



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:53 am BST

PDB ID : 3SDK  
Title : Structure of yeast 20S open-gate proteasome with Compound 34  
Authors : Sintchak, M.D.  
Deposited on : 2011-06-09  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

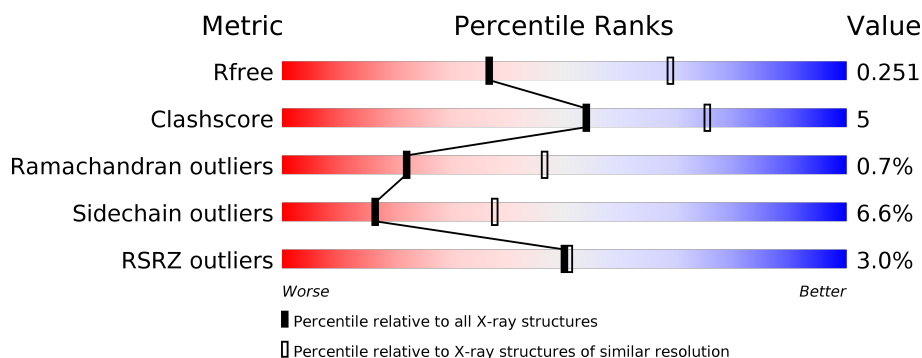
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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>86% 12%</div> </div>
1	O	250	<div> <div>3%</div> <div>85% 13%</div> </div>
2	B	235	<div> <div>3%</div> <div>82% 16%</div> </div>
2	P	235	<div> <div>3%</div> <div>80% 17%</div> </div>
3	C	241	<div> <div>7%</div> <div>84% 14%</div> </div>
3	Q	241	<div> <div>16%</div> <div>76% 22%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	233	
5	S	233	
6	F	242	
6	T	242	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

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	302	-	-	-	X
15	MG	I	201	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49255 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			
2	P	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	0	0
			1794	1123	302	362	7			
4	R	232	Total	C	N	O	S	0	0	0
			1786	1120	298	361	7			

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	236	Total	C	N	O	S	0	0	0
			1840	1171	321	344	4			
6	T	236	Total	C	N	O	S	0	0	0
			1840	1171	321	344	4			

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1582	1003	269	305	5			

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

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

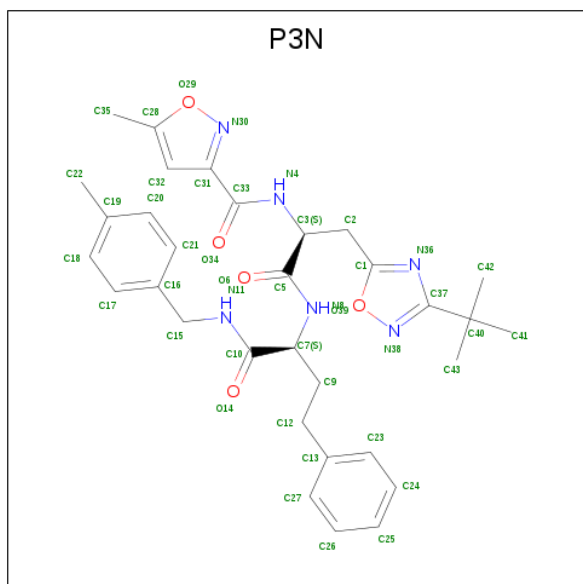
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

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

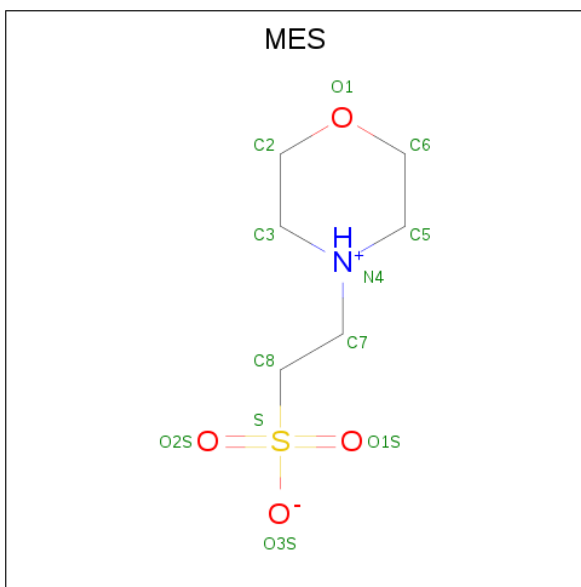
- Molecule 16 is N-[(2S)-3-(3-tert-butyl-1,2,4-oxadiazol-5-yl)-1-({(2S)-1-[(4-methylbenzyl)amino]-1-oxo-4-phenylbutan-2-yl}amino)-1-oxopropan-2-yl]-5-methyl-1,2-oxazole-3-carboxamide (three-letter code: P3N) (formula: C<sub>32</sub>H<sub>38</sub>N<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			43	32	6	5		
16	Y	1	Total	C	N	O	0	0
			43	32	6	5		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



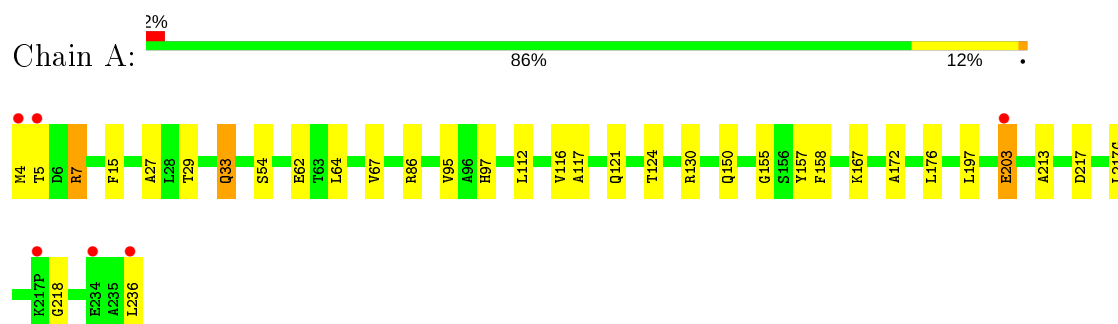


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

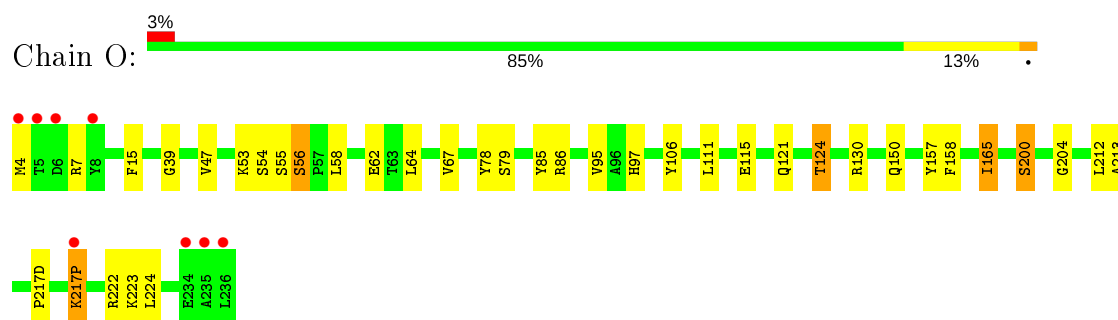
### 3 Residue-property plots [i](#)

