



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:33 PM BST

PDB ID : 4NO9
Title : yCP in complex with Z-Leu-Leu-Leu-epoxyketone
Authors : Stein, M.L.; Cui, H.; Beck, P.; Dubiella, C.; Voss, C.; Krueger, A.; Schmidt, B.; Groll, M.
Deposited on : 2013-11-19
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

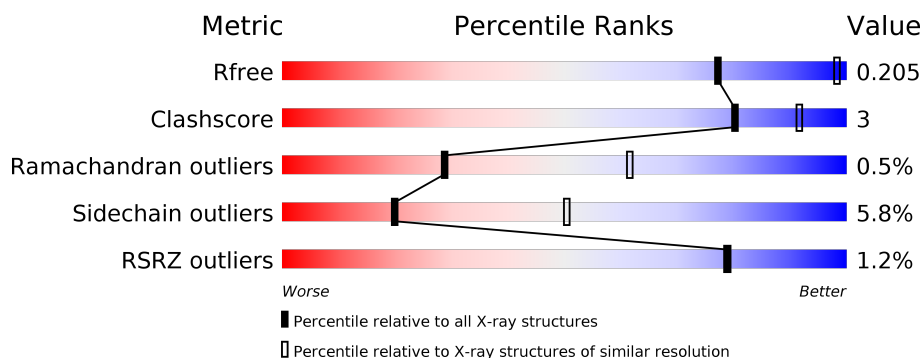
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>2%</div> <div>95%</div> <div>•</div> </div>
1	O	250	<div> <div>2%</div> <div>94%</div> <div>6%</div> </div>
2	B	258	<div> <div>3%</div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>82%</div> <div>11%</div> <div>• 5%</div> </div>
3	C	254	<div> <div>4%</div> <div>82%</div> <div>9%</div> <div>• 6%</div> </div>
3	Q	254	<div> <div>4%</div> <div>82%</div> <div>9%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	% 78% 11% 10%
4	R	260	78% 12% 10%
5	E	234	84% 13% ..
5	S	234	84% 13% ..
6	F	288	76% 7% 16%
6	T	288	% 76% 8% 16%
7	G	252	% 86% 8% . .
7	U	252	% 86% 8% . .
8	H	232	% 84% 10% . .
8	V	232	% 84% 10% . .
9	I	205	91% 8%
9	W	205	92% 8%
10	J	198	% 89% 8% . .
10	X	198	% 89% 8% . .
11	K	212	87% 12% .
11	Y	212	88% 11% .
12	L	222	91% 9% .
12	Z	222	90% 9% .
13	M	246	89% 5% 5%
13	a	246	90% . 5%
14	N	196	93% 7% .
14	b	196	96% .

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49622 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 subunit alpha type-2.

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

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

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

- Molecule 9 is a protein called Proteasome subunit beta type-3.

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1642	1044	280	311	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

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

- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

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

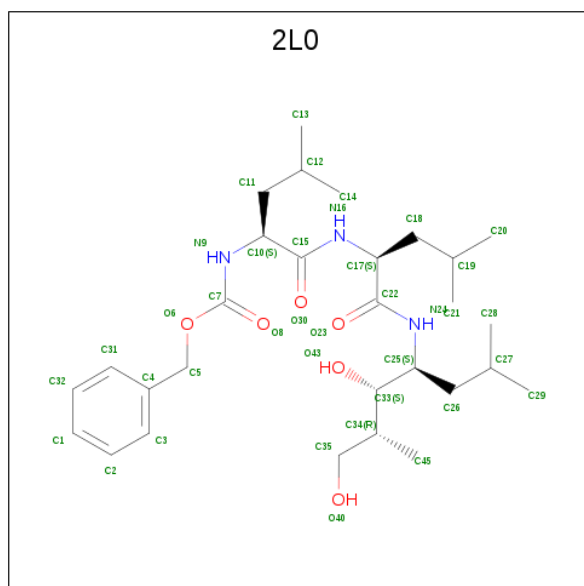
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

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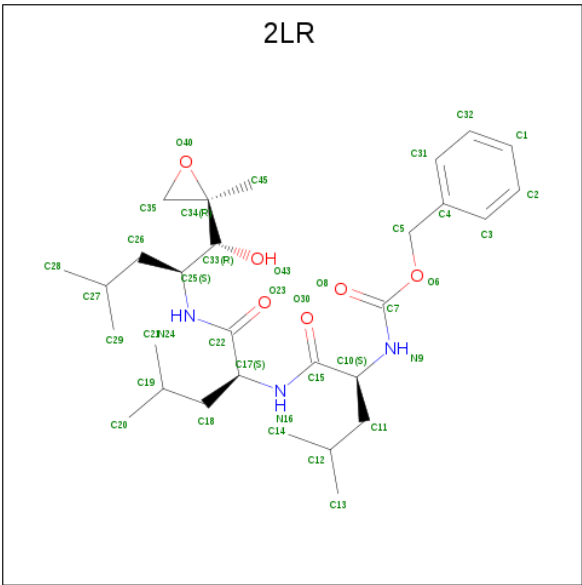
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		

- Molecule 16 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2R,3S,4S)-1,3-dihydroxy-2,6-dimethylheptan-4-yl]-L-leucinamide (three-letter code: 2L0) (formula: $C_{29}H_{49}N_3O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	H	1	Total	C	N	O	0	0
			38	29	3	6		
16	K	1	Total	C	N	O	0	0
			38	29	3	6		
16	Y	1	Total	C	N	O	0	0
			38	29	3	6		

- Molecule 17 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(1R,2S)-1-hydroxy-4-methyl-1-[(2R)-2-methyloxiran-2-yl]pentan-2-yl]-L-leucinamide (three-letter code: 2LR) (formula: $C_{29}H_{47}N_3O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	V	1	Total	C	N	O	0	0
			38	29	3	6		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	3	Total	O	0	0
			3	3		
18	B	4	Total	O	0	0
			4	4		
18	C	1	Total	O	0	0
			1	1		
18	D	4	Total	O	0	0
			4	4		
18	E	2	Total	O	0	0
			2	2		
18	F	6	Total	O	0	0
			6	6		
18	G	6	Total	O	0	0
			6	6		
18	H	7	Total	O	0	0
			7	7		
18	I	5	Total	O	0	0
			5	5		
18	J	10	Total	O	0	0
			10	10		
18	K	12	Total	O	0	0
			12	12		

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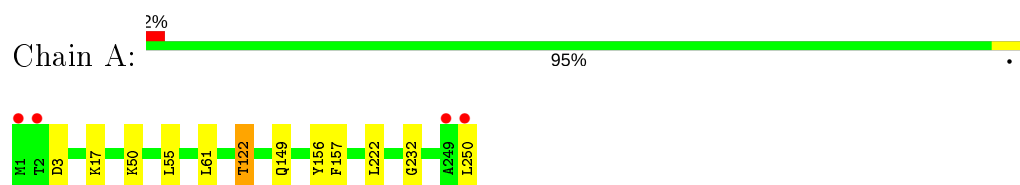
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	11	Total 11	O 11	0	0
18	M	13	Total 13	O 13	0	0
18	N	7	Total 7	O 7	0	0
18	O	4	Total 4	O 4	0	0
18	P	1	Total 1	O 1	0	0
18	Q	1	Total 1	O 1	0	0
18	R	4	Total 4	O 4	0	0
18	S	2	Total 2	O 2	0	0
18	T	6	Total 6	O 6	0	0
18	U	11	Total 11	O 11	0	0
18	V	7	Total 7	O 7	0	0
18	W	3	Total 3	O 3	0	0
18	X	9	Total 9	O 9	0	0
18	Y	10	Total 10	O 10	0	0
18	Z	2	Total 2	O 2	0	0
18	a	8	Total 8	O 8	0	0
18	b	9	Total 9	O 9	0	0

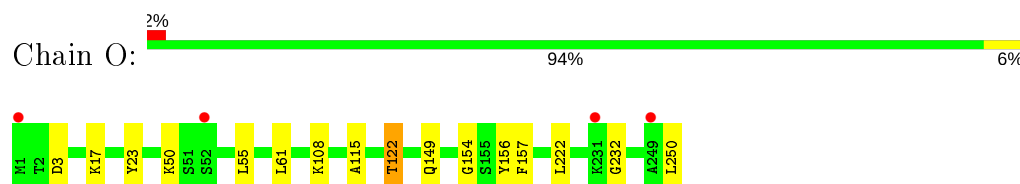
3 Residue-property plots [i](#)

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.

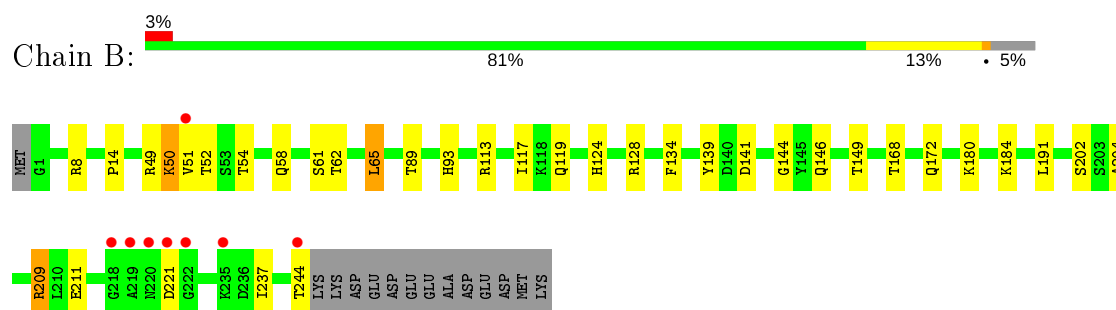
- Molecule 1: Proteasome subunit alpha type-2



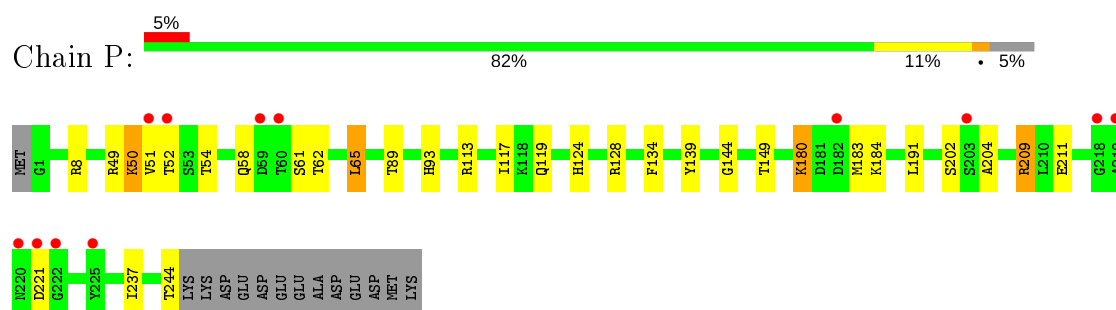
- Molecule 1: Proteasome subunit alpha type-2



