Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 03:24 PM EDT

PDB ID	:	3MG7
Title	:	Structure of yeast 20S open-gate proteasome with Compound 8
Authors	:	Sintchak, M.D.
Deposited on	:	2010-04-05
Resolution	:	2.78 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:

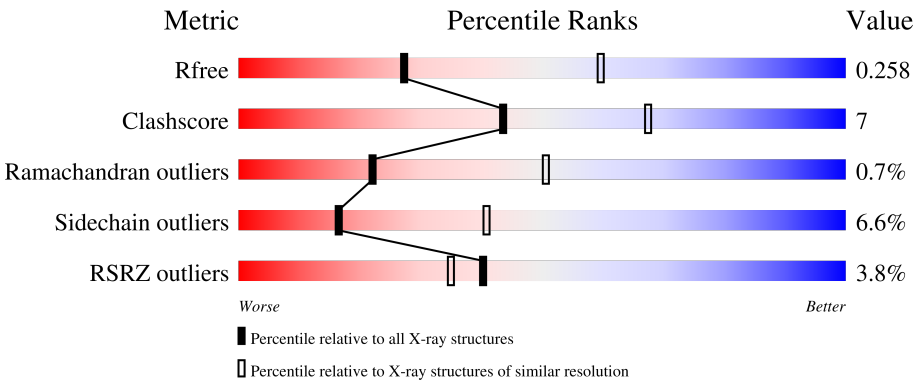
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	3% 86% 12% •
1	O	250	6% 80% 18% •
2	B	245	3% 75% 18% • •
2	P	245	3% 76% 18% • •
3	C	243	11% 83% 15% ••

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Mol	Chain	Length	Quality of chain
3	Q	243	20% 77% 20%
4	D	250	7% 80% 15%
4	R	250	6% 78% 17%
5	E	234	8% 76% 22%
5	S	234	10% 77% 20%
6	F	248	2% 78% 16%
6	T	248	2% 77% 17%
7	G	252	2% 79% 16%
7	U	252	% 82% 12%
8	H	222	80% 18%
8	V	222	78% 21%
9	I	205	% 82% 16%
9	W	205	% 82% 16%
10	J	198	4% 80% 17%
10	X	198	3% 85% 14%
11	K	212	2% 82% 16%
11	Y	212	83% 14%
12	L	241	78% 12% 8%
12	Z	241	2% 75% 15% 8%
13	1	266	% 70% 15% 12%
13	M	266	76% 11% 12%
14	2	196	% 82% 17%
14	N	196	% 84% 16%

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	F	243	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49424 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	235	1829	1158	303	365	3	0	0	0
2	P	235	1829	1158	303	365	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	237	1848	1175	323	346	4	0	0	0
6	T	237	1848	1175	323	346	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	F	2	2	2	0	0
15	G	1	1	1	0	0

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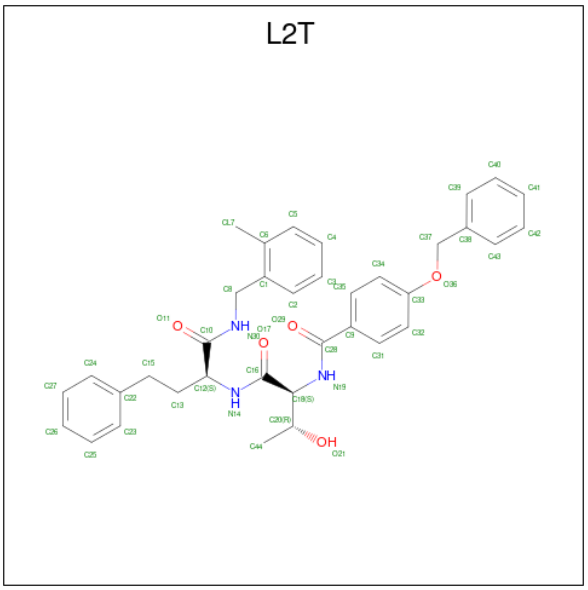
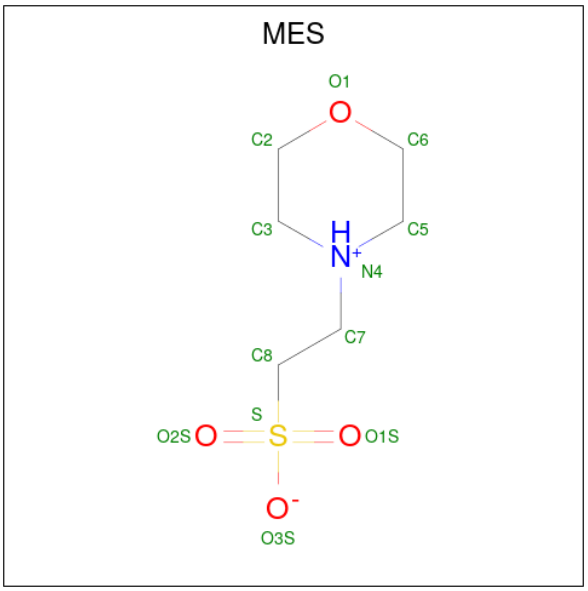
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	H	1	1	1	0	0
			Total	Mg		
15	I	2	2	2	0	0
			Total	Mg		
15	K	1	1	1	0	0
			Total	Mg		
15	L	2	2	2	0	0
			Total	Mg		
15	N	1	1	1	0	0

- Molecule 16 is 4-(benzyloxy)-N-[(1S,2R)-2-hydroxy-1-({(1S)-1-[(2-methylbenzyl)carbamoyl]-3-phenylpropyl}carbamoyl)propyl]benzamide (three-letter code: L2T) (formula: $C_{36}H_{39}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
16	K	1	44	36	3	5	0	0
			Total	C	N	O		
16	Y	1	44	36	3	5	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

- Molecule 18 is water.

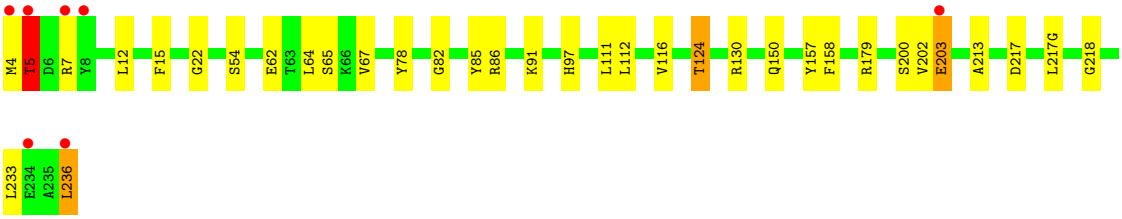
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	L	2	2	2	0	0
			Total	O		
18	Z	2	2	2	0	0

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.

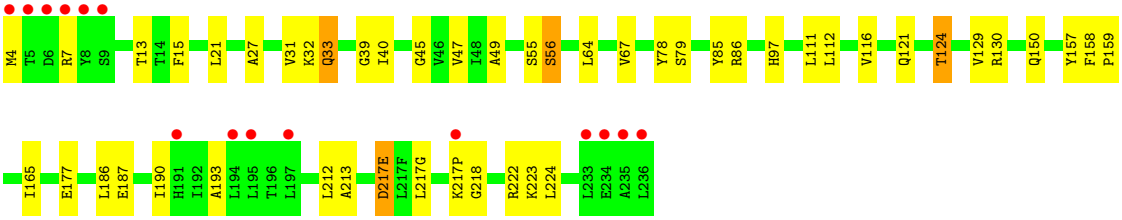
• Molecule 1: Proteasome component Y7

Chain A:



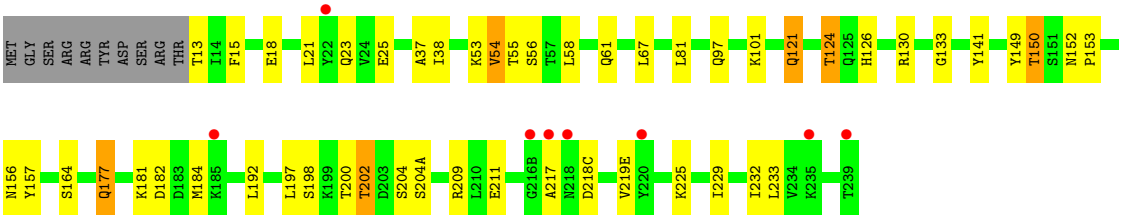
• Molecule 1: Proteasome component Y7

Chain O:



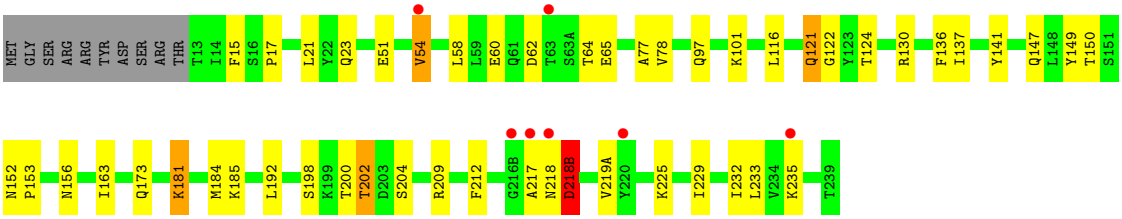
• Molecule 2: Proteasome component Y13

Chain B:



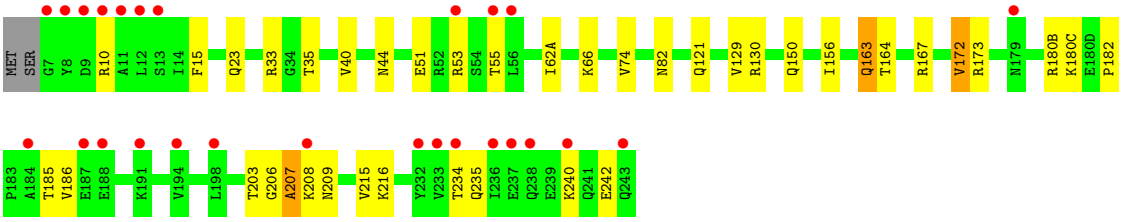
• Molecule 2: Proteasome component Y13

Chain P:



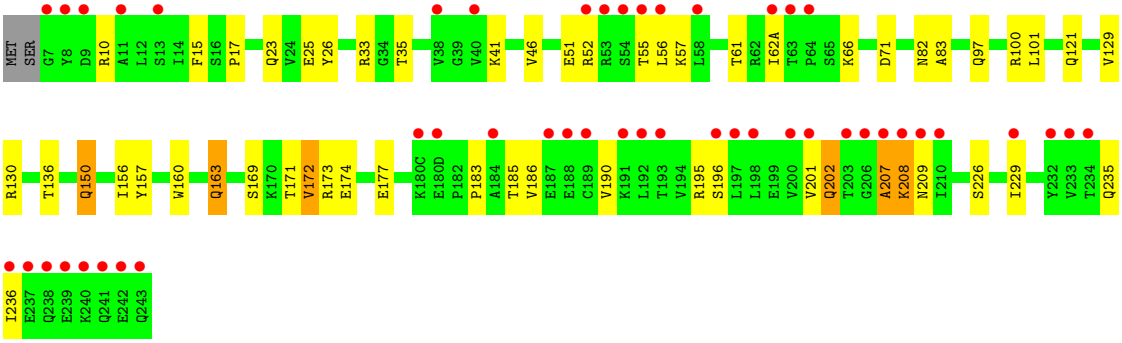
• Molecule 3: Proteasome component PRE6

Chain C:



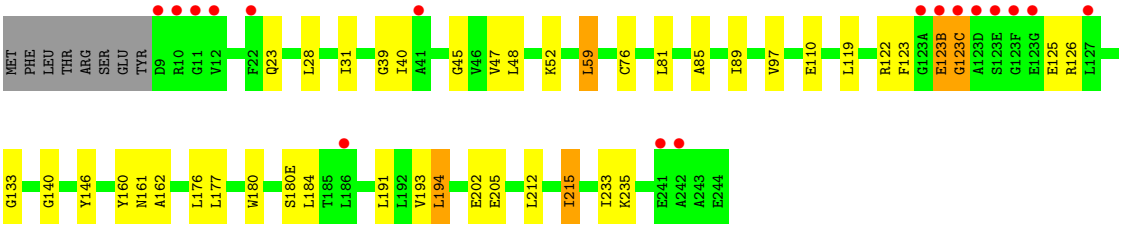
• Molecule 3: Proteasome component PRE6

Chain Q:



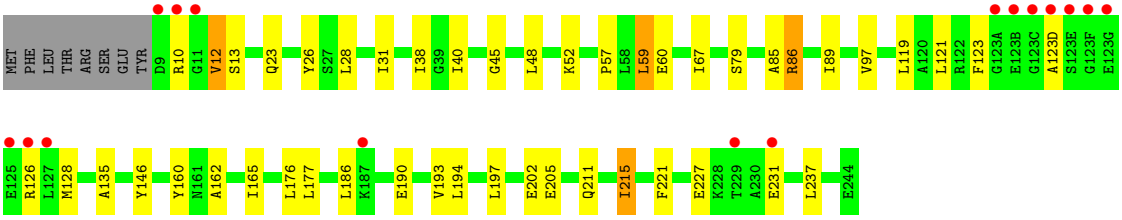
• Molecule 4: Proteasome component PUP2

Chain D:



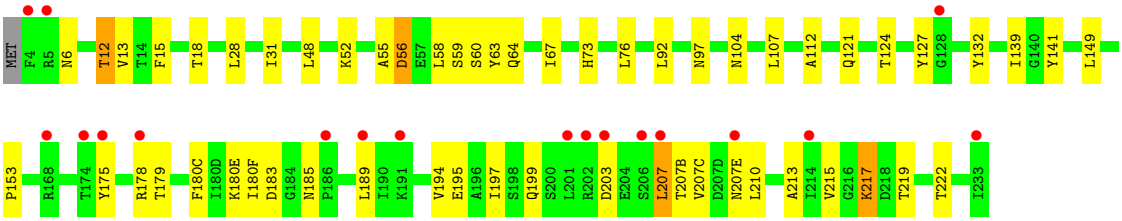
• Molecule 4: Proteasome component PUP2

Chain R:



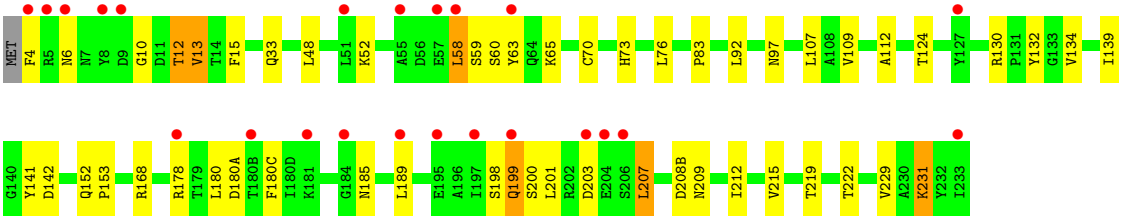
- Molecule 5: Proteasome component PRE5

Chain E:



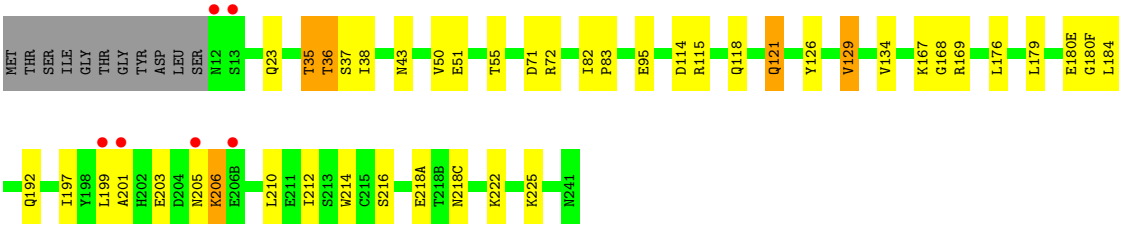
- Molecule 5: Proteasome component PRE5

Chain S:



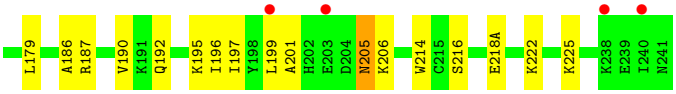
- Molecule 6: Proteasome component C1

Chain F:



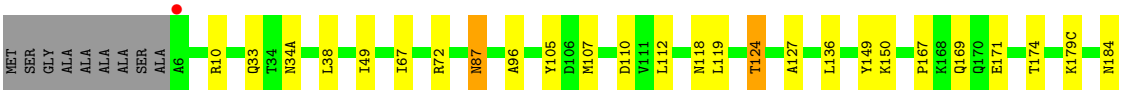
- Molecule 6: Proteasome component C1

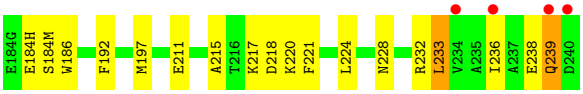
Chain T:



• Molecule 7: Proteasome component C7-alpha

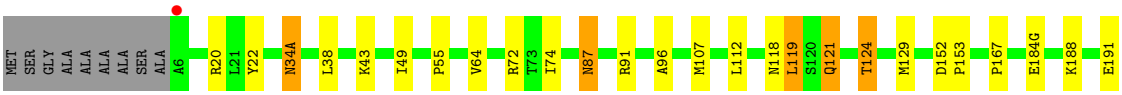
Chain G:

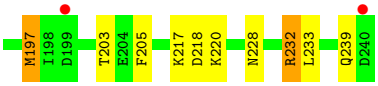




• Molecule 7: Proteasome component C7-alpha

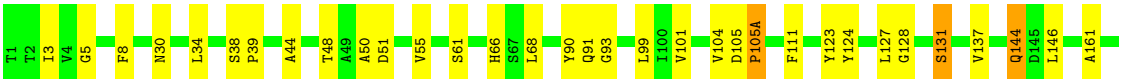
Chain U:

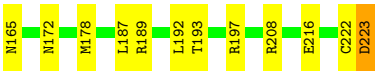




• Molecule 8: Proteasome component PUP1

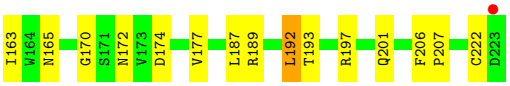
Chain H:





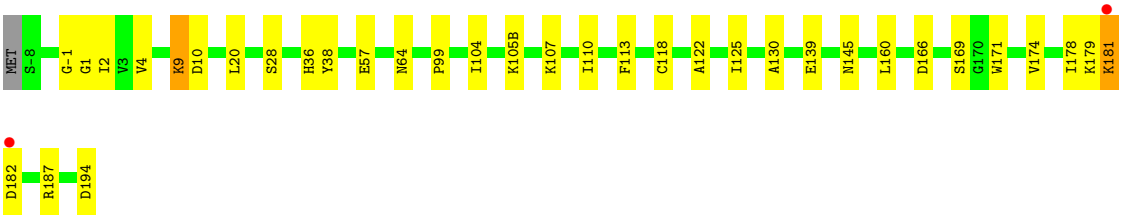
• Molecule 8: Proteasome component PUP1

Chain V:



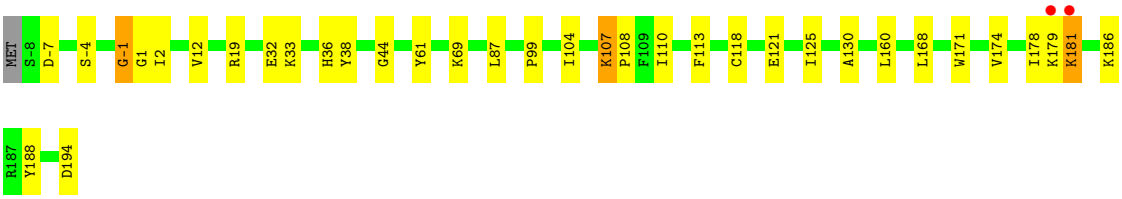
• Molecule 9: Proteasome component PUP3

Chain I:



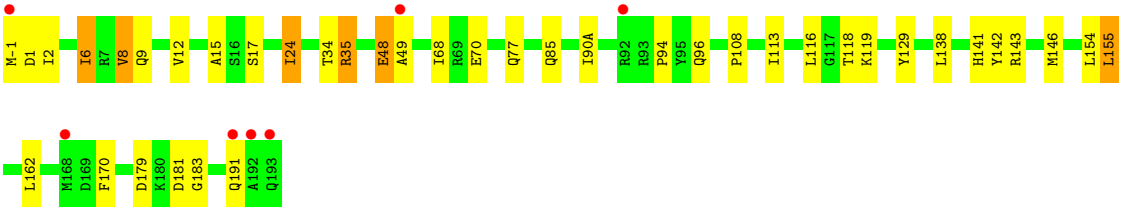
- Molecule 9: Proteasome component PUP3

Chain W:



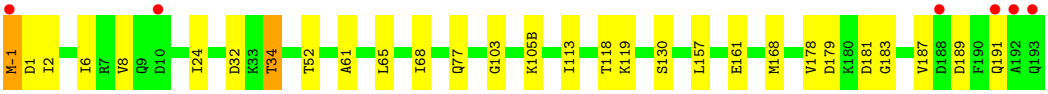
- Molecule 10: Proteasome component C11

Chain J:



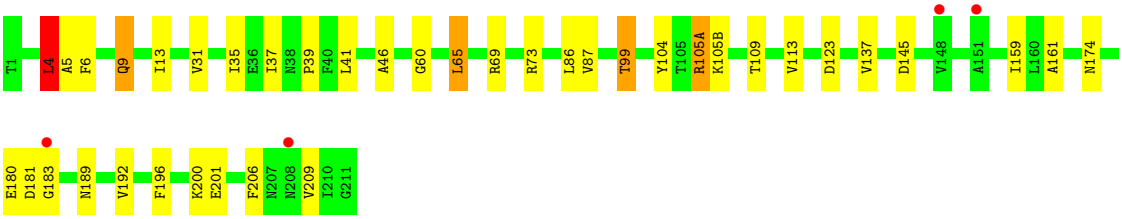
- Molecule 10: Proteasome component C11

Chain X:



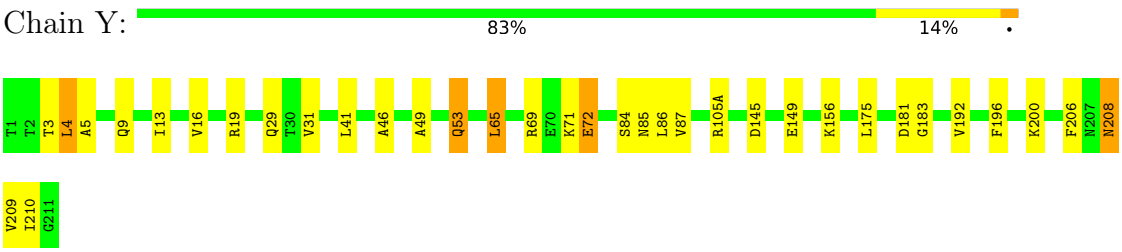
- Molecule 11: Proteasome component PRE2

Chain K:



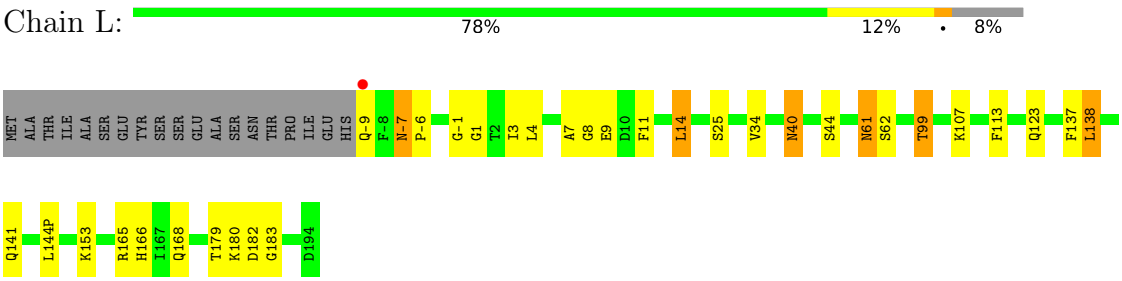
• Molecule 11: Proteasome component PRE2

Chain Y:



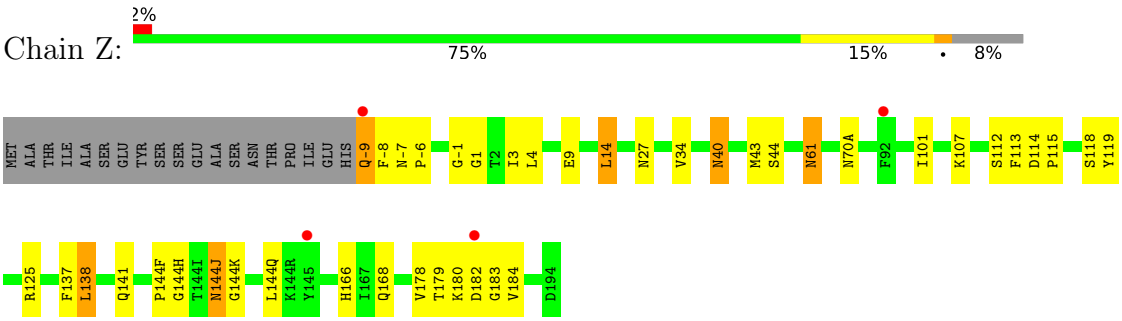
• Molecule 12: Proteasome component C5

Chain L:



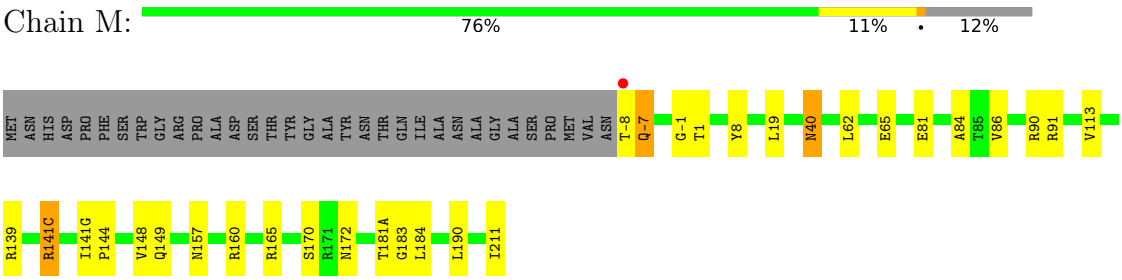
• Molecule 12: Proteasome component C5

Chain Z:



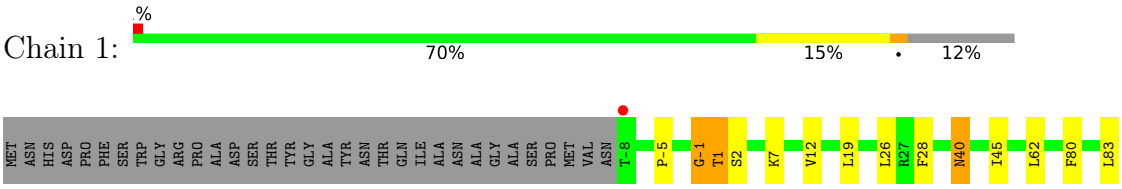
• Molecule 13: Proteasome component PRE4

Chain M:



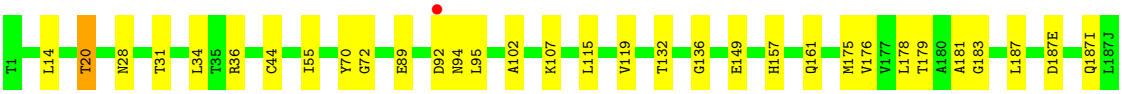
• Molecule 13: Proteasome component PRE4

Chain 1:



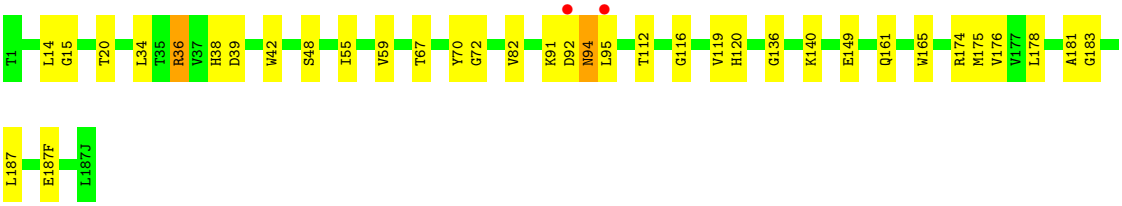
• Molecule 14: Proteasome component PRE3

Chain N:



• Molecule 14: Proteasome component PRE3

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.02Å 300.38Å 145.81Å 90.00° 113.73° 90.00°	Depositor
Resolution (Å)	48.68 – 2.78 48.68 – 2.78	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.68-2.78) 95.8 (48.68-2.78)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.259 0.217 , 0.258	Depositor DCC
R_{free} test set	5191 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49424	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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, L2T

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	0/1951	0.56	0/2639
1	O	0.42	0/1951	0.55	0/2639
2	B	0.42	0/1857	0.57	0/2513
2	P	0.40	0/1857	0.55	0/2513
3	C	0.41	0/1918	0.56	0/2591
3	Q	0.41	0/1918	0.57	0/2591
4	D	0.42	0/1883	0.61	1/2529 (0.0%)
4	R	0.40	0/1884	0.58	1/2532 (0.0%)
5	E	0.40	0/1819	0.57	0/2451
5	S	0.39	0/1821	0.57	0/2457
6	F	0.43	0/1885	0.55	0/2540
6	T	0.43	0/1886	0.57	0/2543
7	G	0.45	0/1956	0.57	0/2643
7	U	0.45	0/1958	0.57	0/2649
8	H	0.40	0/1714	0.56	0/2320
8	V	0.40	0/1714	0.56	0/2320
9	I	0.46	0/1608	0.60	0/2165
9	W	1.03	1/1609 (0.1%)	0.69	1/2168 (0.0%)
10	J	0.43	0/1611	0.58	0/2167
10	X	0.43	0/1611	0.59	0/2167
11	K	0.42	0/1680	0.58	1/2271 (0.0%)
11	Y	0.42	0/1680	0.59	1/2271 (0.0%)
12	L	0.43	0/1793	0.56	0/2414
12	Z	0.43	0/1793	0.57	0/2414
13	1	0.69	1/1853 (0.1%)	0.81	2/2507 (0.1%)
13	M	0.42	0/1852	0.63	0/2504
14	2	0.42	0/1538	0.56	0/2078
14	N	0.45	0/1538	0.54	0/2078
All	All	0.46	2/50138 (0.0%)	0.59	7/67674 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	-1	GLY	C-N	37.20	2.00	1.33
13	1	-1	GLY	C-N	23.09	1.87	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	-1	GLY	O-C-N	-25.36	82.12	122.70
9	W	-1	GLY	O-C-N	-16.35	95.40	123.20
4	D	59	LEU	CA-CB-CG	6.11	129.36	115.30
4	R	59	LEU	CA-CB-CG	5.96	129.02	115.30
11	Y	4	LEU	CA-CB-CG	5.63	128.26	115.30
13	1	-1	GLY	C-N-CA	5.62	135.74	121.70
11	K	4	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1925	24	0
1	O	1915	0	1925	34	0
2	B	1829	0	1828	30	0
2	P	1829	0	1828	30	0
3	C	1891	0	1899	24	0
3	Q	1891	0	1899	36	0
4	D	1862	0	1832	25	0
4	R	1862	0	1833	27	0
5	E	1795	0	1793	29	0
5	S	1795	0	1795	29	0
6	F	1848	0	1842	24	0
6	T	1848	0	1843	30	0
7	G	1921	0	1907	28	0
7	U	1921	0	1909	24	0
8	H	1685	0	1686	29	0
8	V	1685	0	1686	36	0
9	I	1581	0	1574	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	1581	0	1574	26	0
10	J	1585	0	1591	29	0
10	X	1585	0	1591	15	0
11	K	1644	0	1594	23	0
11	Y	1644	0	1594	18	0
12	L	1757	0	1712	23	0
12	Z	1757	0	1712	29	0
13	1	1824	0	1833	31	0
13	M	1824	0	1833	23	0
14	2	1512	0	1478	25	0
14	N	1512	0	1478	22	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	44	0	39	5	0
16	Y	44	0	39	2	0
17	K	12	0	13	1	0
17	Y	12	0	13	1	0
18	L	2	0	0	0	0
18	Z	2	0	0	0	0
All	All	49424	0	49098	660	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 (660) 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)
16:K:213:L2T:C6	16:K:213:L2T:CL7	1.75	1.60
13:1:-1:GLY:C	13:1:1:THR:N	1.87	1.28
11:K:181:ASP:C	11:K:183:GLY:HA2	1.64	1.16
9:W:-1:GLY:C	9:W:1:GLY:N	2.00	1.15
13:1:-1:GLY:C	13:1:1:THR:H1	1.45	1.12
14:N:92:ASP:C	14:N:94:ASN:N	2.04	1.10
9:I:-1:GLY:C	9:I:1:GLY:N	2.05	1.09
13:M:-1:GLY:C	13:M:1:THR:H1	1.57	1.08
12:Z:-1:GLY:O	12:Z:1:GLY:HA3	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:218:ASP:C	7:G:220:LYS:N	2.10	1.03
13:1:-1:GLY:C	13:1:1:THR:H2	1.65	0.99
9:W:36:HIS:C	9:W:38:TYR:N	2.16	0.98
9:I:36:HIS:C	9:I:38:TYR:N	2.17	0.98
7:G:96:ALA:HA	7:G:107:MET:HE2	1.45	0.97
9:I:-1:GLY:C	9:I:1:GLY:H1	1.67	0.97
13:M:141(G):ILE:C	13:M:144:PRO:N	2.18	0.97
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.10	0.96
8:H:91:GLN:C	8:H:93:GLY:N	2.20	0.95
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.46	0.95
13:M:-1:GLY:C	13:M:1:THR:N	2.19	0.94
14:N:70:TYR:C	14:N:72:GLY:N	2.21	0.94
2:P:200:THR:O	2:P:202:THR:N	2.02	0.93
9:W:-1:GLY:C	9:W:1:GLY:H3	1.68	0.92
9:W:-1:GLY:C	9:W:1:GLY:H1	1.65	0.92
8:H:187:LEU:C	8:H:189:ARG:N	2.23	0.90
2:B:200:THR:C	2:B:202:THR:N	2.25	0.90
6:T:192:GLN:NE2	6:T:195:LYS:HE3	1.86	0.89
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.52	0.89
1:O:7:ARG:HG3	6:T:128:SER:HB3	1.55	0.88
13:1:141(G):ILE:C	13:1:144:PRO:N	2.27	0.88
4:D:123(C):GLY:HA2	4:D:126:ARG:H	1.37	0.87
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.40	0.87
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.91	0.84
14:2:70:TYR:C	14:2:72:GLY:N	2.31	0.83
9:I:-1:GLY:C	9:I:1:GLY:H3	1.76	0.83
12:Z:179:THR:HG1	12:Z:182:ASP:N	1.78	0.82
3:C:163:GLN:NE2	3:C:164:THR:H	1.78	0.81
8:V:187:LEU:C	8:V:189:ARG:N	2.33	0.81
6:F:168:GLY:HA3	6:F:201:ALA:HB1	1.61	0.81
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.46	0.80
3:C:163:GLN:HE21	3:C:164:THR:H	1.27	0.80
5:E:15:PHE:H	6:F:23:GLN:HE22	1.30	0.80
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.32	0.77
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.31	0.77
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.48	0.77
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.31	0.77
7:G:184(M):SER:HA	7:G:186:TRP:N	1.99	0.76
7:U:107:MET:HE1	7:U:112:LEU:HD13	1.67	0.76
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.49	0.76
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.69	0.75
14:N:181:ALA:O	14:N:183:GLY:CA	2.35	0.75
2:B:181:LYS:O	2:B:184:MET:HG3	1.87	0.74
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.35	0.74
8:H:128:GLY:O	8:H:131:SER:HB3	1.88	0.74
6:F:35:THR:HG21	6:F:51:GLU:O	1.88	0.73
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.69	0.73
13:1:-1:GLY:O	13:1:1:THR:N	2.09	0.73
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.84	0.73
13:1:181(A):THR:O	13:1:183:GLY:N	2.22	0.72
4:R:123(D):ALA:HB3	4:R:126:ARG:HG3	1.71	0.72
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.54	0.72
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.53	0.72
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.03	0.72
1:A:15:PHE:H	2:B:23:GLN:HE22	1.38	0.71
11:K:181:ASP:C	11:K:183:GLY:CA	2.54	0.71
13:M:40:ASN:H	13:M:40:ASN:HD22	1.37	0.71
14:N:92:ASP:O	14:N:94:ASN:N	2.24	0.71
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.55	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.04	0.71
8:V:30:ASN:O	8:V:189:ARG:NH2	2.23	0.70
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.72	0.70
1:A:200:SER:O	1:A:202:VAL:HA	1.91	0.70
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.55	0.70
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.89	0.70
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.73	0.70
10:J:181:ASP:C	10:J:183:GLY:N	2.46	0.69
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.58	0.69
9:W:36:HIS:CA	9:W:38:TYR:N	2.55	0.69
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.75	0.69
7:U:218:ASP:C	7:U:220:LYS:N	2.46	0.69
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.41	0.68
12:Z:-1:GLY:O	12:Z:1:GLY:CA	2.40	0.68
5:E:12:THR:HG21	5:E:124:THR:HA	1.76	0.68
3:Q:201:VAL:O	3:Q:202:GLN:HB2	1.93	0.68
5:E:132:TYR:O	5:E:153:PRO:HB3	1.93	0.68
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.76	0.68
5:S:13:VAL:HG21	6:T:128:SER:O	1.94	0.68
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.76	0.68
11:Y:208:ASN:H	11:Y:208:ASN:HD22	1.42	0.67
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:179:LYS:C	9:W:181:LYS:N	2.47	0.67
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.77	0.67
8:V:187:LEU:O	8:V:189:ARG:N	2.26	0.67
3:C:163:GLN:HE21	3:C:164:THR:N	1.92	0.67
14:2:92:ASP:O	14:2:94:ASN:N	2.28	0.66
3:C:15:PHE:H	4:D:23:GLN:HE22	1.40	0.66
6:T:199:LEU:C	6:T:201:ALA:N	2.48	0.66
9:I:36:HIS:CA	9:I:38:TYR:N	2.59	0.65
5:S:132:TYR:O	5:S:153:PRO:HB3	1.95	0.65
7:U:107:MET:CE	7:U:112:LEU:HD13	2.27	0.65
5:E:73:HIS:HE1	5:E:107:LEU:O	1.80	0.65
2:P:202:THR:HG22	2:P:204:SER:H	1.59	0.65
4:D:180(E):SER:C	4:D:184:LEU:N	2.50	0.65
9:I:179:LYS:C	9:I:181:LYS:N	2.50	0.65
7:U:96:ALA:HA	7:U:107:MET:HE2	1.79	0.65
10:X:-1:MET:HG3	10:X:1:ASP:H1	1.62	0.64
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.63	0.64
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.46	0.64
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.96	0.64
9:I:179:LYS:O	9:I:181:LYS:N	2.31	0.64
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.80	0.63
1:O:97:HIS:HD2	8:V:61:SER:OG	1.81	0.63
7:U:87:ASN:C	7:U:87:ASN:HD22	2.02	0.63
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.45	0.63
9:W:179:LYS:O	9:W:181:LYS:N	2.32	0.63
10:X:2:ILE:HG12	10:X:130:SER:HB3	1.81	0.63
8:V:91:GLN:O	8:V:93:GLY:HA3	1.99	0.63
1:A:67:VAL:HG11	1:A:213:ALA:HB2	1.80	0.63
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.64	0.63
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.80	0.63
2:B:15:PHE:H	3:C:23:GLN:HE22	1.45	0.63
13:M:181(A):THR:O	13:M:183:GLY:N	2.32	0.62
5:E:180(E):LYS:O	5:E:183:ASP:N	2.33	0.62
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.81	0.62
10:J:143:ARG:O	10:J:146:MET:HG3	2.00	0.62
5:S:73:HIS:HE1	5:S:107:LEU:O	1.82	0.62
4:D:180(E):SER:O	4:D:184:LEU:N	2.32	0.62
12:L:166:HIS:HD2	12:L:168:GLN:H	1.48	0.62
4:R:12:VAL:HG23	4:R:13:SER:H	1.64	0.61
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.65	0.61
13:M:40:ASN:HD22	13:M:40:ASN:N	1.96	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:181:ALA:O	14:N:183:GLY:N	2.33	0.61
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.64	0.61
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.47	0.61
3:Q:171:THR:O	3:Q:174:GLU:HB3	1.98	0.61
6:T:179:LEU:HD11	6:T:192:GLN:HG2	1.83	0.61
2:P:121:GLN:O	2:P:124:THR:HB	1.98	0.61
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.65	0.60
13:1:40:ASN:H	13:1:40:ASN:HD22	1.49	0.60
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.49	0.60
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.66	0.60
5:E:60:SER:C	5:E:63:TYR:N	2.55	0.60
9:W:36:HIS:HA	9:W:38:TYR:N	2.16	0.60
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.83	0.60
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.83	0.60
1:A:7:ARG:HD2	5:E:127:TYR:CD2	2.37	0.60
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.50	0.60
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.65	0.60
10:X:-1:MET:HG3	10:X:1:ASP:N	2.16	0.60
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.83	0.60
5:E:55:ALA:O	5:E:56:ASP:HB2	2.01	0.60
1:O:7:ARG:HG3	6:T:128:SER:CB	2.31	0.60
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.66	0.60
5:S:12:THR:HG21	5:S:124:THR:HA	1.84	0.59
4:D:122:ARG:HA	4:D:126:ARG:HD3	1.84	0.59
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.84	0.59
5:S:15:PHE:H	6:T:23:GLN:HE22	1.48	0.59
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.83	0.59
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.85	0.59
12:L:180:LYS:C	12:L:182:ASP:N	2.56	0.59
4:R:10:ARG:HD2	5:S:10:GLY:HA2	1.84	0.59
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.68	0.58
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.27	0.58
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.83	0.58
10:J:48:GLU:HB3	10:J:96:GLN:HB2	1.84	0.58
13:M:-1:GLY:O	13:M:1:THR:N	2.28	0.58
8:V:172:ASN:HB3	8:V:192:LEU:O	2.03	0.58
3:C:53:ARG:HG3	3:C:167:ARG:HH12	1.69	0.58
7:G:184(M):SER:CA	7:G:186:TRP:N	2.66	0.58
3:Q:71:ASP:OD1	3:Q:100:ARG:NH1	2.35	0.58
4:D:233:ILE:C	4:D:235:LYS:N	2.56	0.58
16:K:213:L2T:CL7	16:K:213:L2T:C5	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.86	0.58
11:Y:49:ALA:O	11:Y:53:GLN:HB2	2.03	0.58
6:T:12:ASN:C	6:T:14:VAL:H	2.07	0.58
6:F:179:LEU:HD11	6:F:192:GLN:HG2	1.86	0.57
5:S:52:LYS:HB2	5:S:63:TYR:CB	2.33	0.57
4:D:202:GLU:O	4:D:205:GLU:N	2.37	0.57
10:J:179:ASP:O	10:J:183:GLY:N	2.38	0.57
10:X:181:ASP:O	10:X:183:GLY:HA3	2.04	0.57
12:Z:180:LYS:O	12:Z:182:ASP:HA	2.04	0.57
12:L:-1:GLY:O	12:L:1:GLY:HA3	2.04	0.57
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.86	0.57
5:S:134:VAL:O	5:S:153:PRO:HG3	2.05	0.57
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.52	0.56
10:X:181:ASP:C	10:X:183:GLY:N	2.58	0.56
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.87	0.56
10:J:6:ILE:HD11	10:J:8:VAL:HG13	1.86	0.56
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.20	0.56
8:V:20:SER:OG	8:V:28:ASP:HB3	2.05	0.56
13:M:211:ILE:HD11	14:2:36:ARG:HD2	1.87	0.56
14:N:181:ALA:O	14:N:183:GLY:HA3	2.06	0.56
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.36	0.56