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

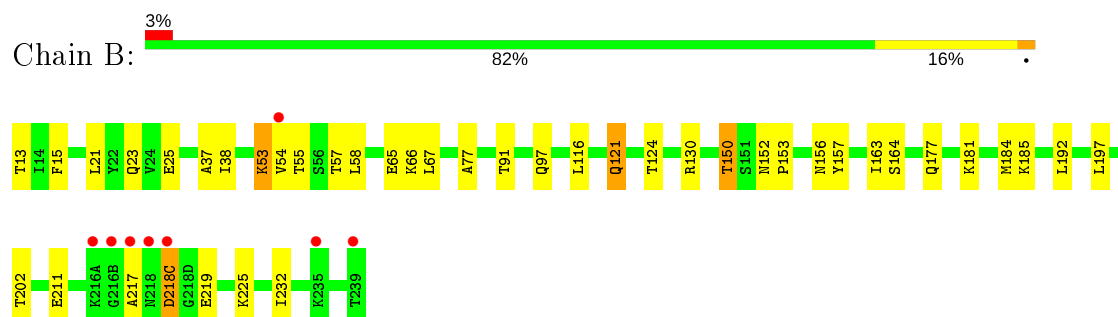
- Molecule 1: Proteasome component Y7



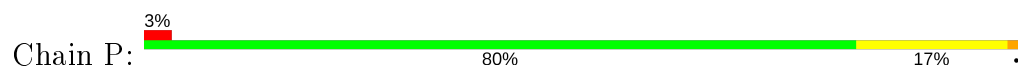
- Molecule 1: Proteasome component Y7

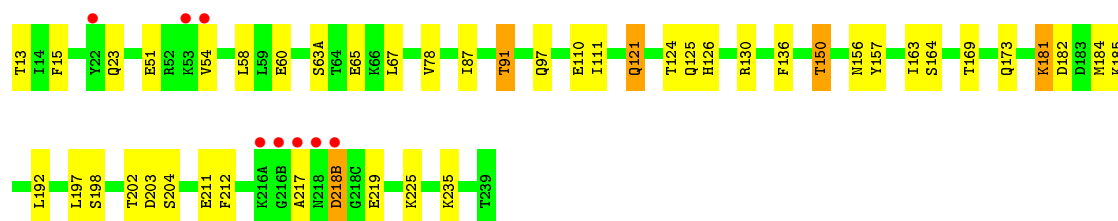


- Molecule 2: Proteasome component Y13

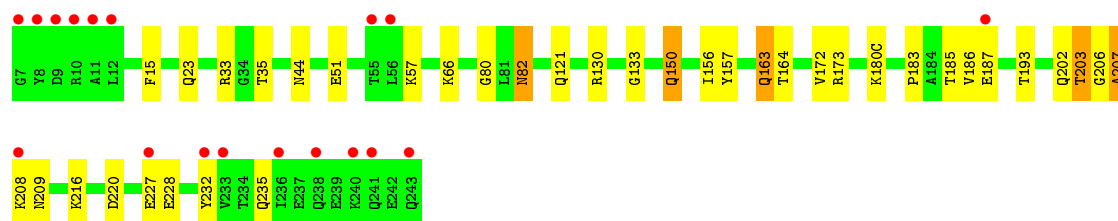
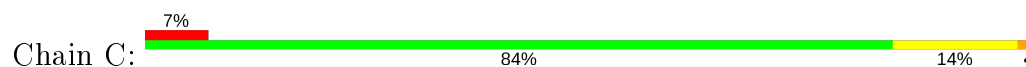


- Molecule 2: Proteasome component Y13

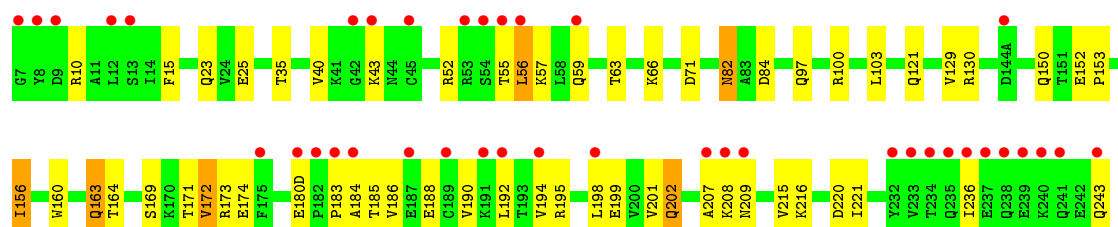
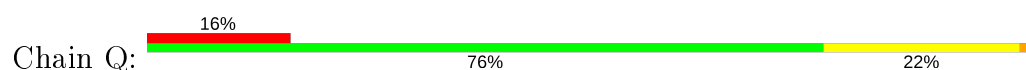




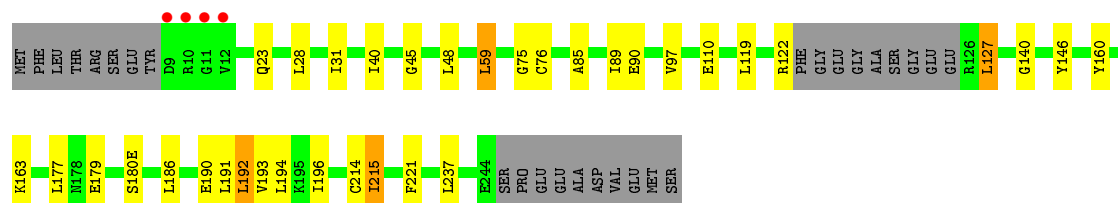
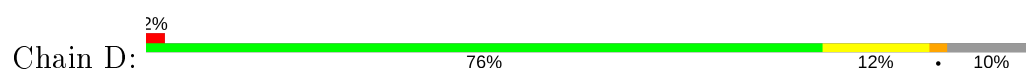
• Molecule 3: Proteasome component PRE6



