wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 07:56 AM EDT

PDB ID	:	3UNF
Title	:	Mouse 20S immunoproteasome in complex with PR-957
Authors	:	Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on	:	2011-11-15
Resolution	:	2.90 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

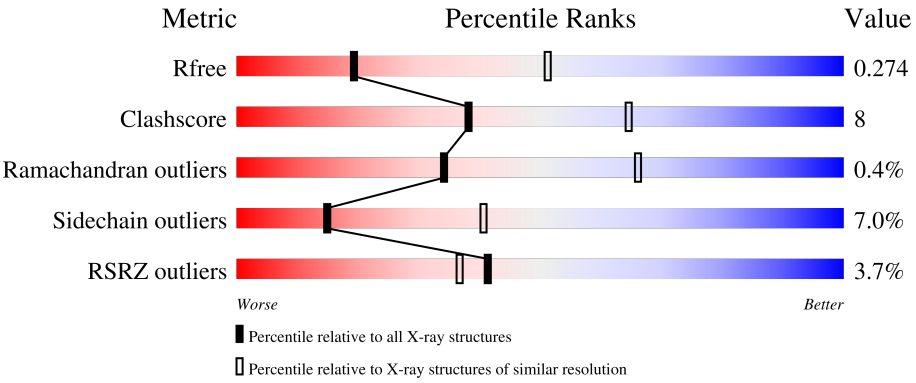
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	5% 73% 24%
1	O	234	2% 75% 21%
2	B	261	6% 75% 18% 5%
2	P	261	5% 76% 17% 5%
3	C	248	12% 67% 25%

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Mol	Chain	Length	Quality of chain
3	Q	248	11% 68% 25%
4	D	241	7% 80% 16%
4	R	241	5% 80% 16%
5	E	263	4% 76% 13% 10%
5	S	263	3% 76% 13% 10%
6	F	255	2% 77% 18%
6	T	255	4% 77% 17%
7	G	246	5% 80% 16%
7	U	246	7% 79% 18%
8	H	234	3% 70% 21% 6%
8	V	234	3% 68% 22% 6%
9	I	205	2% 72% 25%
9	W	205	% 71% 25%
10	J	201	% 82% 13%
10	X	201	82% 13%
11	K	204	% 69% 25%
11	Y	204	2% 70% 25%
12	L	213	% 83% 16%
12	Z	213	81% 18%
13	M	219	84% 14%
13	a	219	93% 5%
14	N	199	% 81% 16%
14	b	199	94% 6%

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
16	K	L	303	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 49805 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	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	6			
1	O	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	P	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	5			
3	Q	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			
4	R	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			
5	S	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	T	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	U	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			

- Molecule 8 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			
8	V	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			

- 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
			1592	1013	265	295	19			
9	W	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

- Molecule 11 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			
11	Y	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	a	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			
14	b	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	3	Total	Cl	0	0
			3	3		
15	D	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	E	1	Total Cl 1 1	0	0
15	H	1	Total Cl 1 1	0	0
15	I	1	Total Cl 1 1	0	0
15	J	1	Total Cl 1 1	0	0
15	L	2	Total Cl 2 2	0	0
15	M	4	Total Cl 4 4	0	0
15	N	1	Total Cl 1 1	0	0
15	O	2	Total Cl 2 2	0	0
15	P	1	Total Cl 1 1	0	0
15	Q	4	Total Cl 4 4	0	0
15	R	3	Total Cl 3 3	0	0
15	S	2	Total Cl 2 2	0	0
15	U	1	Total Cl 1 1	0	0
15	V	4	Total Cl 4 4	0	0
15	W	1	Total Cl 1 1	0	0
15	X	3	Total Cl 3 3	0	0
15	Z	1	Total Cl 1 1	0	0
15	a	4	Total Cl 4 4	0	0

- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total K 1 1	0	0

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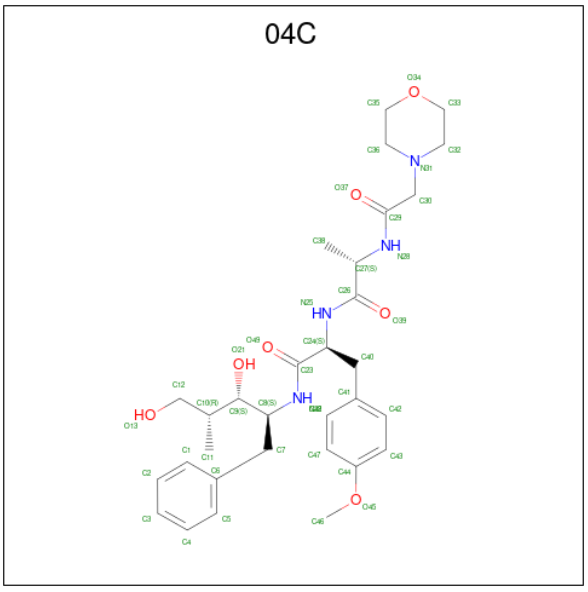
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total K 1 1	0	0
16	I	1	Total K 1 1	0	0
16	K	1	Total K 1 1	0	0
16	L	1	Total K 1 1	0	0
16	M	1	Total K 1 1	0	0
16	S	1	Total K 1 1	0	0
16	X	1	Total K 1 1	0	0
16	Z	3	Total K 3 3	0	0
16	a	1	Total K 1 1	0	0
16	b	1	Total K 1 1	0	0

- Molecule 17 is 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (three-letter code: 04C) (formula: $C_{31}H_{44}N_4O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	1	Total C N O 42 31 4 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	1	Total C N O 42 31 4 7	0	0
17	N	1	Total C N O 42 31 4 7	0	0
17	V	1	Total C N O 42 31 4 7	0	0
17	Y	1	Total C N O 42 31 4 7	0	0
17	b	1	Total C N O 42 31 4 7	0	0

- Molecule 18 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	H	1	Total I 1 1	0	0
18	K	1	Total I 1 1	0	0
18	N	1	Total I 1 1	0	0
18	V	1	Total I 1 1	0	0
18	Y	1	Total I 1 1	0	0
18	b	1	Total I 1 1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	43	Total O 43 43	0	0
19	B	42	Total O 42 42	0	0
19	C	29	Total O 29 29	0	0
19	D	24	Total O 24 24	0	0
19	E	39	Total O 39 39	0	0
19	F	37	Total O 37 37	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	G	44	Total O 44 44	0	0
19	H	40	Total O 40 40	0	0
19	I	25	Total O 25 25	0	0
19	J	28	Total O 28 28	0	0
19	K	32	Total O 32 32	0	0
19	L	43	Total O 43 43	0	0
19	M	50	Total O 50 50	0	0
19	N	29	Total O 29 29	0	0
19	O	44	Total O 44 44	0	0
19	P	38	Total O 38 38	0	0
19	Q	13	Total O 13 13	0	0
19	R	24	Total O 24 24	0	0
19	S	40	Total O 40 40	0	0
19	T	32	Total O 32 32	0	0
19	U	38	Total O 38 38	0	0
19	V	39	Total O 39 39	0	0
19	W	39	Total O 39 39	0	0
19	X	20	Total O 20 20	0	0
19	Y	36	Total O 36 36	0	0
19	Z	49	Total O 49 49	0	0
19	a	35	Total O 35 35	0	0

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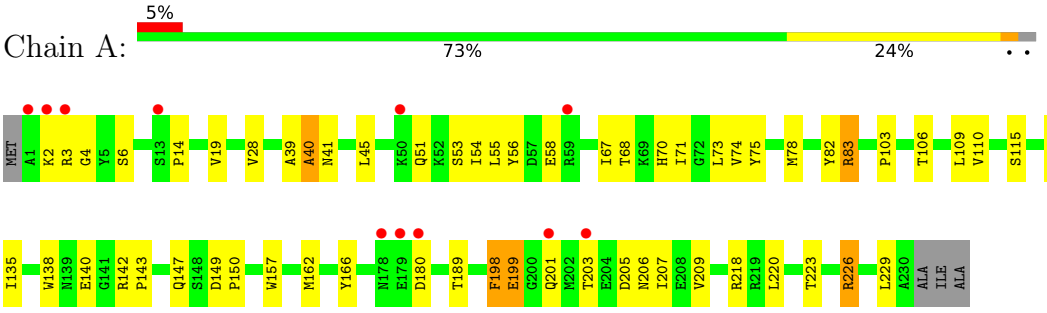
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	b	33	Total	O	0	0
			33	33		

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.

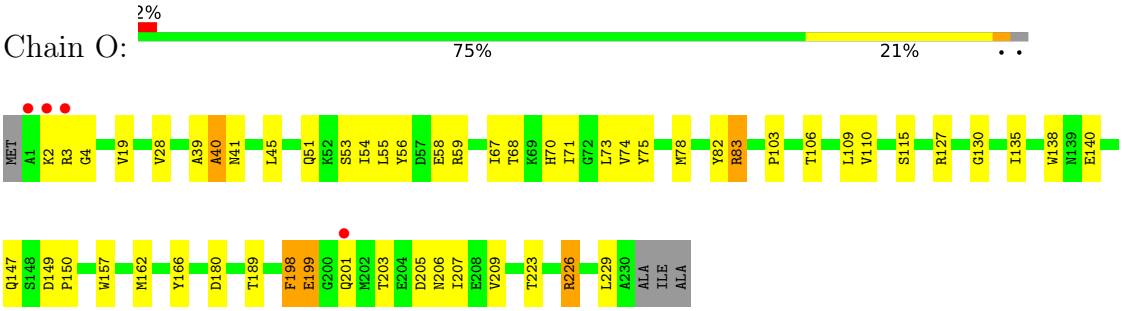
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



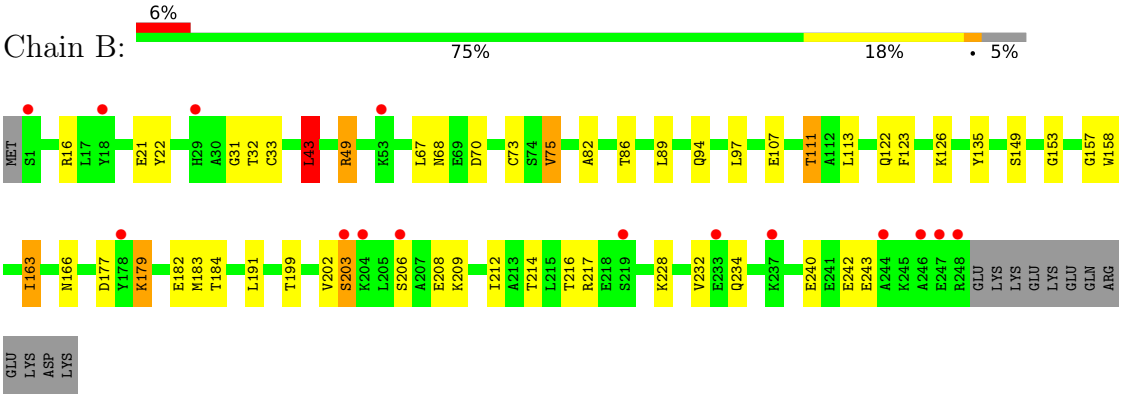
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



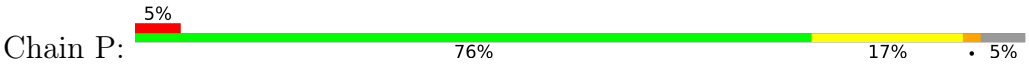
• Molecule 2: Proteasome subunit alpha type-4

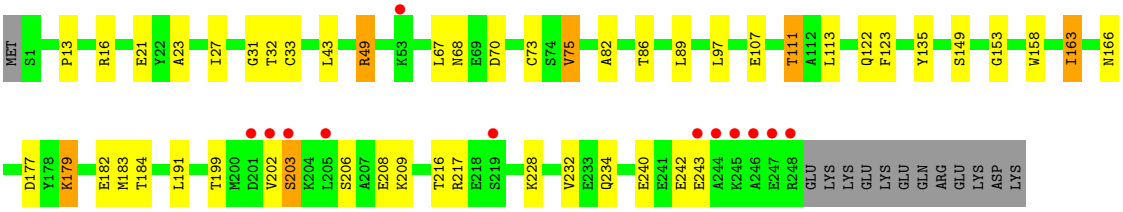
Chain B:



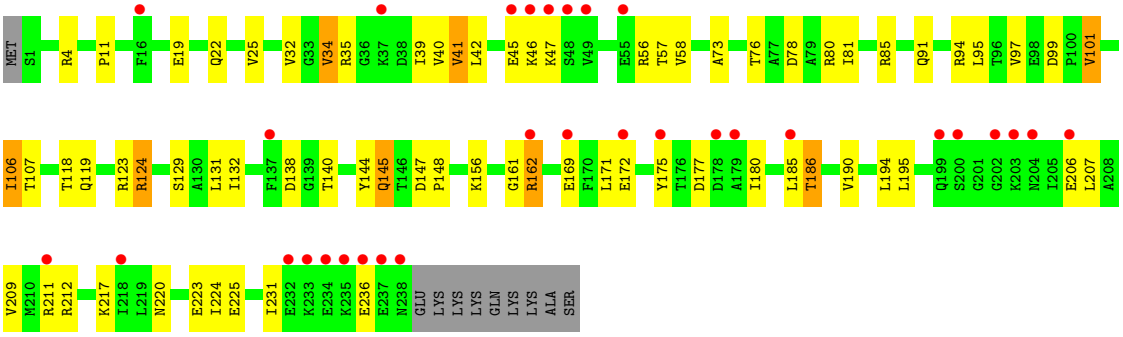
• Molecule 2: Proteasome subunit alpha type-4

Chain P:

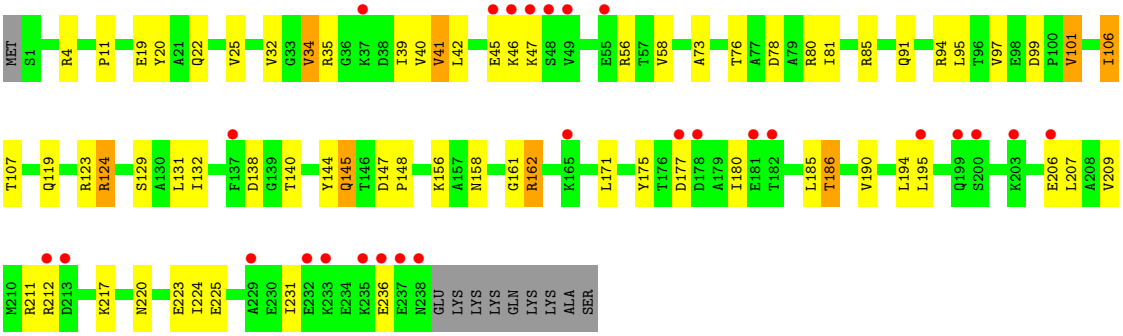




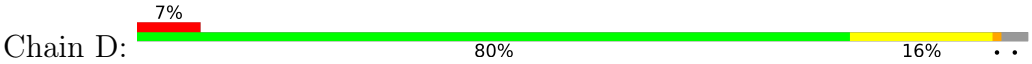
• Molecule 3: Proteasome subunit alpha type-7

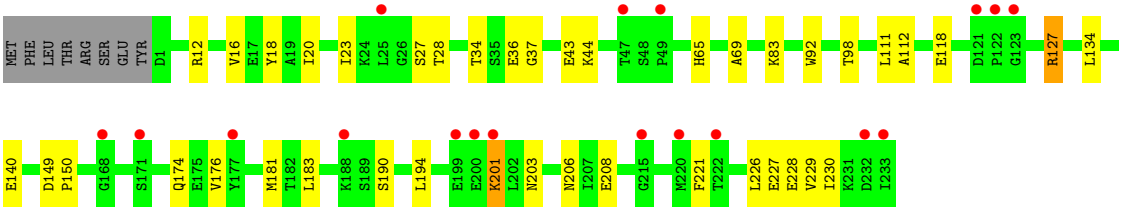


• Molecule 3: Proteasome subunit alpha type-7

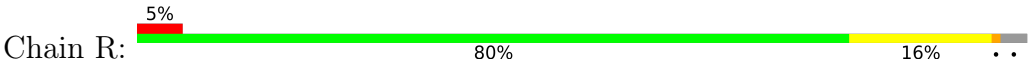


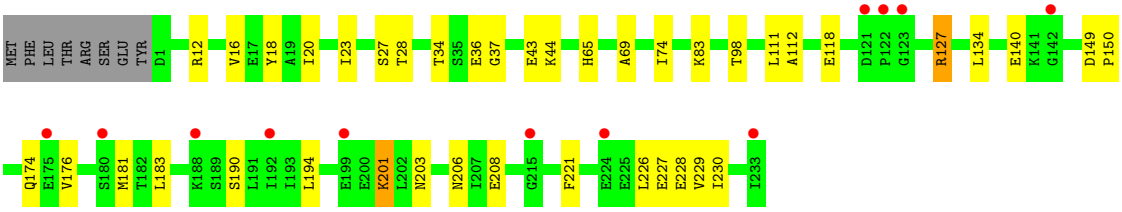
• Molecule 4: Proteasome subunit alpha type-5



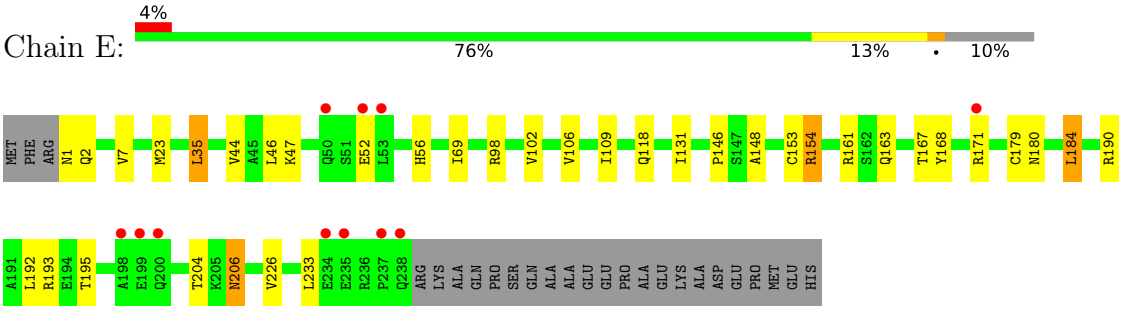


• Molecule 4: Proteasome subunit alpha type-5

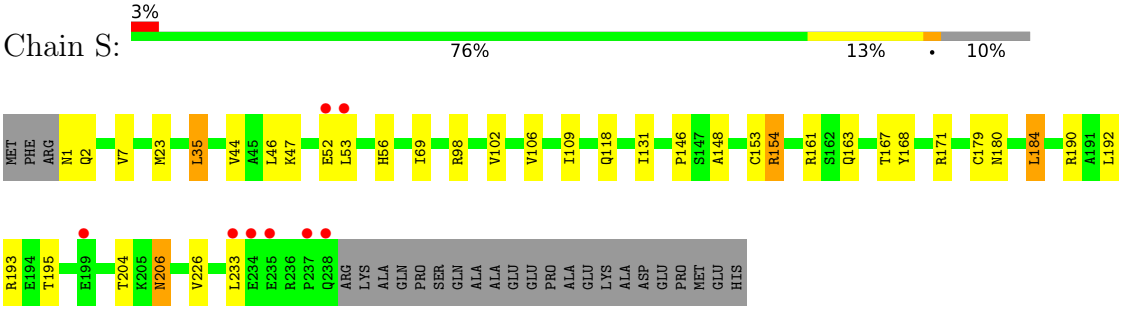




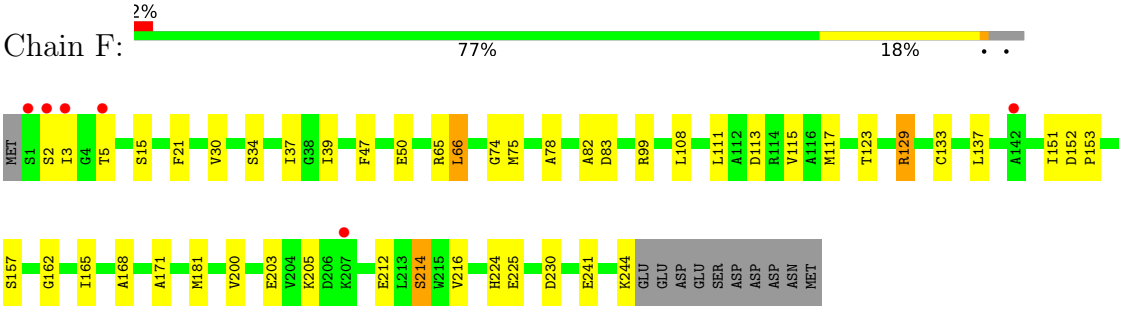
• Molecule 5: Proteasome subunit alpha type-1



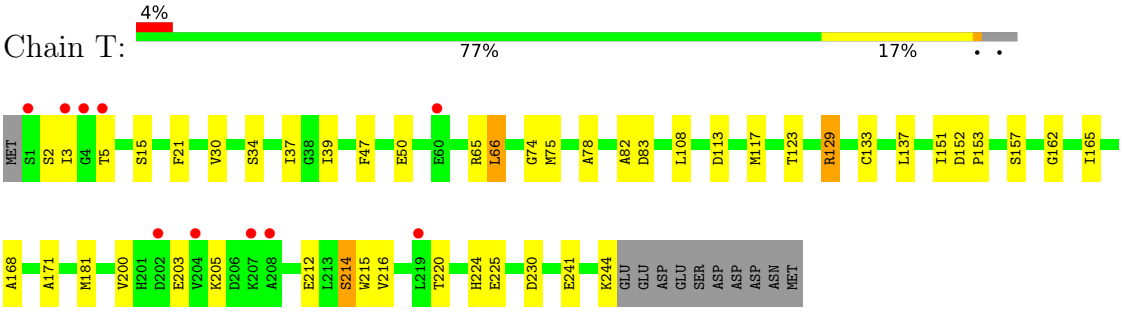
• Molecule 5: Proteasome subunit alpha type-1



• Molecule 6: Proteasome subunit alpha type-3

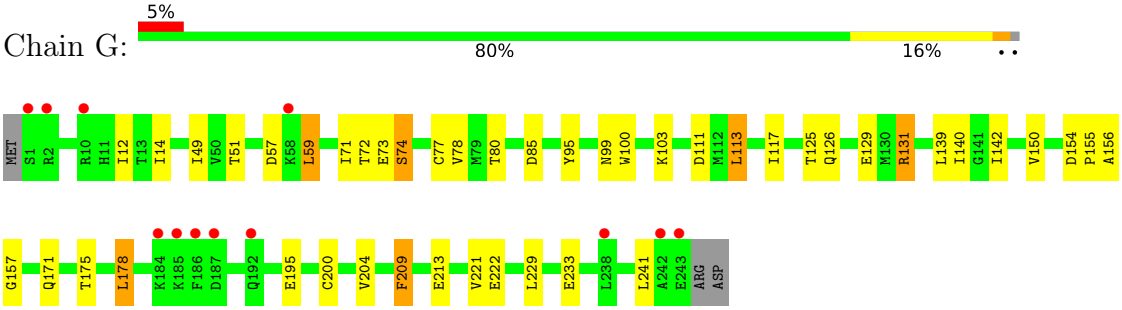


• Molecule 6: Proteasome subunit alpha type-3



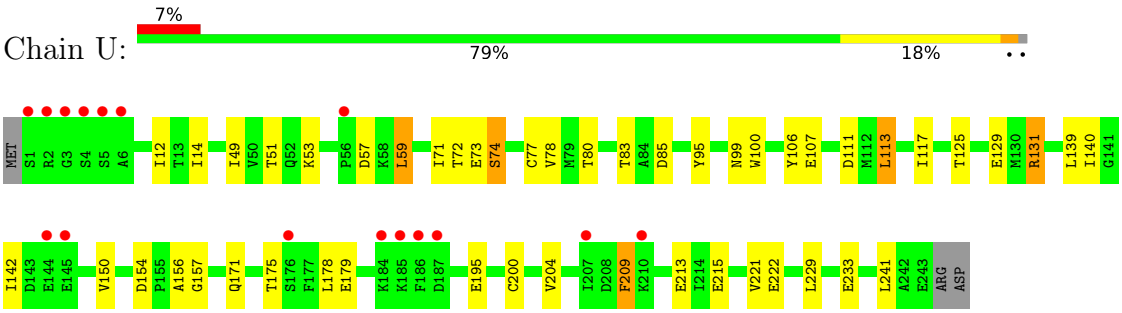
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