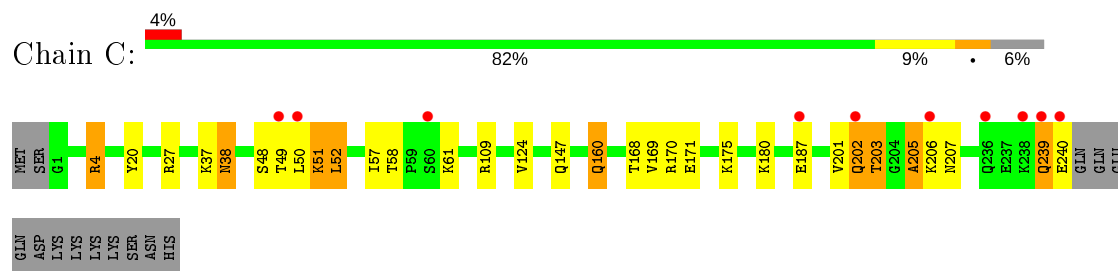
- Molecule 2: Proteasome subunit alpha type-3



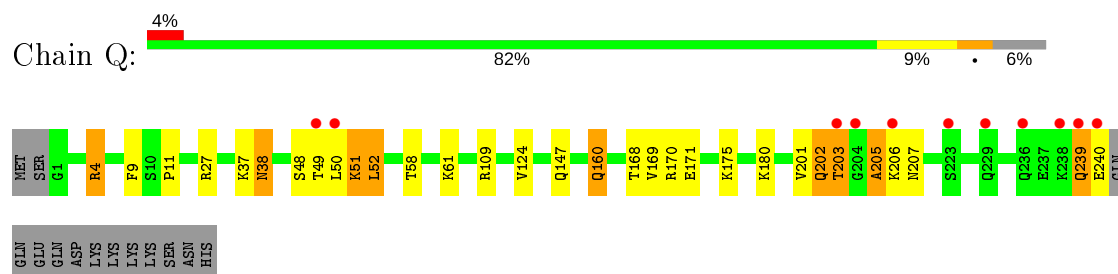
- Molecule 2: Proteasome subunit alpha type-3



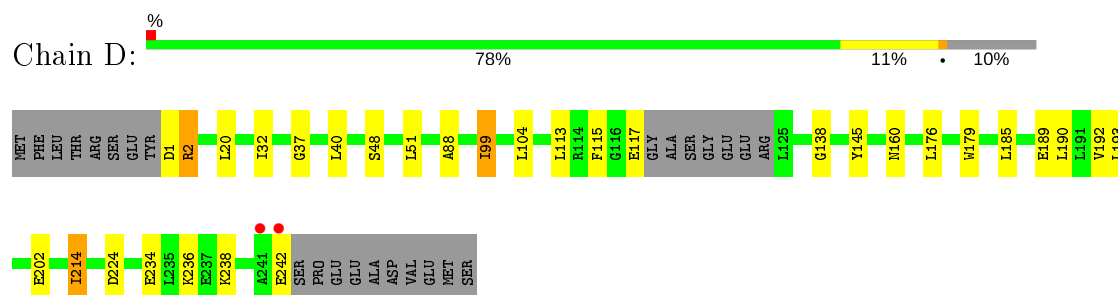
- Molecule 3: Proteasome subunit alpha type-4



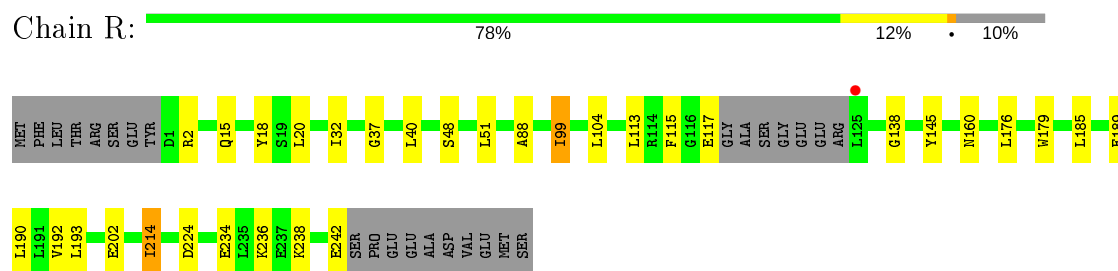
- Molecule 3: Proteasome subunit alpha type-4



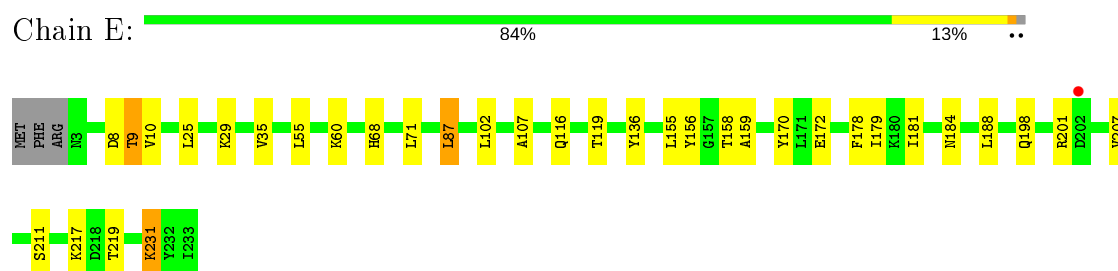
- Molecule 4: Proteasome subunit alpha type-5



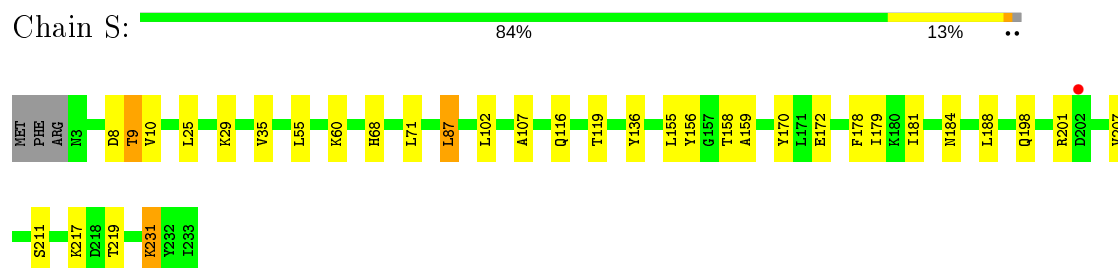
- Molecule 4: Proteasome subunit alpha type-5



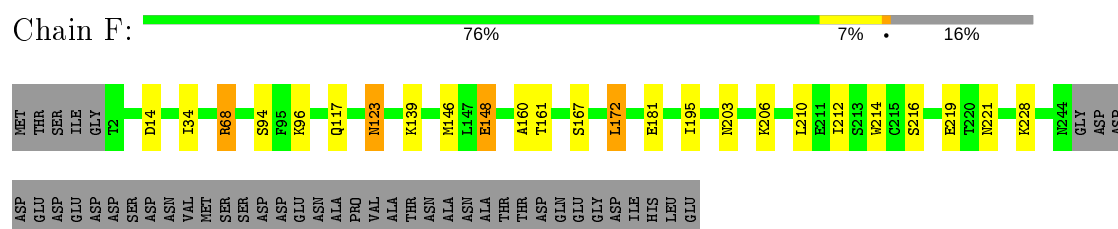
- Molecule 5: Proteasome subunit alpha type-6



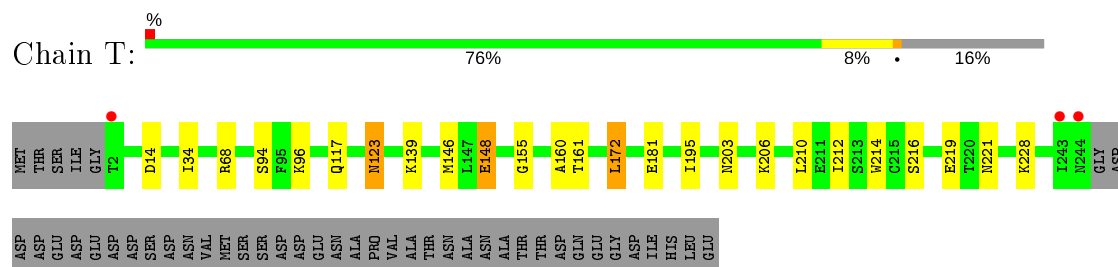
- Molecule 5: Proteasome subunit alpha type-6



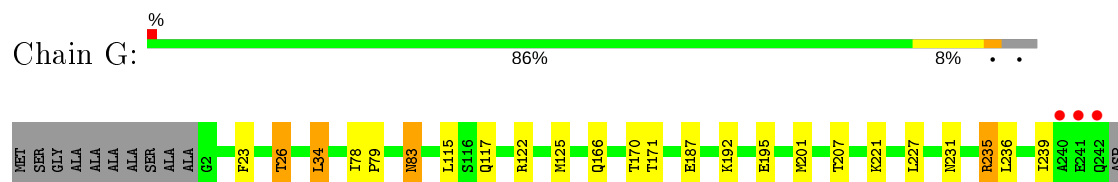
- Molecule 6: Probable proteasome subunit alpha type-7



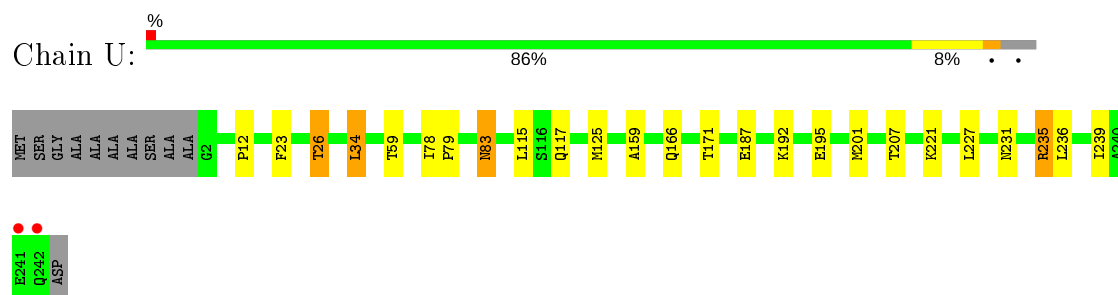
- Molecule 6: Probable proteasome subunit alpha type-7