• Molecule 3: Proteasome component PRE6



• Molecule 4: Proteasome component PUP2

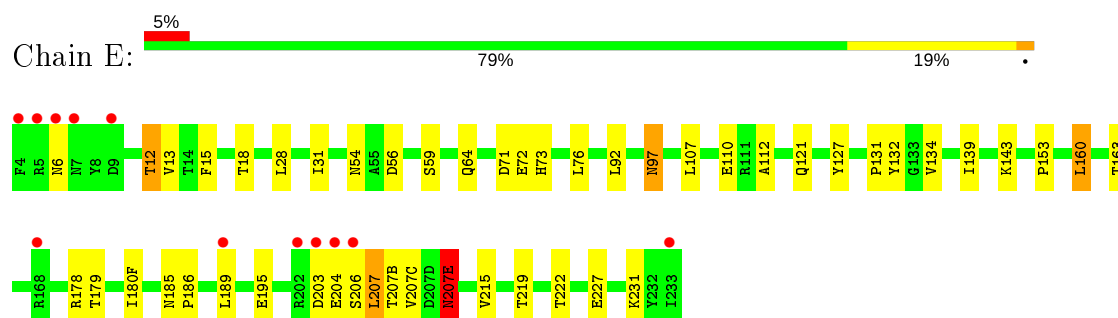


• Molecule 4: Proteasome component PUP2

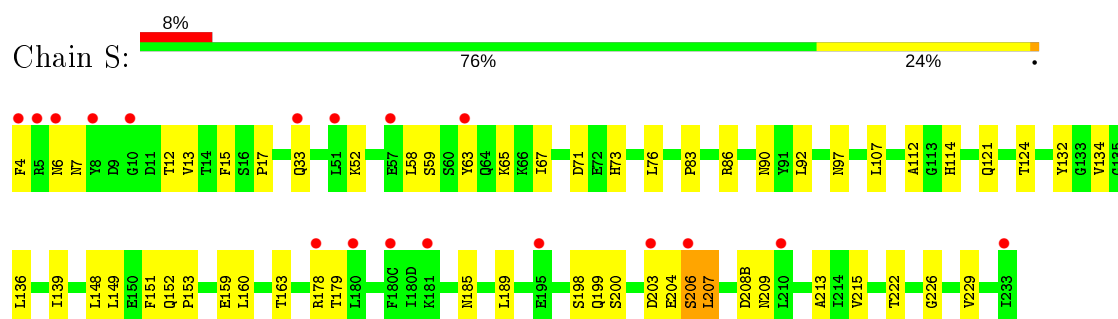




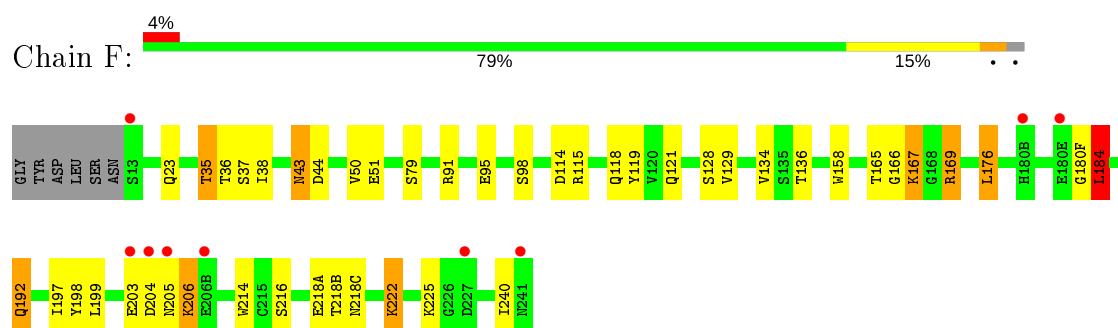
• Molecule 5: Proteasome component PRE5



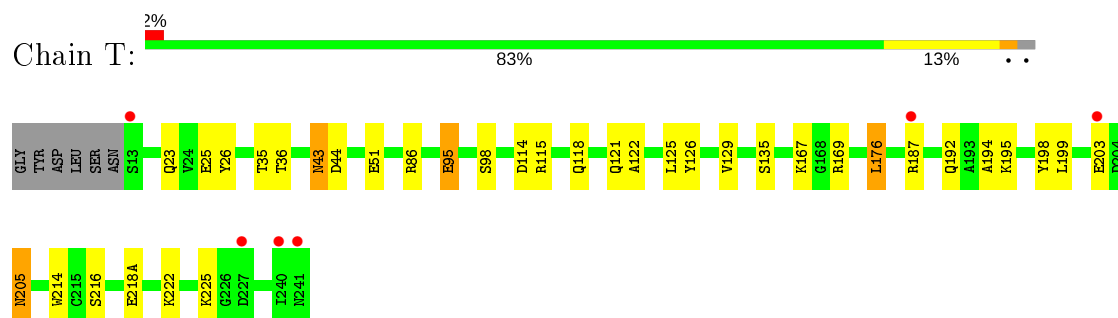
• Molecule 5: Proteasome component PRE5



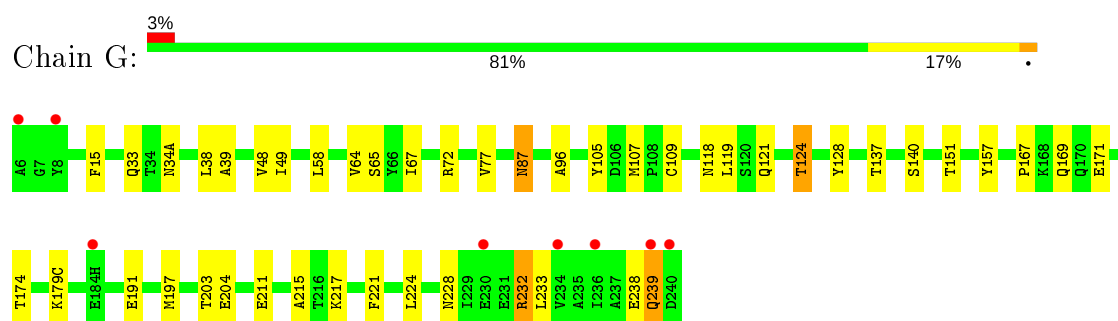
• Molecule 6: Proteasome component C1



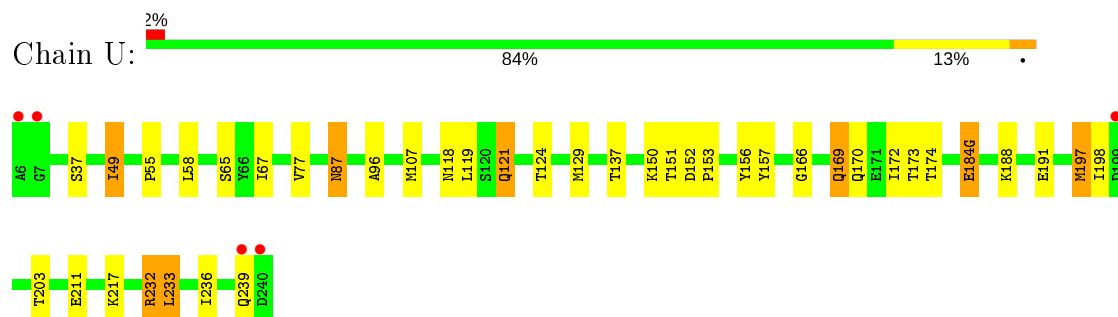
• Molecule 6: Proteasome component C1



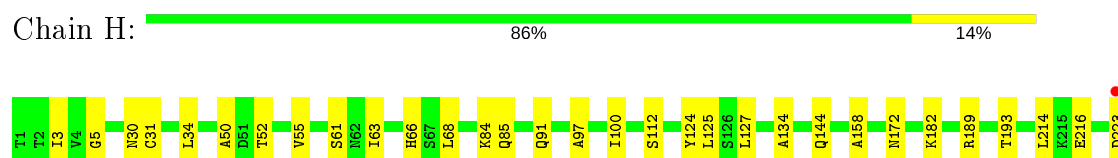
• Molecule 7: Proteasome component C7-alpha



