wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2025 – 01:26 PM EDT

PDB ID	:	9AW6
Title	:	Yeast 20S proteasome soaked with MA9 fraction EF2
Authors	:	Meneghello, R.; Rustiguel, J.K.; Fernandes, A.Z.N.; Trivella, D.B.B.
Deposited on	:	2024-03-05
Resolution	:	3.44 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:

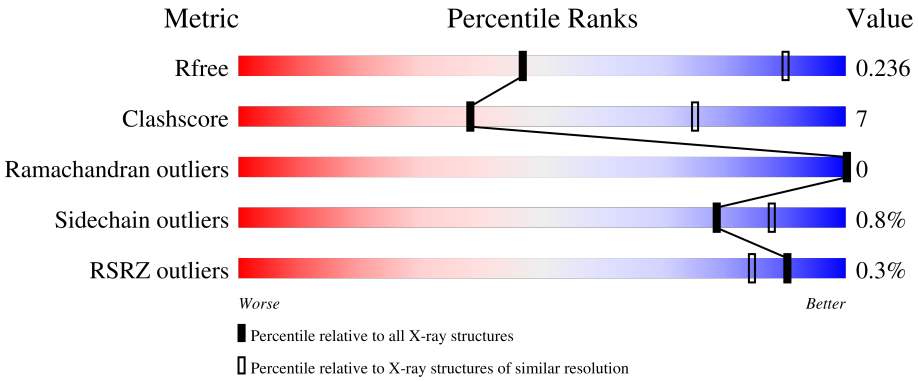
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.44 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}	164625	1587 (3.50-3.38)
Clashscore	180529	1676 (3.50-3.38)
Ramachandran outliers	177936	1665 (3.50-3.38)
Sidechain outliers	177891	1666 (3.50-3.38)
RSRZ outliers	164620	1587 (3.50-3.38)

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

Mol	Chain	Length	Quality of chain
1	A	250	85% 14%
1	O	250	82% 18%
2	B	258	76% 18% 6%
2	P	258	% 79% 15% 5%
3	C	254	79% 18% .

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Mol	Chain	Length	Quality of chain
3	Q	254	73% 21% • 5%
4	D	260	% 78% 13% 8%
4	R	260	% 79% 15% 5%
5	E	234	79% 20% •
5	S	234	78% 21% •
6	F	287	70% 15% • 15%
6	T	287	% 70% 15% 15%
7	G	252	77% 19% •
7	U	252	77% 19% •
8	H	232	81% 15% •
8	V	232	76% 20% •
9	I	205	82% 18%
9	W	205	77% 23%
10	J	198	83% 16% •
10	X	198	83% 16% •
11	K	212	82% 17%
11	Y	212	% 84% 16%
12	L	222	83% 16% •
12	Z	222	% 82% 18%
13	M	233	78% 22%
13	a	233	100%
14	N	196	84% 16%
14	b	196	99% •

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 50447 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	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1905	1204	321	377	3			
2	P	244	Total	C	N	O	S	0	0	0
			1909	1206	322	378	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1934	1206	339	385	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1854	1161	311	375	7			
4	R	246	Total	C	N	O	S	0	0	0
			1898	1186	318	387	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			
5	S	232	Total	C	N	O	S	0	0	0
			1784	1120	311	349	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	245	Total	C	N	O	S	0	0	0
			1904	1211	331	358	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	242	Total	C	N	O	S	0	0	0
			1916	1218	321	369	8			
7	U	242	Total	C	N	O	S	0	0	0
			1916	1218	321	369	8			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	997	266	301	6			

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

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

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

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

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

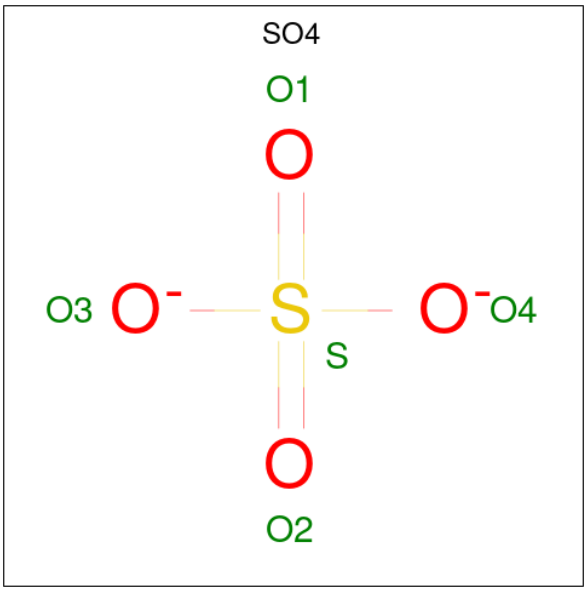
- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

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

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

- Molecule 15 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total O S 5 4 1	0	0
15	C	1	Total O S 5 4 1	0	0
15	D	1	Total O S 5 4 1	0	0
15	E	1	Total O S 5 4 1	0	0
15	E	1	Total O S 5 4 1	0	0
15	F	1	Total O S 5 4 1	0	0
15	F	1	Total O S 5 4 1	0	0
15	G	1	Total O S 5 4 1	0	0
15	G	1	Total O S 5 4 1	0	0
15	P	1	Total O S 5 4 1	0	0
15	Q	1	Total O S 5 4 1	0	0
15	S	1	Total O S 5 4 1	0	0
15	S	1	Total O S 5 4 1	0	0
15	S	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	T	1	Total O S 5 4 1	0	0
15	T	1	Total O S 5 4 1	0	0
15	T	1	Total O S 5 4 1	0	0
15	U	1	Total O S 5 4 1	0	0
15	U	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	H	1	Total O S 5 4 1	0	0
15	I	1	Total O S 5 4 1	0	0
15	I	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0
15	L	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	M	1	Total O S 5 4 1	0	0
15	N	1	Total O S 5 4 1	0	0
15	V	1	Total O S 5 4 1	0	0
15	V	1	Total O S 5 4 1	0	0
15	W	1	Total O S 5 4 1	0	0
15	X	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 5 4 1	0	0
15	Z	1	Total O S 5 4 1	0	0
15	Z	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0

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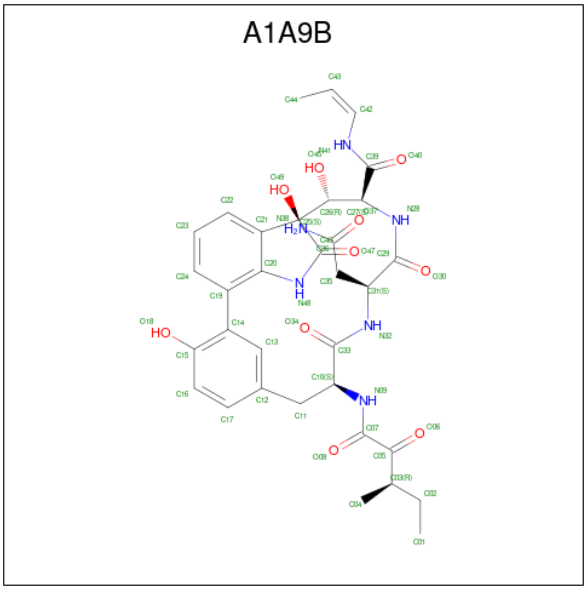
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	b	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0

- Molecule 16 is (10S,11R,12S,15S,18S)-15-(2-amino-2-oxoethyl)-10,11,23-trihydroxy-18-{[(3R)-3-methyl-2-oxopentanoyl]amino}-9,14,17-trioxo-N-[(1Z)-prop-1-en-1-yl]-8,13,16-triazatetracyclo[18.3.1.0(2,7).0(6,10)]tetracosa-1(24),2,4,6,20,22-hexaene-12-carboxamide (three-letter code: A1A9B) (formula: $C_{33}H_{38}N_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	H	1	Total C N O 49 33 6 10	0	0
16	K	1	Total C N O 49 33 6 10	0	0
16	N	1	Total C N O 49 33 6 10	0	0
16	V	1	Total C N O 49 33 6 10	0	0
16	Y	1	Total C N O 49 33 6 10	0	0
16	b	1	Total C N O 49 33 6 10	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	I	1	Total Mg 1 1	0	0
17	L	1	Total Mg 1 1	0	0
17	W	1	Total Mg 1 1	0	0
17	Y	1	Total Mg 1 1	0	0
17	Z	1	Total Mg 1 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	20	Total O 20 20	0	0
18	B	17	Total O 17 17	0	0
18	C	6	Total O 6 6	0	0
18	D	4	Total O 4 4	0	0
18	E	4	Total O 4 4	0	0
18	F	5	Total O 5 5	0	0
18	G	8	Total O 8 8	0	0
18	O	6	Total O 6 6	0	0
18	P	12	Total O 12 12	0	0
18	Q	10	Total O 10 10	0	0
18	R	4	Total O 4 4	0	0
18	S	3	Total O 3 3	0	0
18	T	11	Total O 11 11	0	0
18	U	9	Total O 9 9	0	0
18	H	13	Total O 13 13	0	0

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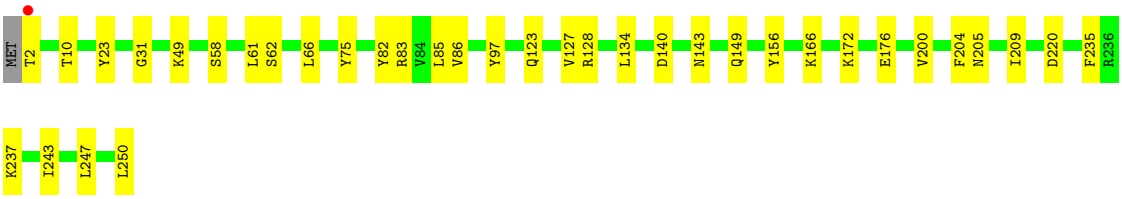
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	I	8	Total O 8 8	0	0
18	J	15	Total O 15 15	0	0
18	K	16	Total O 16 16	0	0
18	L	25	Total O 25 25	0	0
18	M	12	Total O 12 12	0	0
18	N	13	Total O 13 13	0	0
18	V	19	Total O 19 19	0	0
18	W	6	Total O 6 6	0	0
18	X	18	Total O 18 18	0	0
18	Y	8	Total O 8 8	0	0
18	Z	22	Total O 22 22	0	0
18	a	15	Total O 15 15	0	0
18	b	10	Total O 10 10	0	0

3 Residue-property plots (i)

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

• Molecule 1: Proteasome subunit alpha type-2

Chain A:

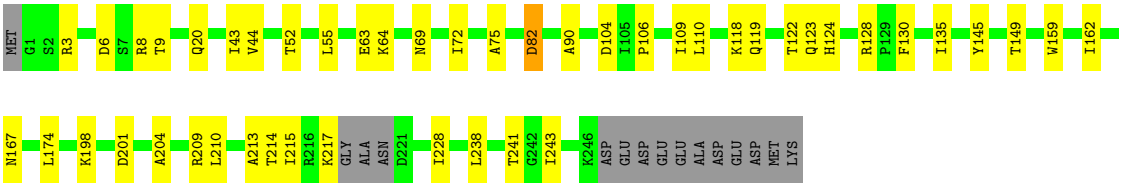


• Molecule 1: Proteasome subunit alpha type-2

Chain O:

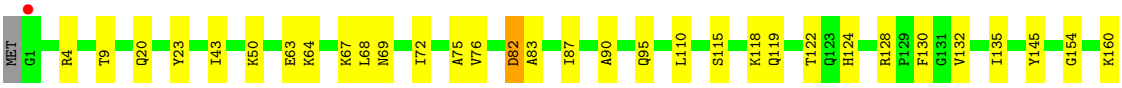
• Molecule 2: Proteasome subunit alpha type-3

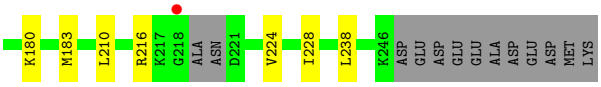
Chain B:



• Molecule 2: Proteasome subunit alpha type-3

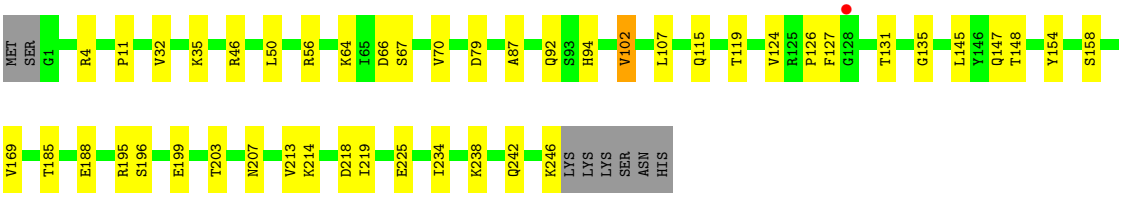
Chain P:





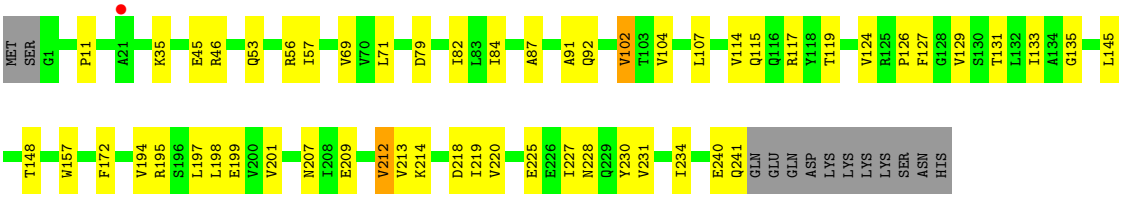
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



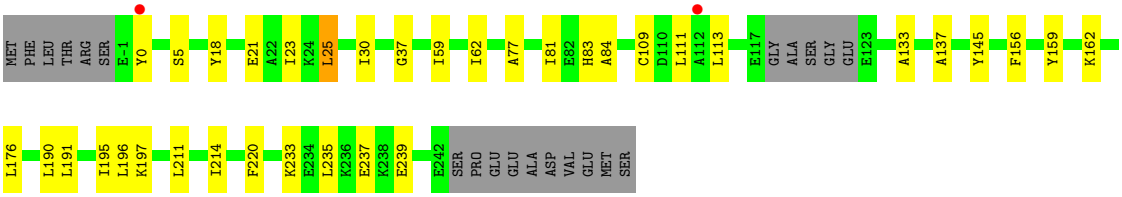
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



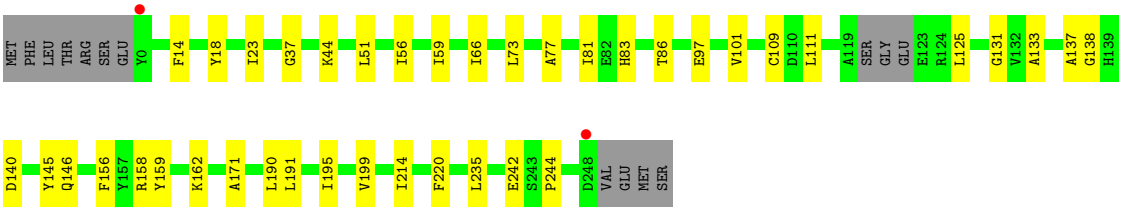
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



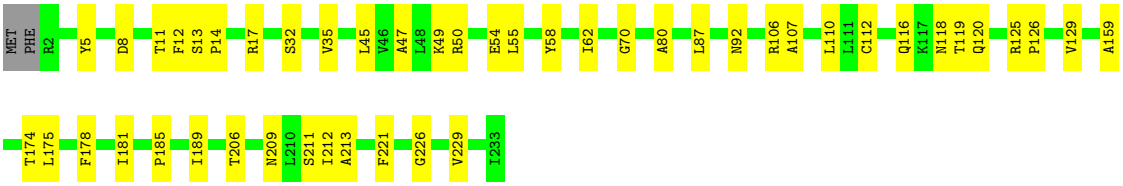
• Molecule 4: Proteasome subunit alpha type-5

Chain R:

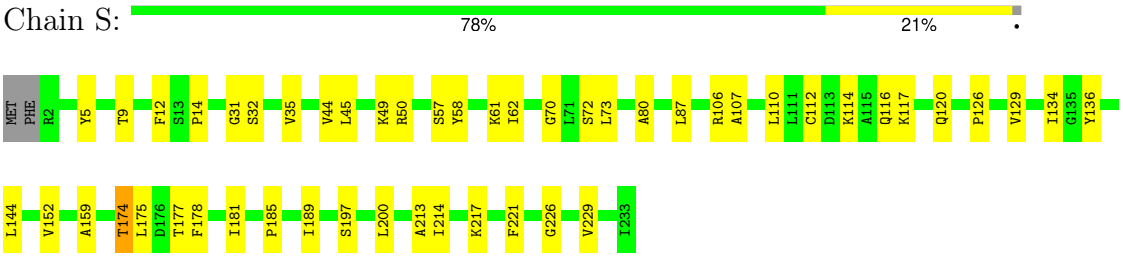


• Molecule 5: Proteasome subunit alpha type-6

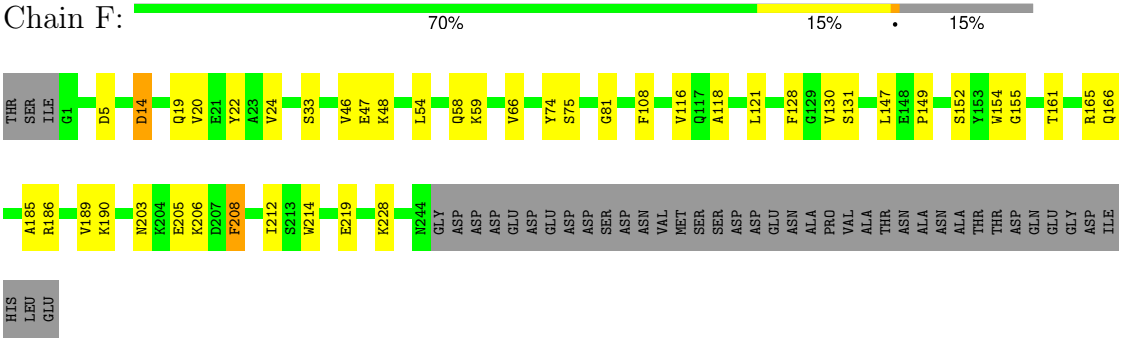
Chain E:



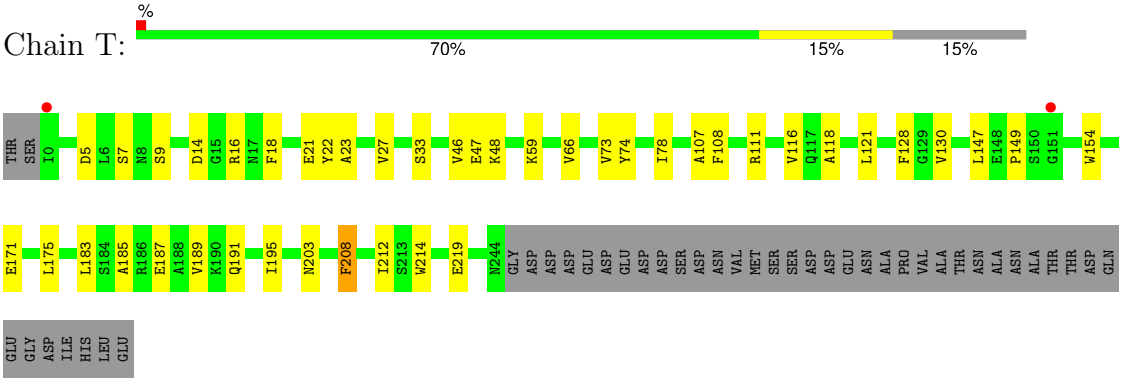
• Molecule 5: Proteasome subunit alpha type-6



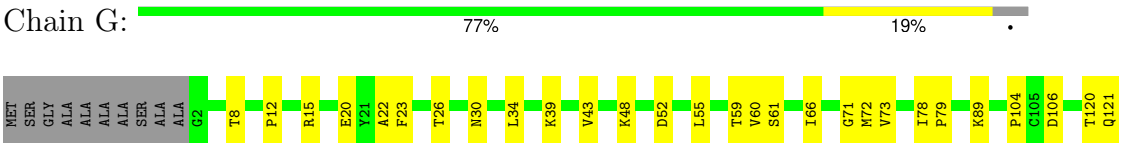
• Molecule 6: Probable proteasome subunit alpha type-7



• Molecule 6: Probable proteasome subunit alpha type-7



• Molecule 7: Proteasome subunit alpha type-1

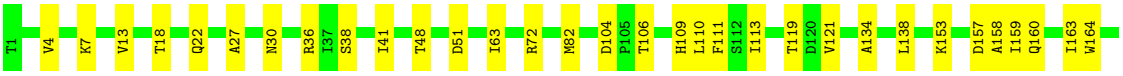


• Molecule 7: Proteasome subunit alpha type-1

Chain U:

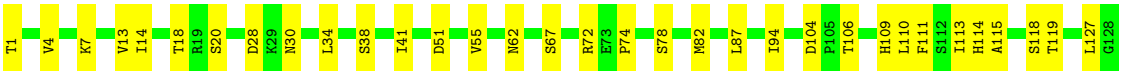
• Molecule 8: Proteasome subunit beta type-2

Chain H:



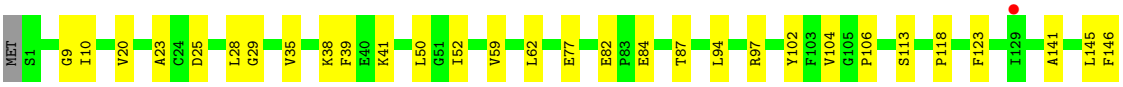
• Molecule 8: Proteasome subunit beta type-2

Chain V:



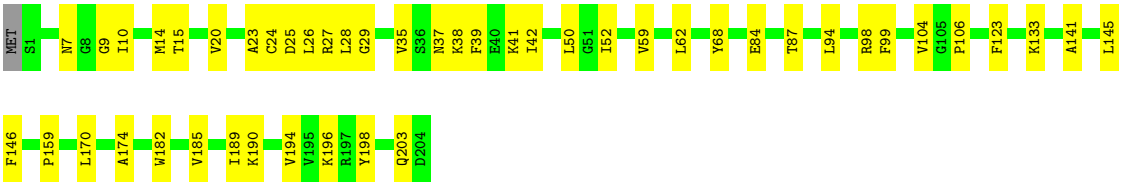
• Molecule 9: Proteasome subunit beta type-3