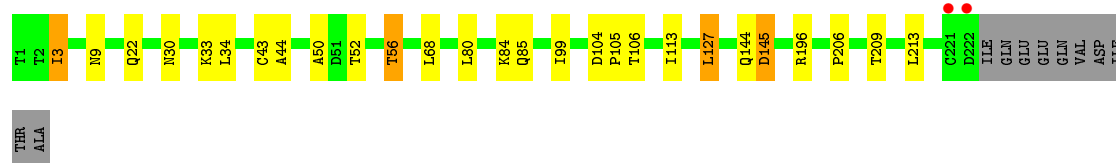
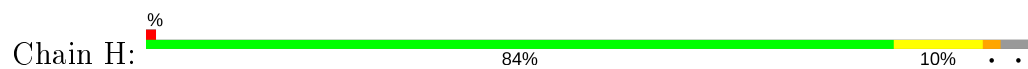
- Molecule 7: Proteasome subunit alpha type-1



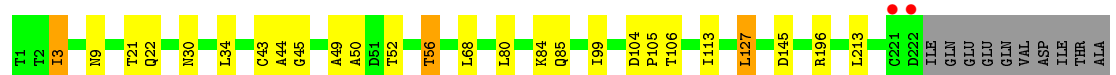
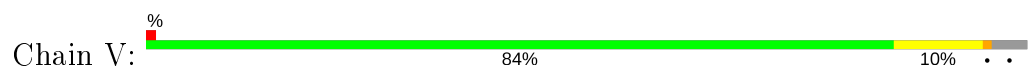
- Molecule 7: Proteasome subunit alpha type-1



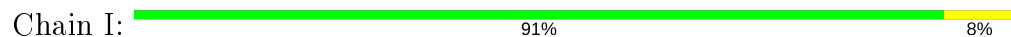
- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2



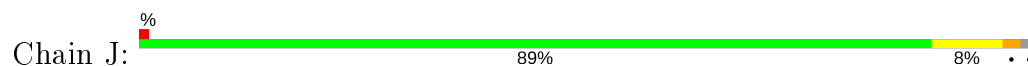
- Molecule 9: Proteasome subunit beta type-3



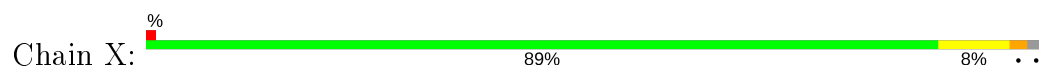
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4

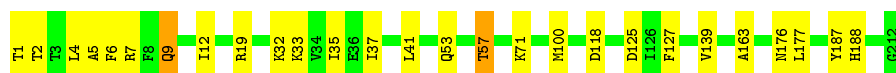


- Molecule 10: Proteasome subunit beta type-4



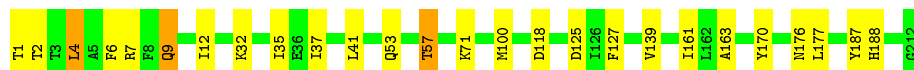
- Molecule 11: Proteasome subunit beta type-5





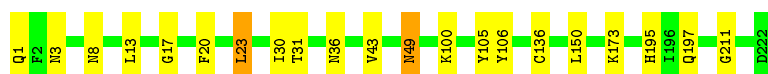
- Molecule 11: Proteasome subunit beta type-5

Chain Y: 88% 11% .



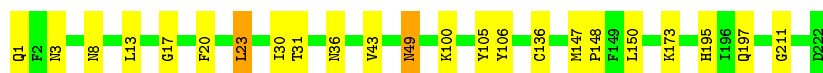
- Molecule 12: Proteasome subunit beta type-6

Chain L: 91% 9% .



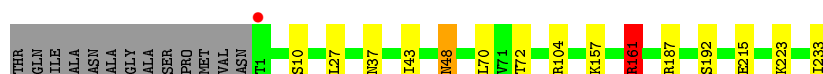
- Molecule 12: Proteasome subunit beta type-6

Chain Z: 90% 9% .



- Molecule 13: Proteasome subunit beta type-7

Chain M: 89% 5% 5% .



- Molecule 13: Proteasome subunit beta type-7

Chain a: 90% 5% .



- Molecule 14: Proteasome subunit beta type-1

Chain N: 93% 7% .



- Molecule 14: Proteasome subunit beta type-1

Chain b: 96% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.49 Å 301.49 Å 144.39 Å 90.00° 114.15° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 14.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-2.90) 99.0 (14.99-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.91 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.203 0.181 , 0.205	Depositor DCC
R_{free} test set	11515 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49622	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 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2L0, 2LR

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	0.28	0/1952	0.52	0/2642
1	O	0.28	0/1952	0.52	0/2642
2	B	0.28	0/1934	0.57	0/2618
2	P	0.28	0/1934	0.57	0/2618
3	C	0.28	0/1910	0.56	0/2586
3	Q	0.29	0/1910	0.56	0/2586
4	D	0.29	0/1837	0.56	0/2475
4	R	0.29	0/1837	0.56	0/2475
5	E	0.28	0/1800	0.53	0/2433
5	S	0.28	0/1800	0.53	0/2433
6	F	0.28	0/1932	0.51	0/2609
6	T	0.29	0/1932	0.51	0/2609
7	G	0.28	0/1945	0.54	0/2634
7	U	0.28	0/1945	0.54	0/2634
8	H	0.26	0/1715	0.54	0/2326
8	V	0.26	0/1715	0.53	0/2326
9	I	0.28	0/1611	0.53	0/2174
9	W	0.28	0/1611	0.53	0/2174
10	J	0.27	0/1589	0.53	0/2142
10	X	0.27	0/1589	0.53	0/2142
11	K	0.27	0/1681	0.53	0/2274
11	Y	0.27	0/1678	0.53	0/2268
12	L	0.28	0/1795	0.51	0/2420
12	Z	0.28	0/1795	0.51	0/2420
13	M	0.28	0/1855	0.58	1/2514 (0.0%)
13	a	0.28	0/1855	0.57	1/2514 (0.0%)
14	N	0.26	0/1541	0.51	0/2087
14	b	0.27	0/1541	0.51	0/2087
All	All	0.28	0/50191	0.54	2/67862 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	161	ARG	NE-CZ-NH1	5.33	122.97	120.30
13	a	161	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1929	5	0
1	O	1915	0	1929	8	0
2	B	1904	0	1904	17	0
2	P	1904	0	1904	14	0
3	C	1881	0	1895	18	0
3	Q	1881	0	1895	18	0
4	D	1813	0	1797	10	0
4	R	1813	0	1797	11	0
5	E	1773	0	1775	9	0
5	S	1773	0	1775	9	0
6	F	1892	0	1883	11	0
6	T	1892	0	1883	11	0
7	G	1907	0	1901	10	0
7	U	1907	0	1901	12	0
8	H	1684	0	1685	14	0
8	V	1684	0	1687	11	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	7	0
11	K	1644	0	1593	19	0
11	Y	1642	0	1589	13	0
12	L	1757	0	1711	9	0
12	Z	1757	0	1711	10	0
13	M	1824	0	1832	4	0
13	a	1824	0	1832	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	5	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	H	38	0	47	4	0
16	K	38	0	47	8	0
16	Y	38	0	47	1	0
17	V	38	0	46	3	0
18	A	3	0	0	1	0
18	B	4	0	0	0	0
18	C	1	0	0	0	0
18	D	4	0	0	0	0
18	E	2	0	0	0	0
18	F	6	0	0	0	0
18	G	6	0	0	0	0
18	H	7	0	0	0	0
18	I	5	0	0	0	0
18	J	10	0	0	0	0
18	K	12	0	0	0	0
18	L	11	0	0	0	0
18	M	13	0	0	0	0
18	N	7	0	0	0	0
18	O	4	0	0	1	0
18	P	1	0	0	0	0
18	Q	1	0	0	0	0
18	R	4	0	0	0	0
18	S	2	0	0	0	0
18	T	6	0	0	0	0
18	U	11	0	0	0	0
18	V	7	0	0	0	0
18	W	3	0	0	0	0
18	X	9	0	0	0	0
18	Y	10	0	0	0	0
18	Z	2	0	0	0	0
18	a	8	0	0	0	0
18	b	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49622	0	49243	255	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 3.