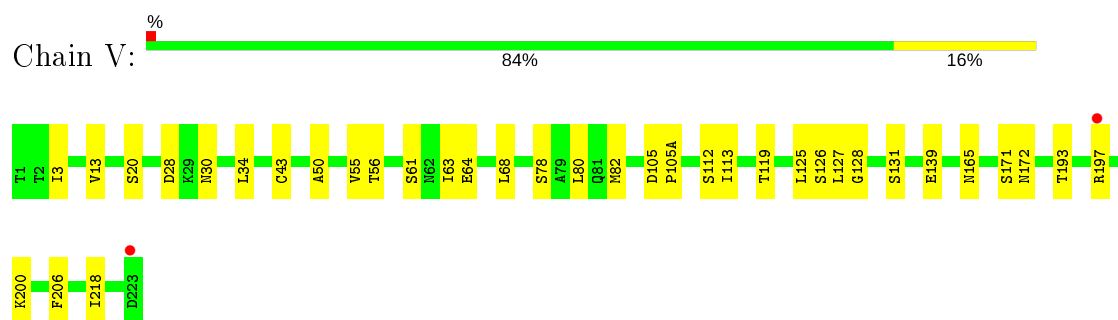
- Molecule 7: Proteasome component C7-alpha



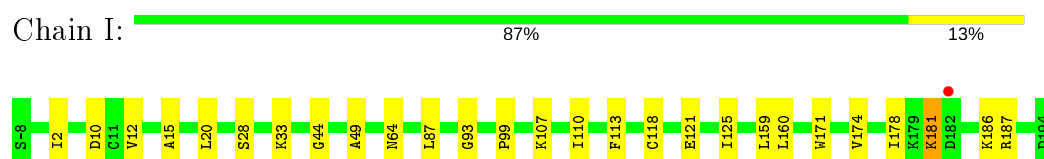
- Molecule 8: Proteasome component PUP1



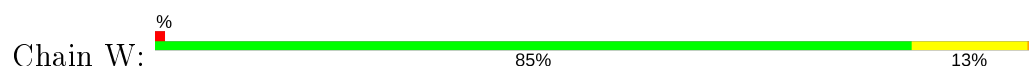
- Molecule 8: Proteasome component PUP1

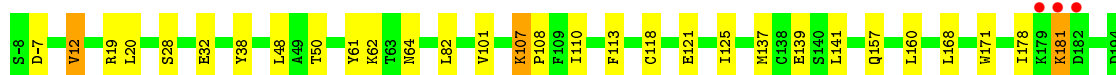


- Molecule 9: Proteasome component PUP3

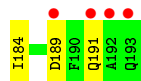
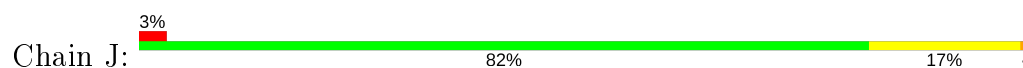


- Molecule 9: Proteasome component PUP3

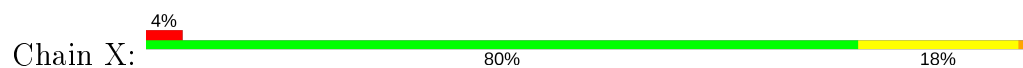




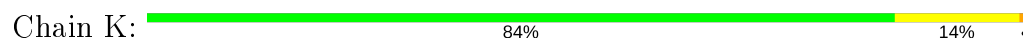
- Molecule 10: Proteasome component C11



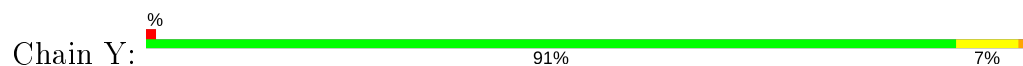
- Molecule 10: Proteasome component C11



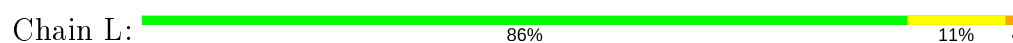
- Molecule 11: Proteasome component PRE2



- Molecule 11: Proteasome component PRE2

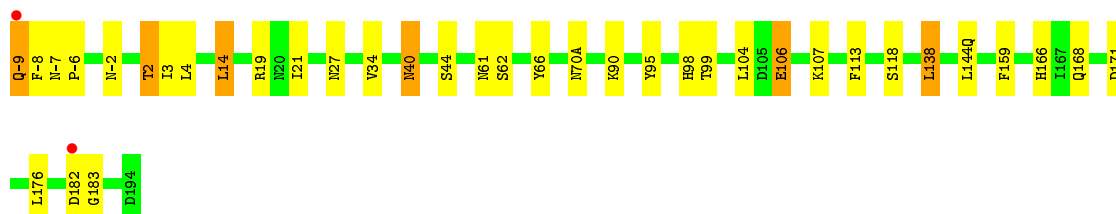
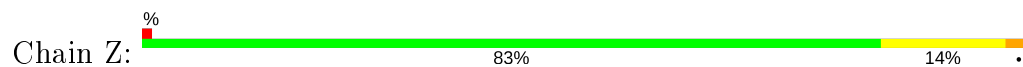


- Molecule 12: Proteasome component C5

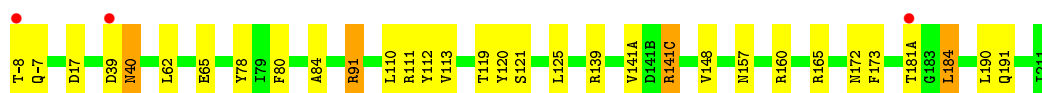
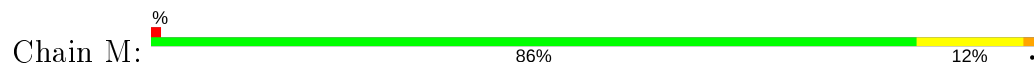