Chain I:

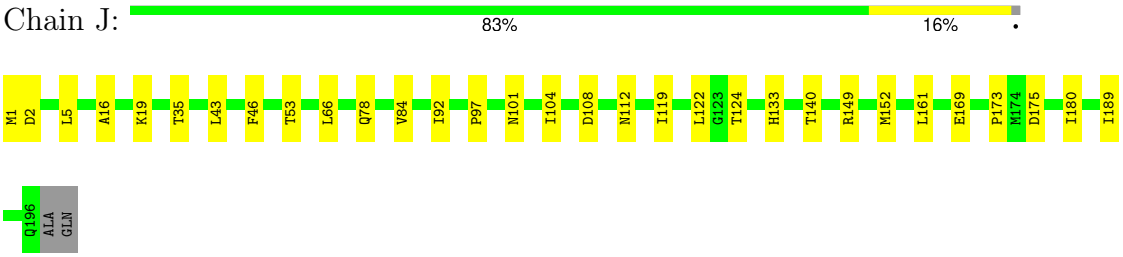


• Molecule 9: Proteasome subunit beta type-3

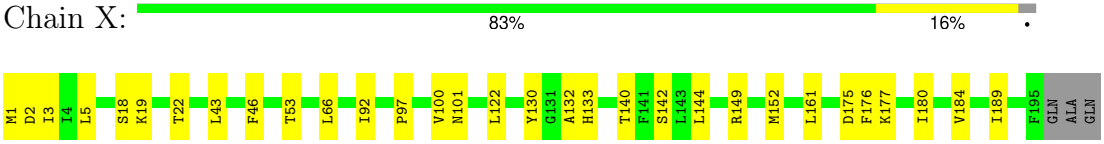
Chain W:



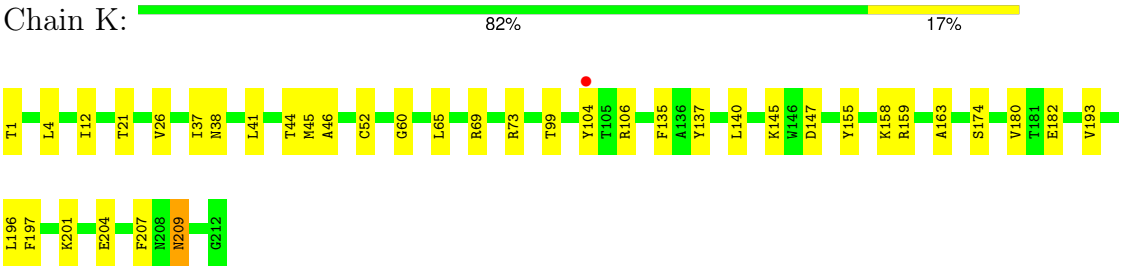
• Molecule 10: Proteasome subunit beta type-4



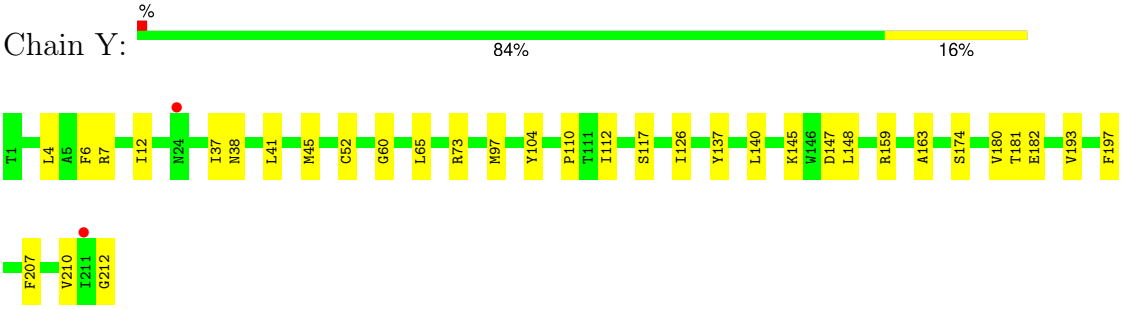
• Molecule 10: Proteasome subunit beta type-4



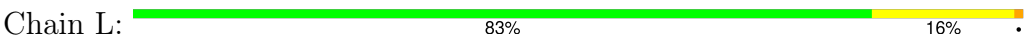
• Molecule 11: Proteasome subunit beta type-5

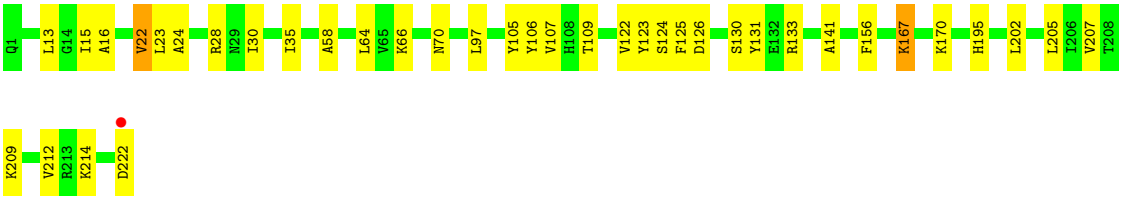


• Molecule 11: Proteasome subunit beta type-5

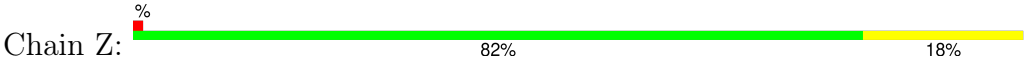


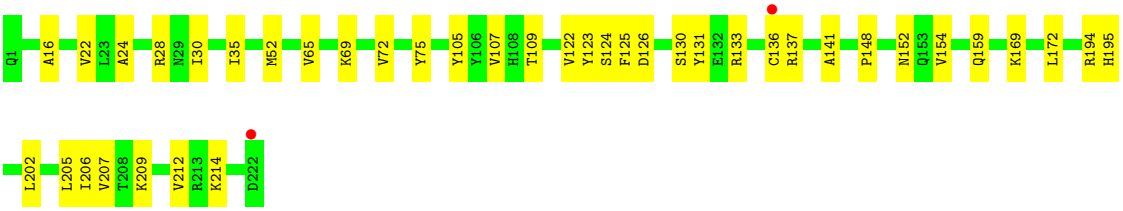
• Molecule 12: Proteasome subunit beta type-6



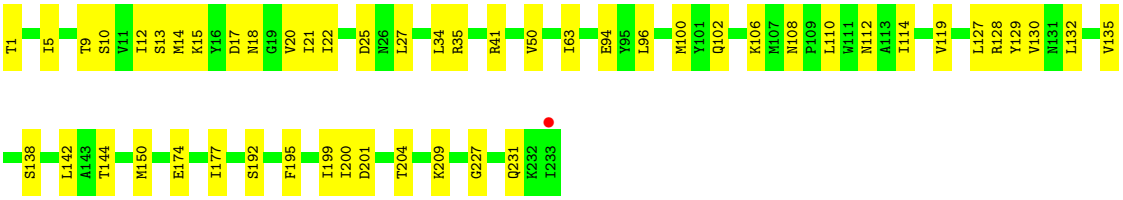


• Molecule 12: Proteasome subunit beta type-6

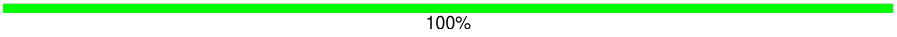




• Molecule 13: Proteasome subunit beta type-7

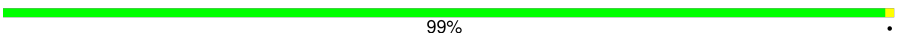


• Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-1

• Molecule 14: Proteasome subunit beta type-1




T1
K83
L196

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.37Å 299.67Å 144.66Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	48.90 – 3.44 48.90 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.90-3.44) 86.9 (48.90-3.44)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.182 , 0.235 0.182 , 0.236	Depositor DCC
R_{free} test set	6810 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	67.4	Xtriage
Anisotropy	0.892	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 85.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	50447	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, A1A9B

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	0.25	0/1944	0.47	0/2632
1	O	0.25	0/1944	0.46	0/2632
2	B	0.25	0/1934	0.49	0/2614
2	P	0.25	0/1938	0.48	0/2619
3	C	0.25	0/1963	0.50	0/2656
3	Q	0.25	0/1919	0.50	0/2598
4	D	0.24	0/1879	0.47	0/2531
4	R	0.24	0/1924	0.47	0/2593
5	E	0.25	0/1811	0.49	0/2447
5	S	0.25	0/1811	0.49	0/2447
6	F	0.26	0/1936	0.46	0/2614
6	T	0.25	0/1944	0.47	0/2625
7	G	0.25	0/1954	0.48	0/2645
7	U	0.25	0/1954	0.47	0/2645
8	H	0.24	0/1715	0.47	0/2326
8	V	0.24	0/1715	0.47	0/2326
9	I	0.25	0/1611	0.47	0/2174
9	W	0.25	0/1611	0.48	0/2174
10	J	0.25	0/1598	0.48	0/2154
10	X	0.25	0/1589	0.49	0/2142
11	K	0.25	0/1681	0.48	0/2274
11	Y	0.25	0/1681	0.48	0/2274
12	L	0.25	0/1795	0.49	0/2420
12	Z	0.26	0/1795	0.49	0/2420
13	M	0.25	0/1855	0.50	0/2514
13	a	0.25	0/1855	0.49	0/2514
14	N	0.24	0/1541	0.48	0/2087
14	b	0.25	0/1541	0.48	0/2087
All	All	0.25	0/50438	0.48	0/68184

