type
12	L	145	TYR
12	L	182	ASP
13	M	2	SER
13	M	21	SER
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	121	SER
13	M	129	PHE
13	M	141(A)	VAL
13	M	141(C)	ARG
13	M	146	THR
13	M	181(A)	THR
13	M	204	LYS
14	N	84	LYS
14	N	105(B)	LYS
14	N	119	VAL
14	N	149	GLU
1	O	4	MET
1	O	29	THR
1	O	33	GLN
1	O	64	LEU
1	O	65	SER
1	O	158	PHE
1	O	165	ILE
1	O	200	SER
1	O	217(P)	LYS
1	O	222	ARG
2	P	58	LEU
2	P	59	LEU
2	P	63	THR
2	P	64	THR
2	P	116	LEU
2	P	121	GLN
2	P	150	THR
2	P	156	ASN
2	P	183	ASP
2	P	185	LYS
2	P	187	ASP
2	P	192	LEU
2	P	202	THR
2	P	206	THR

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Mol	Chain	Res	Type
2	P	212	PHE
2	P	225	LYS
2	P	238	ILE
3	Q	10	ARG
3	Q	33	ARG
3	Q	35	THR
3	Q	43	LYS
3	Q	54	SER
3	Q	56	LEU
3	Q	57	LYS
3	Q	66	LYS
3	Q	82	ASN
3	Q	121	GLN
3	Q	124	THR
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	174	GLU
3	Q	188	GLU
3	Q	208	LYS
3	Q	224	LEU
3	Q	229	ILE
3	Q	235	GLN
4	R	9	ASP
4	R	10	ARG
4	R	12	VAL
4	R	13	SER
4	R	14	THR
4	R	28	LEU
4	R	52	LYS
4	R	61	SER
4	R	86	ARG
4	R	122	ARG
4	R	123(E)	SER
4	R	123(G)	GLU
4	R	125	GLU
4	R	156	THR
4	R	177	LEU
4	R	194	LEU
4	R	215	ILE
4	R	224	TYR
4	R	237	LEU

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Mol	Chain	Res	Type
5	S	12	THR
5	S	13	VAL
5	S	18	THR
5	S	28	LEU
5	S	56	ASP
5	S	58	LEU
5	S	76	LEU
5	S	104	ASN
5	S	121	GLN
5	S	143	LYS
5	S	178	ARG
5	S	179	THR
5	S	185	ASN
5	S	187	ASP
5	S	189	LEU
5	S	207	LEU
5	S	208(B)	ASP
5	S	211	SER
5	S	212	ILE
5	S	222	THR
5	S	231	LYS
6	T	11	SER
6	T	36	THR
6	T	43	ASN
6	T	44	ASP
6	T	56	SER
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	143	LYS
6	T	169	ARG
6	T	171	SER
6	T	187	ARG
6	T	192	GLN
6	T	205	ASN
6	T	206(A)	GLU
6	T	214	TRP
6	T	222	LYS
7	U	13	THR
7	U	62	THR
7	U	73	THR

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Mol	Chain	Res	Type
7	U	87	ASN
7	U	107	MET
7	U	119	LEU
7	U	121	GLN
7	U	151	THR
7	U	157	TYR
7	U	165	THR
7	U	197	MET
7	U	204	GLU
7	U	232	ARG
7	U	239	GLN
8	V	17	ASP
8	V	31	CYS
8	V	34	LEU
8	V	68	LEU
8	V	91	GLN
8	V	106	THR
8	V	135	MET
8	V	156	SER
8	V	182	LYS
8	V	219	VAL
8	V	222	CYS
9	W	61	TYR
9	W	107	LYS
9	W	113	PHE
9	W	122(A)	LYS
9	W	160	LEU
9	W	181	LYS
9	W	182	ASP
9	W	183	GLU
10	X	-1	MET
10	X	6	ILE
10	X	9	GLN
10	X	21	THR
10	X	52	THR
10	X	68	ILE
10	X	77	GLN
10	X	105(B)	LYS
10	X	181	ASP
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE

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Mol	Chain	Res	Type
11	Y	84	SER
11	Y	105(A)	ARG
11	Y	105(B)	LYS
11	Y	127	VAL
11	Y	145	ASP
11	Y	152	LEU
11	Y	181	ASP
12	Z	-9	GLN
12	Z	14	LEU
12	Z	18	THR
12	Z	40	ASN
12	Z	61	ASN
12	Z	62	SER
12	Z	99	THR
12	Z	138	LEU
12	Z	144(A)	LYS
12	Z	144(J)	ASN
12	Z	144(Q)	LEU
12	Z	144(R)	LYS
13	1	-8	THR
13	1	2	SER
13	1	21	SER
13	1	40	ASN
13	1	61	ASP
13	1	62	LEU
13	1	71	ASP
13	1	91	ARG
13	1	111	ARG
13	1	121	SER
13	1	141(A)	VAL
13	1	141(C)	ARG
13	1	148	VAL
13	1	191	GLN
13	1	204	LYS
14	2	10	ASP
14	2	36	ARG
14	2	70	TYR
14	2	84	LYS
14	2	119	VAL
14	2	149	GLU
14	2	168	SER
14	2	187(F)	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
3	C	23	GLN
3	C	82	ASN
3	C	150	GLN
3	C	163	GLN
4	D	23	GLN
4	D	108	ASN
4	D	211	GLN
4	D	226	ASN
5	E	73	HIS
5	E	97	ASN
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	127	ASN
6	F	192	GLN
6	F	237	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
8	H	30	ASN
8	H	66	HIS
8	H	85	GLN

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Mol	Chain	Res	Type
8	H	144	GLN
8	H	172	ASN
8	H	190	ASN
9	I	81	GLN
10	J	9	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	186	GLN
11	K	66	HIS
11	K	85	ASN
11	K	174	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	123	GLN
12	L	140	ASN
12	L	144(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	149	GLN
13	M	157	ASN
14	N	161	GLN
2	P	61	GLN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
3	Q	23	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN

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Mol	Chain	Res	Type
3	Q	209	ASN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	114	GLN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	185	ASN
5	S	209	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
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	184	ASN
7	U	239	GLN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
9	W	29	ASN
9	W	64	ASN
10	X	54	GLN
10	X	85	GLN
10	X	96	GLN
10	X	112	GLN
10	X	140	HIS
11	Y	9	GLN
11	Y	85	ASN

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Mol	Chain	Res	Type
11	Y	131	GLN
11	Y	174	ASN
12	Z	-9	GLN
12	Z	40	ASN
12	Z	61	ASN
12	Z	144(B)	ASN
12	Z	144(C)	GLN
12	Z	166	HIS
13	1	10	ASN
13	1	18	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	28	ASN
14	2	69	GLN
14	2	106	ASN
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	LXT	Y	212	-	48,48,48	0.72	0	62,62,62	0.90	2 (3%)
17	MES	K	214	-	12,12,12	2.16	1 (8%)	14,16,16	1.38	1 (7%)
17	MES	Y	213	-	12,12,12	2.01	1 (8%)	14,16,16	1.69	2 (14%)
16	LXT	K	213	-	48,48,48	0.72	0	62,62,62	0.85	2 (3%)

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	LXT	Y	212	-	-	14/40/40/40	0/4/4/4
17	MES	K	214	-	-	3/6/14/14	0/1/1/1
17	MES	Y	213	-	-	5/6/14/14	0/1/1/1
16	LXT	K	213	-	-	13/40/40/40	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	214	MES	C8-S	-7.12	1.67	1.77
17	Y	213	MES	C8-S	-6.57	1.68	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	213	MES	O3S-S-C8	3.98	112.20	105.77
17	K	214	MES	O3S-S-C8	3.63	111.64	105.77
16	Y	212	LXT	C13-C12-N11	-3.39	105.79	113.05
17	Y	213	MES	O1S-S-C8	3.23	110.81	106.92
16	K	213	LXT	C13-C12-N11	-2.99	106.64	113.05
16	Y	212	LXT	C1-N2-C34	2.76	127.58	121.67
16	K	213	LXT	C1-N2-C34	2.12	126.20	121.67