All (255) 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)
11:Y:170:TYR:O	16:Y:301:2L0:H44	1.63	0.99
11:K:33:LYS:NZ	16:K:301:2L0:H45	1.80	0.96
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.53	0.88
11:K:33:LYS:HZ3	16:K:301:2L0:H45	1.38	0.86
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.58	0.84
11:Y:1:THR:CA	11:Y:2:THR:N	2.43	0.81
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.46	0.81
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.46	0.80
11:K:53:GLN:O	11:K:57:THR:HG23	1.84	0.77
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.84	0.76
7:G:23:PHE:O	7:G:26:THR:HB	1.91	0.71
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.19	0.71
11:K:100:MET:CE	11:K:127:PHE:HB2	2.20	0.71
8:H:33:LYS:NZ	16:H:301:2L0:H45	2.05	0.71
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.91	0.70
7:U:23:PHE:O	7:U:26:THR:HB	1.90	0.70
2:B:50:LYS:HE3	2:B:50:LYS:HA	1.74	0.70
3:C:51:LYS:O	3:C:52:LEU:HB2	1.91	0.69
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.58	0.69
2:P:50:LYS:HA	2:P:50:LYS:HE3	1.74	0.69
3:C:202:GLN:HG3	3:C:203:THR:H	1.58	0.69
10:J:19:LYS:HD3	10:J:180:ILE:HG13	1.77	0.66
8:H:33:LYS:HZ3	16:H:301:2L0:H45	1.63	0.64
10:X:19:LYS:HD3	10:X:180:ILE:HG13	1.78	0.64
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.64	0.62
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.26	0.62
11:K:33:LYS:HZ1	16:K:301:2L0:H45	1.64	0.61
8:V:3:ILE:HG12	8:V:44:ALA:HB1	1.82	0.61
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.66	0.61
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.65	0.60
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.82	0.60
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.82	0.60
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.84	0.60
8:H:3:ILE:HG12	8:H:44:ALA:HB1	1.83	0.59
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.50	0.59
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.85	0.59
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.85	0.58
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.85	0.58
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.85	0.58
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.34	0.58
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.85	0.58
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.50	0.57
3:Q:202:GLN:CG	3:Q:203:THR:H	2.18	0.57
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.04	0.57
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.70	0.57
3:C:201:VAL:O	3:C:202:GLN:HB2	2.04	0.57
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.33	0.57
3:C:202:GLN:CG	3:C:203:THR:H	2.18	0.56
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.87	0.56
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.70	0.56
8:H:52:THR:O	8:H:56:THR:HB	2.06	0.56
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.88	0.56
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.71	0.55
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.88	0.55
3:C:48:SER:HB2	3:C:207:ASN:OD1	2.07	0.55
14:N:20:THR:HG22	14:N:31:THR:OG1	2.07	0.55
11:K:100:MET:HE3	11:K:127:PHE:CB	2.32	0.55
2:P:65:LEU:HD22	2:P:211:GLU:HB3	1.89	0.54
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.88	0.54
8:V:52:THR:O	8:V:56:THR:HB	2.07	0.54
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.41	0.54
2:B:50:LYS:HA	2:B:50:LYS:CE	2.36	0.54
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.88	0.54
3:Q:48:SER:HB2	3:Q:207:ASN:OD1	2.08	0.54
2:B:65:LEU:HD22	2:B:211:GLU:HB3	1.89	0.53
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.89	0.53
2:P:50:LYS:HA	2:P:50:LYS:CE	2.36	0.53
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.91	0.53
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.90	0.53
11:K:33:LYS:NZ	16:K:301:2L0:C45	2.66	0.53
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.91	0.52
14:N:20:THR:CG2	14:N:31:THR:OG1	2.58	0.52
10:J:1:MET:HA	10:J:34:LYS:CE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.25	0.52
8:V:49:ALA:HB2	17:V:301:2LR:H17	1.91	0.52
10:X:1:MET:HA	10:X:34:LYS:CE	2.40	0.52
4:R:234:GLU:O	4:R:238:LYS:HG3	2.10	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.92	0.51
5:E:68:HIS:HE1	5:E:102:LEU:O	1.94	0.51
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.92	0.51
11:K:19:ARG:O	16:K:301:2L0:C45	2.59	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.50
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.41	0.50
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.42	0.50
4:D:234:GLU:O	4:D:238:LYS:HG3	2.11	0.50
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.92	0.50
3:Q:205:ALA:C	3:Q:207:ASN:H	2.14	0.50
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.58	0.50
10:J:1:MET:HA	10:J:34:LYS:HE3	1.94	0.50
12:L:195:HIS:HD2	12:L:197:GLN:H	1.58	0.49
3:C:205:ALA:C	3:C:207:ASN:H	2.15	0.49
5:S:68:HIS:HE1	5:S:102:LEU:O	1.94	0.49
6:F:146:MET:CE	6:F:161:THR:HB	2.42	0.49
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.47	0.49
6:T:146:MET:CE	6:T:161:THR:HB	2.42	0.49
10:X:1:MET:HA	10:X:34:LYS:HE3	1.95	0.49
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.47	0.49
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.47	0.49
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.47	0.49
2:B:49:ARG:HH22	2:B:61:SER:HB3	1.78	0.49
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.28	0.49
7:U:83:ASN:C	7:U:83:ASN:HD22	2.17	0.49
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.47	0.49
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.48	0.49
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.48	0.48
10:J:174:MET:HA	10:X:174:MET:HA	1.94	0.48
11:K:33:LYS:HZ1	16:K:301:2L0:C45	2.26	0.48
2:P:49:ARG:HH22	2:P:61:SER:HB3	1.77	0.48
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.96	0.48
16:H:301:2L0:H36	16:H:301:2L0:H46	1.40	0.48
7:G:83:ASN:C	7:G:83:ASN:HD22	2.17	0.48
11:K:19:ARG:O	16:K:301:2L0:H46	2.15	0.47
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.97	0.47
8:V:45:GLY:O	17:V:301:2LR:H29	2.13	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.47
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.50	0.47
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.49	0.47
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.96	0.47
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.96	0.47
6:T:228:LYS:HB2	6:T:228:LYS:HE3	1.70	0.47
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.62	0.47
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.96	0.47
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.96	0.47
5:S:9:THR:HG21	5:S:119:THR:HA	1.97	0.47
9:W:14:MET:HB3	9:W:162:LEU:HD11	1.96	0.47
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.96	0.47
2:B:141:ASP:O	10:J:110:LYS:NZ	2.48	0.46
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.50	0.46
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.96	0.46
5:S:155:LEU:HD13	5:S:158:THR:HB	1.98	0.46
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.97	0.46
8:V:99:ILE:HG13	8:V:127:LEU:HD22	1.97	0.46
5:E:155:LEU:HD13	5:E:158:THR:HB	1.98	0.46
5:E:9:THR:HG21	5:E:119:THR:HA	1.97	0.46
8:V:21:THR:OG1	17:V:301:2LR:H20	2.15	0.46
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.97	0.45
14:N:152:VAL:HA	14:N:175:MET:HE1	1.97	0.45
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.31	0.45
1:A:222:LEU:HD13	1:A:232:GLY:HA2	1.99	0.45
5:S:170:TYR:HB2	5:S:198:GLN:HG3	1.99	0.45
5:E:170:TYR:HB2	5:E:198:GLN:HG3	1.99	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.99	0.45
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.50	0.45
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.47	0.45
4:D:113:LEU:HD23	4:D:115:PHE:HE1	1.81	0.45
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.99	0.45
8:H:84:LYS:HG3	8:H:85:GLN:N	2.32	0.45
4:R:113:LEU:HD23	4:R:115:PHE:HE1	1.81	0.45
11:Y:7:ARG:HG3	11:Y:12:ILE:HG12	1.99	0.45
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.99	0.45
7:G:34:LEU:HD23	7:G:34:LEU:C	2.37	0.45
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:99:ILE:HG13	8:H:127:LEU:HD22	1.99	0.45
11:K:7:ARG:HG3	11:K:12:ILE:HG12	1.99	0.45
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.99	0.45
7:U:195:GLU:HG2	7:U:239:ILE:HG13	1.99	0.44
7:U:227:LEU:HB3	7:U:231:ASN:HB2	2.00	0.44
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.44
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.47	0.44
8:H:33:LYS:HZ1	16:H:301:2L0:H45	1.78	0.44
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.99	0.44
6:F:146:MET:HE1	6:F:161:THR:HB	1.98	0.44
3:C:201:VAL:HG13	3:C:202:GLN:N	2.32	0.44
1:O:222:LEU:HD13	1:O:232:GLY:HA2	1.99	0.44
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.00	0.44
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.48	0.44
11:K:6:PHE:HA	11:K:125:ASP:O	2.18	0.44
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.44
8:V:84:LYS:HG3	8:V:85:GLN:N	2.32	0.43
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.31	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
6:F:146:MET:HE2	6:F:148:GLU:OE2	2.19	0.43
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.99	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.43
8:H:206:PRO:O	8:H:209:THR:OG1	2.32	0.43
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.51	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
7:G:195:GLU:HG2	7:G:239:ILE:HG13	2.00	0.43
6:T:146:MET:HE3	6:T:161:THR:HB	2.01	0.43
7:U:34:LEU:C	7:U:34:LEU:HD23	2.38	0.43
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.49	0.43
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.18	0.43
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.48	0.43
4:D:185:LEU:O	4:D:189:GLU:HG3	2.19	0.43
6:F:228:LYS:HB2	6:F:228:LYS:HE3	1.71	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.19	0.43
1:O:108:LYS:HG2	18:O:302:HOH:O	2.18	0.42
13:M:48:ASN:H	13:M:48:ASN:HD22	1.66	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
2:P:134:PHE:O	2:P:149:THR:HA	2.20	0.42
3:C:168:THR:O	3:C:171:GLU:HB3	2.19	0.42
4:R:185:LEU:O	4:R:189:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.42
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.02	0.42
1:A:149:GLN:O	1:A:156:TYR:HA	2.20	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.55	0.42
8:H:104:ASP:OD1	8:H:106:THR:HB	2.20	0.42
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.01	0.42
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.02	0.42
10:J:36:ARG:HA	10:J:36:ARG:HD3	1.90	0.42
6:T:146:MET:HE2	6:T:148:GLU:OE2	2.19	0.42
3:Q:27:ARG:HB2	3:Q:27:ARG:CZ	2.50	0.42
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.02	0.42
11:Y:177:LEU:HB3	11:Y:188:HIS:HB2	2.02	0.42
2:B:134:PHE:O	2:B:149:THR:HA	2.20	0.42
5:E:156:TYR:CD1	5:E:179:ILE:HD13	2.55	0.42
16:K:301:2L0:H36	16:K:301:2L0:H46	1.41	0.42
6:T:123:ASN:HD22	6:T:123:ASN:C	2.23	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.42
2:P:204:ALA:O	2:P:209:ARG:NH2	2.53	0.42
5:S:156:TYR:CD1	5:S:179:ILE:HD13	2.55	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.33	0.41
3:C:48:SER:C	3:C:50:LEU:H	2.22	0.41
2:B:168:THR:O	2:B:172:GLN:HB2	2.20	0.41
2:B:204:ALA:O	2:B:209:ARG:NH2	2.53	0.41
8:H:50:ALA:HB2	9:I:128:CYS:HB2	2.02	0.41
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.01	0.41
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.56	0.41
5:E:35:VAL:HG22	5:E:159:ALA:HB2	2.03	0.41
6:F:123:ASN:C	6:F:123:ASN:HD22	2.24	0.41
3:Q:48:SER:C	3:Q:50:LEU:H	2.22	0.41
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.56	0.41
8:H:144:GLN:O	8:H:145:ASP:HB2	2.21	0.41
11:K:177:LEU:HB3	11:K:188:HIS:HB2	2.02	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.19	0.41
8:V:104:ASP:OD1	8:V:106:THR:HB	2.21	0.41
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.02	0.41
11:K:139:VAL:HG21	11:K:163:ALA:CB	2.51	0.41
5:S:35:VAL:HG22	5:S:159:ALA:HB2	2.02	0.41
7:U:83:ASN:C	7:U:83:ASN:ND2	2.74	0.41
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.03	0.41
11:Y:139:VAL:HG21	11:Y:163:ALA:CB	2.51	0.41
9:I:111:ILE:HD12	9:I:189:ILE:HG22	2.03	0.41
11:K:1:THR:HG22	11:K:2:THR:N	2.36	0.41
1:O:115:ALA:HB1	1:O:154:GLY:O	2.21	0.41
2:P:180:LYS:O	2:P:183:MET:HB2	2.21	0.41
3:C:27:ARG:CZ	3:C:27:ARG:HB2	2.50	0.41
3:Q:205:ALA:C	3:Q:207:ASN:N	2.74	0.41
9:W:111:ILE:HD12	9:W:189:ILE:HG22	2.03	0.41
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.86	0.40
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.86	0.40
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.56	0.40
3:C:205:ALA:C	3:C:207:ASN:N	2.74	0.40
18:A:301:HOH:O	7:G:122:ARG:HD2	2.20	0.40
4:D:1:ASP:O	4:D:2:ARG:HB2	2.21	0.40
14:N:35:THR:CG2	14:N:45:ARG:HE	2.34	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
2	B	242/258 (94%)	229 (95%)	10 (4%)	3 (1%)	13	40
2	P	242/258 (94%)	230 (95%)	9 (4%)	3 (1%)	13	40
3	C	238/254 (94%)	227 (95%)	4 (2%)	7 (3%)	4	18
3	Q	238/254 (94%)	227 (95%)	4 (2%)	7 (3%)	4	18
4	D	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	34	66
5	E	229/234 (98%)	220 (96%)	8 (4%)	1 (0%)	34	66
5	S	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	34	66
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	214 (97%)	4 (2%)	2 (1%)	17	48
8	V	220/232 (95%)	214 (97%)	4 (2%)	2 (1%)	17	48
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
11	K	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	29	61
11	Y	209/212 (99%)	202 (97%)	6 (3%)	1 (0%)	29	61
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6275/6614 (95%)	6068 (97%)	173 (3%)	34 (0%)	29	61