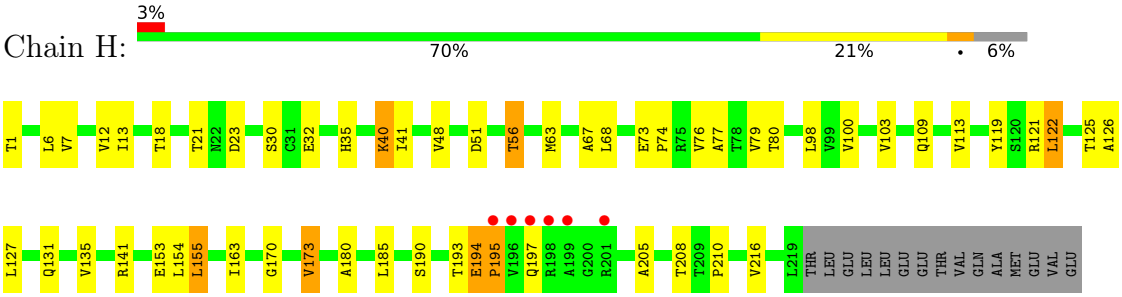
• Molecule 7: Proteasome subunit alpha type-6

Chain U:



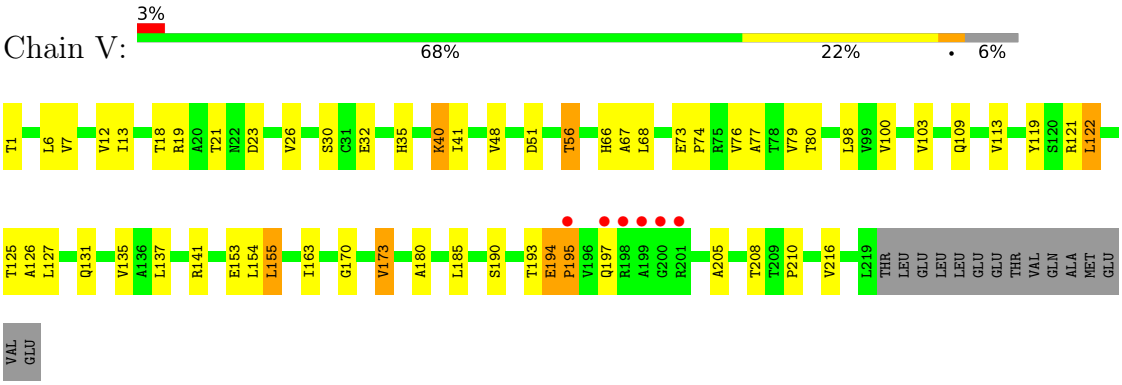
• Molecule 8: Proteasome subunit beta type-10

Chain H:



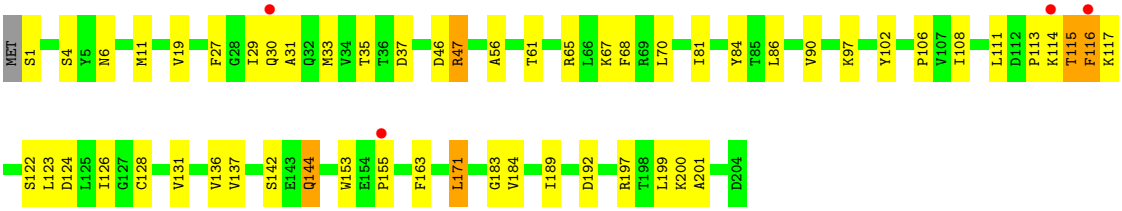
• Molecule 8: Proteasome subunit beta type-10

Chain V:

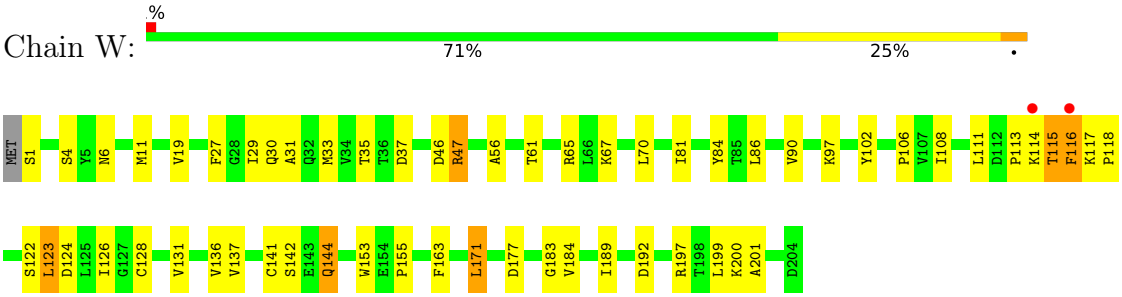


• Molecule 9: Proteasome subunit beta type-3

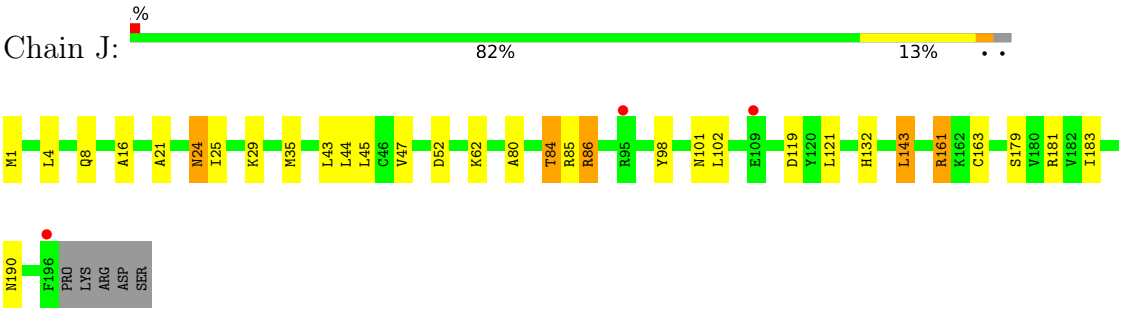
Chain I:



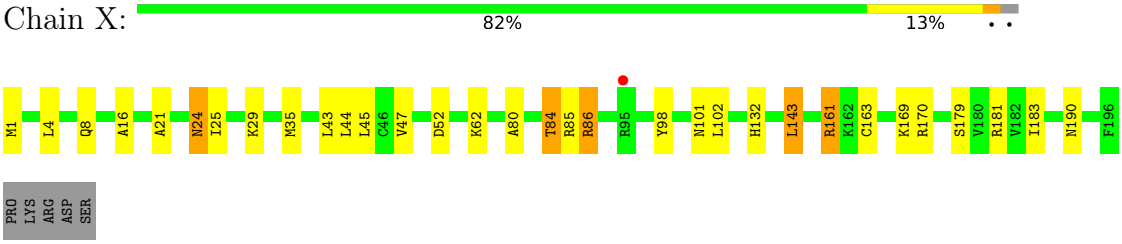
• Molecule 9: Proteasome subunit beta type-3



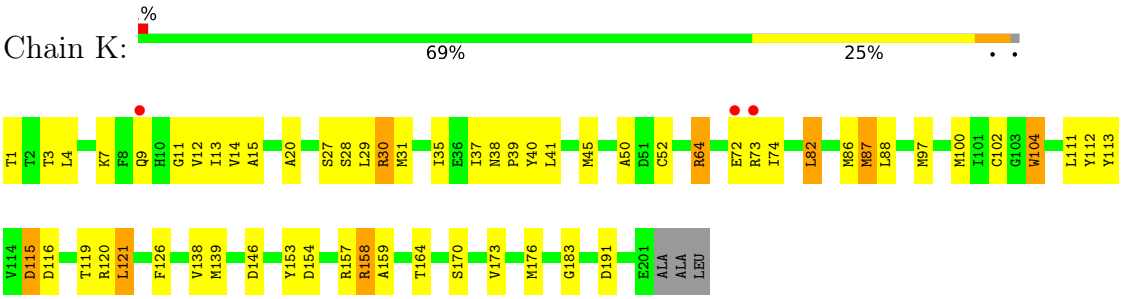
• Molecule 10: Proteasome subunit beta type-2



• Molecule 10: Proteasome subunit beta type-2

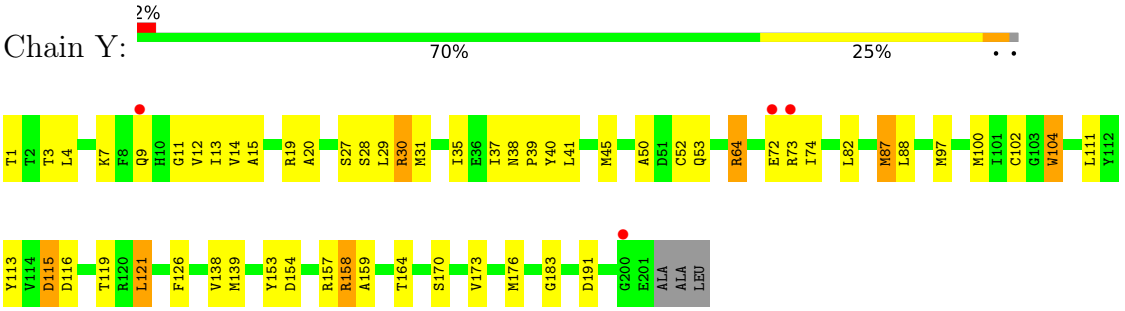


• Molecule 11: Proteasome subunit beta type-8



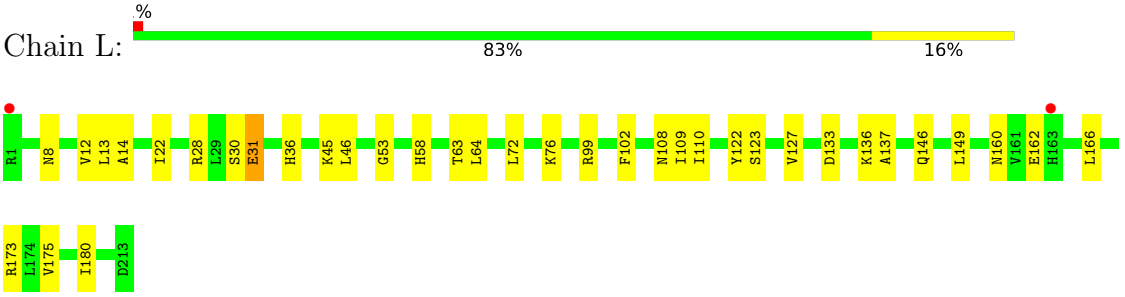
• Molecule 11: Proteasome subunit beta type-8

Chain Y:



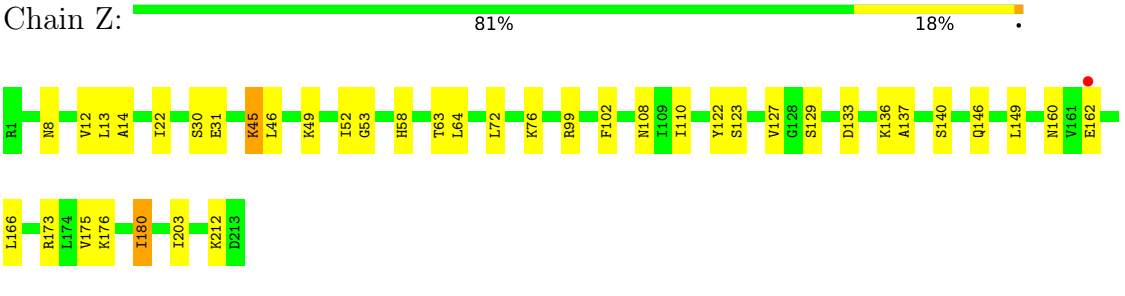
• Molecule 12: Proteasome subunit beta type-1

Chain L:



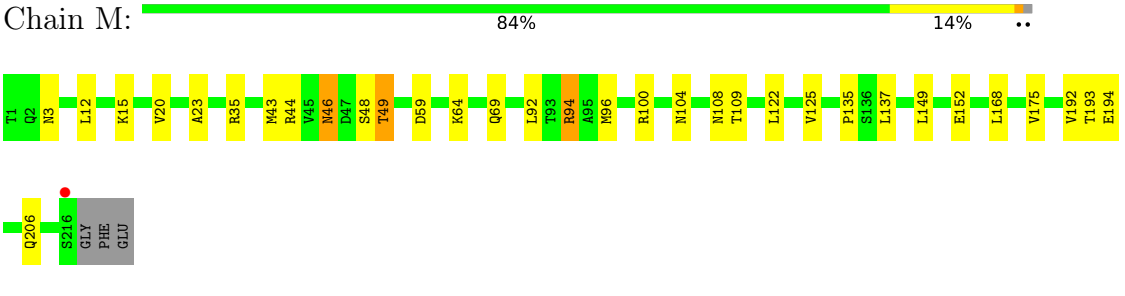
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



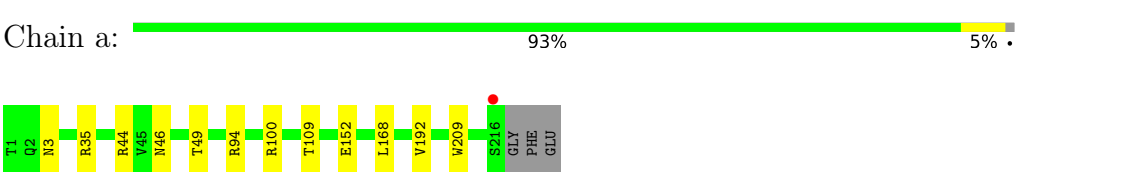
• Molecule 13: Proteasome subunit beta type-4

Chain M:



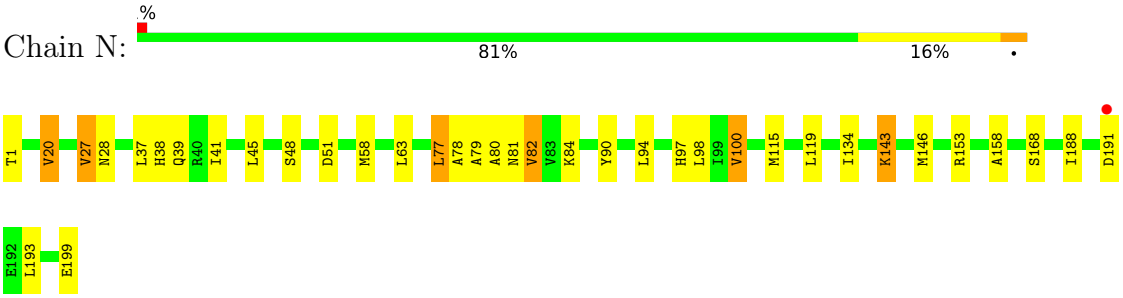
• Molecule 13: Proteasome subunit beta type-4

Chain a:



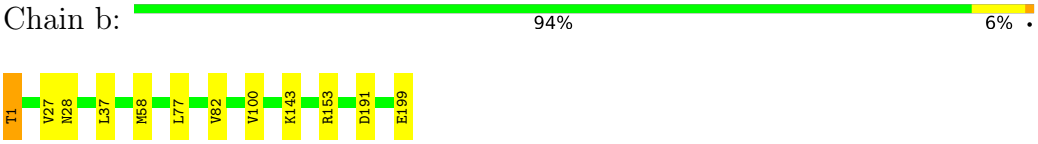
• Molecule 14: Proteasome subunit beta type-9

Chain N:



• Molecule 14: Proteasome subunit beta type-9

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.30Å 194.60Å 157.70Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 29.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (15.00-2.90) 97.2 (29.79-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.235 , 0.275 0.234 , 0.274	Depositor DCC
R_{free} test set	7255 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	49805	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, IOD, CL, 04C

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	0.39	1/1840 (0.1%)	0.50	0/2491
1	O	0.39	1/1840 (0.1%)	0.50	0/2491
2	B	0.37	1/1980 (0.1%)	0.51	1/2667 (0.0%)
2	P	0.37	1/1980 (0.1%)	0.51	0/2667
3	C	0.34	0/1903	0.51	0/2569
3	Q	0.34	0/1903	0.51	0/2569
4	D	0.36	1/1805 (0.1%)	0.47	0/2437
4	R	0.36	0/1805	0.47	0/2437
5	E	0.38	0/1907	0.51	0/2578
5	S	0.37	0/1907	0.51	0/2578
6	F	0.38	0/1938	0.49	0/2608
6	T	0.38	0/1938	0.49	0/2608
7	G	0.37	1/1924 (0.1%)	0.49	0/2600
7	U	0.37	1/1924 (0.1%)	0.49	0/2600
8	H	0.36	1/1645 (0.1%)	0.53	0/2235
8	V	0.37	1/1645 (0.1%)	0.53	0/2235
9	I	0.34	0/1621	0.50	0/2185
9	W	0.34	0/1621	0.50	0/2185
10	J	0.33	0/1602	0.50	0/2167
10	X	0.33	0/1602	0.49	0/2167
11	K	0.43	1/1597 (0.1%)	0.55	0/2151
11	Y	0.43	1/1597 (0.1%)	0.55	0/2151
12	L	0.32	0/1685	0.49	0/2271
12	Z	0.32	0/1685	0.50	0/2271
13	M	0.40	0/1718	0.50	0/2325
13	a	0.40	1/1718 (0.1%)	0.50	0/2325
14	N	0.37	0/1526	0.51	0/2071
14	b	0.37	0/1526	0.51	1/2071 (0.0%)
All	All	0.37	12/49382 (0.0%)	0.50	2/66710 (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
11	K	0	1
11	Y	0	1
14	N	0	2
14	b	0	1
All	All	0	5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	1	THR	C-N	5.77	1.47	1.34
8	H	1	THR	C-N	5.51	1.46	1.34
11	Y	104	TRP	CD2-CE2	5.05	1.47	1.41
7	U	100	TRP	CD2-CE2	5.04	1.47	1.41
1	A	138	TRP	CD2-CE2	5.04	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1	THR	C-N-CA	5.78	136.14	121.70
2	B	43	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	1	THR	Peptide
14	N	1	THR	Mainchain,Peptide
11	Y	1	THR	Peptide
14	b	1	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1801	0	1800	41	0
1	O	1801	0	1800	35	0
2	B	1950	0	1973	29	0
2	P	1950	0	1973	24	0
3	C	1876	0	1902	45	0
3	Q	1876	0	1902	43	0
4	D	1778	0	1767	25	0
4	R	1778	0	1767	27	0
5	E	1872	0	1859	24	0
5	S	1872	0	1859	24	0
6	F	1903	0	1894	30	0
6	T	1903	0	1894	29	0
7	G	1890	0	1900	28	0
7	U	1890	0	1900	31	0
8	H	1619	0	1640	27	0
8	V	1619	0	1640	30	0
9	I	1592	0	1612	32	0
9	W	1592	0	1612	32	0
10	J	1570	0	1573	19	0
10	X	1570	0	1573	18	0
11	K	1566	0	1516	41	1
11	Y	1566	0	1515	40	0
12	L	1654	0	1652	20	0
12	Z	1654	0	1651	25	0
13	M	1685	0	1664	17	1
13	a	1685	0	1664	0	0
14	N	1498	0	1476	20	0
14	b	1498	0	1476	0	0
15	A	3	0	0	0	0
15	D	1	0	0	0	0
15	E	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	L	2	0	0	0	0
15	M	4	0	0	0	0
15	N	1	0	0	0	0
15	O	2	0	0	0	0
15	P	1	0	0	0	0
15	Q	4	0	0	0	0
15	R	3	0	0	0	0
15	S	2	0	0	0	0
15	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	V	4	0	0	0	0
15	W	1	0	0	0	0
15	X	3	0	0	0	0
15	Z	1	0	0	0	0
15	a	4	0	0	0	0
16	B	1	0	0	0	0
16	G	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	S	1	0	0	0	0
16	X	1	0	0	0	0
16	Z	3	0	0	0	0
16	a	1	0	0	0	0
16	b	1	0	0	0	0
17	H	42	0	42	0	0
17	K	42	0	42	3	0
17	N	42	0	42	3	0
17	V	42	0	42	1	0
17	Y	42	0	42	3	0
17	b	42	0	42	0	0
18	H	1	0	0	0	0
18	K	1	0	0	1	0
18	N	1	0	0	0	0
18	V	1	0	0	1	0
18	Y	1	0	0	0	0
18	b	1	0	0	0	0
19	A	43	0	0	2	0
19	B	42	0	0	4	0
19	C	29	0	0	0	0
19	D	24	0	0	0	0
19	E	39	0	0	0	0
19	F	37	0	0	0	0
19	G	44	0	0	1	0
19	H	40	0	0	0	0
19	I	25	0	0	0	0
19	J	28	0	0	0	0
19	K	32	0	0	3	0
19	L	43	0	0	3	0
19	M	50	0	0	1	0
19	N	29	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	44	0	0	0	0
19	P	38	0	0	0	0
19	Q	13	0	0	0	0
19	R	24	0	0	0	0
19	S	40	0	0	0	0
19	T	32	0	0	0	0
19	U	38	0	0	3	0
19	V	39	0	0	0	0
19	W	39	0	0	0	0
19	X	20	0	0	0	0
19	Y	36	0	0	0	0
19	Z	49	0	0	5	0
19	a	35	0	0	0	0
19	b	33	0	0	0	0
All	All	49805	0	48706	700	1

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 8.

The worst 5 of 700 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)
5:S:154:ARG:HG2	5:S:154:ARG:HH11	1.26	0.98
11:Y:31:MET:HG2	17:Y:301:04C:H42	1.45	0.98
5:E:154:ARG:HG2	5:E:154:ARG:HH11	1.27	0.96
5:E:2:GLN:HE22	6:F:5:THR:HA	1.29	0.96
3:C:162:ARG:HG2	3:C:162:ARG:HH11	1.31	0.95

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:146:ASP:O	13:M:206:GLN:NE2[2_655]	2.08	0.12

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	228/234 (97%)	217 (95%)	8 (4%)	3 (1%)	12	37
1	O	228/234 (97%)	217 (95%)	8 (4%)	3 (1%)	12	37
2	B	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	34	66
2	P	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	34	66
3	C	236/248 (95%)	222 (94%)	14 (6%)	0	100	100
3	Q	236/248 (95%)	221 (94%)	15 (6%)	0	100	100
4	D	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	34	66
4	R	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	34	66
5	E	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
5	S	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
6	F	242/255 (95%)	234 (97%)	7 (3%)	1 (0%)	34	66
6	T	242/255 (95%)	234 (97%)	7 (3%)	1 (0%)	34	66
7	G	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
7	U	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
8	H	217/234 (93%)	206 (95%)	9 (4%)	2 (1%)	17	48
8	V	217/234 (93%)	206 (95%)	9 (4%)	2 (1%)	17	48
9	I	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15	45
9	W	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15	45
10	J	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	29	61
10	X	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	29	61
11	K	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
11	Y	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
12	L	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
12	Z	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
13	M	214/219 (98%)	205 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
14	N	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
14	b	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
All	All	6188/6446 (96%)	5953 (96%)	213 (3%)	22 (0%)	34	66

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	216	VAL
9	I	30	GLN
6	T	216	VAL
9	W	30	GLN
1	A	40	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/191 (99%)	175 (93%)	14 (7%)	13	38
1	O	189/191 (99%)	174 (92%)	15 (8%)	12	34
2	B	208/221 (94%)	190 (91%)	18 (9%)	10	30
2	P	208/221 (94%)	190 (91%)	18 (9%)	10	30
3	C	202/211 (96%)	178 (88%)	24 (12%)	5	15
3	Q	202/211 (96%)	178 (88%)	24 (12%)	5	15
4	D	195/203 (96%)	186 (95%)	9 (5%)	27	60
4	R	195/203 (96%)	186 (95%)	9 (5%)	27	60
5	E	204/224 (91%)	191 (94%)	13 (6%)	17	45
5	S	204/224 (91%)	191 (94%)	13 (6%)	17	45
6	F	200/211 (95%)	189 (94%)	11 (6%)	21	53
6	T	200/211 (95%)	189 (94%)	11 (6%)	21	53
7	G	207/210 (99%)	197 (95%)	10 (5%)	25	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	U	207/210 (99%)	197 (95%)	10 (5%)	25 58
8	H	169/183 (92%)	151 (89%)	18 (11%)	6 20
8	V	169/183 (92%)	151 (89%)	18 (11%)	6 20
9	I	174/175 (99%)	163 (94%)	11 (6%)	18 46
9	W	174/175 (99%)	163 (94%)	11 (6%)	18 46
10	J	166/171 (97%)	158 (95%)	8 (5%)	25 58
10	X	166/171 (97%)	158 (95%)	8 (5%)	25 58
11	K	165/166 (99%)	151 (92%)	14 (8%)	10 31
11	Y	165/166 (99%)	151 (92%)	14 (8%)	10 31
12	L	178/178 (100%)	170 (96%)	8 (4%)	27 61
12	Z	178/178 (100%)	168 (94%)	10 (6%)	21 52
13	M	178/180 (99%)	167 (94%)	11 (6%)	18 47
13	a	178/180 (99%)	167 (94%)	11 (6%)	18 47
14	N	155/155 (100%)	143 (92%)	12 (8%)	13 35
14	b	155/155 (100%)	144 (93%)	11 (7%)	14 40
All	All	5180/5358 (97%)	4816 (93%)	364 (7%)	15 41