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Y	212	LXT	N2-C34-C36-N38
16	Y	212	LXT	O35-C34-C36-N38
16	Y	212	LXT	C34-C36-C37-C41
16	Y	212	LXT	N38-C36-C37-C41
17	K	214	MES	C7-C8-S-O1S
17	K	214	MES	C7-C8-S-O3S
17	Y	213	MES	C7-C8-S-O2S
16	K	213	LXT	N5-C7-C8-C20
16	K	213	LXT	C34-C36-C37-C41
16	K	213	LXT	C9-C7-C8-C20
17	Y	213	MES	C7-C8-S-O3S
16	K	213	LXT	C28-C27-C3-C1
16	K	213	LXT	C36-C37-C41-C42
16	K	213	LXT	N2-C34-C36-C37
16	Y	212	LXT	C28-C27-C3-C1
17	Y	213	MES	C8-C7-N4-C5
16	Y	212	LXT	C4-C1-N2-C34
16	Y	212	LXT	N5-C7-C8-C20
16	Y	212	LXT	C21-C20-C8-C7
16	Y	212	LXT	C9-C7-C8-C20
17	K	214	MES	C7-C8-S-O2S
17	Y	213	MES	C7-C8-S-O1S
16	K	213	LXT	O35-C34-C36-N38
16	K	213	LXT	N2-C34-C36-N38
17	Y	213	MES	C8-C7-N4-C3
16	K	213	LXT	C8-C20-C21-C26
16	K	213	LXT	C8-C20-C21-C22
16	K	213	LXT	O35-C34-C36-C37
16	Y	212	LXT	O35-C34-C36-C37
16	Y	212	LXT	N2-C1-C3-C27
16	K	213	LXT	N2-C1-C3-C27
16	Y	212	LXT	C8-C20-C21-C22
16	Y	212	LXT	N2-C34-C36-C37
16	Y	212	LXT	C8-C20-C21-C26
16	K	213	LXT	N38-C36-C37-C41

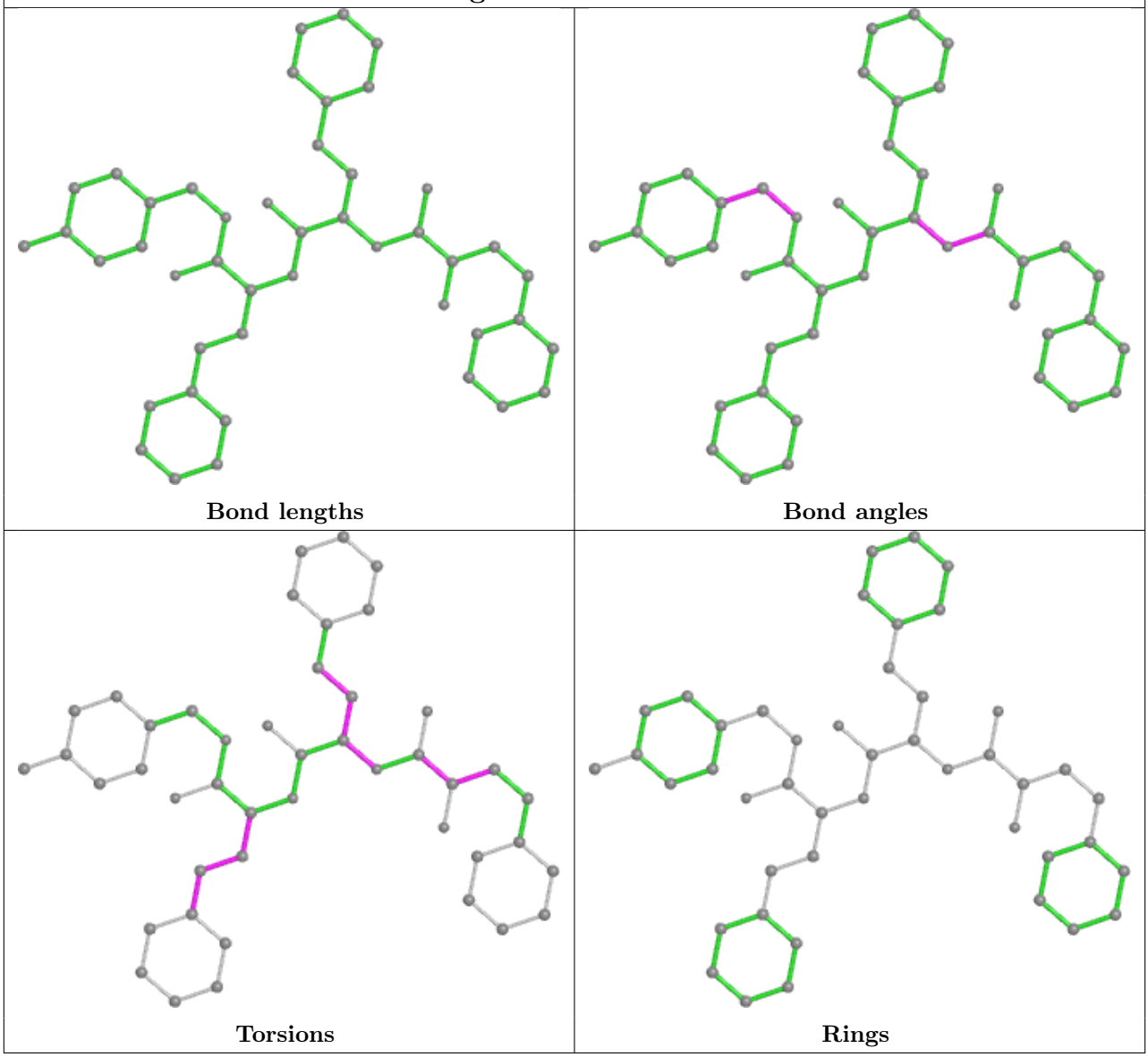
There are no ring outliers.