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1917	25	0
1	O	1907	0	1917	29	0
2	B	1905	0	1915	31	0
2	P	1909	0	1918	28	0
3	C	1934	0	1942	31	0
3	Q	1890	0	1903	41	0
4	D	1854	0	1831	24	0
4	R	1898	0	1866	24	0
5	E	1784	0	1788	31	0
5	S	1784	0	1788	30	0
6	F	1896	0	1889	27	0
6	T	1904	0	1900	28	0
7	G	1916	0	1905	34	0
7	U	1916	0	1905	33	0
8	H	1684	0	1688	19	0
8	V	1684	0	1688	26	0
9	I	1581	0	1574	23	0
9	W	1581	0	1574	30	0
10	J	1570	0	1577	19	0
10	X	1561	0	1569	22	0
11	K	1644	0	1595	23	0
11	Y	1644	0	1595	19	0
12	L	1757	0	1711	21	0
12	Z	1757	0	1711	24	0
13	M	1824	0	1832	33	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	20	0
14	b	1512	0	1481	0	0
15	B	5	0	0	0	0
15	C	5	0	0	0	0
15	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	10	0	0	1	0
15	F	10	0	0	0	0
15	G	10	0	0	0	0
15	H	15	0	0	0	0
15	I	10	0	0	0	0
15	J	10	0	0	0	0
15	K	20	0	0	0	0
15	L	5	0	0	0	0
15	M	40	0	0	0	0
15	N	5	0	0	0	0
15	P	5	0	0	0	0
15	Q	5	0	0	0	0
15	S	15	0	0	0	0
15	T	15	0	0	0	0
15	U	10	0	0	1	0
15	V	10	0	0	0	0
15	W	5	0	0	0	0
15	X	5	0	0	0	0
15	Y	20	0	0	0	0
15	Z	10	0	0	0	0
15	a	25	0	0	0	0
15	b	15	0	0	0	0
16	H	49	0	0	0	0
16	K	49	0	0	1	0
16	N	49	0	0	1	0
16	V	49	0	0	1	0
16	Y	49	0	0	0	0
16	b	49	0	0	0	0
17	I	1	0	0	0	0
17	L	1	0	0	0	0
17	W	1	0	0	0	0
17	Y	1	0	0	0	0
17	Z	1	0	0	0	0
18	A	20	0	0	0	0
18	B	17	0	0	0	0
18	C	6	0	0	0	0
18	D	4	0	0	0	0
18	E	4	0	0	0	0
18	F	5	0	0	0	0
18	G	8	0	0	0	0
18	H	13	0	0	0	0
18	I	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	J	15	0	0	0	0
18	K	16	0	0	0	0
18	L	25	0	0	0	0
18	M	12	0	0	0	0
18	N	13	0	0	0	0
18	O	6	0	0	0	0
18	P	12	0	0	0	0
18	Q	10	0	0	0	0
18	R	4	0	0	0	0
18	S	3	0	0	0	0
18	T	11	0	0	0	0
18	U	9	0	0	2	0
18	V	19	0	0	0	0
18	W	6	0	0	0	0
18	X	18	0	0	0	0
18	Y	8	0	0	0	0
18	Z	22	0	0	0	0
18	a	15	0	0	0	0
18	b	10	0	0	0	0
All	All	50447	0	49292	629	0

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

The worst 5 of 629 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)
3:C:131:THR:HG1	3:C:148:THR:HG1	1.28	0.82
8:H:213:LEU:HD13	11:Y:212:GLY:HA2	1.64	0.79
2:P:4:ARG:HH12	6:T:7:SER:HB2	1.50	0.77
2:B:90:ALA:HB1	2:B:110:LEU:HD21	1.66	0.76
13:M:201:ASP:HB3	13:M:204:THR:HG22	1.67	0.76

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	247/250 (99%)	239 (97%)	8 (3%)	0	100	100
1	O	247/250 (99%)	239 (97%)	8 (3%)	0	100	100
2	B	239/258 (93%)	229 (96%)	10 (4%)	0	100	100
2	P	240/258 (93%)	231 (96%)	9 (4%)	0	100	100
3	C	244/254 (96%)	236 (97%)	8 (3%)	0	100	100
3	Q	239/254 (94%)	229 (96%)	10 (4%)	0	100	100
4	D	235/260 (90%)	225 (96%)	10 (4%)	0	100	100
4	R	242/260 (93%)	230 (95%)	12 (5%)	0	100	100
5	E	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
5	S	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
6	F	242/287 (84%)	234 (97%)	8 (3%)	0	100	100
6	T	243/287 (85%)	235 (97%)	8 (3%)	0	100	100
7	G	240/252 (95%)	233 (97%)	7 (3%)	0	100	100
7	U	240/252 (95%)	233 (97%)	7 (3%)	0	100	100
8	H	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
8	V	220/232 (95%)	212 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	J	194/198 (98%)	188 (97%)	6 (3%)	0	100	100
10	X	193/198 (98%)	186 (96%)	7 (4%)	0	100	100
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
12	L	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
12	Z	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
13	M	231/233 (99%)	221 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6299/6586 (96%)	6052 (96%)	247 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	208/209 (100%)	207 (100%)	1 (0%)	86	92
1	O	208/209 (100%)	207 (100%)	1 (0%)	86	92
2	B	204/216 (94%)	202 (99%)	2 (1%)	73	84
2	P	204/216 (94%)	203 (100%)	1 (0%)	86	92
3	C	218/226 (96%)	216 (99%)	2 (1%)	75	86
3	Q	213/226 (94%)	211 (99%)	2 (1%)	75	86
4	D	198/215 (92%)	197 (100%)	1 (0%)	86	92
4	R	202/215 (94%)	201 (100%)	1 (0%)	86	92
5	E	191/193 (99%)	188 (98%)	3 (2%)	58	76
5	S	191/193 (99%)	188 (98%)	3 (2%)	58	76
6	F	201/238 (84%)	197 (98%)	4 (2%)	50	72
6	T	202/238 (85%)	199 (98%)	3 (2%)	60	77
7	G	207/210 (99%)	206 (100%)	1 (0%)	86	92
7	U	207/210 (99%)	207 (100%)	0	100	100
8	H	181/190 (95%)	180 (99%)	1 (1%)	84	91
8	V	181/190 (95%)	181 (100%)	0	100	100
9	I	172/173 (99%)	170 (99%)	2 (1%)	67	81
9	W	172/173 (99%)	169 (98%)	3 (2%)	56	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	174/175 (99%)	173 (99%)	1 (1%)	84 91
10	X	173/175 (99%)	173 (100%)	0	100 100
11	K	169/169 (100%)	166 (98%)	3 (2%)	54 74
11	Y	169/169 (100%)	167 (99%)	2 (1%)	67 81
12	L	185/185 (100%)	181 (98%)	4 (2%)	47 70
12	Z	185/185 (100%)	184 (100%)	1 (0%)	86 92
13	M	199/199 (100%)	199 (100%)	0	100 100
13	a	199/199 (100%)	198 (100%)	1 (0%)	86 92
14	N	162/162 (100%)	161 (99%)	1 (1%)	84 91
14	b	162/162 (100%)	161 (99%)	1 (1%)	84 91
All	All	5337/5520 (97%)	5292 (99%)	45 (1%)	79 88

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	78	GLN
12	L	209	LYS
11	K	73	ARG
12	L	22	VAL
9	W	37	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	71	ASN
14	b	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 69 ligands modelled in this entry, 5 are monoatomic - leaving 64 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	$\#\|Z\| > 2$
15	SO4	a	305	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.12	0
15	SO4	S	302	-	4,4,4	0.67	0	6,6,6	0.09	0
16	A1A9B	Y	301	-	51,52,52	3.52	19 (37%)	67,76,76	3.33	19 (28%)
15	SO4	T	301	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	S	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Y	306	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	a	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	H	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	I	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	303	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	b	202	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	B	301	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	Q	301	-	4,4,4	0.67	0	6,6,6	0.07	0
16	A1A9B	N	202	-	51,52,52	3.56	19 (37%)	67,76,76	3.33	16 (23%)
15	SO4	V	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	K	303	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	H	304	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	E	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	P	301	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	F	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	K	305	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	M	304	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	U	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	M	305	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	X	201	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	H	303	-	4,4,4	0.67	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SO4	J	201	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	b	203	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	T	302	-	4,4,4	0.67	0	6,6,6	0.11	0
16	A1A9B	H	301	-	51,52,52	3.54	18 (35%)	67,76,76	3.44	18 (26%)
15	SO4	G	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	E	301	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	M	307	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	M	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	L	302	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	N	201	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	Y	303	-	4,4,4	0.67	0	6,6,6	0.09	0
16	A1A9B	b	201	-	51,52,52	3.56	19 (37%)	67,76,76	3.35	16 (23%)
16	A1A9B	V	301	-	51,52,52	3.56	19 (37%)	67,76,76	3.44	18 (26%)
15	SO4	W	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	304	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	K	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	K	304	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	F	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	S	303	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	Y	304	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	V	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	306	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	T	303	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	Z	302	-	4,4,4	0.68	0	6,6,6	0.08	0
16	A1A9B	K	301	-	51,52,52	3.56	19 (37%)	67,76,76	3.45	18 (26%)
15	SO4	G	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	b	204	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	M	303	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	M	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	J	202	-	4,4,4	0.67	0	6,6,6	0.12	0
15	SO4	I	303	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	D	301	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	M	308	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	U	302	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	Y	305	-	4,4,4	0.69	0	6,6,6	0.08	0
15	SO4	Z	303	-	4,4,4	0.67	0	6,6,6	0.10	0

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	A1A9B	Y	301	-	-	11/59/76/76	0/3/4/4
16	A1A9B	H	301	-	-	10/59/76/76	0/3/4/4
16	A1A9B	K	301	-	-	14/59/76/76	0/3/4/4
16	A1A9B	N	202	-	-	11/59/76/76	0/3/4/4
16	A1A9B	b	201	-	-	4/59/76/76	0/3/4/4
16	A1A9B	V	301	-	-	9/59/76/76	0/3/4/4

The worst 5 of 113 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	301	A1A9B	C25-C21	11.90	1.66	1.51
16	b	201	A1A9B	C25-C21	11.84	1.66	1.51
16	N	202	A1A9B	C25-C21	11.81	1.66	1.51
16	H	301	A1A9B	C25-C21	11.76	1.66	1.51
16	K	301	A1A9B	C25-C21	11.52	1.66	1.51

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	301	A1A9B	C20-N48-C46	22.64	129.65	111.26
16	b	201	A1A9B	C20-N48-C46	22.59	129.62	111.26
16	K	301	A1A9B	C20-N48-C46	22.49	129.53	111.26
16	H	301	A1A9B	C20-N48-C46	22.48	129.52	111.26
16	N	202	A1A9B	C20-N48-C46	22.48	129.52	111.26

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	H	301	A1A9B	C01-C02-C03-C05
16	H	301	A1A9B	O40-C39-N41-C42
16	K	301	A1A9B	C05-C07-N09-C10
16	K	301	A1A9B	O08-C07-N09-C10
16	K	301	A1A9B	N32-C31-C35-C36