5 of 364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	195	LEU
8	V	56	THR
4	R	12	ARG
6	T	30	VAL
9	W	67	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	111	GLN
13	a	208	ASN
4	R	106	GLN
13	a	157	GLN
11	Y	117	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 60 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
17	04C	K	301	11	44,44,44	1.20	2 (4%)	56,58,58	1.00	2 (3%)
17	04C	V	301	8	44,44,44	1.18	3 (6%)	56,58,58	0.99	5 (8%)
17	04C	b	201	14	44,44,44	1.28	4 (9%)	56,58,58	1.17	6 (10%)
17	04C	Y	301	11	44,44,44	1.23	2 (4%)	56,58,58	1.36	7 (12%)
17	04C	H	301	8	44,44,44	1.14	2 (4%)	56,58,58	0.96	3 (5%)
17	04C	N	201	14	44,44,44	1.24	3 (6%)	56,58,58	1.19	7 (12%)

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
17	04C	K	301	11	-	12/44/52/52	0/3/3/3
17	04C	V	301	8	-	15/44/52/52	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	04C	b	201	14	-	11/44/52/52	0/3/3/3
17	04C	Y	301	11	-	15/44/52/52	0/3/3/3
17	04C	H	301	8	-	21/44/52/52	0/3/3/3
17	04C	N	201	14	-	12/44/52/52	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	04C	C10-C9	3.39	1.59	1.53
17	K	301	04C	C10-C9	3.19	1.59	1.53
17	K	301	04C	C12-C10	3.09	1.56	1.52
17	b	201	04C	C10-C9	3.07	1.59	1.53
17	b	201	04C	C12-C10	3.06	1.56	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	04C	C32-N31-C36	4.61	119.20	108.83
17	b	201	04C	C11-C10-C12	-4.28	104.25	109.88
17	Y	301	04C	C33-C32-N31	4.27	116.58	110.10
17	K	301	04C	C11-C10-C12	-4.22	104.33	109.88
17	N	201	04C	C11-C10-C12	-3.94	104.70	109.88

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	04C	C6-C7-C8-N22
17	H	301	04C	C6-C7-C8-C9
17	H	301	04C	C11-C10-C9-O21
17	H	301	04C	C9-C10-C12-O13
17	H	301	04C	C11-C10-C12-O13

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	04C	3	0
17	V	301	04C	1	0
17	Y	301	04C	3	0

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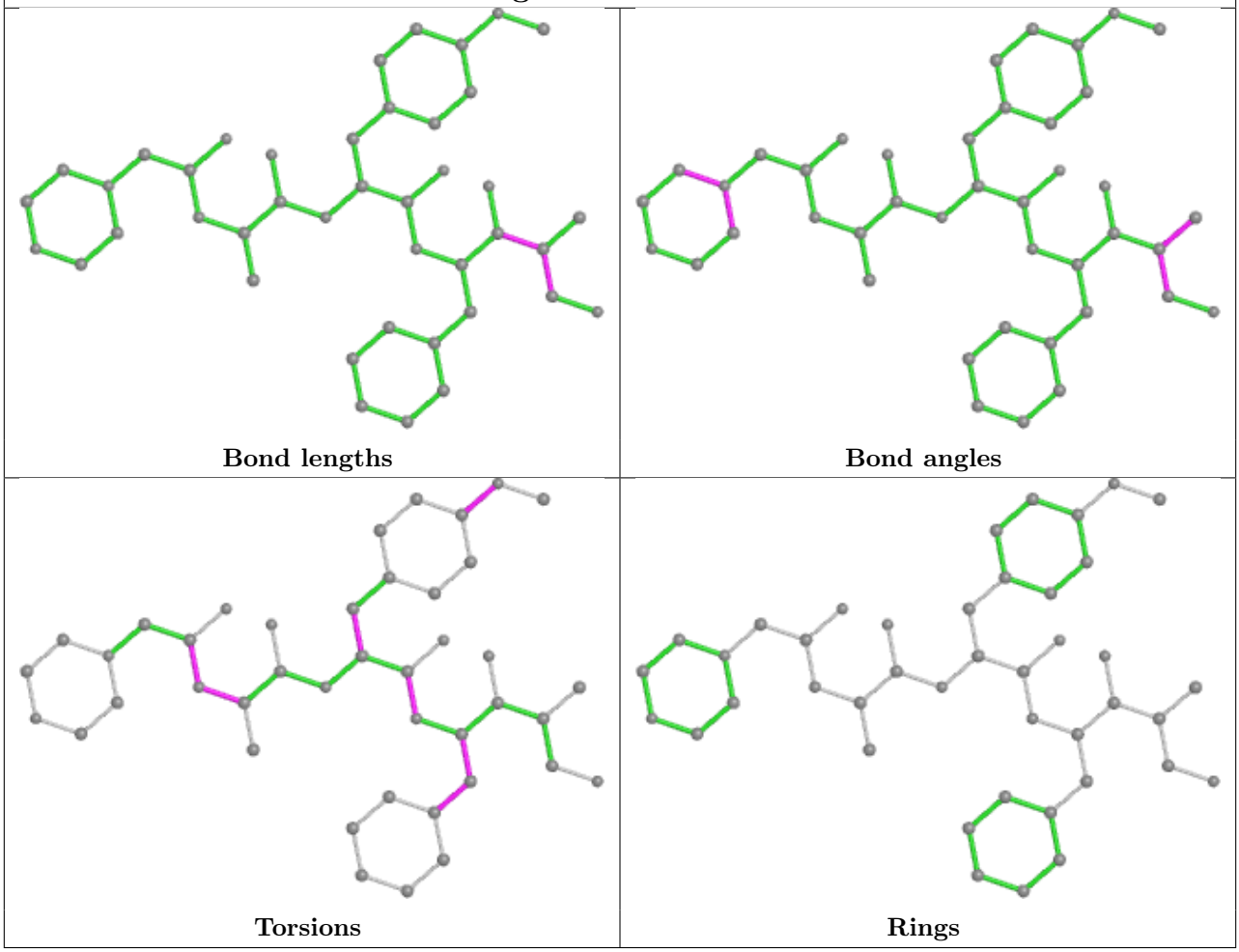
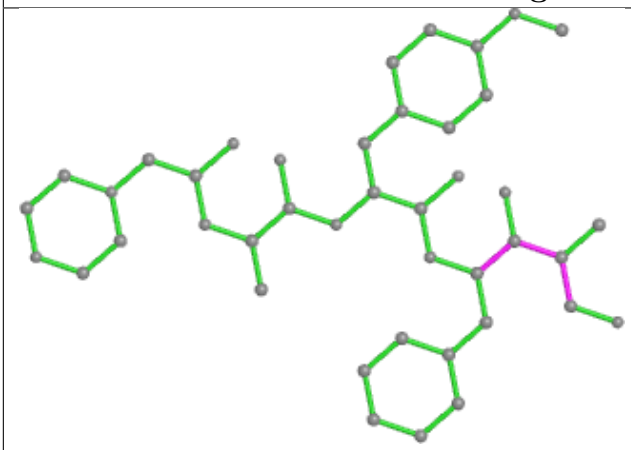
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	201	04C	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