14:2:181:ALA:C	14:2:183:GLY:N	2.59	0.56
4:D:202:GLU:C	4:D:205:GLU:N	2.58	0.56
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.88	0.56
2:B:54:VAL:HG13	2:B:209:ARG:HH22	1.71	0.56
10:J:-1:MET:HG3	10:J:1:ASP:H1	1.71	0.56
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.87	0.56
9:I:36:HIS:HA	9:I:38:TYR:N	2.20	0.56
9:I:110:ILE:HD12	9:I:125:ILE:HG12	1.88	0.56
1:O:55:SER:O	1:O:56:SER:HB3	2.05	0.56
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.20	0.55
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.70	0.55
2:P:54:VAL:HA	2:P:209:ARG:HH12	1.72	0.55
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.88	0.55
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.72	0.55
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.06	0.55
13:1:181(A):THR:C	13:1:183:GLY:N	2.59	0.55
1:O:15:PHE:H	2:P:23:GLN:HE22	1.54	0.55
5:S:180:LEU:HA	5:S:180(C):PHE:CE2	2.42	0.55
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.20	0.55
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180(F):ILE:C	5:E:183:ASP:N	2.61	0.54
6:T:35:THR:HG21	6:T:51:GLU:O	2.06	0.54
14:2:92:ASP:C	14:2:94:ASN:N	2.60	0.54
1:O:121:GLN:O	1:O:124:THR:HB	2.07	0.54
16:K:213:L2T:CL7	16:K:213:L2T:C1	2.73	0.54
9:W:19:ARG:HD3	9:W:168:LEU:O	2.07	0.54
5:S:198:SER:HA	5:S:201:LEU:HD12	1.89	0.54
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.90	0.54
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.88	0.54
5:S:60:SER:HA	5:S:63:TYR:N	2.22	0.54
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.06	0.54
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.89	0.54
4:R:13:SER:HB2	5:S:130:ARG:HD3	1.89	0.54
2:B:101:LYS:HZ1	10:J:85:GLN:NE2	2.05	0.53
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.89	0.53
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.91	0.53
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	1.91	0.53
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.90	0.53
10:J:141:HIS:HB3	10:J:154:LEU:HD11	1.90	0.53
7:U:87:ASN:C	7:U:87:ASN:ND2	2.61	0.53
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.22	0.53
11:K:181:ASP:O	11:K:183:GLY:HA2	2.06	0.53
12:L:180:LYS:O	12:L:182:ASP:N	2.42	0.53
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.73	0.53
7:G:96:ALA:CA	7:G:107:MET:HE2	2.31	0.53
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.90	0.52
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.06	0.52
7:G:238:GLU:O	7:G:239:GLN:HB2	2.10	0.52
8:H:104:VAL:HG13	8:H:178:MET:HB3	1.90	0.52
2:P:97:GLN:NE2	9:W:61:TYR:HA	2.24	0.52
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.91	0.52
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.92	0.52
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.92	0.52
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.90	0.52
1:A:233:LEU:HA	1:A:236:LEU:HB2	1.92	0.52
3:C:15:PHE:N	4:D:23:GLN:HE22	2.07	0.52
6:F:126:TYR:HB2	6:F:129:VAL:HG22	1.91	0.52
11:Y:181:ASP:O	11:Y:183:GLY:HA3	2.09	0.52
5:E:48:LEU:HB2	5:E:213:ALA:HB3	1.92	0.52
5:E:207:LEU:HD12	5:E:210:LEU:HD13	1.91	0.52
3:C:203:THR:HA	3:C:206:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:233:LEU:O	7:G:236:ILE:HG13	2.10	0.52
8:H:91:GLN:O	8:H:93:GLY:HA3	2.10	0.52
12:L:179:THR:HG1	12:L:182:ASP:N	2.08	0.52
8:V:172:ASN:HD22	8:V:193:THR:HA	1.75	0.52
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.57	0.52
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.92	0.52
12:Z:144(H):GLY:C	12:Z:144(J):ASN:H	2.12	0.52
12:L:7:ALA:O	12:L:123:GLN:NE2	2.42	0.52
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.57	0.51
13:M:-1:GLY:C	13:M:1:THR:H2	2.12	0.51
5:E:194:VAL:O	5:E:197:ILE:HG22	2.11	0.51
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.92	0.51
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.45	0.51
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.74	0.51
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.58	0.51
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.46	0.51
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.93	0.51
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.91	0.51
14:2:14:LEU:O	14:2:175:MET:HA	2.11	0.51
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.93	0.51
6:T:192:GLN:HE22	6:T:195:LYS:HE3	1.72	0.51
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.25	0.50
4:R:121:LEU:HD21	5:S:83:PRO:HB3	1.92	0.50
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.37	0.50
5:E:207(E):ASN:O	5:E:210:LEU:N	2.44	0.50
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.20	0.50
6:F:180(F):GLY:O	6:F:184:LEU:N	2.45	0.50
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	1.94	0.50
4:R:85:ALA:O	4:R:89:ILE:HG12	2.12	0.50
14:2:38:HIS:HE1	14:2:67:THR:OG1	1.94	0.50
2:P:163:ILE:HA	2:P:173:GLN:HE22	1.76	0.50
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.93	0.50
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.42	0.50
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.93	0.50
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.75	0.50
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	1.92	0.50
1:A:5:THR:HB	1:A:7:ARG:HH21	1.76	0.50
7:G:87:ASN:C	7:G:87:ASN:HD22	2.15	0.50
1:O:150:GLN:O	1:O:157:TYR:HA	2.12	0.50
13:1:-1:GLY:CA	13:1:1:THR:N	2.71	0.50
11:K:137:VAL:HG21	11:K:161:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.42	0.50
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.93	0.50
3:C:164:THR:HG21	3:C:172:VAL:HG22	1.94	0.50
12:Z:27:ASN:HB3	13:1:120:TYR:CE1	2.47	0.50
4:R:186:LEU:O	4:R:190:GLU:HG3	2.12	0.49
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	1.93	0.49
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.43	0.49
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.42	0.49
3:C:35:THR:HB	3:C:51:GLU:HG3	1.94	0.49
4:R:215:ILE:HG13	4:R:215:ILE:O	2.12	0.49
6:T:114:ASP:O	6:T:118:GLN:HG2	2.12	0.49
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.94	0.49
8:H:48:THR:HB	8:H:51:ASP:HB2	1.93	0.49
13:M:-8:THR:O	13:M:-7:GLN:HB3	2.11	0.49
1:O:79:SER:HB2	1:O:165:ILE:HD12	1.93	0.49
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.94	0.49
8:V:172:ASN:ND2	8:V:193:THR:HA	2.27	0.49
5:E:139:ILE:HD12	5:E:215:VAL:HG12	1.95	0.49
4:R:123:PHE:HA	4:R:128:MET:HB3	1.95	0.49
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.95	0.49
8:V:128:GLY:O	8:V:131:SER:HB2	2.12	0.49
6:F:35:THR:CG2	6:F:51:GLU:O	2.58	0.49
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.77	0.49
7:G:215:ALA:HB2	7:G:221:PHE:HD2	1.78	0.49
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.41	0.49
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.42	0.49
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.26	0.49
10:J:2:ILE:HB	10:J:17:SER:HB3	1.95	0.49
10:J:141:HIS:HB3	10:J:154:LEU:CD1	2.41	0.49
14:N:70:TYR:C	14:N:72:GLY:CA	2.81	0.49
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.61	0.49
2:B:37:ALA:O	2:B:164:SER:HA	2.13	0.49
9:I:181:LYS:HG2	9:I:182:ASP:OD1	2.13	0.49
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.95	0.48
14:N:14:LEU:O	14:N:175:MET:HA	2.13	0.48
7:U:121:GLN:O	7:U:124:THR:HB	2.13	0.48
10:J:-1:MET:HG3	10:J:1:ASP:N	2.28	0.48
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.95	0.48
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.95	0.48
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.96	0.48
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:LEU:HB3	9:I:28:SER:HB3	1.96	0.48
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.48	0.48
10:J:141:HIS:CB	10:J:154:LEU:HD11	2.43	0.48
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.95	0.48
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.49	0.48
2:B:101:LYS:HG3	9:I:57:GLU:HB3	1.96	0.48
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.94	0.48
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.94	0.48
1:A:112:LEU:O	1:A:116:VAL:HG23	2.13	0.48
3:Q:169:SER:HA	3:Q:172:VAL:HG13	1.96	0.48
3:C:242:GLU:CD	3:C:242:GLU:H	2.17	0.48
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.13	0.48
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.95	0.48
2:B:13:THR:O	3:C:130:ARG:HD3	2.14	0.47
3:C:15:PHE:H	4:D:23:GLN:NE2	2.10	0.47
10:J:90(A):ILE:HG12	10:J:116:LEU:HD23	1.95	0.47
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.12	0.47
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.49	0.47
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.14	0.47
12:Z:180:LYS:C	12:Z:182:ASP:N	2.68	0.47
8:H:123:TYR:OH	13:1:202:ASP:HB2	2.14	0.47
9:I:122:ALA:HB3	9:I:125:ILE:HD11	1.97	0.47
11:K:6:PHE:HA	11:K:123:ASP:O	2.14	0.47
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.21	0.47
1:O:13:THR:HG22	1:O:21:LEU:HD22	1.96	0.47
9:W:87:LEU:HD11	9:W:99:PRO:HG2	1.96	0.47
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.78	0.47
6:T:172:ALA:O	6:T:176:LEU:HD22	2.14	0.47
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.45	0.47
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.97	0.47
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.29	0.47
8:V:91:GLN:O	8:V:93:GLY:CA	2.62	0.47
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.44	0.47
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.45	0.47
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.50	0.47
7:U:20:ARG:HH21	7:U:22:TYR:HE1	1.60	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.47
11:Y:181:ASP:C	11:Y:183:GLY:N	2.68	0.47
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.96	0.47
9:I:9:LYS:HD2	9:I:145:ASN:HB3	1.97	0.47
1:O:45:GLY:HA3	1:O:186:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.97	0.47
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.28	0.47
2:P:181:LYS:O	2:P:184:MET:HG3	2.15	0.47
13:1:157:ASN:ND2	13:1:160:ARG:HH11	2.09	0.47
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.46	0.46
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.50	0.46
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.50	0.46
12:Z:43:MET:HG3	12:Z:101:ILE:HG22	1.97	0.46
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.80	0.46
1:A:12:LEU:HD11	7:G:127:ALA:HB2	1.97	0.46
11:K:99:THR:HG22	11:K:113:VAL:HB	1.97	0.46
12:L:3:ILE:HG21	12:L:44:SER:OG	2.15	0.46
12:Z:180:LYS:O	12:Z:182:ASP:CA	2.63	0.46
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.13	0.46
6:F:199:LEU:C	6:F:201:ALA:N	2.68	0.46
8:H:101:VAL:HG13	8:H:111:PHE:HB2	1.97	0.46
8:H:208:ARG:O	12:Z:144(F):PRO:HB3	2.15	0.46
14:N:149:GLU:CD	14:N:149:GLU:H	2.18	0.46
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.49	0.46
10:J:15:ALA:HB2	10:J:155:LEU:HD11	1.97	0.46
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.98	0.46
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	2.31	0.46
4:R:227:GLU:H	4:R:227:GLU:CD	2.19	0.46
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.98	0.46
8:V:3:ILE:O	8:V:126:SER:HA	2.16	0.46
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.98	0.46
6:F:203:GLU:O	6:F:206:LYS:HG3	2.15	0.46
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.14	0.46
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.98	0.46
6:T:206:LYS:HE3	6:T:206:LYS:HB2	1.74	0.46
2:B:150:THR:O	2:B:157:TYR:HA	2.15	0.46
9:I:104:ILE:HD12	9:I:178:ILE:HG22	1.98	0.46
10:J:129:TYR:HB3	10:X:24:ILE:HD11	1.98	0.46
8:V:126:SER:O	8:V:127:LEU:HD23	2.16	0.46
8:H:187:LEU:O	8:H:189:ARG:N	2.48	0.46
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.97	0.45
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.97	0.45
10:J:113:ILE:HA	10:J:118:THR:O	2.16	0.45
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.98	0.45
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.64	0.45
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:52:ARG:HB2	3:Q:209:ASN:HD22	1.82	0.45
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.24	0.45
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.51	0.45
16:K:213:L2T:H24	17:K:214:MES:H82	1.99	0.45
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.98	0.45
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.16	0.45
13:1:83:LEU:O	13:1:87:MET:HG2	2.16	0.45
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.97	0.45
10:J:24:ILE:HG12	10:J:24:ILE:O	2.16	0.45
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.45	0.45
12:Z:-9:GLN:HE21	12:Z:-8:PHE:H	1.64	0.45
8:H:44:ALA:O	8:H:99:LEU:HA	2.16	0.45