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	N	202	A1A9B	1	0

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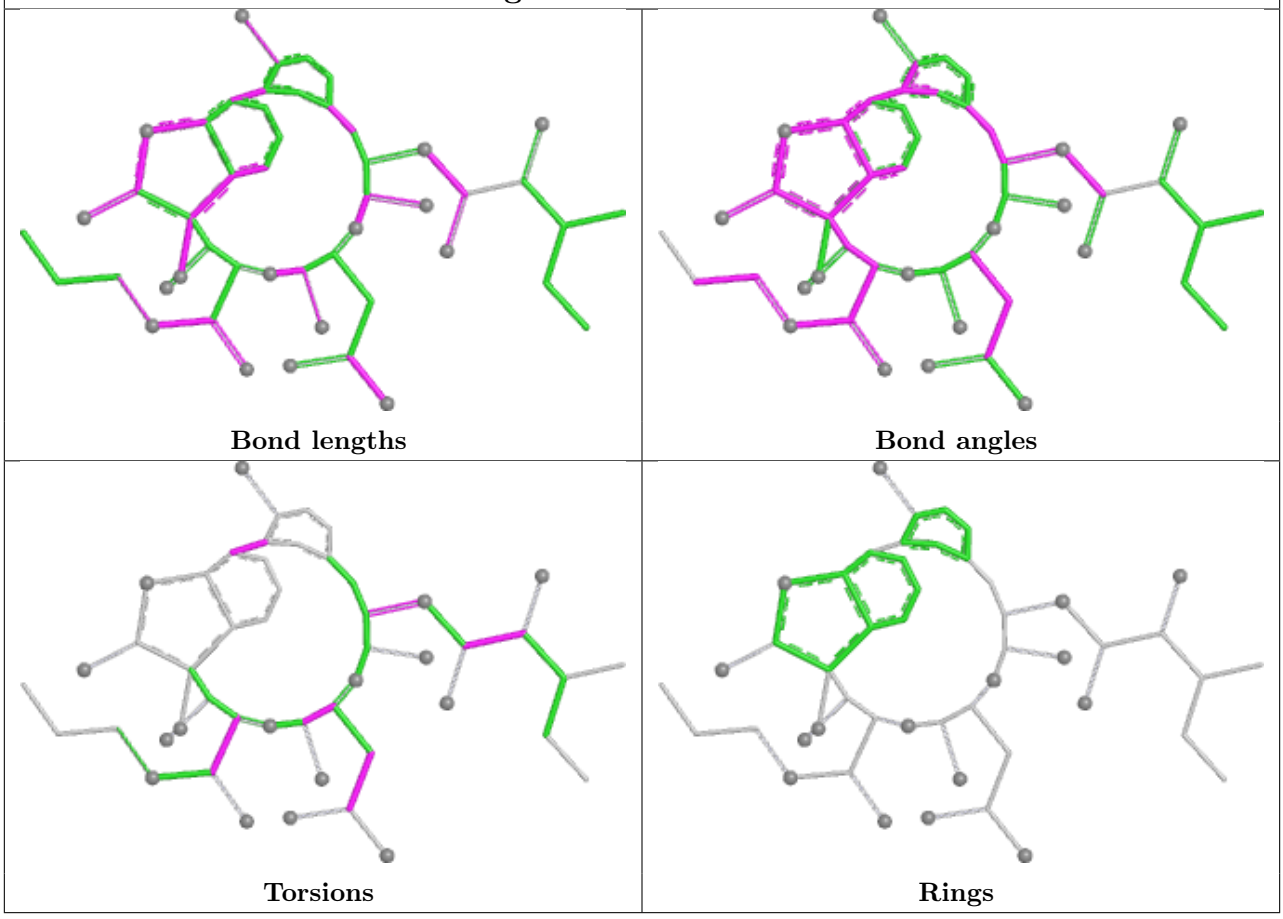
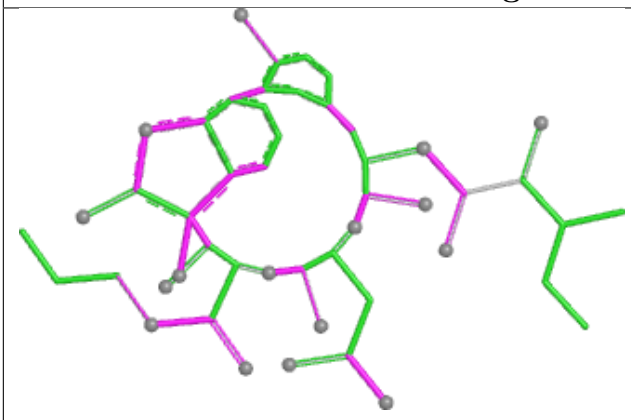
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	302	SO4	1	0
15	U	301	SO4	1	0
16	V	301	A1A9B	1	0
16	K	301	A1A9B	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