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	62	THR
3	C	38	ASN
3	C	202	GLN
3	C	206	LYS
2	P	62	THR
3	Q	38	ASN
3	Q	202	GLN
2	B	51	VAL
3	C	205	ALA

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Mol	Chain	Res	Type
4	D	2	ARG
5	E	231	LYS
8	H	9	ASN
2	P	51	VAL
3	Q	205	ALA
3	Q	206	LYS
4	R	2	ARG
5	S	231	LYS
8	V	9	ASN
2	B	221	ASP
3	C	239	GLN
10	J	2	ASP
2	P	221	ASP
3	Q	239	GLN
10	X	2	ASP
3	C	49	THR
8	H	145	ASP
3	Q	49	THR
8	V	145	ASP
1	A	3	ASP
11	K	9	GLN
1	O	3	ASP
3	Q	52	LEU
3	C	52	LEU
11	Y	9	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	203 (97%)	6 (3%)	42 76
1	O	209/209 (100%)	203 (97%)	6 (3%)	42 76
2	B	203/216 (94%)	190 (94%)	13 (6%)	17 45
2	P	203/216 (94%)	190 (94%)	13 (6%)	17 45
3	C	212/226 (94%)	196 (92%)	16 (8%)	13 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	212/226 (94%)	197 (93%)	15 (7%)	14	40
4	D	194/215 (90%)	180 (93%)	14 (7%)	14	39
4	R	194/215 (90%)	180 (93%)	14 (7%)	14	39
5	E	190/193 (98%)	172 (90%)	18 (10%)	8	26
5	S	190/193 (98%)	172 (90%)	18 (10%)	8	26
6	F	201/239 (84%)	186 (92%)	15 (8%)	13	37
6	T	201/239 (84%)	187 (93%)	14 (7%)	15	41
7	G	206/210 (98%)	193 (94%)	13 (6%)	18	46
7	U	206/210 (98%)	193 (94%)	13 (6%)	18	46
8	H	181/190 (95%)	171 (94%)	10 (6%)	21	53
8	V	181/190 (95%)	171 (94%)	10 (6%)	21	53
9	I	172/173 (99%)	166 (96%)	6 (4%)	36	70
9	W	172/173 (99%)	166 (96%)	6 (4%)	36	70
10	J	173/175 (99%)	163 (94%)	10 (6%)	20	50
10	X	173/175 (99%)	163 (94%)	10 (6%)	20	50
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	64
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	64
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	67
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33	67
13	M	199/208 (96%)	187 (94%)	12 (6%)	19	49
13	a	199/208 (96%)	187 (94%)	12 (6%)	19	49
14	N	162/162 (100%)	154 (95%)	8 (5%)	25	57
14	b	162/162 (100%)	154 (95%)	8 (5%)	25	57
All	All	5312/5540 (96%)	5004 (94%)	308 (6%)	20	50

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	50	LYS
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	250	LEU

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Mol	Chain	Res	Type
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	58	GLN
2	B	65	LEU
2	B	119	GLN
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	202	SER
2	B	209	ARG
2	B	237	ILE
2	B	244	THR
3	C	4	ARG
3	C	37	LYS
3	C	38	ASN
3	C	51	LYS
3	C	58	THR
3	C	61	LYS
3	C	109	ARG
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	239	GLN
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	48	SER
4	D	51	LEU
4	D	99	ILE
4	D	117	GLU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS

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Mol	Chain	Res	Type
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	60	LYS
5	E	71	LEU
5	E	87	LEU
5	E	116	GLN
5	E	172	GLU
5	E	184	ASN
5	E	188	LEU
5	E	201	ARG
5	E	207	VAL
5	E	211	SER
5	E	219	THR
5	E	231	LYS
6	F	14	ASP
6	F	68	ARG
6	F	94	SER
6	F	96	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	148	GLU
6	F	167	SER
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	26	THR
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	171	THR

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Mol	Chain	Res	Type
7	G	201	MET
7	G	207	THR
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	3	ILE
8	H	22	GLN
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
8	H	213	LEU
9	I	37	ASN
9	I	123	PHE
9	I	171	LEU
9	I	182	TRP
9	I	191	LYS
9	I	192	ASP
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	36	ARG
10	J	75	LEU
10	J	78	GLN
10	J	91	SER
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	32	LYS
11	K	35	ILE
11	K	57	THR
11	K	71	LYS
11	K	118	ASP
12	L	1	GLN
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN

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Mol	Chain	Res	Type
12	L	106	TYR
12	L	136	CYS
12	L	173	LYS
13	M	10	SER
13	M	37	ASN
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	157	LYS
13	M	161	ARG
13	M	187	ARG
13	M	215	GLU
13	M	223	LYS
13	M	233	ILE
14	N	9	LYS
14	N	20	THR
14	N	22	THR
14	N	36	ARG
14	N	104	ASP
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	17	LYS
1	O	50	LYS
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	54	THR
2	P	58	GLN
2	P	65	LEU
2	P	119	GLN
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	202	SER
2	P	209	ARG
2	P	237	ILE
2	P	244	THR

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Mol	Chain	Res	Type
3	Q	4	ARG
3	Q	37	LYS
3	Q	38	ASN
3	Q	51	LYS
3	Q	58	THR
3	Q	61	LYS
3	Q	109	ARG
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	203	THR
3	Q	239	GLN
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	48	SER
4	R	51	LEU
4	R	99	ILE
4	R	117	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	60	LYS
5	S	71	LEU
5	S	87	LEU
5	S	116	GLN
5	S	172	GLU
5	S	184	ASN
5	S	188	LEU

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Mol	Chain	Res	Type
5	S	201	ARG
5	S	207	VAL
5	S	211	SER
5	S	219	THR
5	S	231	LYS
6	T	14	ASP
6	T	68	ARG
6	T	94	SER
6	T	96	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	148	GLU
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	26	THR
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	171	THR
7	U	201	MET
7	U	207	THR
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	V	3	ILE
8	V	22	GLN
8	V	30	ASN
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
8	V	213	LEU

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Mol	Chain	Res	Type
9	W	37	ASN
9	W	123	PHE
9	W	171	LEU
9	W	182	TRP
9	W	191	LYS
9	W	192	ASP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	36	ARG
10	X	75	LEU
10	X	78	GLN
10	X	91	SER
10	X	144	LEU
10	X	163	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	32	LYS
11	Y	35	ILE
11	Y	57	THR
11	Y	71	LYS
11	Y	118	ASP
12	Z	1	GLN
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	106	TYR
12	Z	136	CYS
12	Z	173	LYS
13	a	10	SER
13	a	37	ASN
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	157	LYS
13	a	161	ARG
13	a	187	ARG
13	a	215	GLU
13	a	223	LYS
13	a	233	ILE

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Mol	Chain	Res	Type
14	b	9	LYS
14	b	20	THR
14	b	22	THR
14	b	36	ARG
14	b	104	ASP
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	226	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	203	ASN

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Mol	Chain	Res	Type
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	172	ASN
8	H	189	ASN
10	J	55	GLN
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	80	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	69	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	226	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN

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Mol	Chain	Res	Type
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	203	ASN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
8	V	30	ASN
8	V	57	GLN
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN
10	X	86	GLN
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 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	2L0	Y	301	11	38,38,38	1.54	2 (5%)	47,50,50	2.64	5 (10%)
16	2L0	H	301	8	38,38,38	1.29	2 (5%)	47,50,50	1.65	6 (12%)
16	2L0	K	301	11	38,38,38	1.02	2 (5%)	47,50,50	1.60	3 (6%)
17	2LR	V	301	8	38,39,39	1.62	4 (10%)	49,54,54	2.66	8 (16%)

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	2L0	Y	301	11	-	6/47/47/47	0/1/1/1
16	2L0	H	301	8	-	8/47/47/47	0/1/1/1
16	2L0	K	301	11	-	8/47/47/47	0/1/1/1
17	2LR	V	301	8	-	6/47/51/51	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	2L0	C45-C34	7.44	1.71	1.53
17	V	301	2LR	C45-C34	-6.93	1.36	1.52
16	H	301	2L0	C45-C34	-5.07	1.40	1.53
16	H	301	2L0	C5-C4	-4.38	1.40	1.50
16	K	301	2L0	C5-C4	-4.33	1.40	1.50
17	V	301	2LR	C5-C4	-4.11	1.40	1.50
16	Y	301	2L0	C5-C4	-4.11	1.40	1.50
17	V	301	2LR	C35-C34	2.80	1.53	1.46
16	K	301	2L0	C34-C33	2.16	1.57	1.53
17	V	301	2LR	O40-C35	-2.05	1.39	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	2L0	C45-C34-C35	-14.62	90.68	109.88
17	V	301	2LR	C45-C34-C35	-11.37	97.95	119.48
17	V	301	2LR	O40-C34-C45	-10.42	94.42	113.72
16	K	301	2L0	C45-C34-C33	-8.52	95.75	111.54
16	Y	301	2L0	C45-C34-C33	7.90	126.18	111.54
16	H	301	2L0	C26-C25-N24	-6.00	102.43	110.18
17	V	301	2LR	C35-O40-C34	5.42	65.86	60.44
16	H	301	2L0	C45-C34-C33	-5.17	101.95	111.54
17	V	301	2LR	C34-C33-C25	-4.45	105.33	115.71
17	V	301	2LR	O6-C7-N9	4.40	119.45	110.50
16	Y	301	2L0	O6-C7-N9	4.35	119.34	110.50
16	H	301	2L0	O6-C7-N9	4.34	119.32	110.50
16	K	301	2L0	O6-C7-N9	4.25	119.14	110.50
16	H	301	2L0	C45-C34-C35	-3.93	104.72	109.88
16	H	301	2L0	O8-C7-N9	-2.99	119.95	124.85
17	V	301	2LR	O8-C7-N9	-2.97	119.97	124.85
16	K	301	2L0	O8-C7-N9	-2.76	120.33	124.85
16	Y	301	2L0	O8-C7-N9	-2.73	120.37	124.85
17	V	301	2LR	O40-C34-C35	-2.11	56.12	59.78
16	Y	301	2L0	O6-C7-O8	-2.07	120.28	124.25
17	V	301	2LR	C12-C11-C10	-2.06	109.76	115.43
16	H	301	2L0	C19-C18-C17	-2.02	109.87	115.43