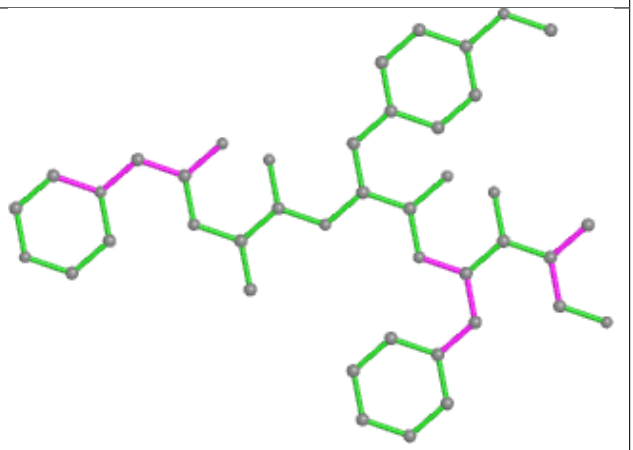
Ligand 04C K 301



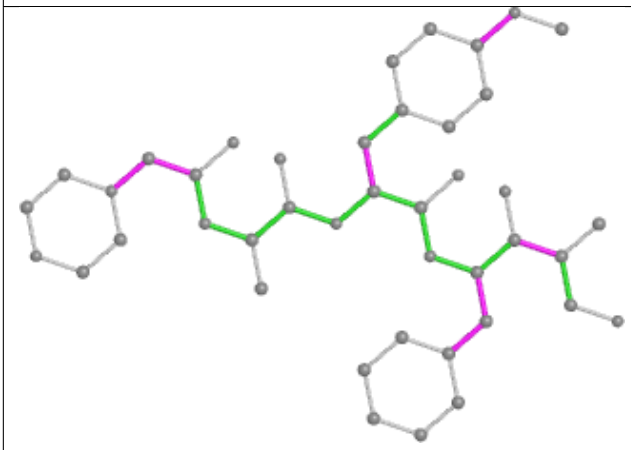
Ligand 04C V 301



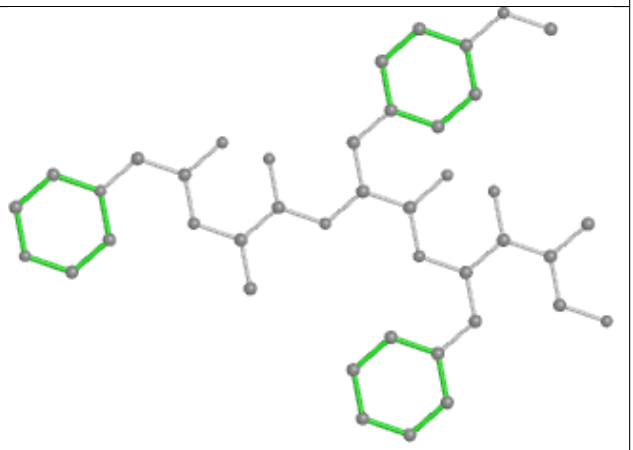
Bond lengths



Bond angles

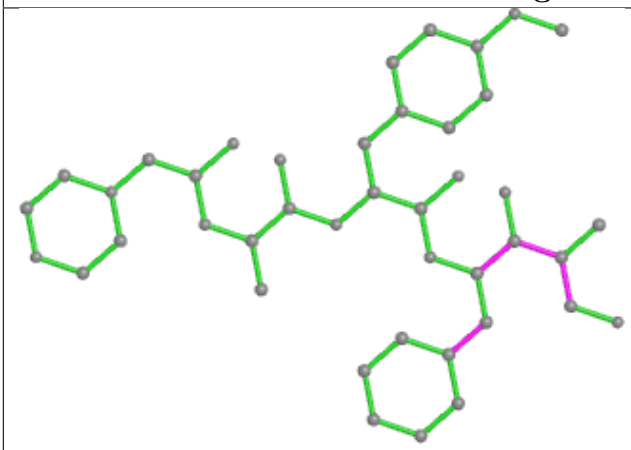


Torsions

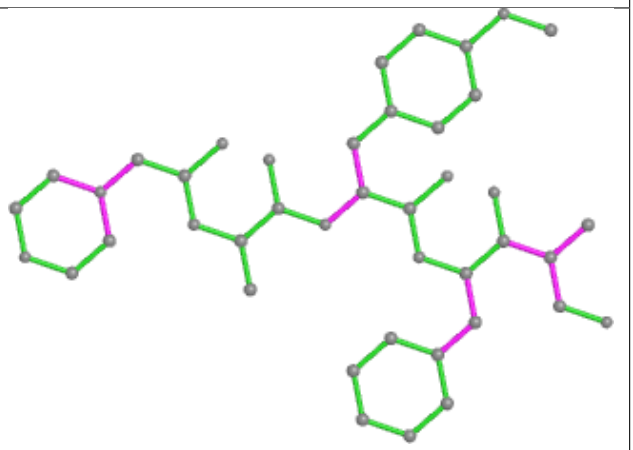


Rings

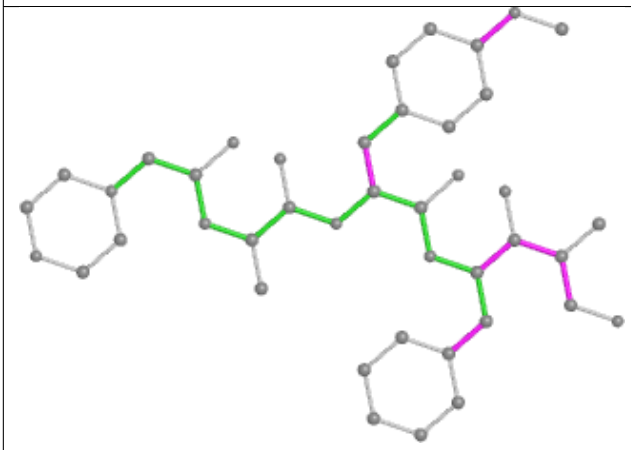
Ligand 04C b 201



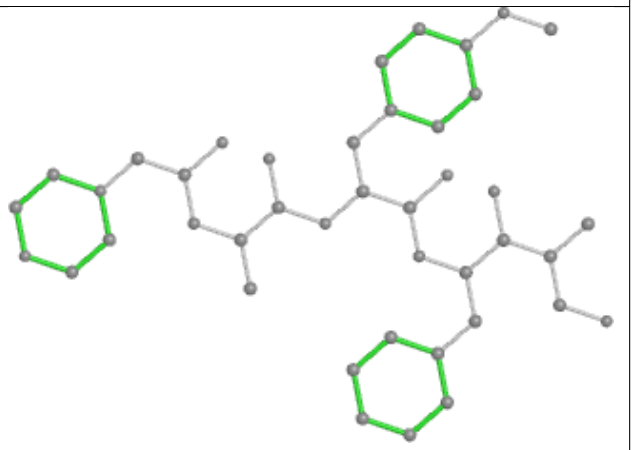
Bond lengths



Bond angles

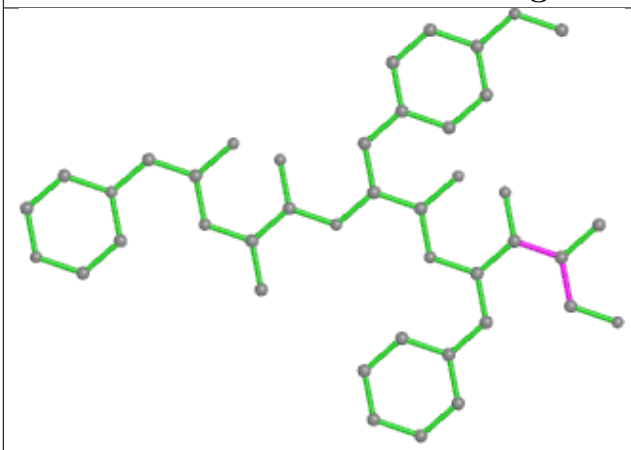


Torsions

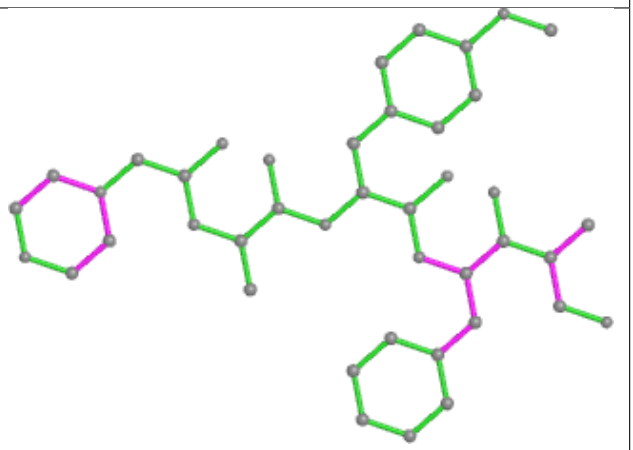


Rings

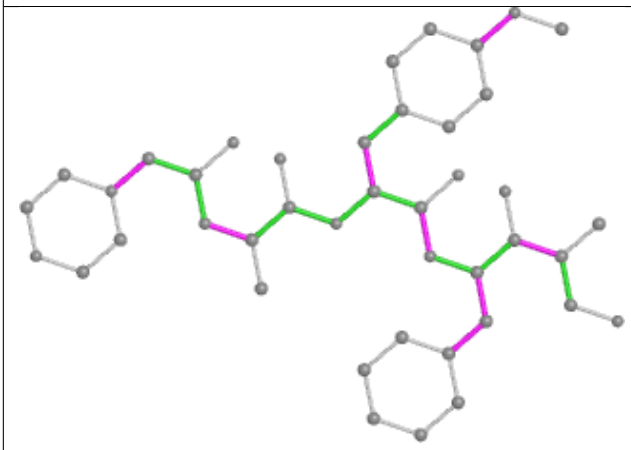
Ligand 04C Y 301



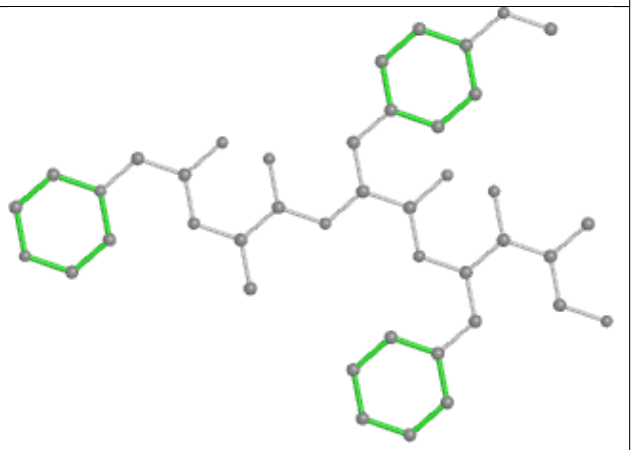
Bond lengths



Bond angles

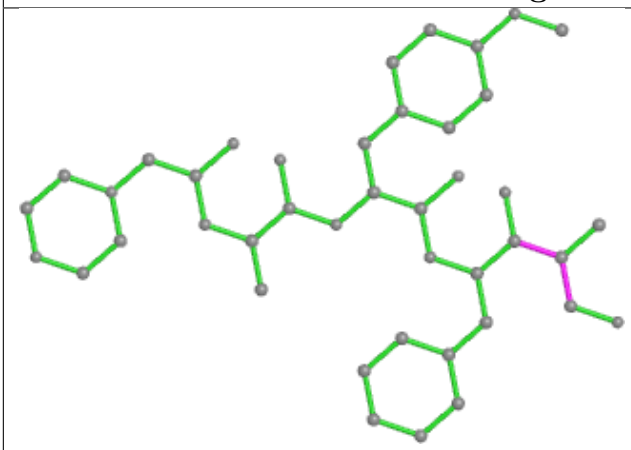


Torsions



Rings

Ligand 04C H 301



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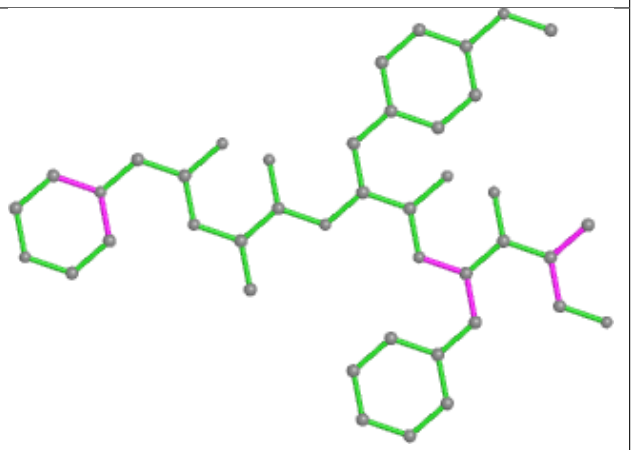
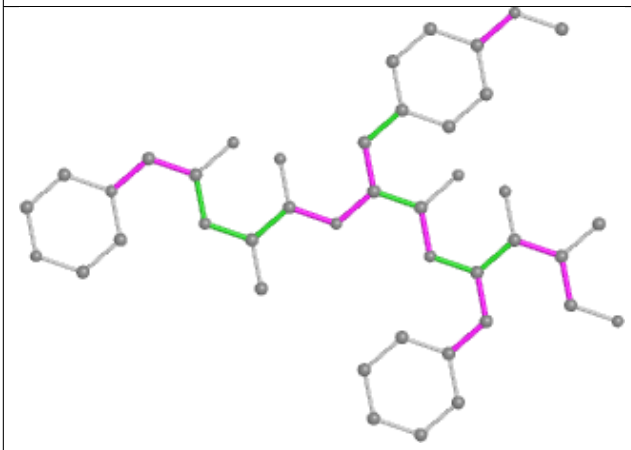
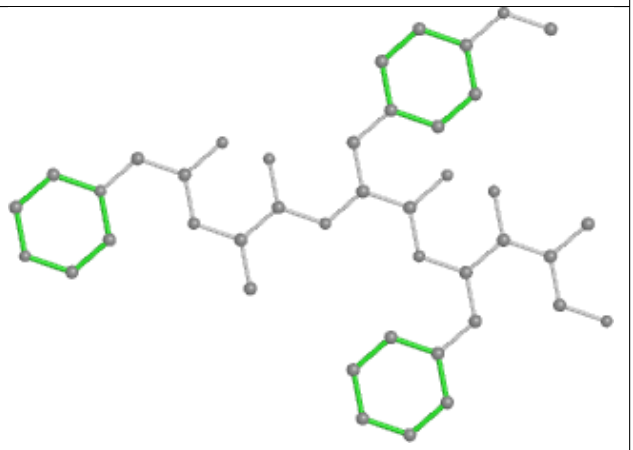