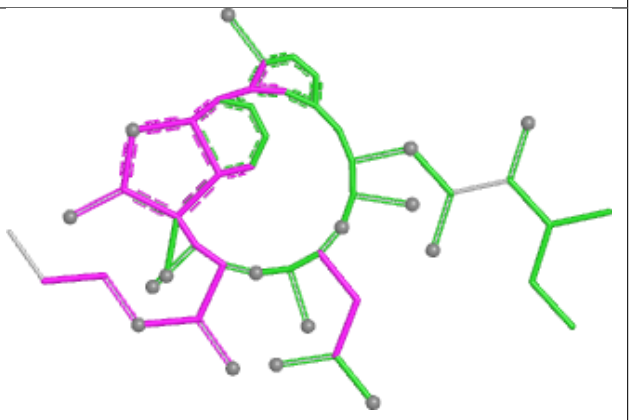
Ligand A1A9B Y 301



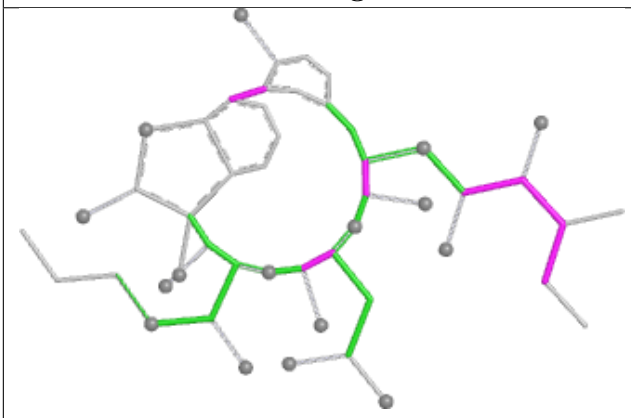
Ligand A1A9B N 202



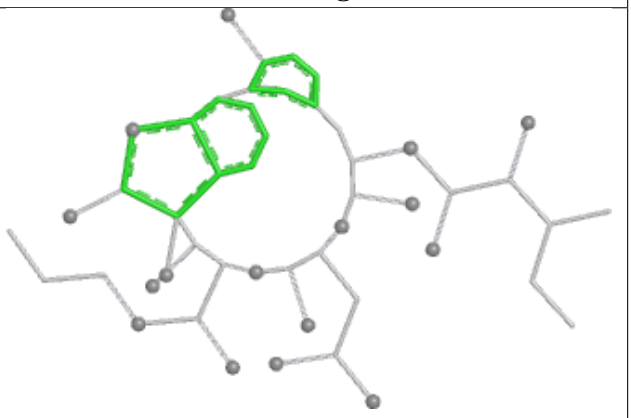
Bond lengths



Bond angles

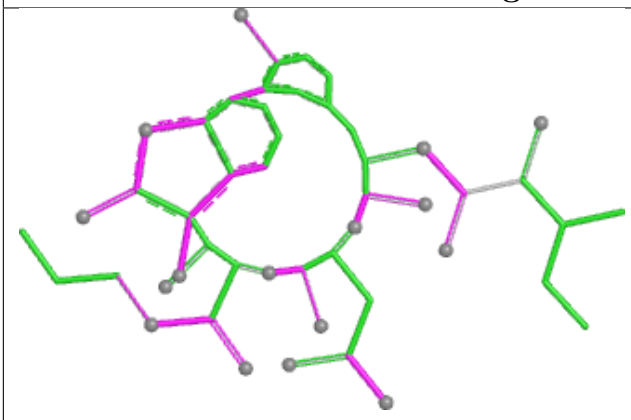


Torsions

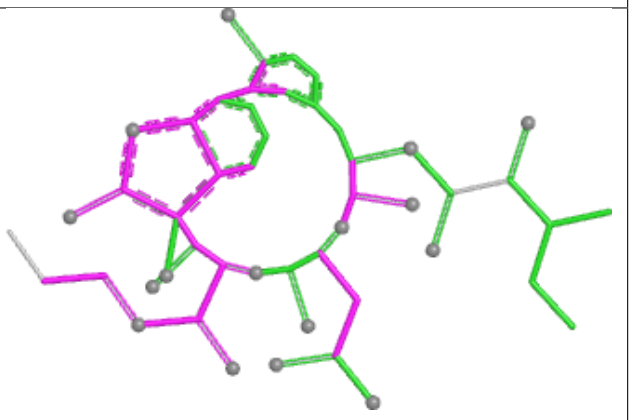


Rings

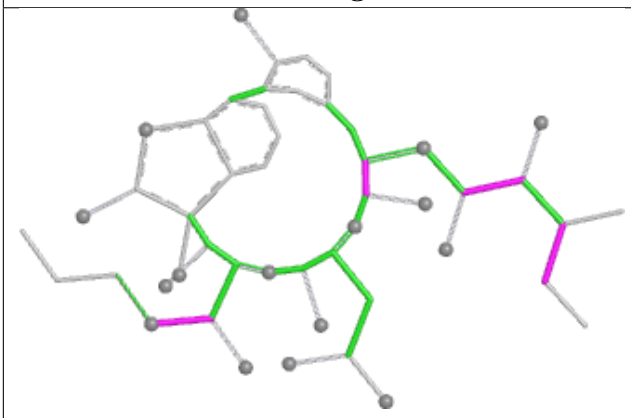
Ligand A1A9B H 301



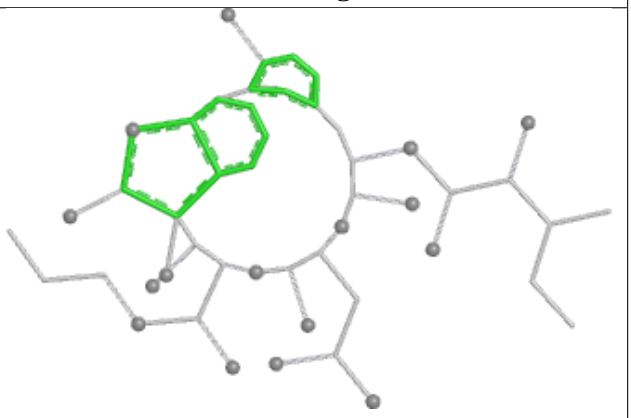
Bond lengths



Bond angles

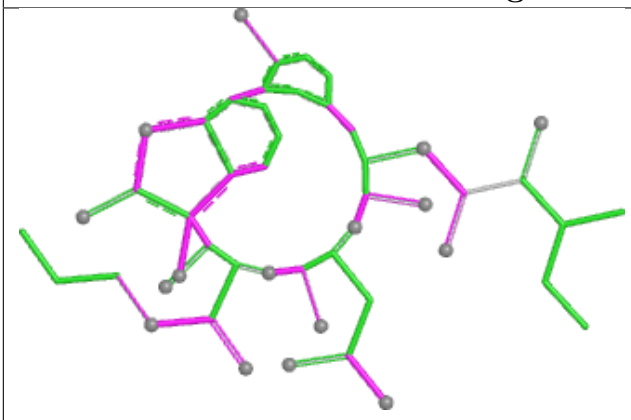


Torsions

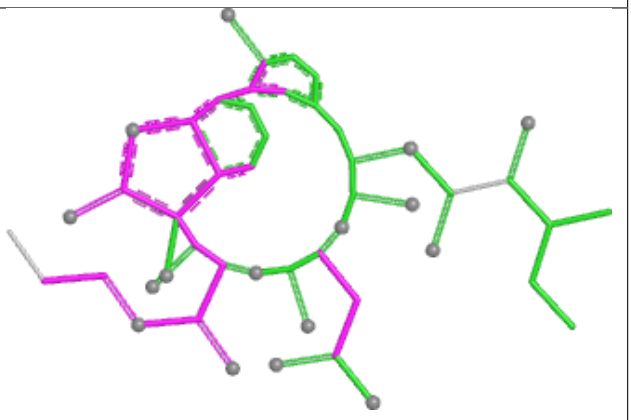


Rings

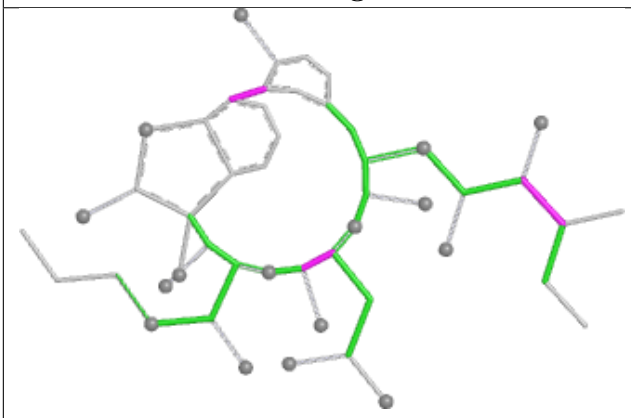
Ligand A1A9B b 201



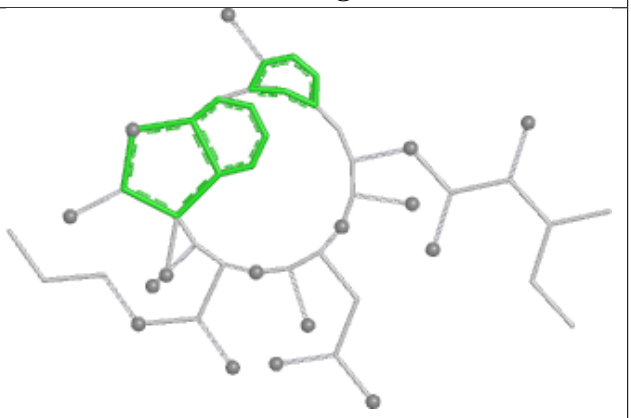
Bond lengths



Bond angles

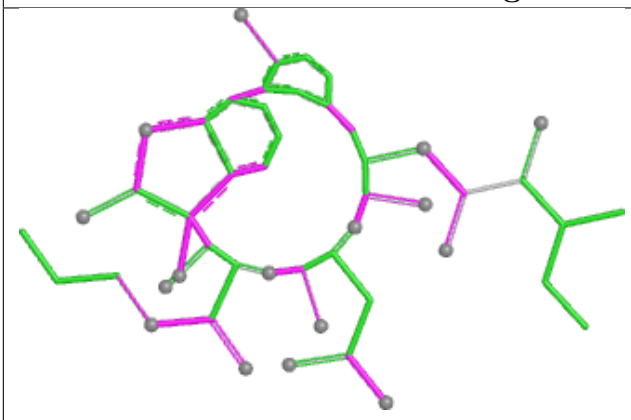


Torsions

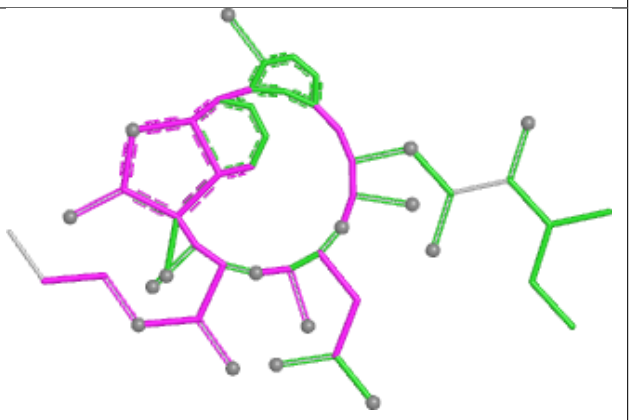


Rings

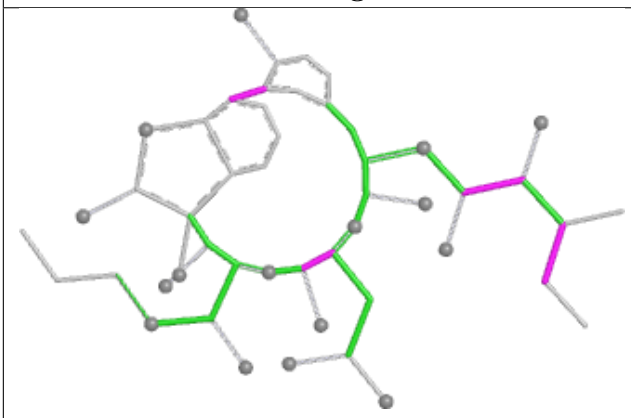
Ligand A1A9B V 301



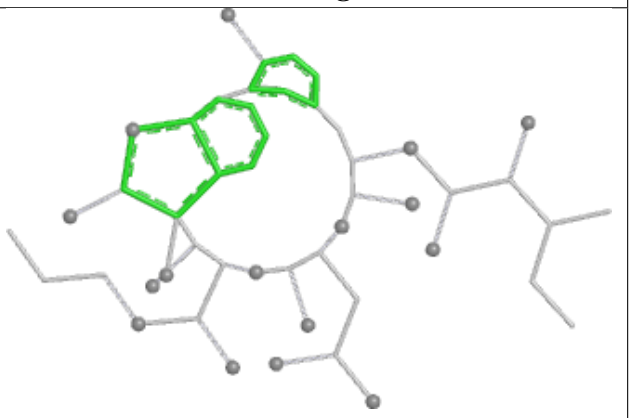
Bond lengths



Bond angles

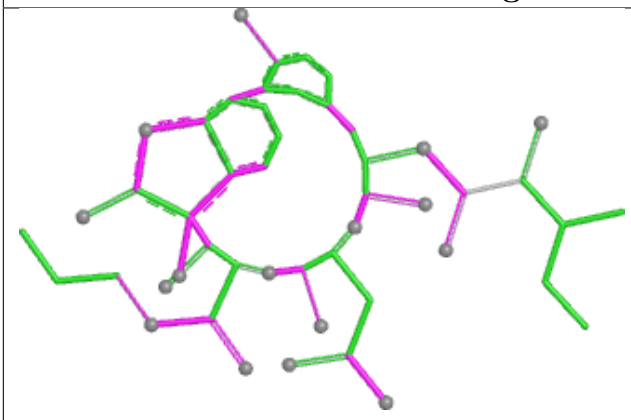


Torsions

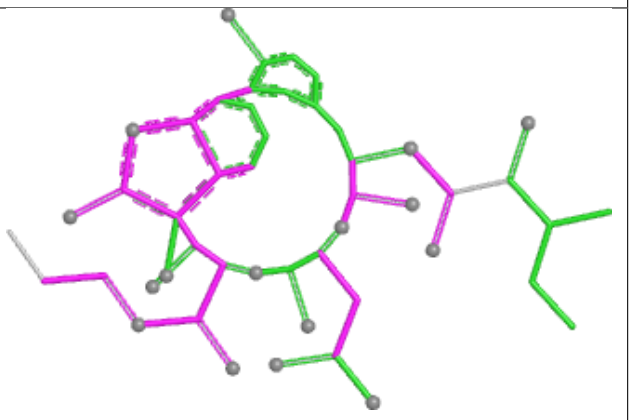


Rings

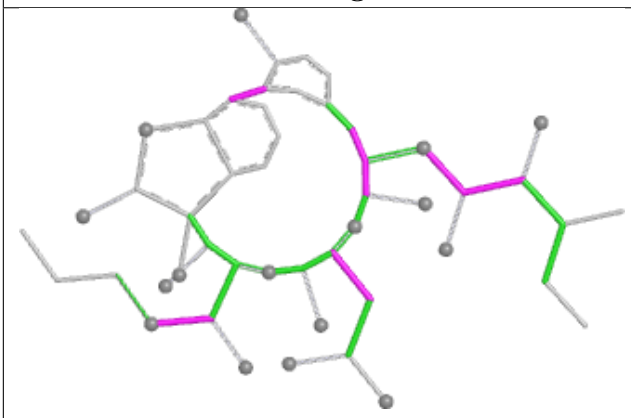
Ligand A1A9B K 301



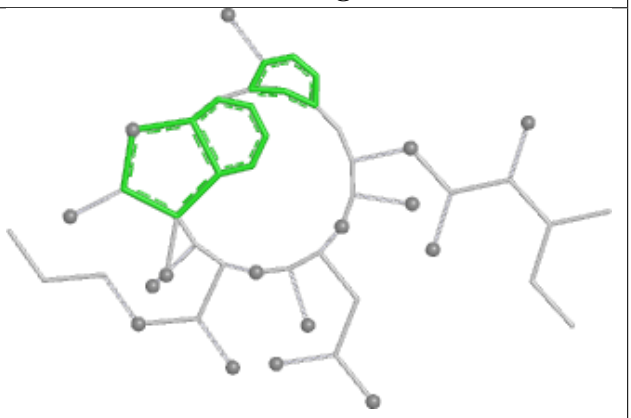
Bond lengths



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^{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	249/250 (99%)	-0.25	1 (0%) 89 81	50, 78, 117, 143	0
1	O	249/250 (99%)	-0.16	0 100 100	55, 84, 115, 131	0
2	B	243/258 (94%)	-0.15	0 100 100	56, 83, 116, 143	0
2	P	244/258 (94%)	-0.11	2 (0%) 82 70	52, 82, 120, 146	0
3	C	246/254 (96%)	-0.11	1 (0%) 89 81	54, 89, 142, 189	0
3	Q	241/254 (94%)	-0.06	1 (0%) 89 81	60, 95, 146, 170	0
4	D	239/260 (91%)	-0.12	2 (0%) 82 70	59, 85, 115, 172	0
4	R	246/260 (94%)	-0.16	2 (0%) 82 70	60, 89, 132, 178	0
5	E	232/234 (99%)	-0.08	0 100 100	61, 95, 126, 139	0
5	S	232/234 (99%)	0.08	0 100 100	59, 96, 133, 154	0
6	F	244/287 (85%)	-0.00	0 100 100	59, 87, 124, 151	0
6	T	245/287 (85%)	-0.08	2 (0%) 82 70	57, 86, 122, 137	0
7	G	242/252 (96%)	-0.21	0 100 100	57, 82, 112, 175	0
7	U	242/252 (96%)	-0.15	0 100 100	55, 81, 107, 132	0
8	H	222/232 (95%)	-0.15	0 100 100	56, 79, 100, 156	0
8	V	222/232 (95%)	-0.23	0 100 100	56, 79, 100, 140	0
9	I	204/205 (99%)	-0.18	1 (0%) 87 78	52, 76, 102, 132	0
9	W	204/205 (99%)	-0.15	0 100 100	51, 75, 107, 130	0
10	J	196/198 (98%)	-0.28	0 100 100	54, 76, 105, 138	0
10	X	195/198 (98%)	-0.17	0 100 100	56, 76, 99, 156	0
11	K	212/212 (100%)	-0.28	1 (0%) 87 78	58, 76, 104, 134	0
11	Y	212/212 (100%)	-0.20	2 (0%) 81 67	56, 80, 113, 134	0
12	L	222/222 (100%)	-0.26	1 (0%) 87 78	55, 78, 97, 120	0
12	Z	222/222 (100%)	-0.13	2 (0%) 81 67	59, 78, 107, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	-0.18	1 (0%) 89 81	58, 79, 105, 141	0
13	a	233/233 (100%)	-0.25	0 100 100	55, 74, 98, 115	0
14	N	196/196 (100%)	-0.22	0 100 100	55, 76, 99, 126	0
14	b	196/196 (100%)	-0.29	0 100 100	58, 75, 99, 120	0
All	All	6363/6586 (96%)	-0.16	19 (0%) 90 84	50, 81, 118, 189	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	248	ASP	3.7
4	D	112	ALA	2.9
4	D	0	TYR	2.5
4	R	0	TYR	2.3
12	Z	222	ASP	2.3