2 monomers are involved in 5 short contacts:

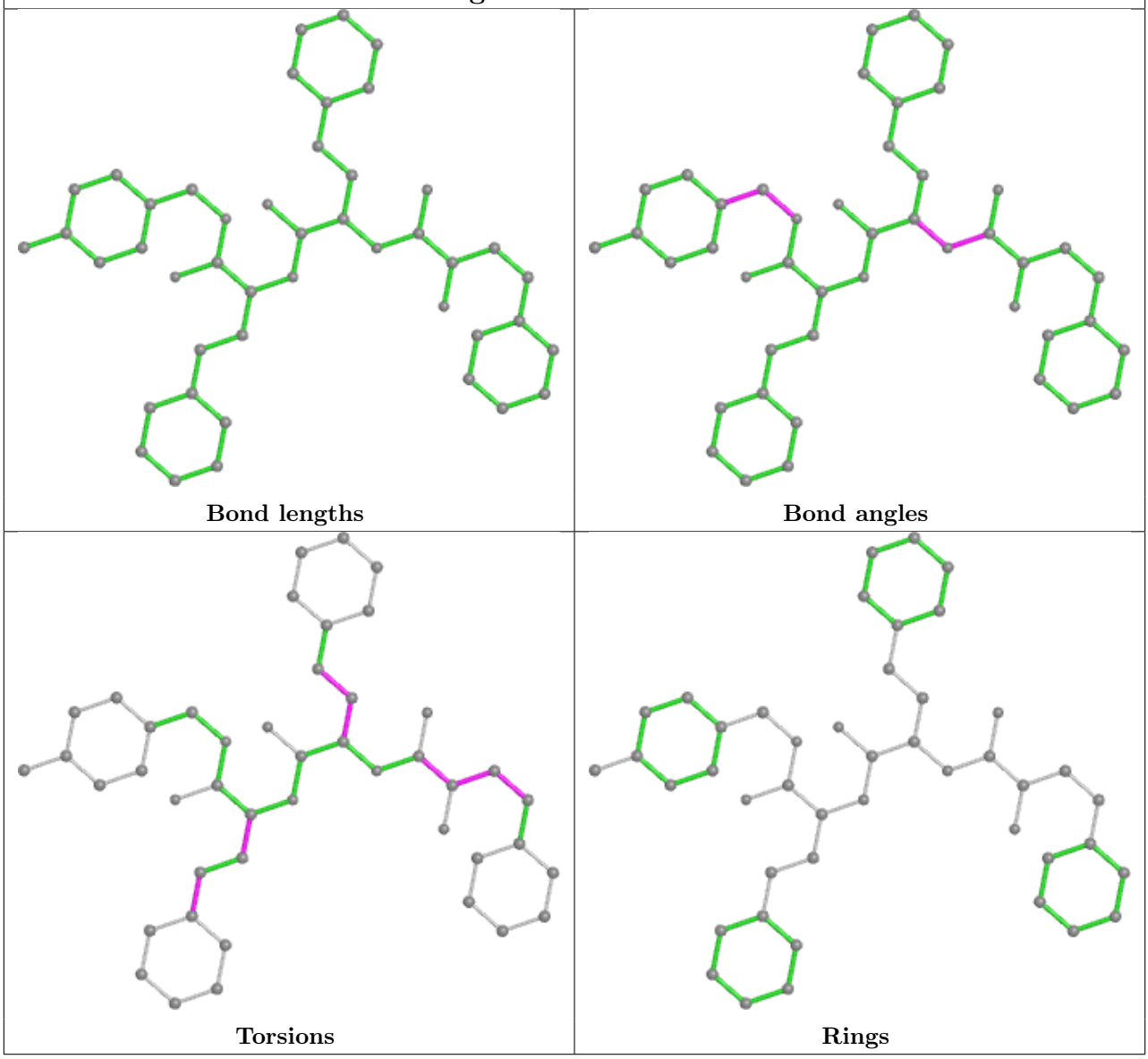
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	212	LXT	4	0
17	Y	213	MES	1	0