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.98	0.45
10:J:-1:MET:HA	10:J:1:ASP:N	2.31	0.45
2:P:17:PRO:HA	3:Q:26:TYR:CE1	2.52	0.45
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.46	0.45
6:T:168:GLY:HA3	6:T:201:ALA:HB1	1.98	0.45
2:B:202:THR:HG22	2:B:204:SER:H	1.81	0.45
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.98	0.45
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.98	0.45
1:O:97:HIS:HD2	8:V:61:SER:HG	1.65	0.45
8:V:35:HIS:HB2	8:V:56:THR:HG21	1.99	0.45
13:1:19:LEU:HD12	13:1:28:PHE:O	2.17	0.45
8:H:90:TYR:O	8:H:91:GLN:C	2.54	0.45
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.85	0.45
14:2:181:ALA:O	14:2:183:GLY:HA3	2.17	0.45
4:D:162:ALA:HB1	4:D:176:LEU:HD22	1.98	0.45
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.99	0.45
11:K:5:ALA:HA	11:K:13:ILE:O	2.16	0.45
1:O:112:LEU:O	1:O:116:VAL:HG23	2.17	0.45
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.98	0.45
6:F:71:ASP:OD2	6:F:72:ARG:N	2.48	0.45
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.99	0.45
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.97	0.45
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.99	0.45
14:2:15:GLY:HA2	14:2:174:ARG:O	2.16	0.45
9:W:-1:GLY:O	9:W:1:GLY:N	2.44	0.45
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.17	0.45
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.99	0.45
13:1:141(G):ILE:C	13:1:144:PRO:CA	2.85	0.45
9:I:36:HIS:O	9:I:38:TYR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.98	0.44
5:S:73:HIS:HB2	5:S:141:TYR:O	2.17	0.44
11:Y:71:LYS:O	11:Y:72:GLU:HB2	2.16	0.44
14:2:91:LYS:HE2	14:2:116:GLY:O	2.16	0.44
1:A:130:ARG:NH2	7:G:124:THR:CG2	2.72	0.44
9:I:99:PRO:HB2	9:I:113:PHE:HD2	1.81	0.44
12:Z:3:ILE:HG21	12:Z:44:SER:OG	2.16	0.44
13:1:7:LYS:HB3	13:1:12:VAL:HG12	1.99	0.44
13:1:80:PHE:CZ	13:1:111:ARG:HG2	2.52	0.44
2:B:121:GLN:O	2:B:124:THR:HB	2.18	0.44
2:B:229:ILE:O	2:B:233:LEU:HB2	2.18	0.44
8:H:30:ASN:O	8:H:189:ARG:NH2	2.51	0.44
11:K:196:PHE:CZ	11:K:209:VAL:HG21	2.52	0.44
4:R:79:SER:HB3	4:R:165:ILE:HD12	1.98	0.44
1:A:97:HIS:HD2	8:H:61:SER:OG	2.00	0.44
2:B:55:THR:HB	2:B:56:SER:H	1.65	0.44
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.13	0.44
7:U:129:MET:HB3	7:U:129:MET:HE2	1.87	0.44
8:V:41:ILE:HG12	8:V:76:VAL:HG22	2.00	0.44
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.98	0.44
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.84	0.44
12:Z:27:ASN:HB3	13:1:120:TYR:CZ	2.53	0.44
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.52	0.44
13:1:111:ARG:HH11	13:1:121:SER:HB2	1.83	0.44
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.00	0.44
1:O:40:ILE:HD12	1:O:193:ALA:HB2	2.00	0.44
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.98	0.44
11:K:86:LEU:C	11:K:86:LEU:HD13	2.39	0.44
13:M:84:ALA:HA	13:M:113:VAL:HG21	2.00	0.44
7:U:74:ILE:HD11	7:U:107:MET:O	2.18	0.44
8:V:91:GLN:O	8:V:93:GLY:N	2.51	0.44
1:A:150:GLN:O	1:A:157:TYR:HA	2.18	0.44
5:E:180(F):ILE:O	5:E:183:ASP:HA	2.18	0.44
6:F:167:LYS:HG2	6:F:205:ASN:HD21	1.83	0.44
8:H:223:ASP:N	8:H:223:ASP:OD2	2.50	0.44
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	1.99	0.44
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.62	0.44
5:S:109:VAL:HG23	5:S:142:ASP:OD1	2.18	0.44
6:T:35:THR:CG2	6:T:51:GLU:O	2.66	0.44
11:Y:46:ALA:HA	16:Y:212:L2T:HL7A	2.00	0.44
8:H:8:PHE:HB2	8:H:146:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.18	0.43
13:1:112:TYR:O	13:1:119:THR:HA	2.18	0.43
6:F:179:LEU:CD1	6:F:192:GLN:HG2	2.48	0.43
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.18	0.43
5:S:198:SER:C	5:S:200:SER:H	2.21	0.43
8:V:84:LYS:HG3	8:V:85:GLN:N	2.33	0.43
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	2.01	0.43
2:P:229:ILE:O	2:P:233:LEU:HB2	2.18	0.43
3:Q:226:SER:HA	3:Q:229:ILE:HD12	2.00	0.43
7:U:197:MET:HG2	7:U:205:PHE:CE1	2.53	0.43
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.53	0.43
1:A:130:ARG:HH21	7:G:124:THR:HG23	1.77	0.43
8:H:38:SER:HB2	8:H:39:PRO:HD2	2.01	0.43
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.99	0.43
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.83	0.43
13:1:19:LEU:HD21	13:1:26:LEU:HD22	2.00	0.43
6:F:95:GLU:HG2	6:F:115:ARG:CB	2.45	0.43
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.99	0.43
8:H:5:GLY:O	8:H:124:TYR:HA	2.18	0.43
1:O:39:GLY:HA2	1:O:47:VAL:O	2.19	0.43
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.39	0.43
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.24	0.43
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.19	0.43
7:G:238:GLU:O	7:G:239:GLN:CB	2.67	0.43
8:V:90:TYR:O	8:V:91:GLN:C	2.57	0.43
9:W:104:ILE:HD12	9:W:178:ILE:HG22	2.01	0.43
6:T:216:SER:HB3	6:T:218(A):GLU:HB2	2.01	0.43
8:V:128:GLY:O	8:V:131:SER:CB	2.67	0.43
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.59	0.43
2:P:122:GLY:C	2:P:124:THR:H	2.23	0.43
11:Y:181:ASP:C	11:Y:183:GLY:HA3	2.38	0.43
6:F:121:GLN:HE21	6:F:121:GLN:HB3	1.67	0.42
2:B:177:GLN:HE21	2:B:177:GLN:HB2	1.53	0.42
8:H:172:ASN:ND2	8:H:193:THR:HA	2.34	0.42
8:V:91:GLN:C	8:V:93:GLY:N	2.72	0.42
10:J:-1:MET:HA	10:J:1:ASP:H3	1.84	0.42
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.16	0.42
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.68	0.42
6:T:12:ASN:C	6:T:14:VAL:N	2.73	0.42
7:G:107:MET:CE	7:G:112:LEU:HD13	2.49	0.42
7:G:136:LEU:O	7:G:150:LYS:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ILE:HD13	10:J:162:LEU:HD13	2.01	0.42
1:O:111:LEU:HD21	9:W:69:LYS:HB3	2.00	0.42
3:Q:207:ALA:C	3:Q:209:ASN:H	2.23	0.42
5:S:48:LEU:HG	5:S:139:ILE:HG12	2.02	0.42
5:S:139:ILE:HD12	5:S:215:VAL:HG12	2.01	0.42
5:S:212:ILE:HD12	5:S:229:VAL:HG12	2.01	0.42
6:T:186:ALA:O	6:T:190:VAL:HG23	2.19	0.42
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.54	0.42
10:J:90(A):ILE:HA	10:J:94:PRO:HB3	2.02	0.42
12:L:9:GLU:O	12:L:107:LYS:HA	2.18	0.42
2:P:116:LEU:HD23	2:P:116:LEU:HA	1.93	0.42
13:1:45:ILE:HG12	13:1:99:ILE:HG12	2.00	0.42
5:E:15:PHE:H	6:F:23:GLN:NE2	2.06	0.42
7:G:192:PHE:CD1	7:G:192:PHE:C	2.93	0.42
9:I:194:ASP:HB3	11:Y:192:VAL:HG11	2.00	0.42
3:Q:41:LYS:HA	3:Q:46:VAL:HA	2.02	0.42
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.54	0.42
2:P:218:ASN:O	2:P:218(B):ASP:HB2	2.18	0.42
11:Y:3:THR:HG22	11:Y:16:VAL:HG12	2.02	0.42
13:1:84:ALA:HA	13:1:113:VAL:HG21	2.02	0.42
4:D:123(C):GLY:HA2	4:D:126:ARG:N	2.19	0.42
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.55	0.42
11:K:104:TYR:OH	11:K:105(A):ARG:NH1	2.53	0.42
2:P:147:GLN:HG2	3:Q:62(A):ILE:HG21	2.01	0.42
9:W:107:LYS:HE2	9:W:107:LYS:HB3	1.74	0.42
4:D:85:ALA:O	4:D:89:ILE:HG12	2.20	0.42
8:H:144:GLN:HE21	8:H:144:GLN:HB2	1.67	0.42
10:J:2:ILE:HD12	10:J:170:PHE:CG	2.55	0.42
11:K:46:ALA:HA	16:K:213:L2T:HL7A	2.02	0.42
1:O:27:ALA:O	1:O:31:VAL:HG23	2.19	0.42
3:Q:57:LYS:HD2	3:Q:57:LYS:HA	1.75	0.42
6:T:12:ASN:ND2	6:T:126:TYR:O	2.46	0.42
9:W:113:PHE:HA	9:W:118:CYS:O	2.20	0.42
1:A:82:GLY:O	1:A:85:TYR:HB3	2.20	0.41
2:B:21:LEU:O	2:B:25:GLU:HG2	2.20	0.41
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.85	0.41
14:2:38:HIS:O	14:2:39:ASP:C	2.58	0.41
1:O:217(E):ASP:OD1	1:O:217(E):ASP:N	2.49	0.41
2:P:17:PRO:HA	3:Q:26:TYR:CD1	2.55	0.41
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.55	0.41
10:X:103:GLY:HA2	10:X:178:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:LEU:HA	4:D:31:ILE:HD12	2.02	0.41
13:M:19:LEU:HB2	13:M:170:SER:HB2	2.03	0.41
3:Q:150:GLN:HE21	3:Q:160:TRP:HE1	1.68	0.41
11:Y:208:ASN:H	11:Y:208:ASN:ND2	2.12	0.41
16:Y:212:L2T:H24	17:Y:213:MES:H71	2.01	0.41
12:Z:113:PHE:HA	12:Z:118:SER:O	2.20	0.41
7:G:184(M):SER:C	7:G:186:TRP:N	2.73	0.41
10:J:138:LEU:O	10:J:142:TYR:HB3	2.21	0.41
2:P:147:GLN:HB3	2:P:149:TYR:CE2	2.55	0.41
6:T:179:LEU:HD21	6:T:192:GLN:HG2	2.01	0.41
14:2:36:ARG:HG3	14:2:42:TRP:NE1	2.35	0.41
3:C:207:ALA:C	3:C:209:ASN:H	2.23	0.41
6:F:38:ILE:HG12	6:F:197:ILE:HD11	2.02	0.41
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.87	0.41
6:T:176:LEU:HD13	6:T:196:ILE:HD13	2.02	0.41
11:Y:19:ARG:HH21	11:Y:29:GLN:HE22	1.67	0.41
5:S:152:GLN:HA	5:S:153:PRO:HD3	1.94	0.41
4:D:97:VAL:HG11	11:K:65:LEU:HD22	2.03	0.41
6:F:36:THR:HB	6:F:168:GLY:H	1.85	0.41
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.02	0.41
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.60	0.41
5:S:231:LYS:HE3	5:S:231:LYS:HB2	1.95	0.41
6:T:38:ILE:HG12	6:T:197:ILE:HD11	2.01	0.41
8:V:152:ILE:HD11	8:V:177:VAL:HG21	2.02	0.41
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.21	0.41
4:D:123:PHE:O	4:D:126:ARG:HD2	2.19	0.41
11:K:39:PRO:O	11:K:183:GLY:N	2.53	0.41
12:L:14:LEU:HD23	12:L:14:LEU:HA	1.92	0.41
4:R:52:LYS:HE3	4:R:211:GLN:HB2	2.02	0.41
9:W:-1:GLY:C	9:W:1:GLY:CA	2.86	0.41
9:W:186:LYS:HE2	9:W:188:TYR:CE1	2.55	0.41
11:Y:85:ASN:HD22	11:Y:85:ASN:HA	1.64	0.41
12:Z:114:ASP:HB2	12:Z:115:PRO:CD	2.51	0.41
4:D:39:GLY:HA2	4:D:47:VAL:O	2.21	0.41
5:E:175:TYR:HB2	5:E:199:GLN:HG2	2.03	0.41
10:J:181:ASP:O	10:J:183:GLY:HA3	2.20	0.41
1:O:33:GLN:H	1:O:33:GLN:HG2	1.64	0.41
2:P:77:ALA:HB3	2:P:137:ILE:HB	2.03	0.41
3:Q:101:LEU:HD13	10:X:61:ALA:HB2	2.02	0.41
3:Q:177:GLU:HG2	4:R:57:PRO:HG2	2.03	0.41
4:R:162:ALA:HB3	5:S:58:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:150:MET:HB3	6:T:160:TYR:CE1	2.56	0.41
10:X:113:ILE:HA	10:X:118:THR:O	2.21	0.41
6:F:210:LEU:HD21	6:F:212:ILE:HD11	2.03	0.41
9:I:130:ALA:HB2	9:I:166:ASP:CB	2.51	0.41
9:W:33:LYS:O	9:W:44:GLY:HA2	2.21	0.41
10:X:179:ASP:O	10:X:183:GLY:N	2.53	0.41
2:B:152:ASN:HB2	2:B:153:PRO:HD2	2.02	0.40
13:M:86:VAL:O	13:M:90:ARG:HG2	2.21	0.40
3:Q:157:TYR:OH	4:R:86:ARG:NH2	2.54	0.40
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.56	0.40
14:N:179:THR:O	14:N:183:GLY:N	2.54	0.40
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.56	0.40
1:O:187:GLU:HA	1:O:190:ILE:HD12	2.03	0.40
7:U:91:ARG:CZ	7:U:119:LEU:HD21	2.50	0.40
13:1:40:ASN:HD22	13:1:40:ASN:N	2.11	0.40
8:H:172:ASN:HD22	8:H:193:THR:HA	1.86	0.40
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	2.03	0.40
4:R:202:GLU:O	4:R:205:GLU:N	2.55	0.40
8:V:34:LEU:HD22	8:V:174:ASP:HB3	2.03	0.40
8:V:206:PHE:HA	8:V:207:PRO:HD2	1.95	0.40
1:A:78:TYR:HB3	1:A:85:TYR:CD1	2.57	0.40
3:C:180(B):ARG:O	3:C:182:PRO:HD3	2.21	0.40
4:D:81:LEU:HD12	4:D:133:GLY:HA3	2.04	0.40
6:F:114:ASP:O	6:F:118:GLN:HG2	2.22	0.40
9:I:-1:GLY:O	9:I:1:GLY:N	2.44	0.40
12:L:4:LEU:HD11	12:L:138:LEU:HD21	2.02	0.40
12:L:180:LYS:O	12:L:182:ASP:CA	2.69	0.40
10:X:181:ASP:O	10:X:183:GLY:CA	2.70	0.40
12:Z:112:SER:HB3	12:Z:125:ARG:HG2	2.03	0.40
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.57	0.40
9:I:166:ASP:HB3	9:I:169:SER:HB2	2.03	0.40
11:K:192:VAL:HG11	9:W:194:ASP:HB3	2.04	0.40
13:M:40:ASN:N	13:M:40:ASN:ND2	2.66	0.40
2:P:156:ASN:OD1	3:Q:82:ASN:HB2	2.21	0.40
3:Q:136:THR:O	3:Q:150:GLN:HA	2.22	0.40
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.50	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%)	234 (95%)	9 (4%)	3 (1%)	13	36
1	O	246/250 (98%)	235 (96%)	10 (4%)	1 (0%)	34	64
2	B	231/245 (94%)	216 (94%)	10 (4%)	5 (2%)	6	20
2	P	231/245 (94%)	218 (94%)	8 (4%)	5 (2%)	6	20
3	C	235/243 (97%)	229 (97%)	5 (2%)	1 (0%)	34	64
3	Q	235/243 (97%)	228 (97%)	3 (1%)	4 (2%)	9	27
4	D	232/250 (93%)	219 (94%)	11 (5%)	2 (1%)	17	44
4	R	234/250 (94%)	216 (92%)	17 (7%)	1 (0%)	34	64
5	E	223/234 (95%)	211 (95%)	8 (4%)	4 (2%)	8	25
5	S	227/234 (97%)	211 (93%)	12 (5%)	4 (2%)	8	25
6	F	231/248 (93%)	217 (94%)	14 (6%)	0	100	100
6	T	233/248 (94%)	222 (95%)	10 (4%)	1 (0%)	34	64
7	G	235/252 (93%)	224 (95%)	10 (4%)	1 (0%)	34	64
7	U	239/252 (95%)	234 (98%)	3 (1%)	2 (1%)	19	47
8	H	216/222 (97%)	207 (96%)	8 (4%)	1 (0%)	29	58
8	V	216/222 (97%)	205 (95%)	11 (5%)	0	100	100
9	I	196/205 (96%)	188 (96%)	8 (4%)	0	100	100
9	W	198/205 (97%)	190 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	183 (95%)	8 (4%)	2 (1%)	15	41
10	X	193/198 (98%)	184 (95%)	6 (3%)	3 (2%)	9	28
11	K	208/212 (98%)	202 (97%)	5 (2%)	1 (0%)	29	58
11	Y	208/212 (98%)	198 (95%)	9 (4%)	1 (0%)	29	58
12	L	216/241 (90%)	212 (98%)	4 (2%)	0	100	100
12	Z	216/241 (90%)	208 (96%)	7 (3%)	1 (0%)	29	58
13	1	227/266 (85%)	217 (96%)	9 (4%)	1 (0%)	34	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	225/266 (85%)	215 (96%)	9 (4%)	1 (0%)	34	64
14	2	188/196 (96%)	181 (96%)	7 (4%)	0	100	100
14	N	188/196 (96%)	181 (96%)	7 (4%)	0	100	100
All	All	6166/6524 (94%)	5885 (95%)	236 (4%)	45 (1%)	22	50