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	H	301	2L0	N24-C25-C26-C27
16	H	301	2L0	C33-C25-C26-C27
16	Y	301	2L0	N24-C25-C33-C34
16	Y	301	2L0	N24-C25-C33-O43
16	Y	301	2L0	C26-C25-C33-C34
16	Y	301	2L0	C26-C25-C33-O43
17	V	301	2LR	C33-C25-C26-C27
16	K	301	2L0	N24-C25-C33-C34
16	K	301	2L0	N24-C25-C33-O43
16	K	301	2L0	C26-C25-C33-C34
16	K	301	2L0	C26-C25-C33-O43
16	K	301	2L0	C33-C34-C35-O40
16	K	301	2L0	C45-C34-C35-O40
16	Y	301	2L0	O8-C7-O6-C5
16	Y	301	2L0	N9-C7-O6-C5
17	V	301	2LR	N16-C17-C18-C19
17	V	301	2LR	C22-C17-C18-C19
16	H	301	2L0	N16-C17-C18-C19
16	H	301	2L0	C22-C17-C18-C19
17	V	301	2LR	N24-C25-C26-C27
16	K	301	2L0	O8-C7-O6-C5
16	K	301	2L0	N9-C7-O6-C5
16	H	301	2L0	N16-C17-C22-O23
16	H	301	2L0	N16-C17-C22-N24
17	V	301	2LR	C25-C33-C34-O40
17	V	301	2LR	C25-C26-C27-C28
16	H	301	2L0	N24-C25-C33-O43
16	H	301	2L0	N24-C25-C33-C34

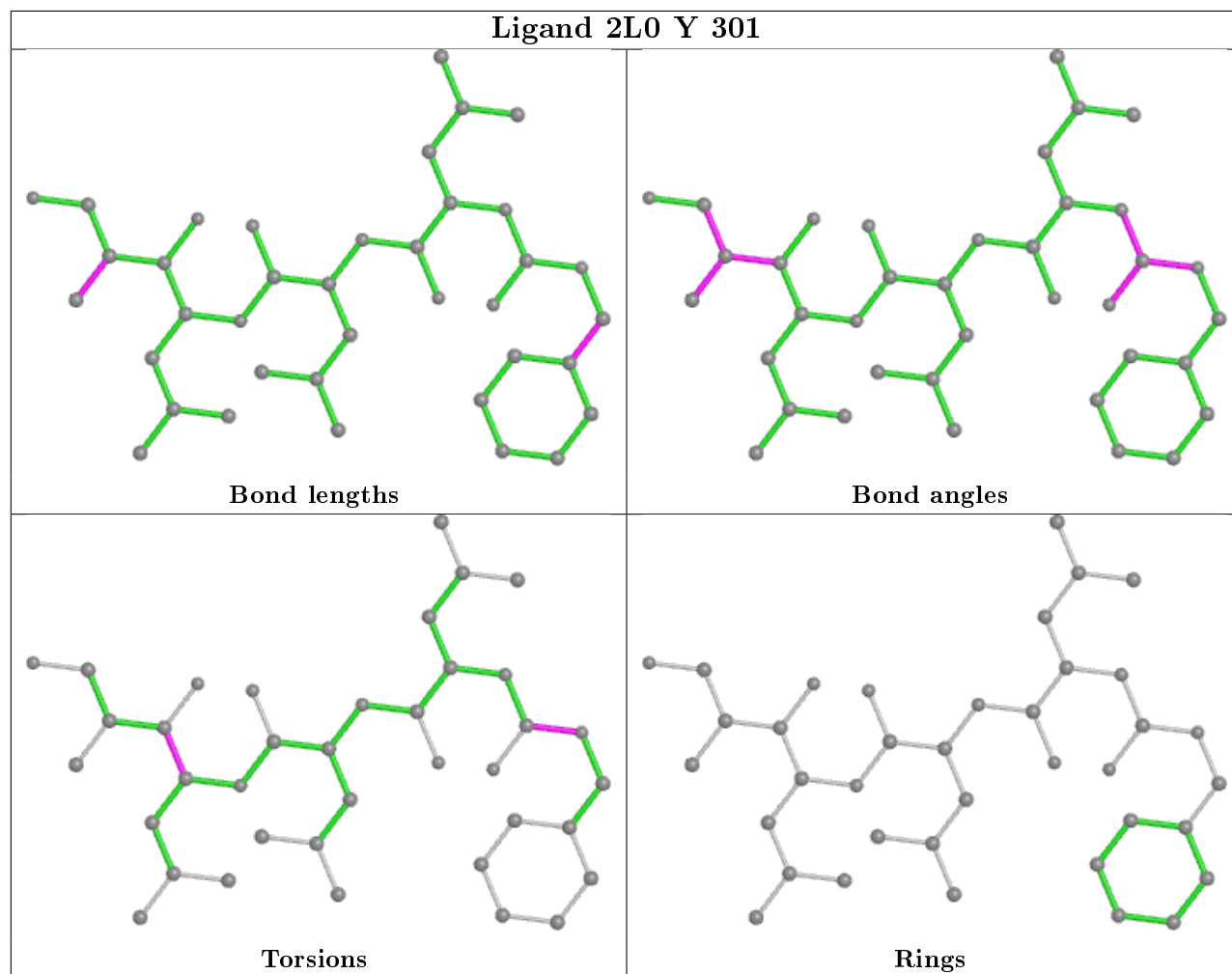
There are no ring outliers.

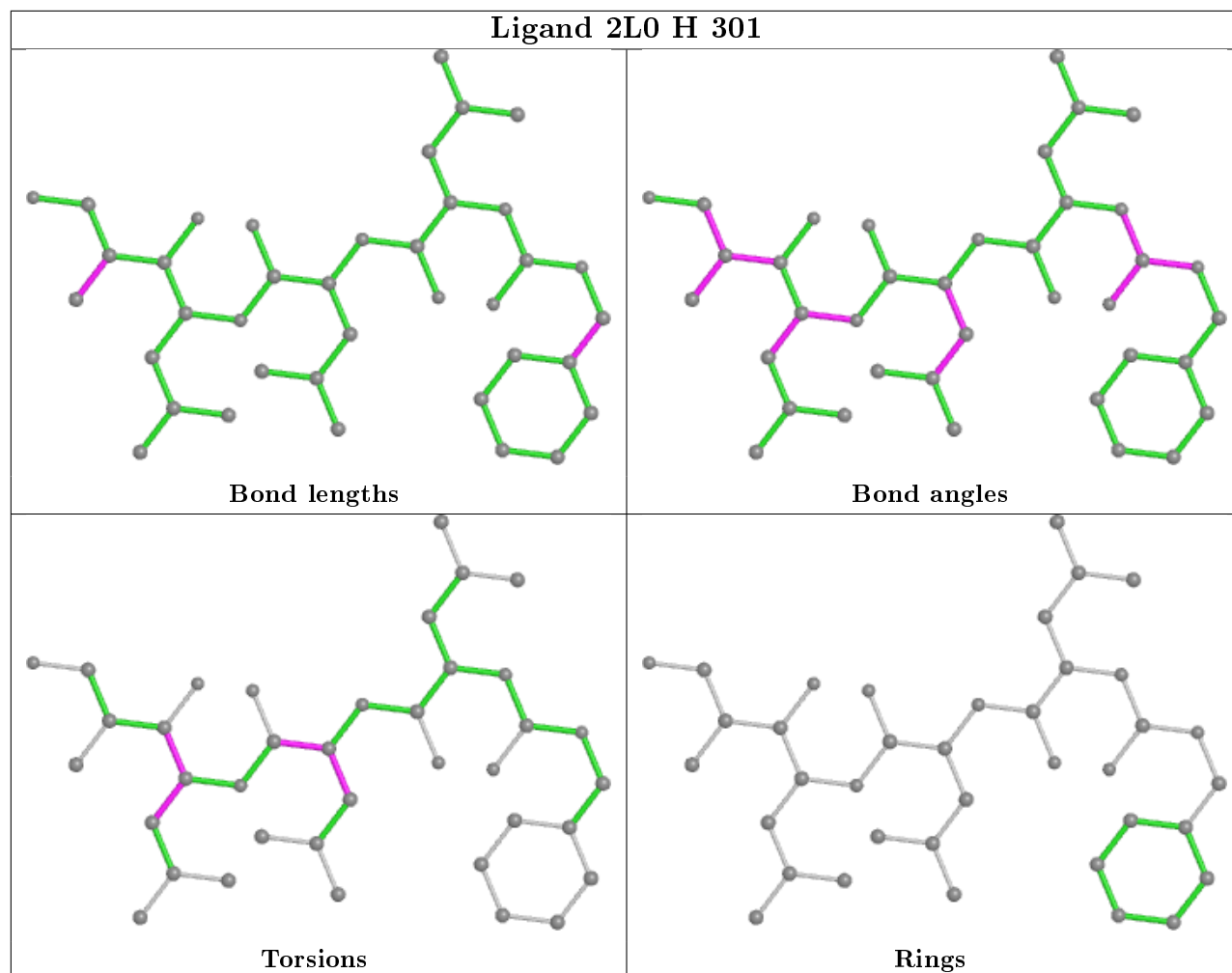
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	301	2L0	1	0
16	H	301	2L0	4	0
16	K	301	2L0	8	0
17	V	301	2LR	3	0