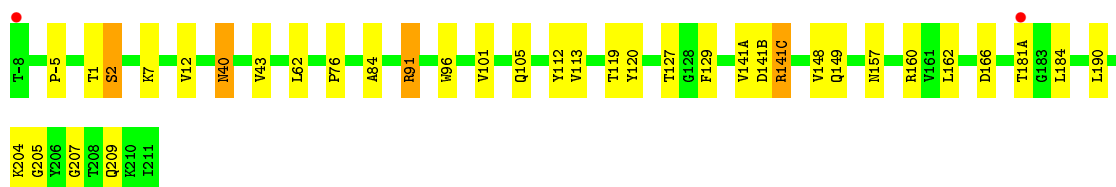
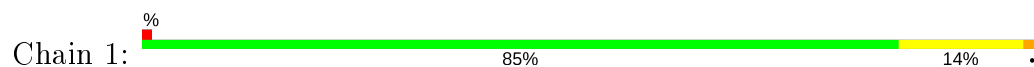
- Molecule 12: Proteasome component C5



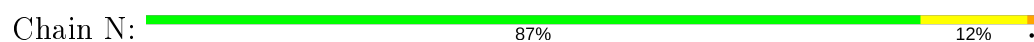
- Molecule 13: Proteasome component PRE4



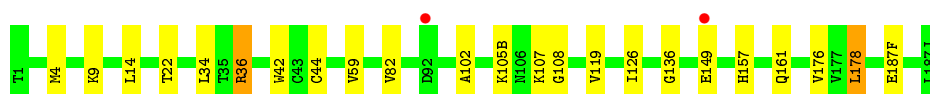
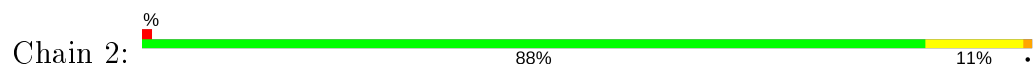
- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.12Å 299.40Å 146.24Å 90.00° 112.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.70) 95.0 (49.21-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.223 , 0.259 0.218 , 0.251	Depositor DCC
$R_{free}$ test set	5652 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	49255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, P3N, MES

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	0.44	0/1952	0.58	0/2642
1	O	0.51	1/1952 (0.1%)	0.58	0/2642
2	B	0.44	0/1858	0.59	0/2516
2	P	0.45	0/1858	0.57	0/2516
3	C	0.45	0/1920	0.59	0/2598
3	Q	0.46	1/1920 (0.1%)	0.59	2/2598 (0.1%)
4	D	0.46	0/1817	0.62	1/2449 (0.0%)
4	R	0.45	0/1810	0.59	0/2440
5	E	0.51	1/1823 (0.1%)	0.60	0/2463
5	S	0.47	0/1823	0.57	0/2463
6	F	0.44	0/1879	0.57	1/2535 (0.0%)
6	T	0.46	0/1879	0.58	0/2535
7	G	0.49	0/1959	0.58	0/2652
7	U	0.46	0/1959	0.58	0/2652
8	H	0.44	0/1716	0.57	0/2326
8	V	0.50	0/1716	0.57	0/2326
9	I	0.55	0/1611	0.60	0/2174
9	W	0.57	1/1611 (0.1%)	0.60	0/2174
10	J	0.50	0/1613	0.61	0/2173
10	X	0.46	0/1610	0.60	0/2170
11	K	0.47	0/1681	0.64	1/2274 (0.0%)
11	Y	0.45	0/1681	0.61	1/2274 (0.0%)
12	L	0.49	0/1795	0.59	0/2420
12	Z	0.50	0/1795	0.59	0/2420
13	1	0.50	0/1855	0.63	0/2514
13	M	0.49	0/1855	0.64	0/2514
14	2	0.57	0/1541	0.59	0/2087
14	N	0.59	1/1541 (0.1%)	0.60	0/2087
All	All	0.48	5/50030 (0.0%)	0.59	6/67634 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
5	E	0	2
5	S	0	1
14	N	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	207(E)	ASN	C-O	8.61	1.39	1.23
1	O	200	SER	C-O	8.24	1.39	1.23
3	Q	180(D)	GLU	C-O	6.81	1.36	1.23
14	N	181	ALA	C-O	5.73	1.34	1.23
9	W	38	TYR	CD1-CE1	-5.10	1.31	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	LEU	CA-CB-CG	5.58	128.15	115.30
6	F	184	LEU	CA-CB-CG	5.22	127.31	115.30
11	Y	4	LEU	CA-CB-CG	5.22	127.31	115.30
3	Q	56	LEU	CA-CB-CG	5.16	127.17	115.30
3	Q	103	LEU	CA-CB-CG	5.12	127.09	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	204	GLU	Peptide
5	E	207(E)	ASN	Mainchain
14	N	181	ALA	Mainchain
1	O	200	SER	Mainchain
5	S	204	GLU	Peptide

## 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	1926	28	0
1	O	1915	0	1926	22	0
2	B	1829	0	1829	25	0
2	P	1829	0	1829	27	0
3	C	1891	0	1900	26	0
3	Q	1891	0	1900	38	0
4	D	1794	0	1778	21	0
4	R	1786	0	1763	19	0
5	E	1795	0	1797	20	0
5	S	1795	0	1797	27	0
6	F	1840	0	1838	30	0
6	T	1840	0	1838	22	0
7	G	1921	0	1910	28	0
7	U	1921	0	1910	33	0
8	H	1685	0	1688	16	0
8	V	1685	0	1688	20	0
9	I	1581	0	1574	15	0
9	W	1581	0	1574	19	0
10	J	1585	0	1590	14	0
10	X	1582	0	1583	20	0
11	K	1644	0	1595	15	0
11	Y	1644	0	1595	10	0
12	L	1757	0	1711	19	0
12	Z	1757	0	1711	24	0
13	1	1824	0	1832	22	0
13	M	1824	0	1832	25	0
14	2	1512	0	1481	13	0
14	N	1512	0	1481	14	0
15	F	2	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
16	K	43	0	38	2	0
16	Y	43	0	38	1	0
17	K	12	0	13	1	0
17	Y	12	0	13	1	0
All	All	49255	0	48978	519	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 5.

The worst 5 of 519 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)
4:D:127:LEU:N	4:D:127:LEU:HD12	1.53	1.02
4:D:127:LEU:H	4:D:127:LEU:CD1	1.70	1.01
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.78	0.97
4:D:127:LEU:H	4:D:127:LEU:HD12	0.81	0.95
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.29	0.94