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
17	MG	I	301	1/1	0.70	0.32	65,65,65,65	0
15	SO4	B	301	5/5	0.74	0.17	97,119,137,147	5
15	SO4	Y	306	5/5	0.76	0.10	108,111,131,135	5
15	SO4	b	203	5/5	0.77	0.23	75,98,114,128	5
15	SO4	T	303	5/5	0.77	0.13	69,84,95,113	5
15	SO4	F	302	5/5	0.78	0.20	75,76,95,108	5
15	SO4	M	306	5/5	0.81	0.14	91,100,124,129	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	P	301	5/5	0.81	0.21	104,116,142,162	5
15	SO4	M	304	5/5	0.83	0.16	63,88,112,114	5
15	SO4	S	302	5/5	0.84	0.18	73,88,91,114	5
15	SO4	E	302	5/5	0.84	0.14	86,91,100,101	5
15	SO4	Y	304	5/5	0.84	0.21	68,73,88,98	5
15	SO4	H	302	5/5	0.84	0.20	94,94,109,127	5
15	SO4	a	302	5/5	0.84	0.20	86,90,101,116	5
15	SO4	I	303	5/5	0.84	0.16	72,76,107,128	5
15	SO4	J	202	5/5	0.84	0.19	93,107,121,137	5
17	MG	W	301	1/1	0.84	0.39	65,65,65,65	0
15	SO4	a	301	5/5	0.85	0.12	92,105,120,135	5
16	A1A9B	V	301	49/49	0.85	0.16	57,105,128,138	0
15	SO4	M	301	5/5	0.86	0.13	91,96,100,108	5
15	SO4	M	302	5/5	0.86	0.19	73,84,95,111	5
15	SO4	T	301	5/5	0.86	0.24	83,101,130,147	0
15	SO4	K	304	5/5	0.86	0.10	60,60,74,97	5
15	SO4	L	302	5/5	0.87	0.17	88,90,130,139	5
15	SO4	Y	303	5/5	0.87	0.17	94,103,113,123	5
15	SO4	S	303	5/5	0.87	0.13	84,91,102,114	5
15	SO4	a	304	5/5	0.87	0.15	113,121,160,164	0
17	MG	Y	302	1/1	0.87	0.10	87,87,87,87	1
17	MG	Z	301	1/1	0.87	0.09	60,60,60,60	0
15	SO4	a	305	5/5	0.88	0.18	74,90,113,116	5
15	SO4	I	302	5/5	0.88	0.14	75,79,91,97	5
15	SO4	T	302	5/5	0.88	0.18	102,103,141,142	5
15	SO4	S	301	5/5	0.88	0.28	64,75,94,104	5
15	SO4	K	302	5/5	0.88	0.23	52,75,78,84	5
15	SO4	D	301	5/5	0.88	0.20	81,87,90,90	5
15	SO4	V	302	5/5	0.88	0.18	97,98,101,129	5
16	A1A9B	N	202	49/49	0.89	0.13	55,79,103,123	0
15	SO4	V	303	5/5	0.89	0.11	72,84,105,116	5
16	A1A9B	b	201	49/49	0.89	0.12	55,74,92,103	0
15	SO4	W	302	5/5	0.89	0.19	74,79,100,108	5
15	SO4	E	301	5/5	0.89	0.11	86,95,99,120	5
15	SO4	N	201	5/5	0.89	0.18	78,81,98,102	5
15	SO4	K	305	5/5	0.89	0.18	95,96,119,136	5
16	A1A9B	H	301	49/49	0.90	0.12	64,90,125,148	0
15	SO4	K	303	5/5	0.90	0.09	69,84,93,95	5
15	SO4	H	304	5/5	0.90	0.17	77,82,108,112	5
15	SO4	Y	305	5/5	0.90	0.11	66,77,95,117	5
15	SO4	a	303	5/5	0.91	0.15	67,69,87,98	5
15	SO4	b	204	5/5	0.91	0.14	70,72,77,83	5

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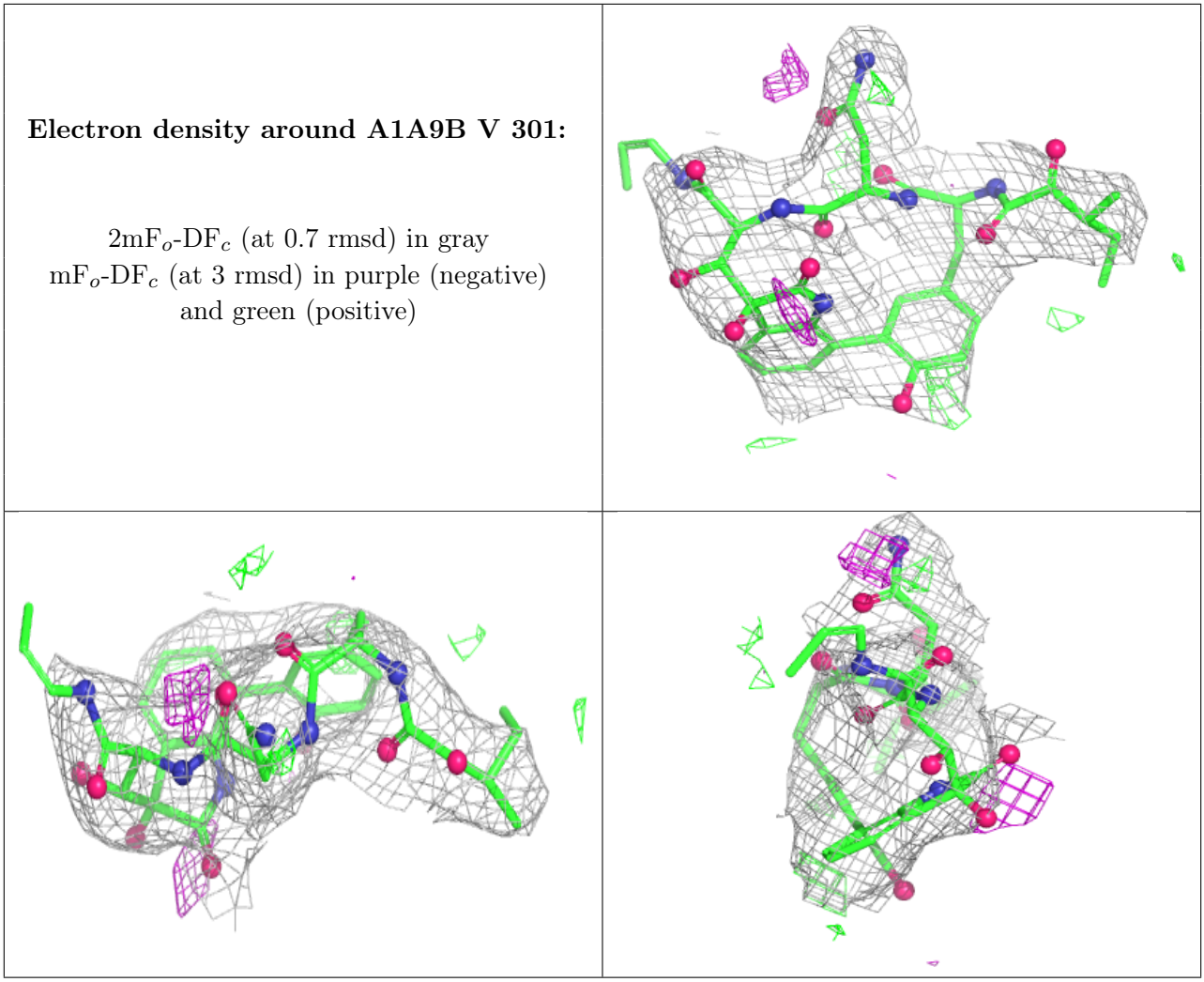
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	F	301	5/5	0.91	0.19	72,80,91,101	5
15	SO4	U	302	5/5	0.91	0.17	68,81,90,104	5
15	SO4	b	202	5/5	0.91	0.14	64,70,85,87	5
15	SO4	Z	302	5/5	0.92	0.20	65,75,86,89	5
15	SO4	Z	303	5/5	0.92	0.12	63,83,107,108	5
15	SO4	M	303	5/5	0.92	0.22	70,98,109,133	5
15	SO4	H	303	5/5	0.92	0.13	75,75,79,93	5
15	SO4	Q	301	5/5	0.92	0.17	77,78,95,97	5
15	SO4	M	308	5/5	0.92	0.13	94,104,112,130	5
16	A1A9B	K	301	49/49	0.93	0.12	52,74,103,108	0
15	SO4	G	301	5/5	0.93	0.17	83,87,99,119	5
15	SO4	G	302	5/5	0.94	0.12	79,80,92,114	5
17	MG	L	301	1/1	0.94	0.09	53,53,53,53	0
15	SO4	X	201	5/5	0.94	0.15	76,77,83,108	5
16	A1A9B	Y	301	49/49	0.94	0.10	51,73,93,99	0
15	SO4	C	301	5/5	0.94	0.15	55,62,91,98	5
15	SO4	M	307	5/5	0.95	0.15	51,63,72,78	5
15	SO4	J	201	5/5	0.95	0.15	47,63,78,86	5
15	SO4	M	305	5/5	0.96	0.14	63,67,77,80	5
15	SO4	U	301	5/5	0.96	0.15	81,96,103,118	5

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.

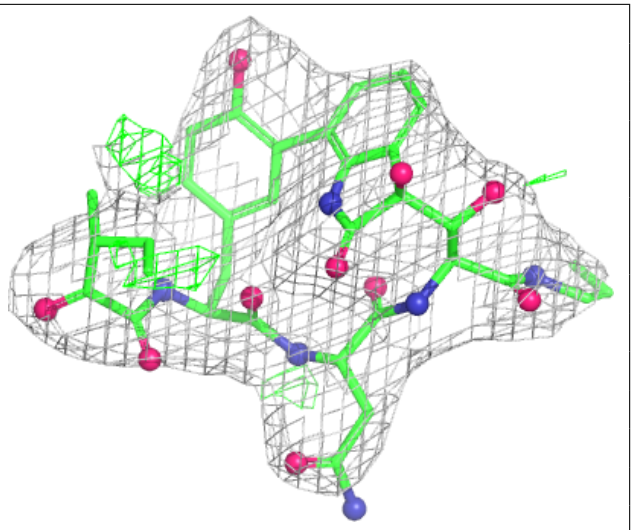
Electron density around A1A9B V 301:

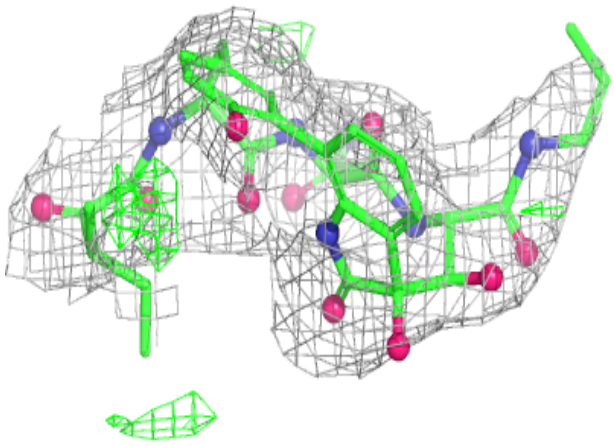
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