Bond angles

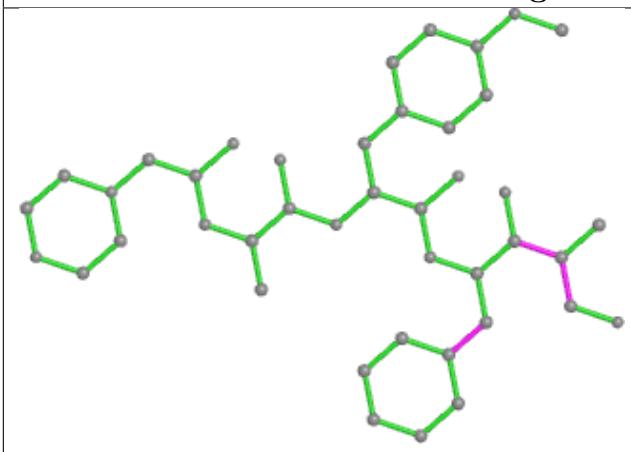


Torsions

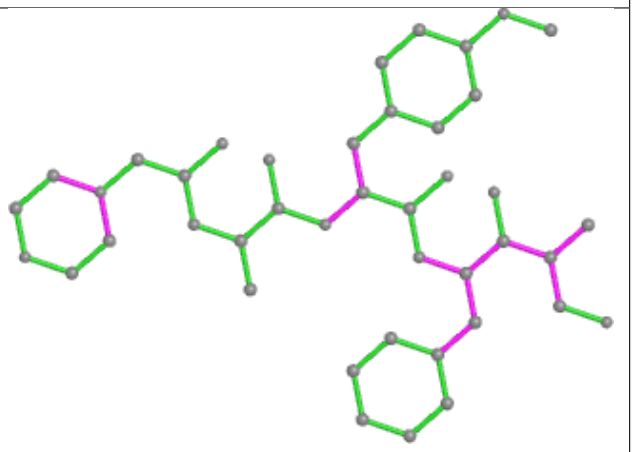


Rings

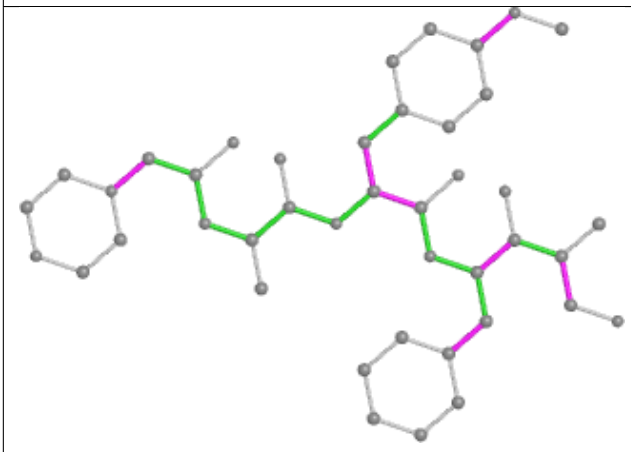
Ligand 04C N 201



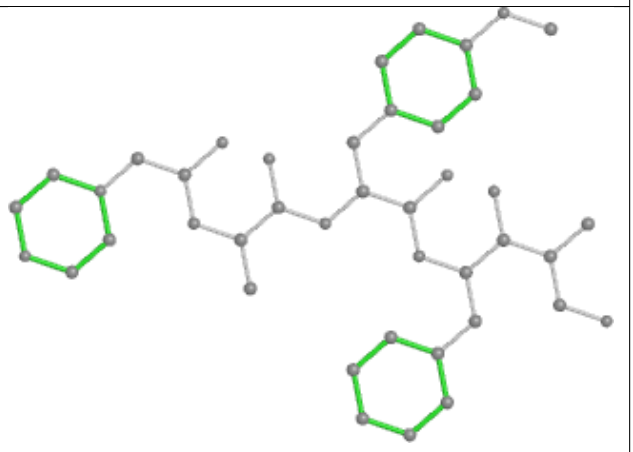
Bond lengths



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/234 (98%)	0.10	11 (4%)	30	27	44, 68, 95, 106	0
1	O	230/234 (98%)	0.03	4 (1%)	70	69	35, 52, 86, 96	0
2	B	248/261 (95%)	0.24	15 (6%)	21	18	45, 72, 121, 149	0
2	P	248/261 (95%)	0.00	12 (4%)	30	27	32, 57, 99, 142	0
3	C	238/248 (95%)	0.64	31 (13%)	3	2	51, 87, 150, 194	0
3	Q	238/248 (95%)	0.47	27 (11%)	5	4	41, 74, 132, 174	0
4	D	233/241 (96%)	0.55	18 (7%)	13	10	41, 91, 150, 200	0
4	R	233/241 (96%)	0.39	12 (5%)	27	23	43, 83, 125, 154	0
5	E	238/263 (90%)	0.19	11 (4%)	32	29	34, 66, 107, 128	0
5	S	238/263 (90%)	0.08	8 (3%)	45	40	35, 61, 102, 122	0
6	F	244/255 (95%)	0.17	6 (2%)	57	55	37, 67, 103, 117	0
6	T	244/255 (95%)	0.09	10 (4%)	37	32	34, 57, 93, 111	0
7	G	243/246 (98%)	0.21	12 (4%)	29	26	47, 70, 108, 129	0
7	U	243/246 (98%)	0.08	16 (6%)	18	14	32, 57, 99, 117	0
8	H	219/234 (93%)	-0.12	6 (2%)	54	50	11, 50, 94, 125	0
8	V	219/234 (93%)	-0.24	6 (2%)	54	50	4, 41, 78, 103	0
9	I	204/205 (99%)	-0.08	4 (1%)	65	63	33, 55, 82, 101	0
9	W	204/205 (99%)	-0.25	2 (0%)	82	82	27, 42, 64, 82	0
10	J	196/201 (97%)	-0.16	3 (1%)	73	73	38, 50, 72, 83	0
10	X	196/201 (97%)	-0.26	1 (0%)	91	91	32, 48, 67, 83	0
11	K	201/204 (98%)	-0.08	3 (1%)	73	73	9, 47, 72, 87	0
11	Y	201/204 (98%)	0.15	4 (1%)	65	63	5, 57, 82, 94	0
12	L	213/213 (100%)	-0.20	2 (0%)	84	84	29, 42, 64, 86	0
12	Z	213/213 (100%)	-0.14	1 (0%)	91	91	41, 49, 67, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	216/219 (98%)	-0.30	1 (0%) 91 91	29, 38, 61, 82	0
13	a	216/219 (98%)	-0.24	1 (0%) 91 91	36, 44, 61, 82	0
14	N	199/199 (100%)	-0.19	1 (0%) 91 91	4, 43, 61, 72	0
14	b	199/199 (100%)	-0.20	0 100 100	3, 41, 61, 70	0
All	All	6244/6446 (96%)	0.05	228 (3%) 41 37	3, 56, 111, 200	0

The worst 5 of 228 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	5	THR	7.7
3	C	49	VAL	7.7
4	D	123	GLY	7.4
4	R	123	GLY	7.3
6	F	1	SER	6.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	K	L	303	1/1	0.70	0.69	31,31,31,31	0
16	K	B	301	1/1	0.72	0.32	55,55,55,55	0
16	K	K	303	1/1	0.74	0.18	51,51,51,51	0
15	CL	V	305	1/1	0.81	0.23	44,44,44,44	0
15	CL	a	303	1/1	0.82	0.14	44,44,44,44	0
15	CL	U	301	1/1	0.82	0.14	45,45,45,45	0
15	CL	S	302	1/1	0.82	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CL	X	302	1/1	0.82	0.19	51,51,51,51	0
16	K	b	203	1/1	0.84	0.38	45,45,45,45	0
16	K	G	301	1/1	0.85	0.22	56,56,56,56	0
15	CL	R	302	1/1	0.85	0.22	59,59,59,59	0
16	K	Z	302	1/1	0.86	0.14	47,47,47,47	0
15	CL	P	301	1/1	0.86	0.19	39,39,39,39	0
16	K	S	303	1/1	0.88	0.27	50,50,50,50	0
15	CL	A	303	1/1	0.89	0.13	45,45,45,45	0
17	04C	Y	301	42/42	0.89	0.30	2,16,29,34	0
16	K	X	304	1/1	0.90	0.24	70,70,70,70	0
15	CL	a	304	1/1	0.90	0.12	44,44,44,44	0
15	CL	R	303	1/1	0.90	0.11	45,45,45,45	0
15	CL	L	302	1/1	0.90	0.15	24,24,24,24	0
15	CL	X	303	1/1	0.91	0.17	72,72,72,72	0
15	CL	M	304	1/1	0.91	0.09	48,48,48,48	0
17	04C	N	201	42/42	0.91	0.23	2,3,8,11	0
15	CL	E	301	1/1	0.91	0.20	42,42,42,42	0
17	04C	K	301	42/42	0.92	0.26	7,14,28,32	0
16	K	Z	304	1/1	0.92	0.21	40,40,40,40	0
15	CL	J	301	1/1	0.92	0.07	35,35,35,35	0
17	04C	b	201	42/42	0.93	0.22	2,3,12,17	0
17	04C	V	301	42/42	0.94	0.16	3,5,24,25	0
15	CL	X	301	1/1	0.94	0.24	46,46,46,46	0
17	04C	H	301	42/42	0.94	0.20	6,13,19,20	0
15	CL	V	306	1/1	0.95	0.12	40,40,40,40	0
15	CL	A	302	1/1	0.95	0.12	32,32,32,32	0
16	K	M	305	1/1	0.95	0.20	37,37,37,37	0
16	K	Z	303	1/1	0.95	0.07	24,24,24,24	0
15	CL	R	301	1/1	0.96	0.12	32,32,32,32	0
15	CL	D	301	1/1	0.96	0.10	35,35,35,35	0
16	K	a	305	1/1	0.96	0.43	37,37,37,37	0
15	CL	Q	301	1/1	0.96	0.16	39,39,39,39	0
15	CL	Q	302	1/1	0.96	0.09	37,37,37,37	0
15	CL	S	301	1/1	0.97	0.18	35,35,35,35	0
15	CL	M	301	1/1	0.97	0.08	39,39,39,39	0
15	CL	O	301	1/1	0.97	0.09	33,33,33,33	0
15	CL	O	302	1/1	0.97	0.08	44,44,44,44	0
16	K	I	302	1/1	0.97	0.45	41,41,41,41	0
15	CL	a	301	1/1	0.97	0.10	33,33,33,33	0
15	CL	a	302	1/1	0.97	0.07	29,29,29,29	0
15	CL	Z	301	1/1	0.98	0.19	26,26,26,26	0
15	CL	Q	304	1/1	0.98	0.04	29,29,29,29	0

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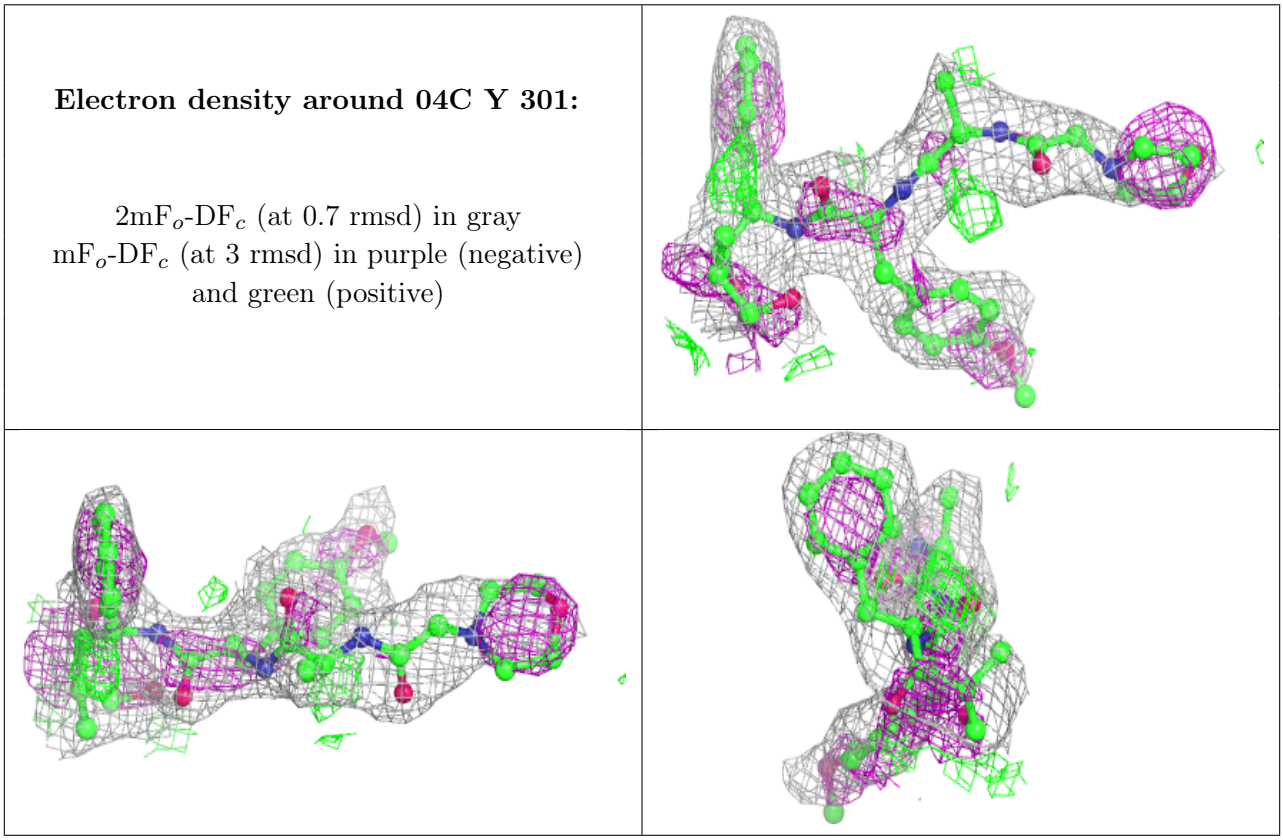
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CL	V	304	1/1	0.98	0.09	33,33,33,33	0
15	CL	M	302	1/1	0.98	0.14	30,30,30,30	0
15	CL	I	301	1/1	0.98	0.06	28,28,28,28	0
15	CL	N	203	1/1	0.98	0.09	36,36,36,36	0
15	CL	A	301	1/1	0.98	0.08	34,34,34,34	0
15	CL	Q	303	1/1	0.98	0.03	32,32,32,32	0
15	CL	H	303	1/1	0.99	0.07	31,31,31,31	0
15	CL	M	303	1/1	0.99	0.06	25,25,25,25	0
15	CL	W	301	1/1	0.99	0.12	28,28,28,28	0
15	CL	V	303	1/1	0.99	0.12	30,30,30,30	0
15	CL	L	301	1/1	0.99	0.05	32,32,32,32	0
18	IOD	H	302	1/1	0.99	0.07	49,49,49,49	0
18	IOD	N	202	1/1	0.99	0.02	48,48,48,48	0
18	IOD	Y	302	1/1	0.99	0.02	55,55,55,55	0
18	IOD	b	202	1/1	0.99	0.03	46,46,46,46	0
18	IOD	K	302	1/1	1.00	0.03	53,53,53,53	0
18	IOD	V	302	1/1	1.00	0.13	17,17,17,17	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.