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	6 (2%)	3 (1%)	13	32
1	O	248/250 (99%)	234 (94%)	12 (5%)	2 (1%)	19	43
2	B	233/235 (99%)	223 (96%)	7 (3%)	3 (1%)	12	30
2	P	233/235 (99%)	218 (94%)	11 (5%)	4 (2%)	9	23
3	C	239/241 (99%)	229 (96%)	6 (2%)	4 (2%)	9	23
3	Q	239/241 (99%)	230 (96%)	6 (2%)	3 (1%)	12	30
4	D	229/260 (88%)	218 (95%)	11 (5%)	0	100	100
4	R	228/260 (88%)	219 (96%)	9 (4%)	0	100	100
5	E	231/233 (99%)	217 (94%)	9 (4%)	5 (2%)	6	17
5	S	231/233 (99%)	216 (94%)	11 (5%)	4 (2%)	9	23
6	F	234/242 (97%)	223 (95%)	10 (4%)	1 (0%)	34	60
6	T	234/242 (97%)	221 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	241/243 (99%)	234 (97%)	6 (2%)	1 (0%)	34	60
7	U	241/243 (99%)	232 (96%)	7 (3%)	2 (1%)	19	43
8	H	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	29	54
8	V	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	29	54
9	I	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29	54
9	W	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
10	J	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	29	54
10	X	196/198 (99%)	185 (94%)	8 (4%)	3 (2%)	10	26
11	K	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	29	54
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	1	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	34	60
13	M	231/233 (99%)	214 (93%)	17 (7%)	0	100	100
14	2	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6255/6382 (98%)	5981 (96%)	233 (4%)	41 (1%)	22	46

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
3	C	203	THR
3	C	207	ALA
5	E	6	ASN
6	F	184	LEU

### 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%)	198 (95%)	11 (5%)	22	48
1	O	209/209 (100%)	196 (94%)	13 (6%)	18	40
2	B	195/195 (100%)	182 (93%)	13 (7%)	16	37
2	P	195/195 (100%)	180 (92%)	15 (8%)	13	30
3	C	213/213 (100%)	196 (92%)	17 (8%)	12	27
3	Q	213/213 (100%)	200 (94%)	13 (6%)	18	41
4	D	192/215 (89%)	177 (92%)	15 (8%)	12	29
4	R	191/215 (89%)	172 (90%)	19 (10%)	8	18
5	E	192/192 (100%)	171 (89%)	21 (11%)	6	14
5	S	192/192 (100%)	175 (91%)	17 (9%)	9	22
6	F	195/200 (98%)	177 (91%)	18 (9%)	9	21
6	T	195/200 (98%)	180 (92%)	15 (8%)	13	30
7	G	207/207 (100%)	191 (92%)	16 (8%)	13	30
7	U	207/207 (100%)	197 (95%)	10 (5%)	25	53
8	H	181/181 (100%)	174 (96%)	7 (4%)	32	61
8	V	181/181 (100%)	172 (95%)	9 (5%)	24	51
9	I	172/172 (100%)	166 (96%)	6 (4%)	36	65
9	W	172/172 (100%)	164 (95%)	8 (5%)	26	54
10	J	175/175 (100%)	163 (93%)	12 (7%)	15	35
10	X	174/175 (99%)	162 (93%)	12 (7%)	15	35
11	K	169/169 (100%)	156 (92%)	13 (8%)	13	30
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26	54
12	L	185/185 (100%)	175 (95%)	10 (5%)	22	47
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	38
13	1	199/199 (100%)	187 (94%)	12 (6%)	19	42
13	M	199/199 (100%)	190 (96%)	9 (4%)	27	55
14	2	162/162 (100%)	154 (95%)	8 (5%)	25	52
14	N	162/162 (100%)	154 (95%)	8 (5%)	25	52
All	All	5290/5348 (99%)	4943 (93%)	347 (7%)	16	38

5 of 347 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	98	HIS
2	P	121	GLN
12	Z	70(A)	ASN
13	M	65	GLU
1	O	4	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	157	ASN
4	R	23	GLN
12	Z	166	HIS
14	N	69	GLN
2	P	125	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 carbohydrates 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	P3N	Y	301	-	40,46,46	1.44	5 (12%)	50,64,64	1.52	1 (2%)
16	P3N	K	302	-	40,46,46	1.52	4 (10%)	50,64,64	1.35	2 (4%)
17	MES	K	303	-	12,12,12	2.23	1 (8%)	14,16,16	1.32	1 (7%)
17	MES	Y	302	-	12,12,12	2.26	1 (8%)	14,16,16	1.46	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	P3N	Y	301	-	-	0/35/40/40	0/4/4/4
16	P3N	K	302	-	-	4/35/40/40	0/4/4/4
17	MES	K	303	-	-	1/6/14/14	0/1/1/1
17	MES	Y	302	-	-	3/6/14/14	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	302	MES	C8-S	-7.57	1.66	1.77
17	K	303	MES	C8-S	-7.45	1.66	1.77
16	K	302	P3N	C2-C1	6.02	1.53	1.49
16	Y	301	P3N	C2-C1	4.97	1.52	1.49
16	K	302	P3N	C35-C28	4.48	1.53	1.48

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	P3N	C37-N36-C1	9.35	109.02	104.11
16	K	302	P3N	C37-N36-C1	7.57	108.08	104.11
17	Y	302	MES	O3S-S-C8	3.41	111.29	105.77
17	K	303	MES	O3S-S-C8	3.41	111.28	105.77
16	K	302	P3N	C1-C2-C3	-2.39	107.82	113.90

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	Y	302	MES	C7-C8-S-O1S
17	Y	302	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
16	K	302	P3N	N36-C37-C40-C43
17	K	303	MES	C7-C8-S-O3S
17	Y	302	MES	C7-C8-S-O2S

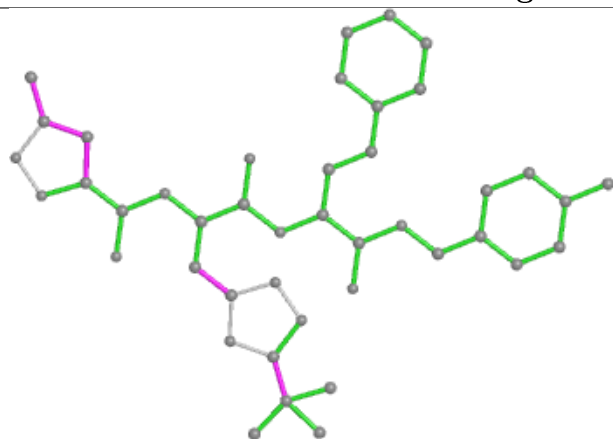
There are no ring outliers.

4 monomers are involved in 4 short contacts:

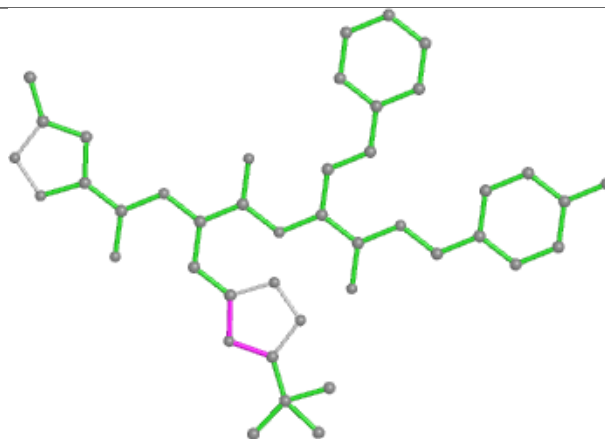
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	301	P3N	1	0
16	K	302	P3N	2	0
17	K	303	MES	1	0
17	Y	302	MES	1	0

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 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.