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
5	E	6	ASN
5	E	203	ASP
5	E	217	LYS
7	G	239	GLN
2	P	54	VAL
2	P	218(B)	ASP
3	Q	202	GLN
5	S	203	ASP
13	1	1	THR
1	A	5	THR
2	B	204(A)	SER
2	B	217	ALA
5	E	56	ASP
13	M	-7	GLN
2	P	217	ALA
3	Q	207	ALA
3	Q	208	LYS
5	S	199	GLN
7	U	239	GLN
11	Y	72	GLU
2	B	218(C)	ASP
3	C	207	ALA
11	K	9	GLN
2	P	62	ASP
5	S	6	ASN
10	X	189	ASP
1	A	203	GLU
4	D	123(B)	GLU
10	J	49	ALA
2	P	65	GLU
6	T	205	ASN
12	Z	144(K)	GLY

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Mol	Chain	Res	Type
4	D	123(C)	GLY
5	S	231	LYS
7	U	55	PRO
2	B	182	ASP
1	O	56	SER
1	A	22	GLY
3	Q	183	PRO
8	H	105(A)	PRO
10	J	8	VAL
10	X	8	VAL
10	X	187	VAL
4	R	12	VAL

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%)	195 (93%)	14 (7%)	16	40
1	O	209/209 (100%)	198 (95%)	11 (5%)	22	51
2	B	195/204 (96%)	181 (93%)	14 (7%)	14	36
2	P	195/204 (96%)	180 (92%)	15 (8%)	13	32
3	C	213/215 (99%)	193 (91%)	20 (9%)	8	23
3	Q	213/215 (99%)	200 (94%)	13 (6%)	18	45
4	D	198/206 (96%)	186 (94%)	12 (6%)	18	45
4	R	198/206 (96%)	187 (94%)	11 (6%)	21	48
5	E	192/193 (100%)	174 (91%)	18 (9%)	8	23
5	S	192/193 (100%)	175 (91%)	17 (9%)	9	26
6	F	196/205 (96%)	181 (92%)	15 (8%)	13	32
6	T	196/205 (96%)	181 (92%)	15 (8%)	13	32
7	G	207/210 (99%)	189 (91%)	18 (9%)	10	27
7	U	207/210 (99%)	192 (93%)	15 (7%)	14	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	181/181 (100%)	173 (96%)	8 (4%)	28	58
8	V	181/181 (100%)	172 (95%)	9 (5%)	24	53
9	I	172/173 (99%)	164 (95%)	8 (5%)	26	56
9	W	172/173 (99%)	163 (95%)	9 (5%)	23	52
10	J	175/175 (100%)	164 (94%)	11 (6%)	18	43
10	X	175/175 (100%)	165 (94%)	10 (6%)	20	48
11	K	169/169 (100%)	154 (91%)	15 (9%)	9	26
11	Y	169/169 (100%)	155 (92%)	14 (8%)	11	29
12	L	185/201 (92%)	175 (95%)	10 (5%)	22	50
12	Z	185/201 (92%)	177 (96%)	8 (4%)	29	59
13	1	199/224 (89%)	184 (92%)	15 (8%)	13	34
13	M	199/224 (89%)	190 (96%)	9 (4%)	27	58
14	2	162/162 (100%)	155 (96%)	7 (4%)	29	59
14	N	162/162 (100%)	152 (94%)	10 (6%)	18	44
All	All	5306/5454 (97%)	4955 (93%)	351 (7%)	16	41

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	THR
1	A	54	SER
1	A	62	GLU
1	A	64	LEU
1	A	65	SER
1	A	91	LYS
1	A	111	LEU
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
1	A	203	GLU
1	A	217	ASP
1	A	236	LEU
2	B	18	GLU
2	B	53	LYS
2	B	58	LEU
2	B	61	GLN

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Mol	Chain	Res	Type
2	B	121	GLN
2	B	124	THR
2	B	150	THR
2	B	156	ASN
2	B	177	GLN
2	B	192	LEU
2	B	198	SER
2	B	202	THR
2	B	225	LYS
2	B	232	ILE
3	C	10	ARG
3	C	33	ARG
3	C	40	VAL
3	C	44	ASN
3	C	55	THR
3	C	66	LYS
3	C	74	VAL
3	C	82	ASN
3	C	121	GLN
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	180(C)	LYS
3	C	185	THR
3	C	208	LYS
3	C	215	VAL
3	C	234	THR
3	C	235	GLN
3	C	240	LYS
4	D	48	LEU
4	D	52	LYS
4	D	59	LEU
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	191	LEU
4	D	194	LEU
4	D	215	ILE

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Mol	Chain	Res	Type
5	E	12	THR
5	E	13	VAL
5	E	18	THR
5	E	28	LEU
5	E	58	LEU
5	E	64	GLN
5	E	76	LEU
5	E	121	GLN
5	E	149	LEU
5	E	178	ARG
5	E	179	THR
5	E	185	ASN
5	E	189	LEU
5	E	195	GLU
5	E	207	LEU
5	E	207(C)	VAL
5	E	219	THR
5	E	222	THR
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	55	THR
6	F	121	GLN
6	F	129	VAL
6	F	134	VAL
6	F	169	ARG
6	F	176	LEU
6	F	180(E)	GLU
6	F	206	LYS
6	F	214	TRP
6	F	218(C)	ASN
6	F	222	LYS
6	F	225	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
7	G	169	GLN

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Mol	Chain	Res	Type
7	G	171	GLU
7	G	174	THR
7	G	179(C)	LYS
7	G	184	ASN
7	G	184(H)	GLU
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
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	222	CYS
8	H	223	ASP
9	I	4	VAL
9	I	9	LYS
9	I	105(B)	LYS
9	I	107	LYS
9	I	160	LEU
9	I	171	TRP
9	I	174	VAL
9	I	181	LYS
10	J	6	ILE
10	J	9	GLN
10	J	24	ILE
10	J	34	THR
10	J	35	ARG
10	J	48	GLU
10	J	68	ILE
10	J	70	GLU
10	J	77	GLN
10	J	155	LEU
10	J	191	GLN
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	65	LEU
11	K	69	ARG

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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	109	THR
11	K	145	ASP
11	K	180	GLU
11	K	201	GLU
12	L	-9	GLN
12	L	-7	ASN
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	61	ASN
12	L	62	SER
12	L	99	THR
12	L	138	LEU
12	L	144(P)	LEU
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	141(C)	ARG
13	M	149	GLN
13	M	172	ASN
13	M	184	LEU
13	M	190	LEU
14	N	20	THR
14	N	31	THR
14	N	36	ARG
14	N	89	GLU
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	132	THR
14	N	187(E)	ASP
14	N	187(I)	GLN
1	O	4	MET
1	O	33	GLN
1	O	64	LEU
1	O	124	THR

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Mol	Chain	Res	Type
1	O	129	VAL
1	O	158	PHE
1	O	177	GLU
1	O	217(E)	ASP
1	O	217(P)	LYS
1	O	222	ARG
1	O	223	LYS
2	P	58	LEU
2	P	64	THR
2	P	101	LYS
2	P	121	GLN
2	P	150	THR
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	10	ARG
3	Q	25	GLU
3	Q	61	THR
3	Q	66	LYS
3	Q	121	GLN
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	208	LYS
3	Q	235	GLN
4	R	28	LEU
4	R	48	LEU
4	R	59	LEU
4	R	60	GLU
4	R	86	ARG
4	R	119	LEU
4	R	177	LEU

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Mol	Chain	Res	Type
4	R	194	LEU
4	R	215	ILE
4	R	231	GLU
4	R	237	LEU
5	S	4	PHE
5	S	12	THR
5	S	13	VAL
5	S	33	GLN
5	S	58	LEU
5	S	65	LYS
5	S	76	LEU
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	207	LEU
5	S	208(B)	ASP
5	S	219	THR
5	S	222	THR
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	63	LYS
6	T	98	SER
6	T	121	GLN
6	T	129	VAL
6	T	143	LYS
6	T	169	ARG
6	T	176	LEU
6	T	187	ARG
6	T	205	ASN
6	T	214	TRP
6	T	222	LYS
6	T	225	LYS
7	U	34(A)	ASN
7	U	38	LEU
7	U	43	LYS
7	U	49	ILE
7	U	72	ARG
7	U	87	ASN

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Mol	Chain	Res	Type
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	197	MET
7	U	203	THR
7	U	217	LYS
7	U	228	ASN
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	144	GLN
8	V	149	GLU
8	V	192	LEU
8	V	197	ARG
8	V	222	CYS
9	W	-7	ASP
9	W	-4	SER
9	W	32	GLU
9	W	107	LYS
9	W	121	GLU
9	W	160	LEU
9	W	171	TRP
9	W	174	VAL
9	W	181	LYS
10	X	-1	MET
10	X	6	ILE
10	X	34	THR
10	X	52	THR
10	X	68	ILE
10	X	77	GLN
10	X	105(B)	LYS
10	X	157	LEU
10	X	168	MET
10	X	191	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	41	LEU
11	Y	53	GLN

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Mol	Chain	Res	Type
11	Y	65	LEU
11	Y	69	ARG
11	Y	84	SER
11	Y	87	VAL
11	Y	105(A)	ARG
11	Y	145	ASP
11	Y	149	GLU
11	Y	208	ASN
11	Y	210	ILE
12	Z	-9	GLN
12	Z	14	LEU
12	Z	40	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	138	LEU
12	Z	144(J)	ASN
12	Z	144(Q)	LEU
13	1	2	SER
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	141(B)	ASP
13	1	141(C)	ARG
13	1	148	VAL
13	1	181(A)	THR
13	1	184	LEU
13	1	190	LEU
13	1	191	GLN
13	1	194	ASN
13	1	204	LYS
13	1	211	ILE
14	2	20	THR
14	2	36	ARG
14	2	48	SER
14	2	94	ASN
14	2	119	VAL
14	2	149	GLU
14	2	187(F)	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
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	23	GLN
3	C	44	ASN
3	C	82	ASN
3	C	150	GLN
3	C	163	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
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	169	GLN
7	G	178	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN

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Mol	Chain	Res	Type
8	H	190	ASN
9	I	29	ASN
10	J	9	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	160	GLN
10	J	186	GLN
11	K	85	ASN
11	K	174	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70	HIS
12	L	70(A)	ASN
12	L	144(C)	GLN
12	L	144(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
14	N	38	HIS
14	N	141	ASN
14	N	157	HIS
14	N	161	GLN
1	O	97	HIS
2	P	23	GLN
2	P	121	GLN
2	P	125	GLN
2	P	177	GLN
2	P	218	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
4	R	23	GLN
4	R	108	ASN

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Mol	Chain	Res	Type
4	R	147	GLN
4	R	161	ASN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
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	199	GLN
5	S	209	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	192	GLN
6	T	205	ASN
6	T	241	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	170	GLN
7	U	178	ASN
7	U	182	HIS
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	112	GLN
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	174	ASN