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 LXT Y 212



Ligand LXT K 213



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.31	3 (1%)	79	63	42, 61, 89, 102	0
1	O	250/250 (100%)	-0.26	6 (2%)	59	37	43, 62, 89, 102	0
2	B	244/244 (100%)	-0.17	3 (1%)	79	63	47, 67, 100, 107	0
2	P	244/244 (100%)	-0.18	3 (1%)	79	63	47, 67, 100, 108	0
3	C	241/241 (100%)	-0.04	4 (1%)	70	50	49, 69, 118, 142	0
3	Q	241/241 (100%)	0.10	14 (5%)	23	10	49, 70, 118, 142	0
4	D	242/242 (100%)	-0.07	9 (3%)	41	21	50, 69, 104, 113	0
4	R	242/242 (100%)	-0.10	7 (2%)	51	29	50, 69, 103, 113	0
5	E	233/233 (100%)	-0.07	6 (2%)	56	33	53, 74, 104, 111	0
5	S	233/233 (100%)	0.03	6 (2%)	56	33	53, 75, 104, 111	0
6	F	244/244 (100%)	-0.17	1 (0%)	92	85	46, 66, 97, 109	0
6	T	244/244 (100%)	-0.12	2 (0%)	86	74	46, 66, 97, 109	0
7	G	243/243 (100%)	-0.24	1 (0%)	92	85	44, 61, 84, 105	0
7	U	243/243 (100%)	-0.29	1 (0%)	92	85	45, 61, 83, 105	0
8	H	222/222 (100%)	-0.39	0	100	100	44, 57, 76, 107	0
8	V	222/222 (100%)	-0.42	1 (0%)	91	82	45, 57, 76, 107	0
9	I	204/204 (100%)	-0.43	0	100	100	44, 57, 69, 77	0
9	W	204/204 (100%)	-0.38	0	100	100	43, 56, 69, 77	0
10	J	198/198 (100%)	-0.32	2 (1%)	82	69	43, 59, 72, 115	0
10	X	198/198 (100%)	-0.21	3 (1%)	73	56	43, 59, 73, 115	0
11	K	212/212 (100%)	-0.28	0	100	100	45, 60, 78, 89	0
11	Y	212/212 (100%)	-0.37	0	100	100	44, 60, 79, 89	0
12	L	222/222 (100%)	-0.37	1 (0%)	91	82	40, 57, 84, 90	0
12	Z	222/222 (100%)	-0.27	0	100	100	41, 57, 84, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/233 (100%)	-0.32	1 (0%) 92 85	42, 55, 72, 82	0
13	M	233/233 (100%)	-0.42	1 (0%) 92 85	42, 55, 73, 83	0
14	2	196/196 (100%)	-0.38	1 (0%) 91 82	45, 53, 72, 79	0
14	N	196/196 (100%)	-0.38	0 100 100	45, 53, 72, 79	0
All	All	6368/6368 (100%)	-0.24	76 (1%) 79 63	40, 61, 97, 142	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	123(A)	GLY	7.3
4	D	123(C)	GLY	6.9
13	1	-8	THR	6.8
4	R	123(E)	SER	6.3
4	R	123(F)	GLY	6.2
4	R	123(D)	ALA	6.1
4	D	123(D)	ALA	5.8
13	M	-8	THR	5.5
4	D	123(F)	GLY	5.1
4	D	123(E)	SER	5.0
4	D	123(B)	GLU	4.9
8	V	223	ASP	4.8
10	X	192	ALA	4.7
10	X	193	GLN	4.5
3	Q	54	SER	4.3
2	B	218	ASN	4.2
4	R	123(C)	GLY	4.1
7	U	240	ASP	4.0
2	P	218	ASN	4.0
4	R	126	ARG	3.8
10	X	191	GLN	3.7
10	J	192	ALA	3.5
2	B	217	ALA	3.4
3	Q	240	LYS	3.4
1	A	4	MET	3.3
6	F	5	GLY	3.3
4	R	123(B)	GLU	3.3
3	Q	236	ILE	3.2
3	Q	207	ALA	3.2
5	E	4	PHE	3.2
6	T	5	GLY	3.2
10	J	193	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
5	E	5	ARG	3.1
3	Q	56	LEU	3.0
6	T	6	THR	3.0
2	P	4	GLY	3.0
1	O	236	LEU	3.0
5	S	206	SER	3.0
3	C	55	THR	3.0
3	Q	203	THR	2.9
3	Q	55	THR	2.9
12	L	-9	GLN	2.8
2	P	217	ALA	2.7
1	O	234	GLU	2.7
1	O	5	THR	2.7
3	C	56	LEU	2.7
4	D	126	ARG	2.6
5	S	233	ILE	2.6
5	E	233	ILE	2.6
7	G	240	ASP	2.5
5	E	206	SER	2.5
4	D	123(G)	GLU	2.5
1	O	4	MET	2.5
1	A	234	GLU	2.4
3	Q	233	VAL	2.4
1	O	217(P)	LYS	2.4
3	Q	235	GLN	2.4
3	Q	187	GLU	2.4
5	S	178	ARG	2.4
3	Q	7	GLY	2.4
3	C	240	LYS	2.4
1	O	235	ALA	2.4
5	E	127	TYR	2.3
4	R	123(G)	GLU	2.3
2	B	216(B)	GLY	2.3
5	S	11	ASP	2.2
3	Q	238	GLN	2.1
3	C	243	GLN	2.1
5	E	191	LYS	2.1
5	S	183	ASP	2.1
14	2	92	ASP	2.1
5	S	195	GLU	2.1
4	D	10	ARG	2.1
1	A	236	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	Q	239	GLU	2.0
3	Q	234	THR	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)