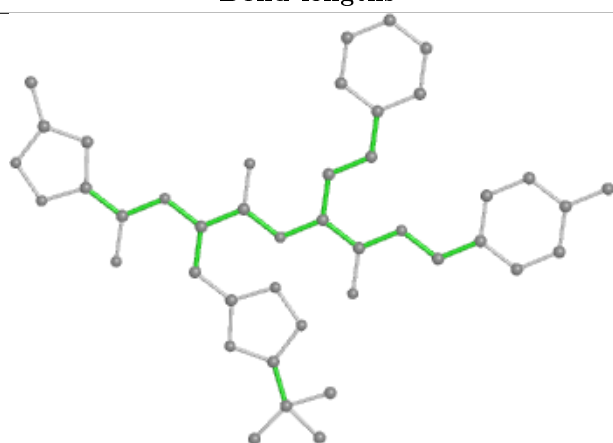
## Ligand P3N Y 301



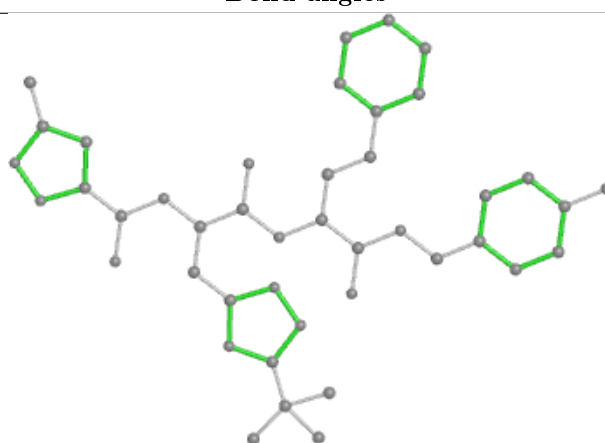
Bond lengths



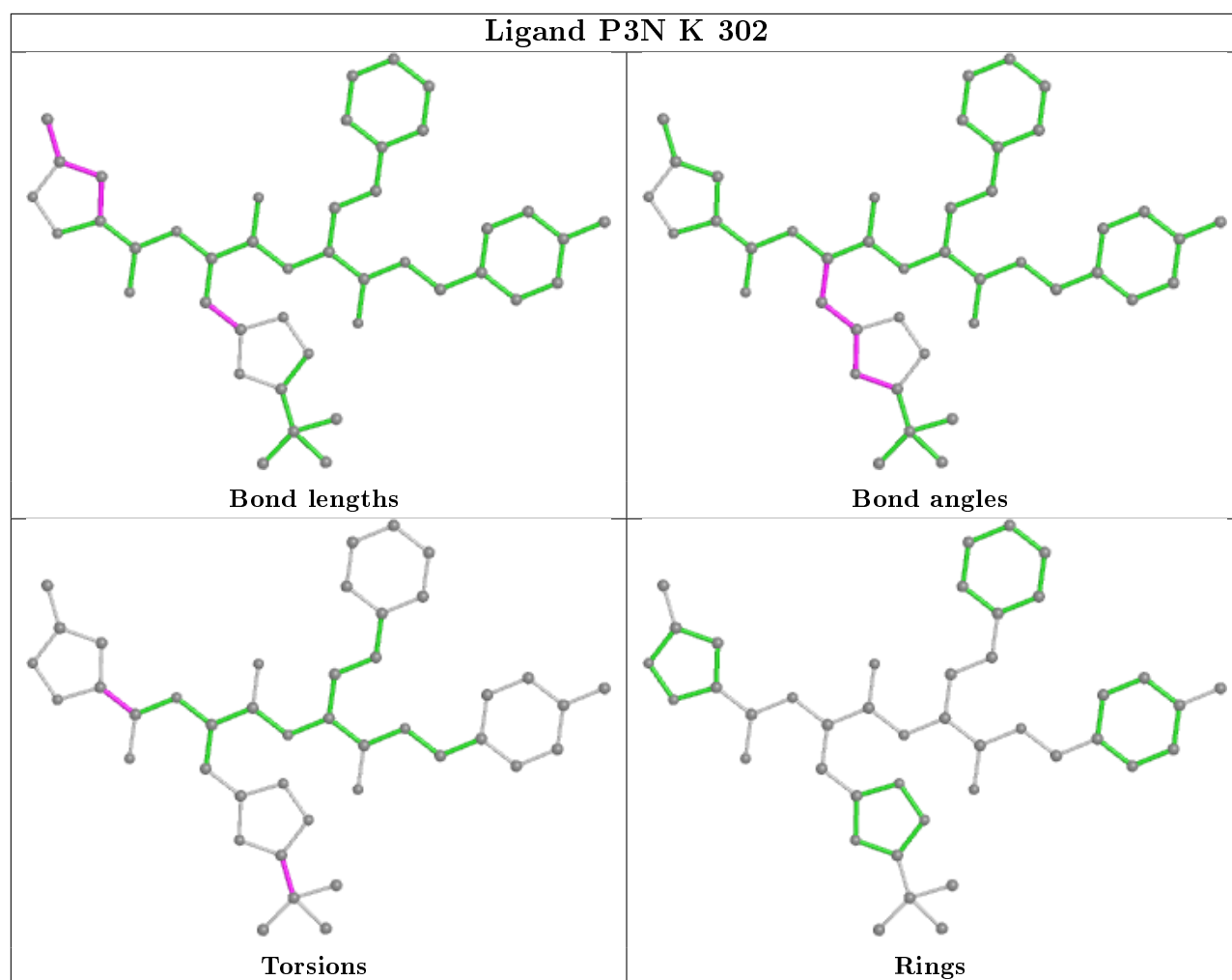
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	0.09	6 (2%) 59 60	35, 50, 71, 89	0
1	O	250/250 (100%)	0.07	8 (3%) 47 48	37, 55, 83, 94	0
2	B	235/235 (100%)	0.16	8 (3%) 45 45	34, 53, 86, 91	0
2	P	235/235 (100%)	0.23	8 (3%) 45 45	33, 55, 85, 94	0
3	C	241/241 (100%)	0.35	18 (7%) 14 12	38, 61, 100, 118	0
3	Q	241/241 (100%)	0.77	39 (16%) 1 1	42, 65, 110, 128	0
4	D	233/260 (89%)	0.10	4 (1%) 70 72	36, 56, 81, 97	0
4	R	232/260 (89%)	0.04	7 (3%) 50 51	35, 57, 80, 94	0
5	E	233/233 (100%)	0.23	12 (5%) 27 25	42, 58, 84, 94	0
5	S	233/233 (100%)	0.44	18 (7%) 13 11	40, 60, 90, 102	0
6	F	236/242 (97%)	0.01	9 (3%) 40 39	33, 51, 80, 88	0
6	T	236/242 (97%)	0.05	6 (2%) 57 59	32, 52, 77, 98	0
7	G	243/243 (100%)	-0.04	8 (3%) 46 46	30, 47, 72, 96	0
7	U	243/243 (100%)	-0.06	5 (2%) 63 65	31, 47, 70, 86	0
8	H	222/222 (100%)	-0.17	1 (0%) 91 92	34, 44, 61, 88	0
8	V	222/222 (100%)	-0.08	2 (0%) 84 85	37, 47, 64, 87	0
9	I	204/204 (100%)	-0.25	1 (0%) 91 92	31, 43, 57, 64	0
9	W	204/204 (100%)	-0.01	3 (1%) 73 76	31, 44, 61, 66	0
10	J	198/198 (100%)	-0.07	6 (3%) 50 51	33, 45, 58, 110	0
10	X	198/198 (100%)	0.00	7 (3%) 44 44	36, 46, 62, 111	0
11	K	212/212 (100%)	-0.15	1 (0%) 91 92	33, 42, 59, 72	0
11	Y	212/212 (100%)	-0.17	2 (0%) 84 85	32, 44, 60, 65	0
12	L	222/222 (100%)	-0.12	1 (0%) 91 92	32, 44, 65, 72	0
12	Z	222/222 (100%)	-0.15	2 (0%) 84 85	32, 44, 64, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	1	233/233 (100%)	-0.10	2 (0%)	84	85	31, 43, 59, 64	0
13	M	233/233 (100%)	-0.14	3 (1%)	77	78	33, 45, 59, 62	0
14	2	196/196 (100%)	-0.17	2 (1%)	82	83	33, 41, 58, 72	0
14	N	196/196 (100%)	-0.17	0	100	100	32, 41, 57, 71	0
All	All	6315/6382 (98%)	0.03	189 (2%)	50	51	30, 48, 83, 128	0