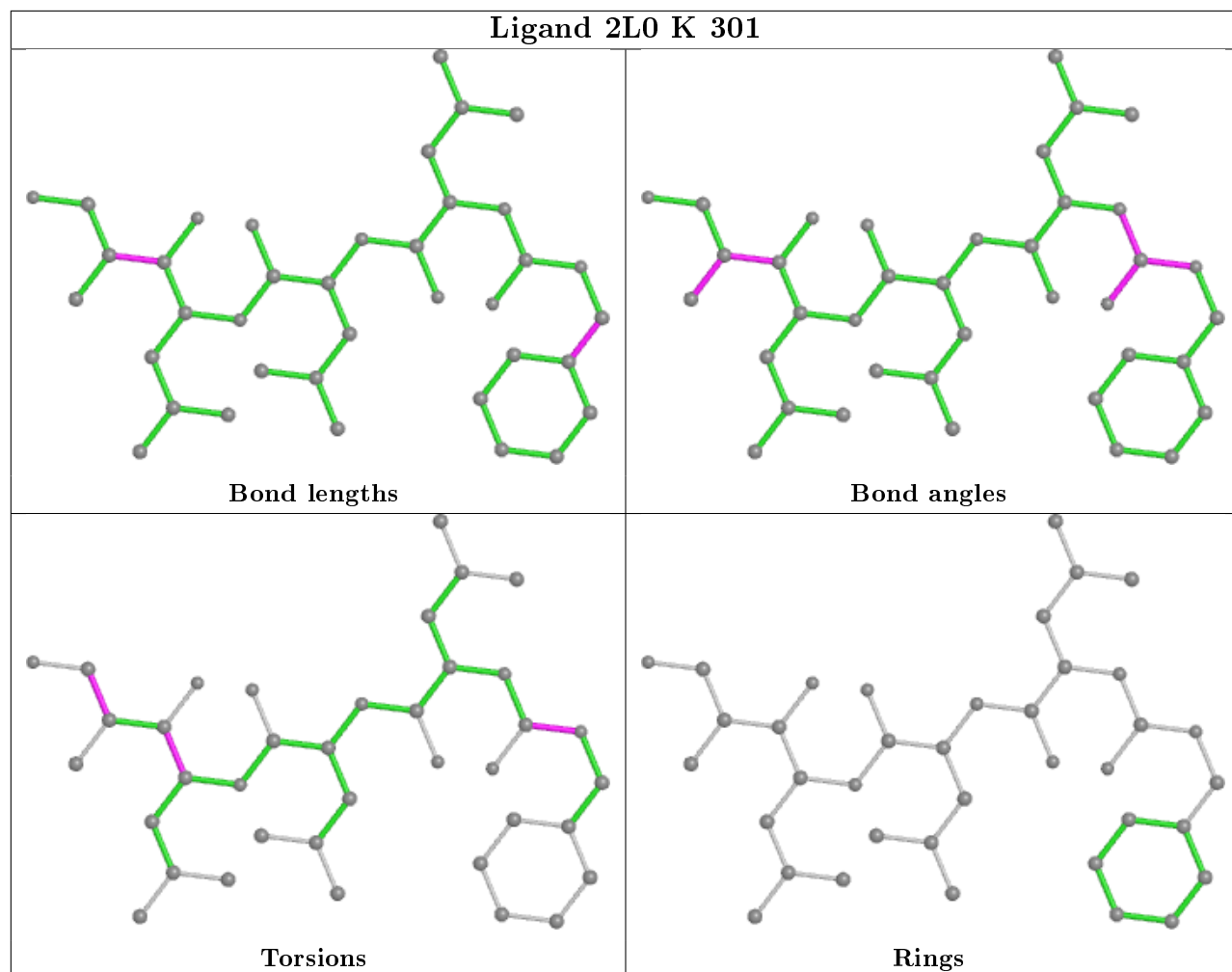
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

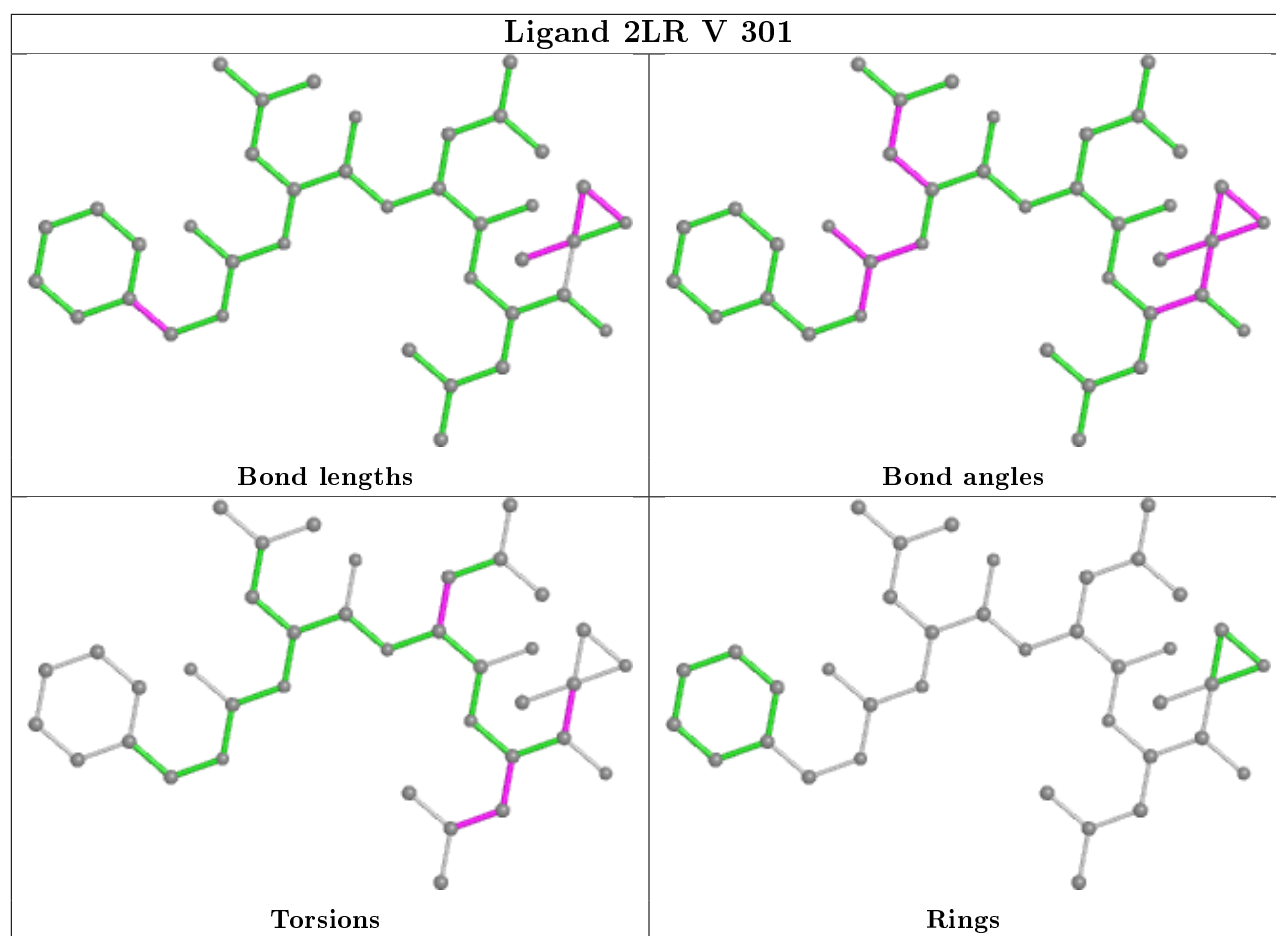
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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 2L0 K 301





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%)	-0.54	4 (1%) 72 71	33, 52, 88, 132	0
1	O	250/250 (100%)	-0.49	4 (1%) 72 71	40, 59, 98, 123	0
2	B	244/258 (94%)	-0.38	8 (3%) 46 41	37, 59, 111, 142	0
2	P	244/258 (94%)	-0.28	12 (4%) 29 26	39, 61, 112, 150	0
3	C	240/254 (94%)	-0.33	10 (4%) 36 32	35, 59, 117, 138	0
3	Q	240/254 (94%)	-0.15	11 (4%) 32 29	41, 72, 135, 151	0
4	D	235/260 (90%)	-0.49	2 (0%) 84 84	36, 59, 90, 116	0
4	R	235/260 (90%)	-0.46	1 (0%) 92 93	41, 65, 95, 124	0
5	E	231/234 (98%)	-0.48	1 (0%) 92 93	38, 61, 88, 116	0
5	S	231/234 (98%)	-0.48	1 (0%) 92 93	38, 62, 91, 117	0
6	F	243/288 (84%)	-0.57	0 100 100	36, 54, 97, 122	0
6	T	243/288 (84%)	-0.56	3 (1%) 79 79	36, 55, 91, 120	0
7	G	241/252 (95%)	-0.57	3 (1%) 79 79	30, 51, 88, 126	0
7	U	241/252 (95%)	-0.59	2 (0%) 86 86	31, 52, 82, 120	0
8	H	222/232 (95%)	-0.62	2 (0%) 84 84	33, 49, 74, 116	0
8	V	222/232 (95%)	-0.64	2 (0%) 84 84	34, 51, 79, 119	0
9	I	204/205 (99%)	-0.80	1 (0%) 91 91	33, 47, 69, 101	0
9	W	204/205 (99%)	-0.75	1 (0%) 91 91	32, 50, 74, 107	0
10	J	195/198 (98%)	-0.66	2 (1%) 82 82	32, 50, 75, 123	0
10	X	195/198 (98%)	-0.67	2 (1%) 82 82	36, 52, 77, 135	0
11	K	212/212 (100%)	-0.68	0 100 100	30, 49, 72, 104	0
11	Y	212/212 (100%)	-0.69	0 100 100	34, 51, 77, 103	0
12	L	222/222 (100%)	-0.73	0 100 100	32, 49, 70, 96	0
12	Z	222/222 (100%)	-0.71	0 100 100	32, 48, 71, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.72	1 (0%) 92 93	33, 47, 67, 77	0
13	a	233/246 (94%)	-0.75	1 (0%) 92 93	31, 46, 66, 80	0
14	N	196/196 (100%)	-0.77	0 100 100	29, 45, 66, 88	0
14	b	196/196 (100%)	-0.75	0 100 100	30, 46, 70, 90	0
All	All	6336/6614 (95%)	-0.57	74 (1%) 79 79	29, 53, 92, 151	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	6.5
2	P	51	VAL	5.9
3	Q	49	THR	5.6
2	P	220	ASN	5.3
2	P	218	GLY	5.1
2	P	219	ALA	5.1
9	W	1	SER	5.0
3	C	206	LYS	4.7
2	P	221	ASP	4.6
3	Q	236	GLN	4.4
2	B	221	ASP	4.1
8	V	222	ASP	3.8
2	B	222	GLY	3.8
2	P	60	THR	3.7
2	B	220	ASN	3.6
3	Q	238	LYS	3.6
8	H	221	CYS	3.6
3	Q	239	GLN	3.6
1	O	249	ALA	3.5
6	T	244	ASN	3.5
3	Q	206	LYS	3.4
8	H	222	ASP	3.4
2	P	59	ASP	3.4
3	C	50	LEU	3.3
5	E	202	ASP	3.2
1	O	1	MET	3.2
1	A	2	THR	3.1
10	X	194	ASP	3.1
13	a	1	THR	3.1
2	P	222	GLY	3.0
7	U	242	GLN	3.0
2	B	51	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	Q	204	GLY	2.9
9	I	1	SER	2.9
4	D	241	ALA	2.9
1	O	231	LYS	2.8
2	B	219	ALA	2.8
2	P	182	ASP	2.8
1	A	1	MET	2.8
3	C	239	GLN	2.8
5	S	202	ASP	2.8
4	D	242	GLU	2.8
3	Q	240	GLU	2.7
10	J	1	MET	2.7
3	C	60	SER	2.6
3	C	238	LYS	2.5
1	A	249	ALA	2.5
13	M	1	THR	2.5
2	B	235	LYS	2.5
2	P	203	SER	2.5
6	T	2	THR	2.4
8	V	221	CYS	2.4
1	O	52	SER	2.4
3	C	202	GLN	2.4
2	P	225	TYR	2.3
3	Q	203	THR	2.3
7	G	240	ALA	2.3
2	B	218	GLY	2.3
7	G	242	GLN	2.3
3	C	49	THR	2.3
3	C	187	GLU	2.3
3	C	236	GLN	2.3
7	U	241	GLU	2.2
10	J	194	ASP	2.2
2	B	244	THR	2.2
2	P	52	THR	2.2
3	C	240	GLU	2.2
7	G	241	GLU	2.1
6	T	243	ILE	2.1
1	A	250	LEU	2.0
3	Q	223	SER	2.0
4	R	125	LEU	2.0
3	Q	229	GLN	2.0
10	X	1	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