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Mol	Chain	Res	Type
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	144(J)	ASN
12	Z	166	HIS
13	1	-7	GLN
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	38	HIS
14	2	62	HIS
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	L2T	K	213	-	47,47,47	1.95	2 (4%)	61,62,62	0.81	1 (1%)
16	L2T	Y	212	-	47,47,47	1.86	2 (4%)	61,62,62	0.81	2 (3%)
17	MES	K	214	-	12,12,12	2.02	1 (8%)	14,16,16	1.45	1 (7%)
17	MES	Y	213	-	12,12,12	2.19	1 (8%)	14,16,16	1.48	2 (14%)

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	L2T	K	213	-	-	2/39/39/39	0/4/4/4
16	L2T	Y	212	-	-	6/39/39/39	0/4/4/4
17	MES	K	214	-	-	5/6/14/14	0/1/1/1
17	MES	Y	213	-	-	1/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	213	L2T	CL7-C6	12.01	1.75	1.51
16	Y	212	L2T	CL7-C6	11.35	1.73	1.51
17	Y	213	MES	C8-S	-7.21	1.67	1.77
17	K	214	MES	C8-S	-6.57	1.68	1.77
16	K	213	L2T	C37-C38	-4.71	1.39	1.50
16	Y	212	L2T	C37-C38	-4.15	1.40	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	214	MES	O3S-S-C8	3.75	111.83	105.77
17	Y	213	MES	O3S-S-C8	3.29	111.09	105.77
16	Y	212	L2T	O36-C37-C38	3.27	118.96	109.16
17	Y	213	MES	O2S-S-C8	2.85	110.34	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	K	213	L2T	O36-C37-C38	2.26	115.95	109.16
16	Y	212	L2T	CL7-C6-C1	-2.00	119.58	121.99

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	214	MES	C8-C7-N4-C3
17	K	214	MES	C8-C7-N4-C5
17	K	214	MES	C7-C8-S-O1S
17	K	214	MES	C7-C8-S-O2S
17	K	214	MES	C7-C8-S-O3S
16	Y	212	L2T	N19-C28-C9-C31
16	Y	212	L2T	O29-C28-C9-C31
16	Y	212	L2T	N19-C28-C9-C35
16	Y	212	L2T	C34-C33-O36-C37
16	Y	212	L2T	C32-C33-O36-C37
16	Y	212	L2T	O29-C28-C9-C35
17	Y	213	MES	N4-C7-C8-S
16	K	213	L2T	O29-C28-C9-C31
16	K	213	L2T	N19-C28-C9-C31

There are no ring outliers.

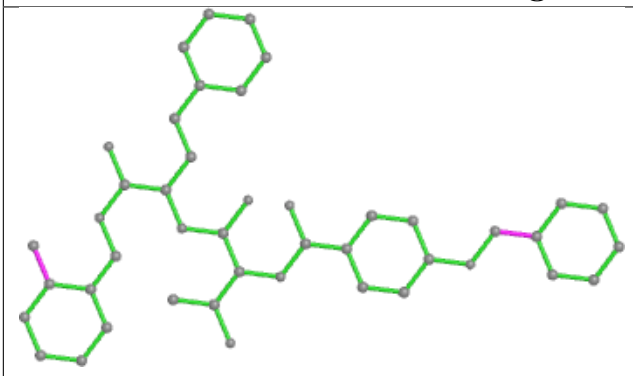
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	213	L2T	5	0
16	Y	212	L2T	2	0
17	K	214	MES	1	0
17	Y	213	MES	1	0

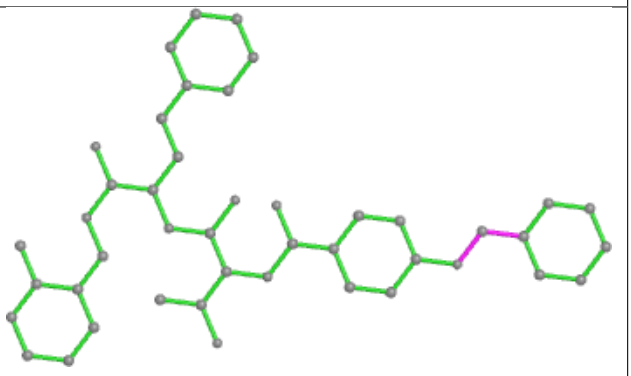
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

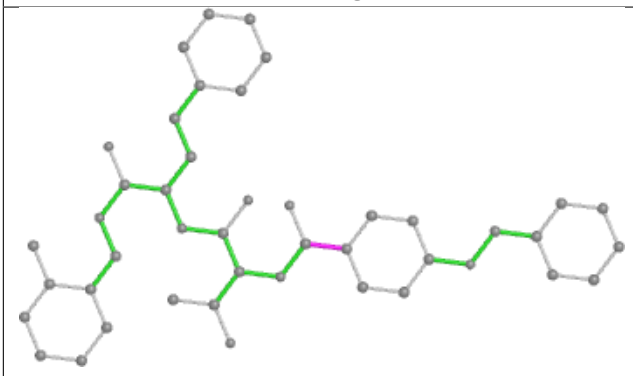
Ligand L2T K 213



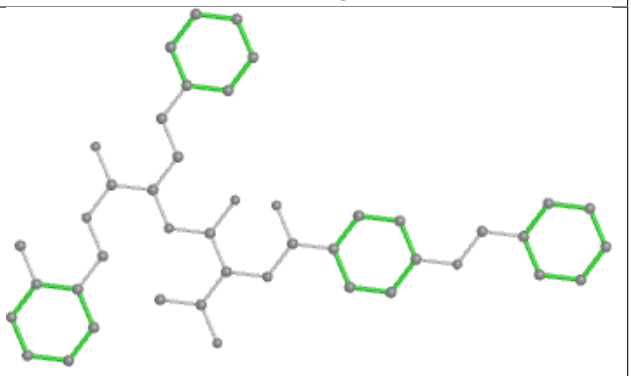
Bond lengths



Bond angles

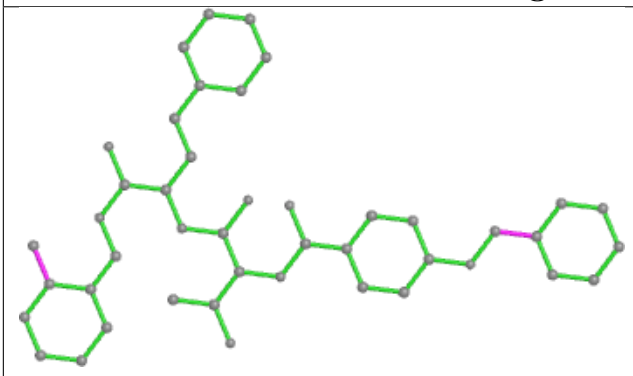


Torsions

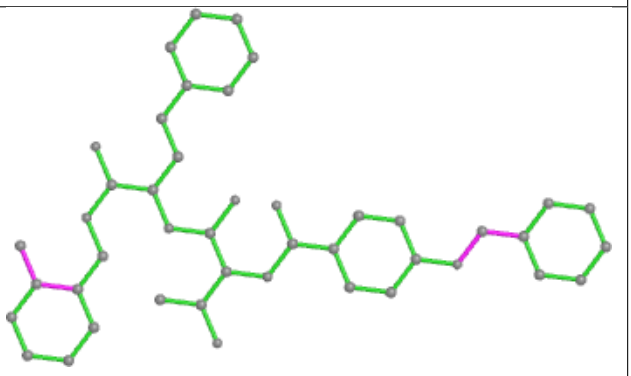


Rings

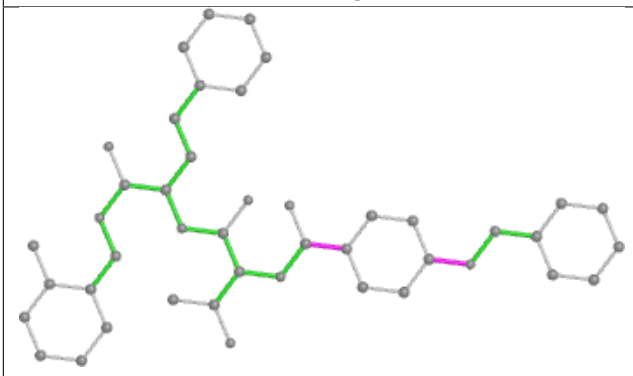
Ligand L2T Y 212



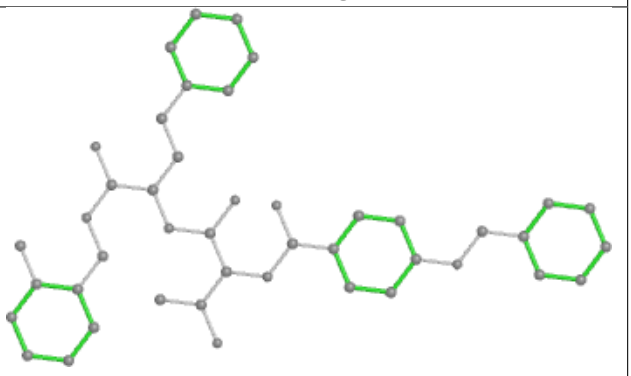
Bond lengths



Bond angles



Torsions



Rings

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
7	G	3
14	2	3
13	1	3
9	I	3
9	W	3
3	C	2
10	J	2
10	X	2
3	Q	2
5	S	2
6	F	2
12	Z	2
12	L	2
8	V	2
8	H	2
11	K	1
1	A	1
1	O	1
2	P	1
11	Y	1
6	T	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	4.65
1	C	203:THR	C	206:GLY	N	4.56
1	R	123(G):GLU	C	125:GLU	N	4.48

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	-1:MET	C	1:ASP	N	4.02
1	X	-1:MET	C	1:ASP	N	3.71
1	Q	180(D):GLU	C	182:PRO	N	3.30
1	S	204:GLU	C	206:SER	N	3.24
1	M	181(A):THR	C	183:GLY	N	3.20
1	K	181:ASP	C	183:GLY	N	3.19
1	Q	203:THR	C	206:GLY	N	3.18
1	E	204:GLU	C	206:SER	N	3.11
1	C	180(D):GLU	C	182:PRO	N	3.08
1	F	180(F):GLY	C	184:LEU	N	3.02
1	S	60:SER	C	63:TYR	N	3.01
1	A	200:SER	C	202:VAL	N	3.00
1	N	181:ALA	C	183:GLY	N	3.00
1	O	200:SER	C	202:VAL	N	3.00
1	E	207(E):ASN	C	210:LEU	N	2.96
1	R	233:ILE	C	235:LYS	N	2.96
1	Z	-1:GLY	C	1:GLY	N	2.87
1	G	180(D):ILE	C	184:ASN	N	2.83
1	L	-1:GLY	C	1:GLY	N	2.83
1	R	202:GLU	C	205:GLU	N	2.80
1	P	200:THR	C	202:THR	N	2.75
1	G	184(M):SER	C	186:TRP	N	2.73
1	V	91:GLN	C	93:GLY	N	2.72
1	F	199:LEU	C	201:ALA	N	2.68
1	Y	181:ASP	C	183:GLY	N	2.68
1	Z	180:LYS	C	182:ASP	N	2.68
1	E	180(F):ILE	C	183:ASP	N	2.61
1	2	92:ASP	C	94:ASN	N	2.60
1	1	181(A):THR	C	183:GLY	N	2.59
1	2	181:ALA	C	183:GLY	N	2.59
1	D	202:GLU	C	205:GLU	N	2.58
1	X	181:ASP	C	183:GLY	N	2.58
1	D	233:ILE	C	235:LYS	N	2.56
1	L	180:LYS	C	182:ASP	N	2.56
1	E	60:SER	C	63:TYR	N	2.55
1	D	180(E):SER	C	184:LEU	N	2.50
1	I	179:LYS	C	181:LYS	N	2.50
1	T	199:LEU	C	201:ALA	N	2.48
1	W	179:LYS	C	181:LYS	N	2.47
1	J	181:ASP	C	183:GLY	N	2.46
1	U	218:ASP	C	220:LYS	N	2.46
1	V	187:LEU	C	189:ARG	N	2.33

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	70:TYR	C	72:GLY	N	2.31
1	1	141(G):ILE	C	144:PRO	N	2.27
1	B	200:THR	C	202:THR	N	2.25
1	H	187:LEU	C	189:ARG	N	2.23
1	N	70:TYR	C	72:GLY	N	2.21
1	H	91:GLN	C	93:GLY	N	2.20
1	M	-1:GLY	C	1:THR	N	2.19
1	M	141(G):ILE	C	144:PRO	N	2.18
1	I	36:HIS	C	38:TYR	N	2.17
1	W	36:HIS	C	38:TYR	N	2.16
1	G	218:ASP	C	220:LYS	N	2.10
1	I	-1:GLY	C	1:GLY	N	2.05
1	N	92:ASP	C	94:ASN	N	2.04
1	W	-1:GLY	C	1:GLY	N	2.00
1	1	-1:GLY	C	1:THR	N	1.87