The worst 5 of 189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	7	GLY	10.0
2	P	217	ALA	9.5
2	P	218	ASN	8.9
3	Q	55	THR	8.0
2	B	218	ASN	7.2

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
15	MG	L	201	1/1	0.67	0.18	56,56,56,56	0
15	MG	I	201	1/1	0.72	0.45	58,58,58,58	0
15	MG	F	302	1/1	0.73	1.34	107,107,107,107	0
15	MG	L	202	1/1	0.89	0.17	54,54,54,54	0
15	MG	N	201	1/1	0.90	0.19	47,47,47,47	0
15	MG	I	202	1/1	0.90	0.46	57,57,57,57	0
15	MG	H	301	1/1	0.90	0.12	66,66,66,66	0

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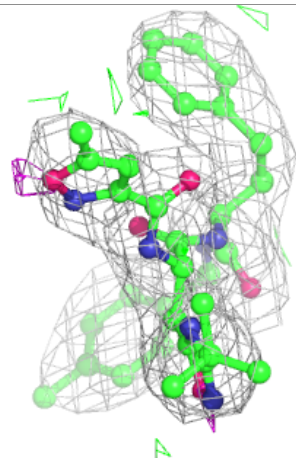
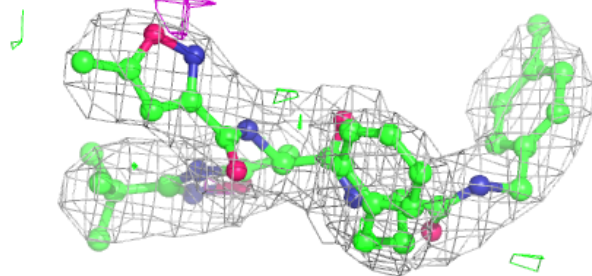
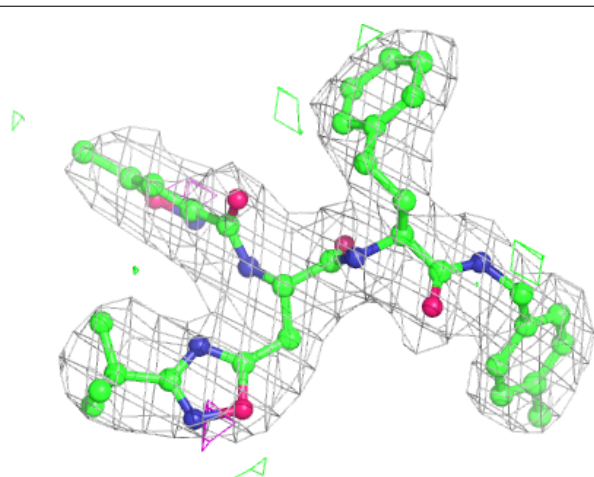
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	G	301	1/1	0.92	0.14	59,59,59,59	0
15	MG	F	301	1/1	0.95	0.16	61,61,61,61	0
16	P3N	Y	301	43/43	0.95	0.17	40,45,58,59	0
16	P3N	K	302	43/43	0.95	0.18	38,45,57,58	0
17	MES	K	303	12/12	0.96	0.19	62,66,69,69	0
15	MG	K	301	1/1	0.97	0.16	53,53,53,53	0
17	MES	Y	302	12/12	0.97	0.16	66,69,71,71	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.

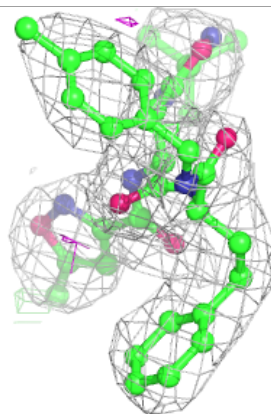
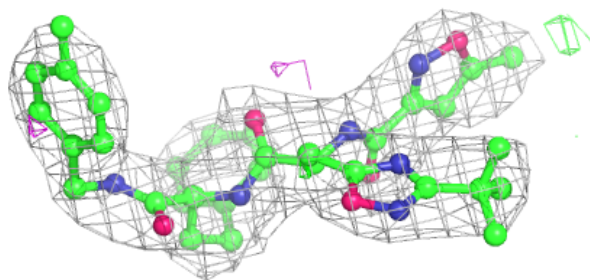
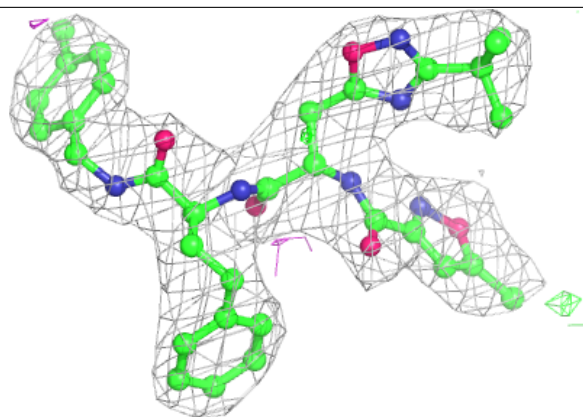
**Electron density around P3N Y 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around P3N K 302:**

$2mF_o-DF_c$  (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.