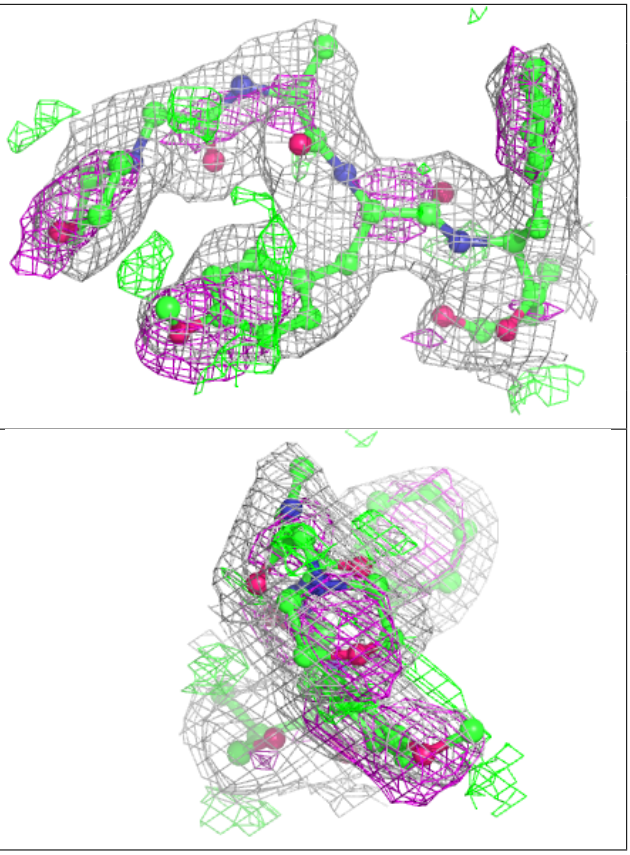
Electron density around 04C Y 301:

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



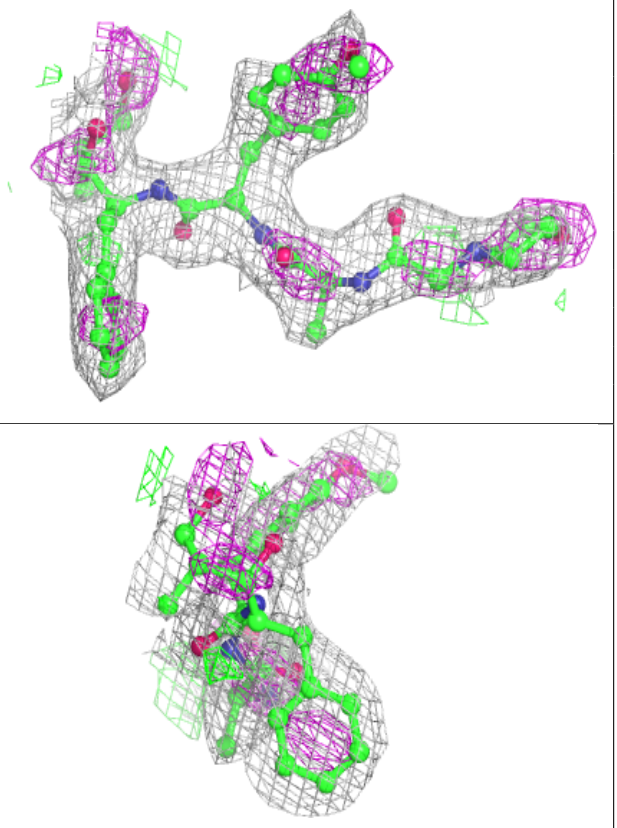
Electron density around 04C N 201:

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



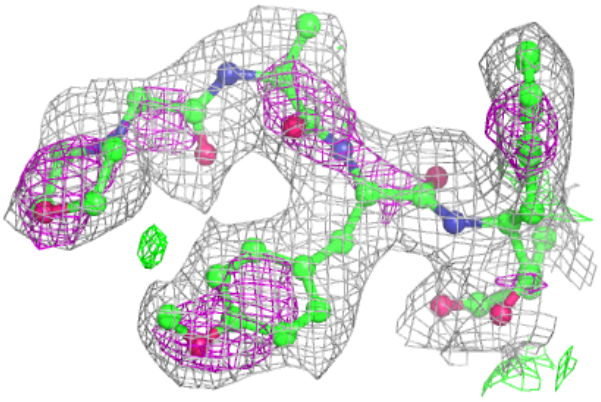
Electron density around 04C K 301:

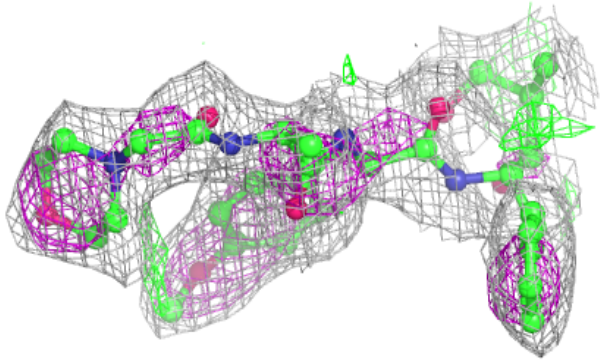
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

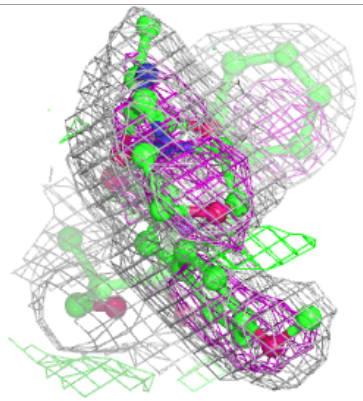


Electron density around 04C b 201:

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

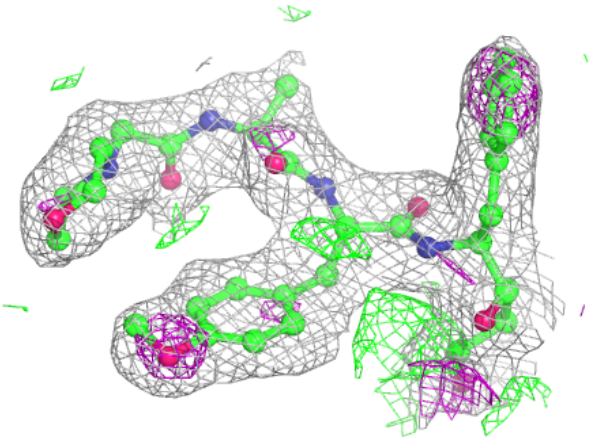


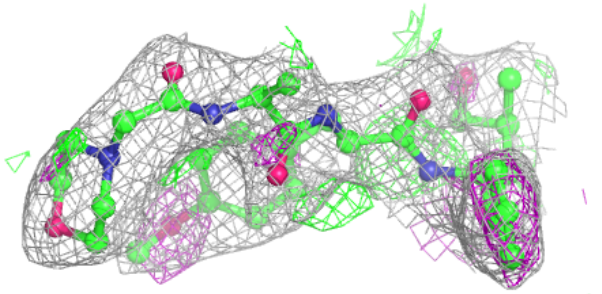


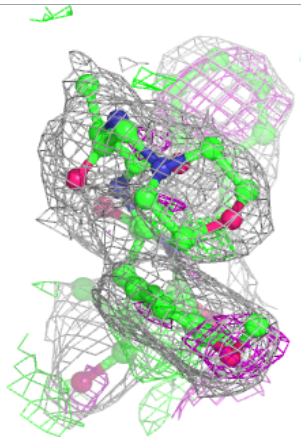


Electron density around 04C V 301:

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

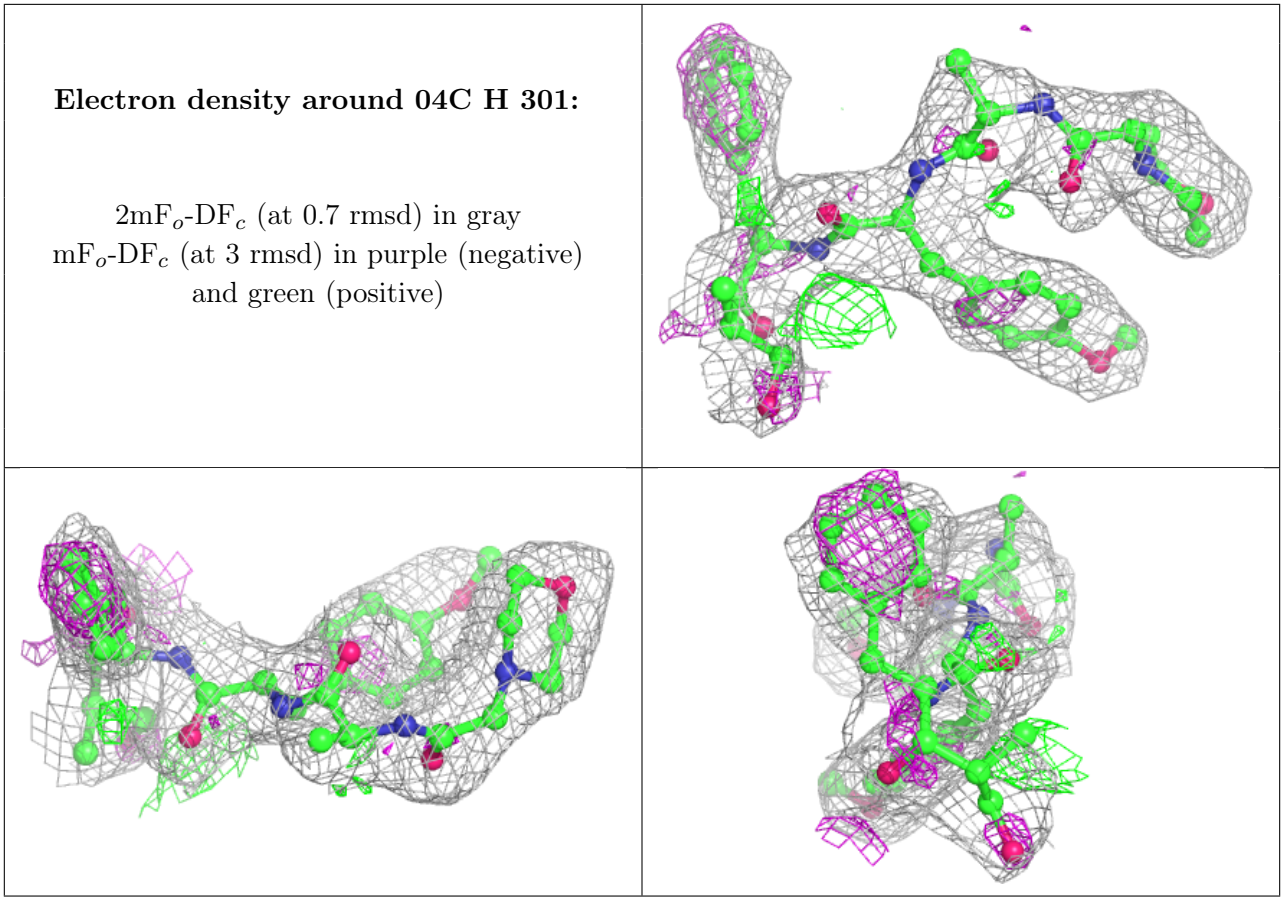






Electron density around 04C H 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.