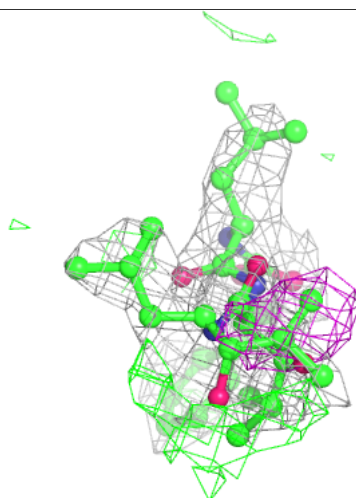
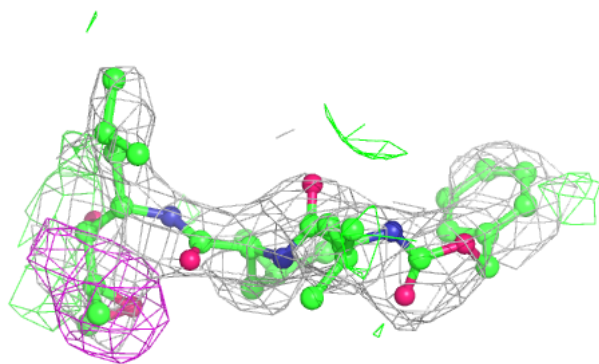
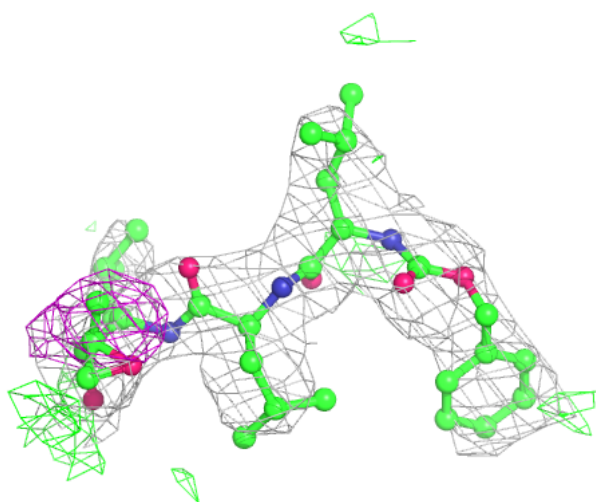
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	2LR	V	301	38/38	0.85	0.28	32,83,104,107	0
16	2L0	H	301	38/38	0.88	0.24	63,87,110,111	0
16	2L0	Y	301	38/38	0.92	0.20	36,44,56,56	0
16	2L0	K	301	38/38	0.92	0.20	44,58,76,76	0
15	MG	N	201	1/1	0.95	0.09	38,38,38,38	0
15	MG	I	301	1/1	0.95	0.22	60,60,60,60	0
15	MG	K	302	1/1	0.96	0.09	50,50,50,50	0
15	MG	G	301	1/1	0.96	0.11	58,58,58,58	0
15	MG	V	302	1/1	0.96	0.10	59,59,59,59	0
15	MG	H	302	1/1	0.96	0.13	44,44,44,44	0
15	MG	Y	302	1/1	0.97	0.08	51,51,51,51	0
15	MG	Z	301	1/1	0.98	0.17	45,45,45,45	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.

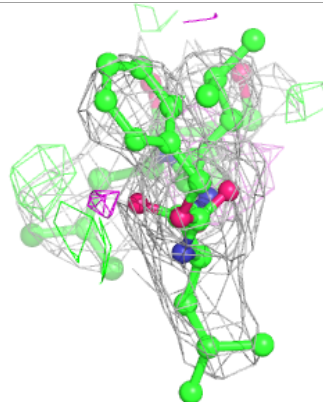
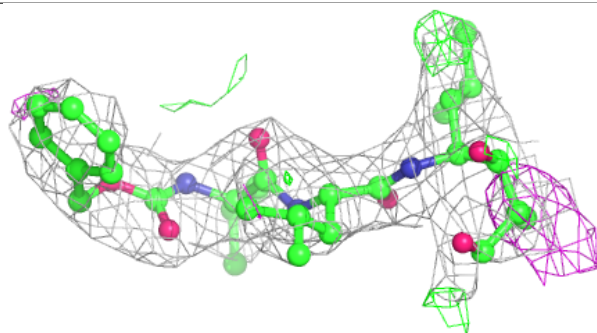
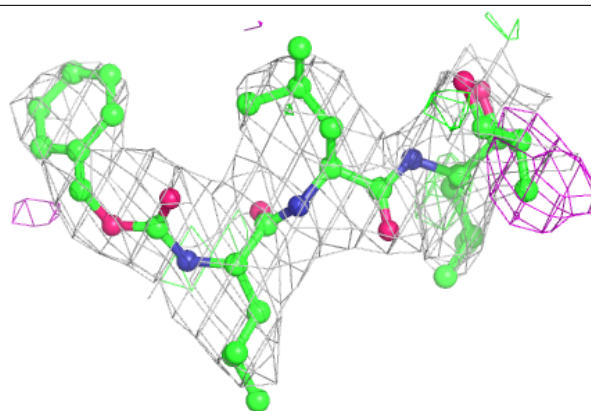
Electron density around 2LR V 301:

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

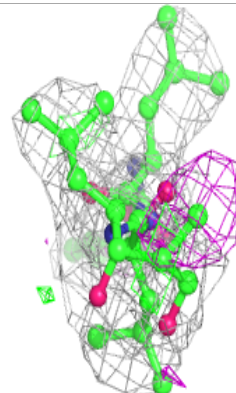
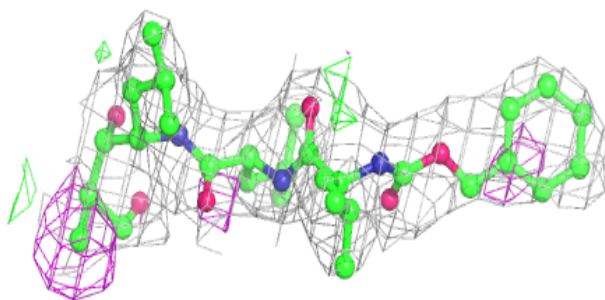
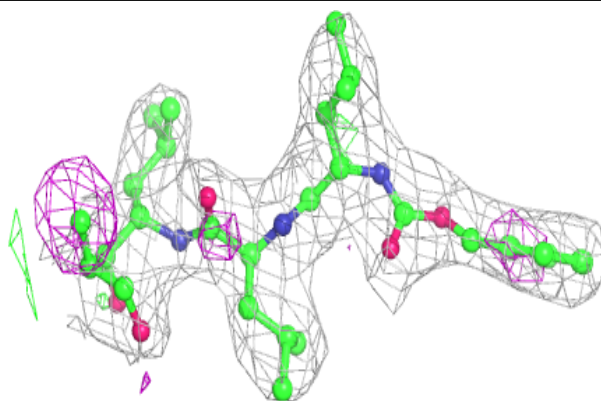


Electron density around 2L0 H 301:

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

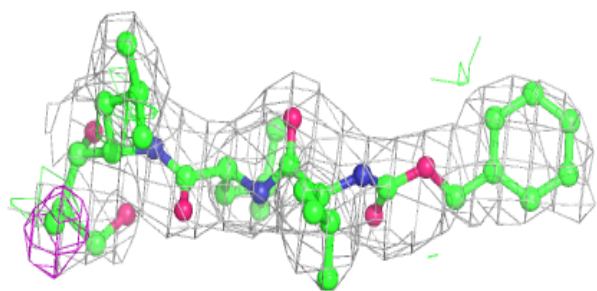
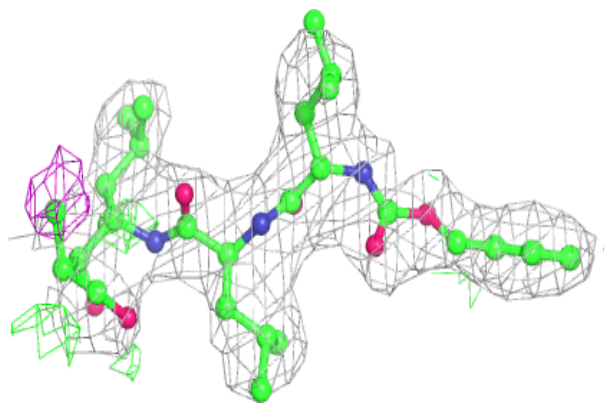
**Electron density around 2L0 Y 301:**

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



Electron density around 2L0 K 301:

$2mF_o-DF_c$ (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.