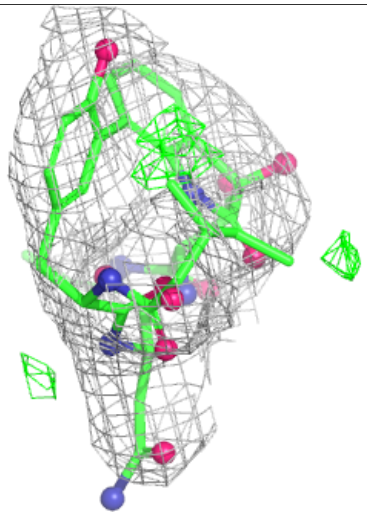


Electron density around A1A9B N 202:

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

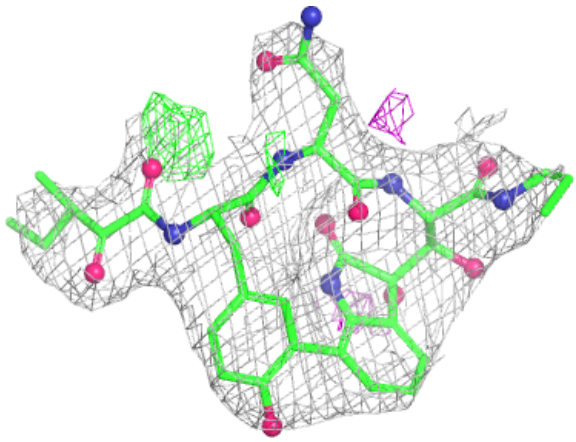


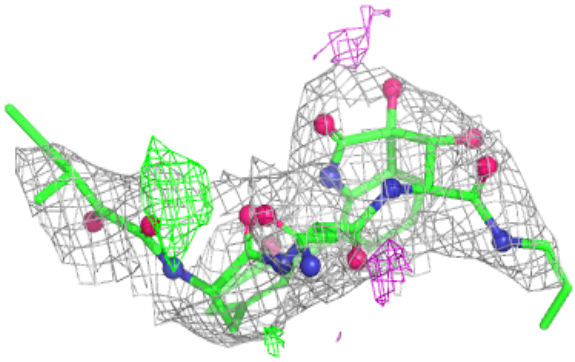


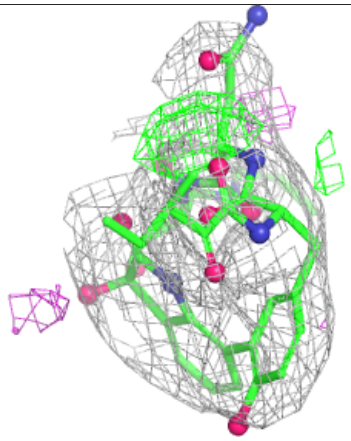


Electron density around A1A9B b 201:

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

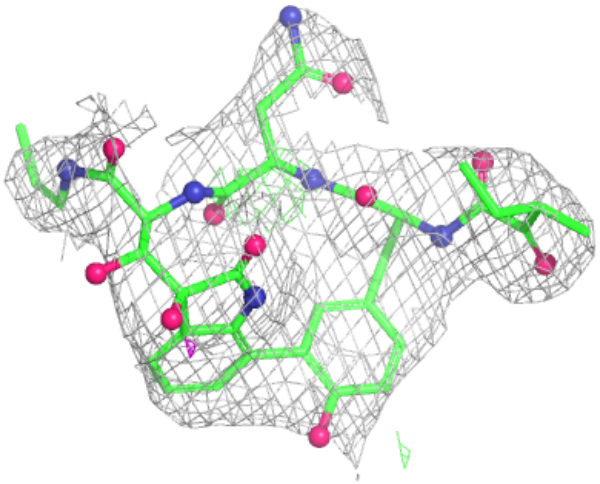


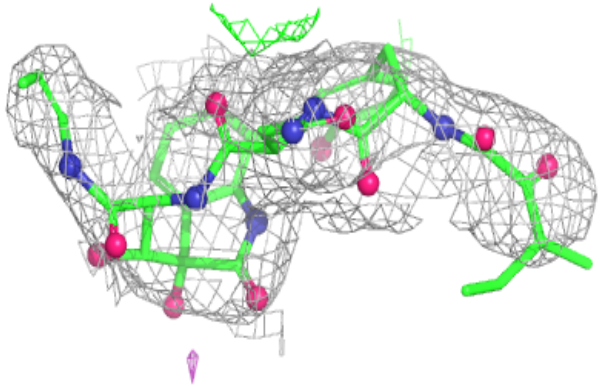


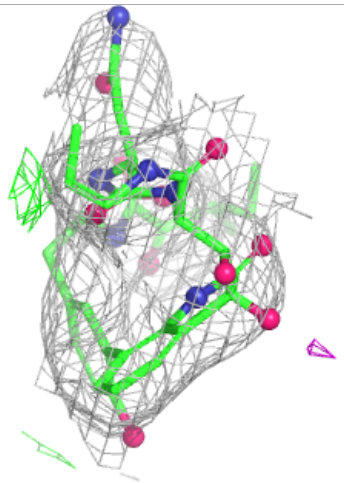


Electron density around A1A9B H 301:

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

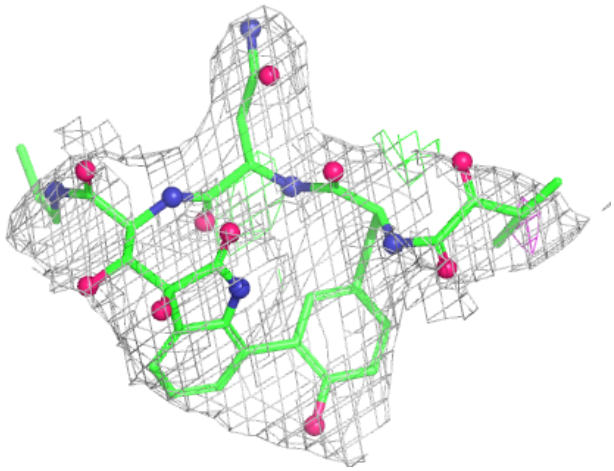


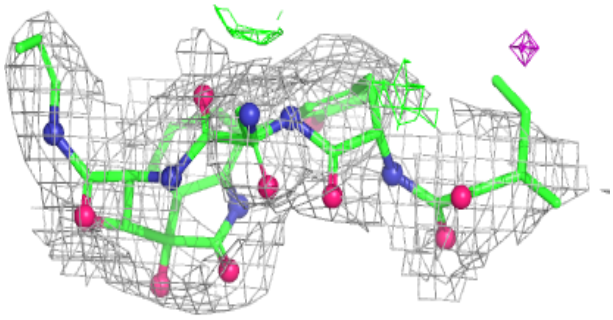


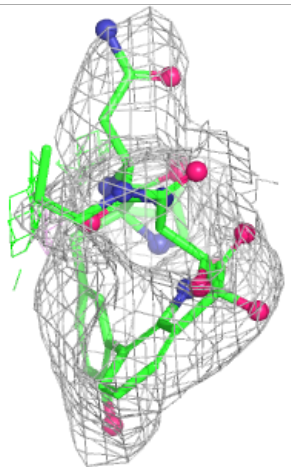


Electron density around A1A9B K 301:

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

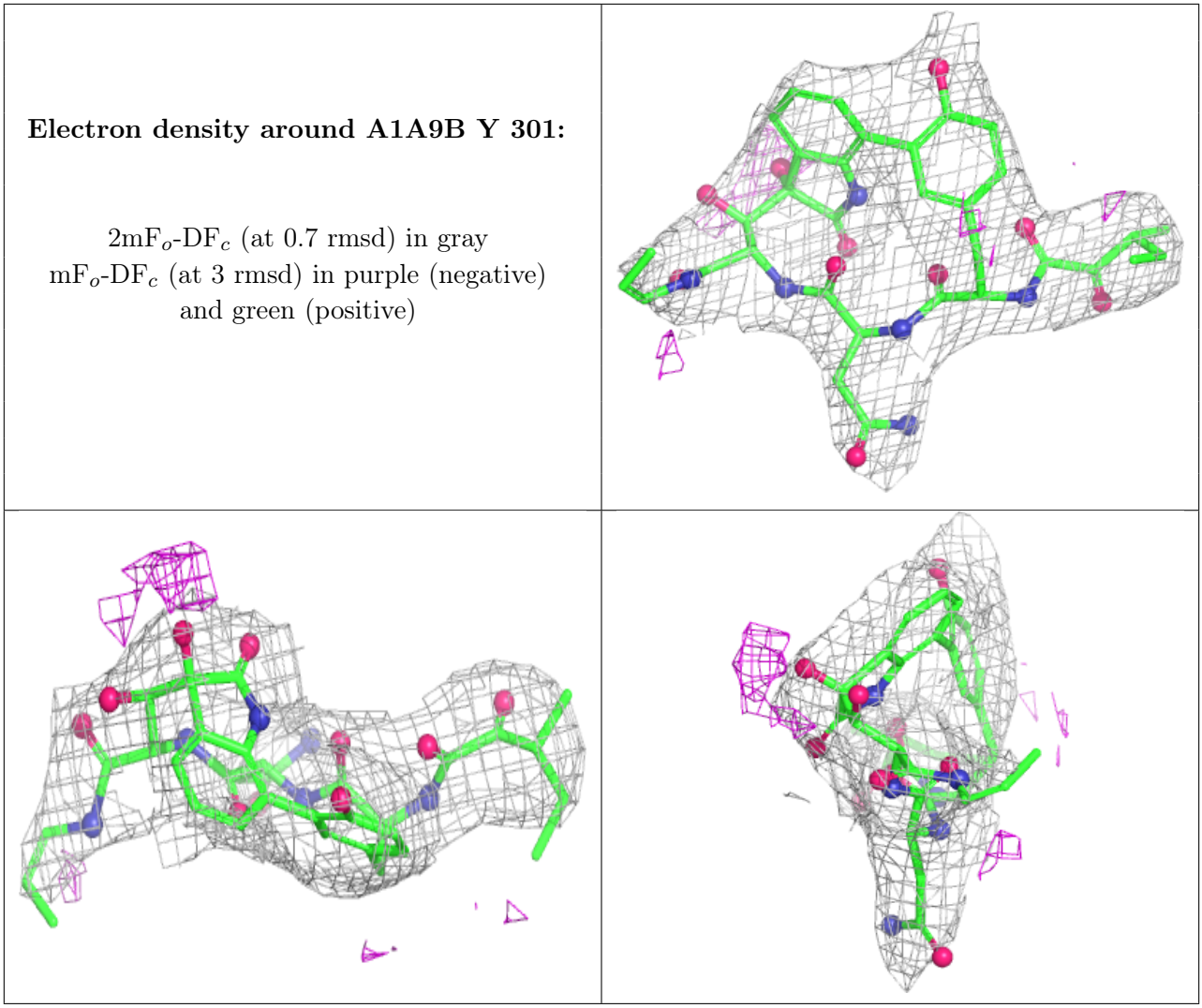






Electron density around A1A9B Y 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.