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%)	0.13	7 (2%)	53	48	37, 54, 80, 110	0
1	O	250/250 (100%)	0.27	15 (6%)	21	16	41, 62, 88, 115	0
2	B	235/245 (95%)	0.21	8 (3%)	45	39	41, 60, 92, 106	0
2	P	235/245 (95%)	0.29	7 (2%)	50	45	39, 63, 97, 108	0
3	C	241/243 (99%)	0.54	26 (10%)	5	4	43, 69, 110, 125	0
3	Q	241/243 (99%)	0.90	48 (19%)	1	0	45, 74, 121, 140	0
4	D	242/250 (96%)	0.42	17 (7%)	16	11	40, 65, 101, 122	0
4	R	242/250 (96%)	0.43	16 (6%)	18	13	41, 65, 101, 129	0
5	E	233/234 (99%)	0.34	18 (7%)	13	9	48, 63, 91, 111	0
5	S	233/234 (99%)	0.48	23 (9%)	7	5	46, 64, 97, 125	0
6	F	237/248 (95%)	0.06	6 (2%)	57	52	39, 57, 95, 107	0
6	T	237/248 (95%)	0.12	6 (2%)	57	52	38, 58, 85, 109	0
7	G	243/252 (96%)	0.08	5 (2%)	63	59	36, 51, 80, 111	0
7	U	243/252 (96%)	-0.05	3 (1%)	79	76	35, 51, 73, 101	0
8	H	222/222 (100%)	-0.07	0	100	100	34, 48, 65, 99	0
8	V	222/222 (100%)	-0.06	1 (0%)	91	90	39, 52, 72, 107	0
9	I	204/205 (99%)	-0.03	2 (0%)	82	80	36, 48, 66, 82	0
9	W	204/205 (99%)	0.06	2 (0%)	82	80	35, 51, 69, 86	0
10	J	198/198 (100%)	0.09	7 (3%)	44	38	38, 51, 68, 127	0
10	X	198/198 (100%)	0.10	6 (3%)	50	45	39, 53, 68, 125	0
11	K	212/212 (100%)	-0.04	4 (1%)	66	63	36, 50, 69, 88	0
11	Y	212/212 (100%)	-0.13	0	100	100	36, 51, 70, 77	0
12	L	222/241 (92%)	-0.05	1 (0%)	91	90	36, 51, 71, 82	0
12	Z	222/241 (92%)	0.02	4 (1%)	68	65	34, 50, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1	233/266 (87%)	-0.10	2 (0%)	84	82	34, 48, 63, 67	0
13	M	233/266 (87%)	-0.06	1 (0%)	92	92	36, 51, 65, 71	0
14	2	196/196 (100%)	-0.12	2 (1%)	82	80	34, 46, 64, 79	0
14	N	196/196 (100%)	-0.13	1 (0%)	91	90	37, 45, 60, 76	0
All	All	6336/6524 (97%)	0.14	238 (3%)	40	35	34, 54, 91, 140	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	123(C)	GLY	12.0
4	R	123(E)	SER	11.5
4	R	123(F)	GLY	11.1
3	C	7	GLY	10.9
4	R	123(C)	GLY	10.8
4	R	123(D)	ALA	9.8
4	D	123(B)	GLU	8.8
4	D	123(E)	SER	8.7
2	P	217	ALA	8.2
10	J	192	ALA	8.0
3	C	9	ASP	7.9
4	D	123(F)	GLY	7.7
3	C	11	ALA	7.7
7	G	240	ASP	7.5
3	C	8	TYR	7.5
2	P	218	ASN	7.4
4	R	123(B)	GLU	7.4
13	1	-8	THR	7.3
2	B	218	ASN	7.1
1	O	4	MET	6.8
13	M	-8	THR	6.8
3	Q	56	LEU	6.7
4	D	123(D)	ALA	6.7
3	Q	55	THR	6.5
5	E	4	PHE	6.2
4	R	10	ARG	6.2
10	J	193	GLN	6.1
2	B	217	ALA	6.1
5	S	4	PHE	6.1
7	U	6	ALA	6.0
7	G	6	ALA	5.8
7	U	240	ASP	5.7

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Mol	Chain	Res	Type	RSRZ
2	P	216(B)	GLY	5.7
6	F	12	ASN	5.7
3	Q	236	ILE	5.7
4	D	10	ARG	5.6
3	Q	237	GLU	5.6
2	B	216(B)	GLY	5.5
10	J	-1	MET	5.5
3	Q	233	VAL	5.3
1	A	236	LEU	5.2
1	O	5	THR	5.2
10	J	191	GLN	5.1
3	Q	54	SER	4.9
3	Q	206	GLY	4.9
10	X	-1	MET	4.9
4	D	9	ASP	4.8
5	S	206	SER	4.8
3	Q	8	TYR	4.7
1	O	6	ASP	4.6
3	Q	238	GLN	4.6
3	Q	209	ASN	4.6
4	D	11	GLY	4.5
10	X	191	GLN	4.4
6	T	12	ASN	4.3
4	D	127	LEU	4.3
1	A	5	THR	4.3
3	Q	7	GLY	4.3
5	S	57	GLU	4.3
10	X	193	GLN	4.2
4	R	9	ASP	4.2
1	A	4	MET	4.1
3	C	208	LYS	3.9
3	Q	243	GLN	3.9
1	O	236	LEU	3.9
4	R	127	LEU	3.8
5	E	206	SER	3.8
3	Q	203	THR	3.7
3	C	12	LEU	3.7
8	V	223	ASP	3.7
3	Q	241	GLN	3.7
3	Q	192	LEU	3.6
6	T	13	SER	3.6
4	D	22	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
3	Q	234	THR	3.6
3	Q	240	LYS	3.6
12	Z	-9	GLN	3.6
1	A	8	TYR	3.5
3	C	236	ILE	3.5
4	R	123(A)	GLY	3.5
3	Q	198	LEU	3.5
10	J	92	ARG	3.5
6	F	199	LEU	3.4
5	S	51	LEU	3.4
3	Q	11	ALA	3.4
3	Q	197	LEU	3.4
5	E	189	LEU	3.4
3	Q	9	ASP	3.3
1	O	235	ALA	3.3
3	Q	210	ILE	3.2
4	D	12	VAL	3.2
5	E	5	ARG	3.2
5	S	58	LEU	3.2
6	F	13	SER	3.2
10	X	192	ALA	3.2
5	S	181	LYS	3.2
3	C	198	LEU	3.2
3	Q	201	VAL	3.1
3	Q	184	ALA	3.1
3	C	191	LYS	3.1
3	C	243	GLN	3.1
3	C	53	ARG	3.1
1	A	203	GLU	3.1
3	C	232	TYR	3.1
3	C	194	VAL	3.1
2	P	54	VAL	3.0
7	G	234	VAL	3.0
6	T	199	LEU	3.0
5	E	203	ASP	3.0
3	Q	180(D)	GLU	2.9
5	S	5	ARG	2.9
7	G	239	GLN	2.9
11	K	208	ASN	2.9
3	C	13	SER	2.9
3	C	10	ARG	2.9
5	S	8	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
3	Q	229	ILE	2.9
3	C	234	THR	2.9
1	O	197	LEU	2.9
4	R	11	GLY	2.8
1	O	217(P)	LYS	2.8
1	O	191	HIS	2.8
5	S	233	ILE	2.8
5	S	203	ASP	2.8
3	Q	53	ARG	2.8
1	A	234	GLU	2.8
5	S	127	TYR	2.8
5	E	233	ILE	2.8
3	Q	208	LYS	2.8
4	R	123(G)	GLU	2.8
3	Q	187	GLU	2.8
10	J	168	MET	2.7
5	S	63	TYR	2.7
3	Q	232	TYR	2.7
3	C	240	LYS	2.7
5	S	6	ASN	2.7
3	Q	62(A)	ILE	2.7
7	U	199	ASP	2.7
14	2	92	ASP	2.7
3	C	237	GLU	2.7
4	R	187	LYS	2.7
4	D	123(A)	GLY	2.6
9	W	181	LYS	2.6
1	O	234	GLU	2.6
2	B	239	THR	2.6
5	E	178	ARG	2.6
1	O	194	LEU	2.6
3	Q	64	PRO	2.5
10	X	188	ASP	2.5
2	B	185	LYS	2.5
10	J	49	ALA	2.5
1	O	195	LEU	2.5
9	I	181	LYS	2.5
3	Q	193	THR	2.5
4	D	123(G)	GLU	2.4
1	A	7	ARG	2.4
3	Q	52	ARG	2.4
5	E	175	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	207(E)	ASN	2.4
12	L	-9	GLN	2.4
3	Q	180(C)	LYS	2.4
3	Q	63	THR	2.4
6	T	240	ILE	2.4
3	Q	40	VAL	2.4
3	Q	188	GLU	2.4
4	D	241	GLU	2.4
5	E	191	LYS	2.4
5	S	197	ILE	2.4
7	G	236	ILE	2.4
3	Q	207	ALA	2.4
1	O	8	TYR	2.4
3	C	55	THR	2.4
3	C	56	LEU	2.4
3	Q	13	SER	2.3
3	Q	196	SER	2.3
4	D	242	ALA	2.3
1	O	233	LEU	2.3
14	N	92	ASP	2.3
3	Q	58	LEU	2.3
5	E	128	GLY	2.3
3	C	184	ALA	2.3
5	E	168	ARG	2.3
9	I	182	ASP	2.3
5	S	184	GLY	2.3
2	B	235	LYS	2.3
5	S	178	ARG	2.3
9	W	179	LYS	2.3
14	2	95	LEU	2.3
5	S	180(B)	THR	2.3
3	C	233	VAL	2.3
6	F	206(B)	GLU	2.2
1	O	7	ARG	2.2
2	B	220	TYR	2.2
3	Q	191	LYS	2.2
3	Q	239	GLU	2.2
5	E	201	LEU	2.2
2	P	220	TYR	2.2
3	C	187	GLU	2.2
5	S	204	GLU	2.2
4	R	126	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	41	ALA	2.2
4	R	229	THR	2.2
11	K	151	ALA	2.2
1	O	9	SER	2.2
6	F	205	ASN	2.2
11	K	148	VAL	2.2
6	T	203	GLU	2.2
11	K	183	GLY	2.2
3	Q	200	VAL	2.1
5	E	174	THR	2.1
3	C	179	ASN	2.1
12	Z	182	ASP	2.1
3	Q	189	CYS	2.1
5	S	195	GLU	2.1
4	D	186	LEU	2.1
5	S	189	LEU	2.1
12	Z	92	PHE	2.1
4	R	231	GLU	2.1
6	F	201	ALA	2.1
5	S	9	ASP	2.1
3	C	188	GLU	2.1
5	E	186	PRO	2.1
12	Z	145	TYR	2.1
5	S	199	GLN	2.1
6	T	238	LYS	2.1
2	P	63	THR	2.1
13	1	181(A)	THR	2.1
3	Q	38	VAL	2.1
2	P	235	LYS	2.1
5	E	207	LEU	2.0
2	B	22	TYR	2.0
5	E	202	ARG	2.0
5	E	214	ILE	2.0
3	Q	242	GLU	2.0
10	X	10	ASP	2.0
3	C	238	GLN	2.0
4	R	125	GLU	2.0
5	S	55	ALA	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)

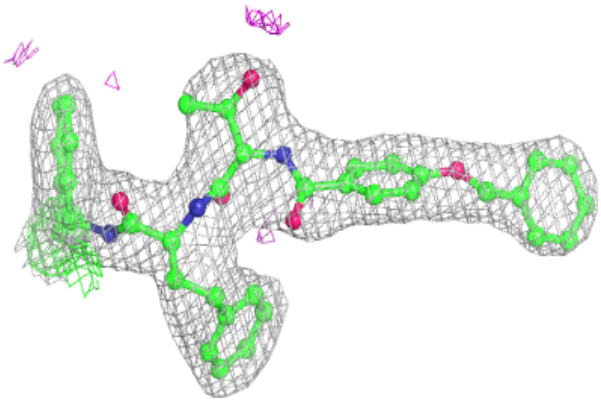
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

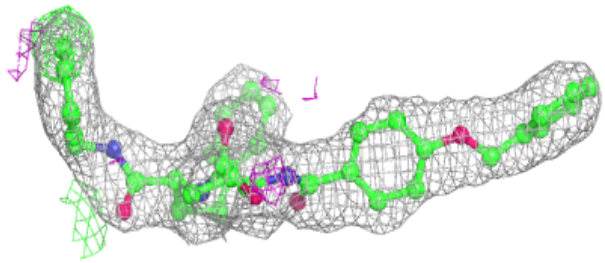
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	F	242	1/1	0.69	0.41	74,74,74,74	0
15	MG	I	196	1/1	0.69	0.31	68,68,68,68	0
15	MG	F	243	1/1	0.80	0.81	118,118,118,118	0
15	MG	L	195	1/1	0.81	0.24	66,66,66,66	0
15	MG	I	195	1/1	0.87	0.58	72,72,72,72	0
15	MG	L	196	1/1	0.88	0.20	52,52,52,52	0
16	L2T	K	213	44/44	0.92	0.21	45,47,55,55	1
17	MES	K	214	12/12	0.92	0.20	90,90,90,90	0
15	MG	H	224	1/1	0.93	0.15	57,57,57,57	0
15	MG	N	188	1/1	0.93	0.11	50,50,50,50	0
15	MG	K	212	1/1	0.93	0.28	55,55,55,55	0
16	L2T	Y	212	44/44	0.93	0.22	49,51,56,57	1
15	MG	G	241	1/1	0.93	0.10	54,54,54,54	0
17	MES	Y	213	12/12	0.95	0.20	97,98,98,98	0

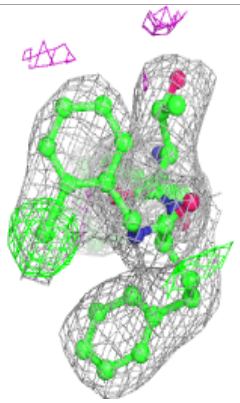
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L2T 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)

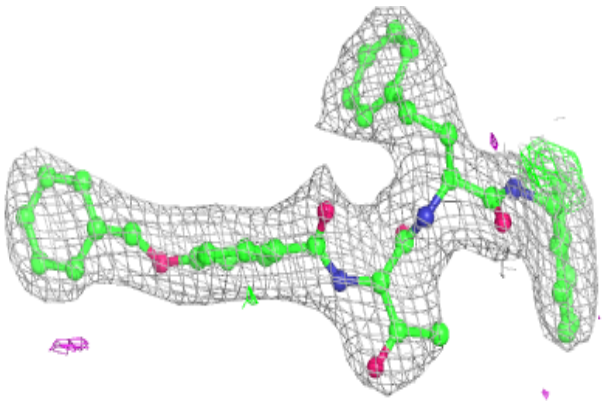


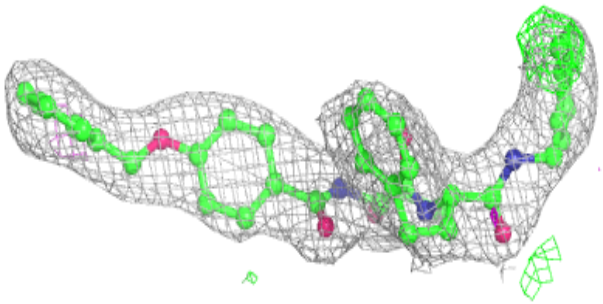


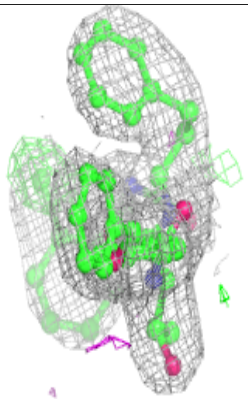


Electron density around L2T Y 212:

$2mF_o$-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.