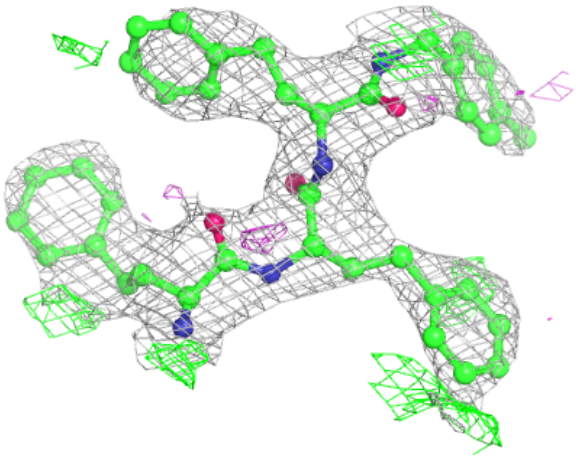
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

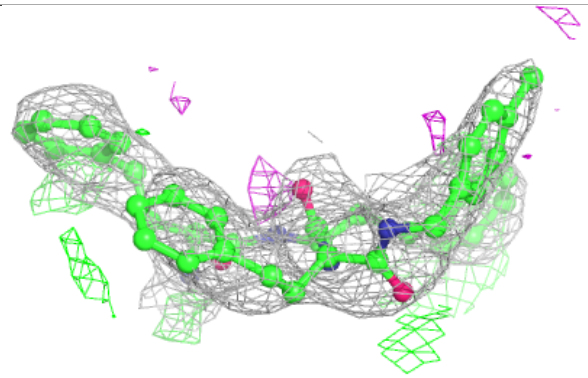
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	F	242	1/1	0.71	0.41	60,60,60,60	0
15	MG	G	241	1/1	0.72	0.83	85,85,85,85	0
16	LXT	Y	212	45/45	0.85	0.31	78,84,89,90	0
16	LXT	K	213	45/45	0.87	0.31	66,77,88,88	0
15	MG	I	196	1/1	0.90	0.18	57,57,57,57	0
15	MG	N	188	1/1	0.92	0.23	49,49,49,49	0
15	MG	H	224	1/1	0.92	0.12	56,56,56,56	0
15	MG	D	2	1/1	0.92	0.08	55,55,55,55	0
15	MG	K	212	1/1	0.93	0.17	56,56,56,56	0
17	MES	Y	213	12/12	0.93	0.23	90,91,92,92	0
15	MG	I	195	1/1	0.94	0.34	53,53,53,53	0
17	MES	K	214	12/12	0.96	0.17	84,86,87,87	0
15	MG	L	195	1/1	0.96	0.28	58,58,58,58	0
15	MG	G	1	1/1	0.98	0.06	54,54,54,54	0

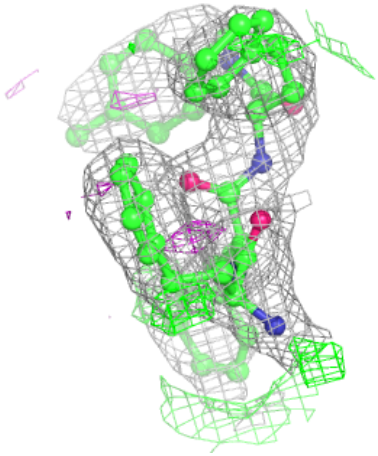
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

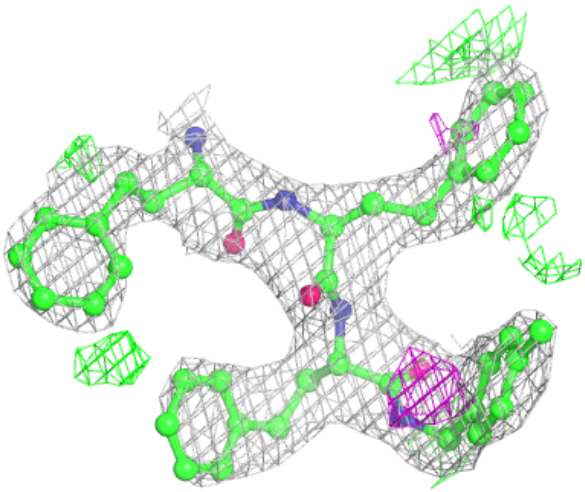
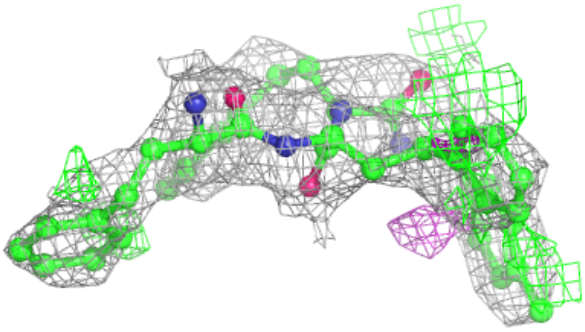
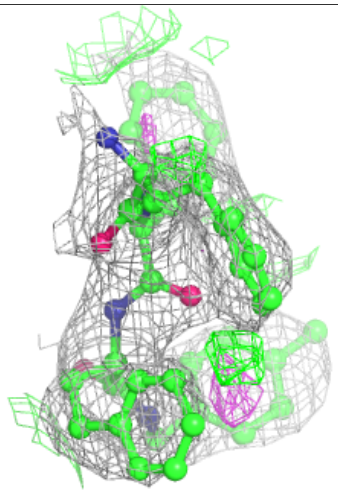
Electron density around LXT Y 212:

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







Electron density around LXT 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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.