Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2025 – 01:18 PM EDT

PDB ID	:	9AW5
Title	:	Yeast 20S proteasome soaked with MA9 fraction E/F
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

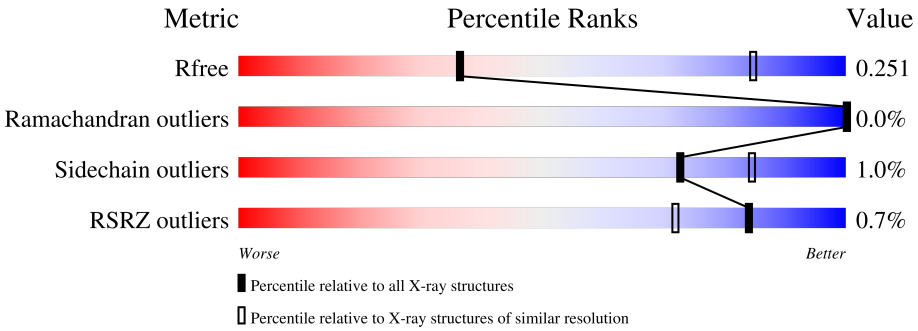
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (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)
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	100%
1	O	250	99%
2	B	258	2% 93% 6%
2	P	258	% 94% 5%
3	C	254	97%
3	Q	254	% 95% 5%

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Mol	Chain	Length	Quality of chain
4	D	260	92% 8%
4	R	260	3% 95%
5	E	234	97%
5	S	234	% 97%
6	F	287	% 84% 15%
6	T	287	84% 15%
7	G	252	96%
7	U	252	96%
8	H	232	% 95%
8	V	232	94%
9	I	205	% 99%
9	W	205	99%
10	J	198	% 98%
10	X	198	2% 98%
11	K	212	99%
11	Y	212	98%
12	L	222	% 99%
12	Z	222	99%
13	M	233	99%
13	a	233	98%
14	N	196	% 99%
14	b	196	99%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 50274 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	249	Total	C	N	O	S	0	0	0
			1920	1199	321	393	7			

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

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

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

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

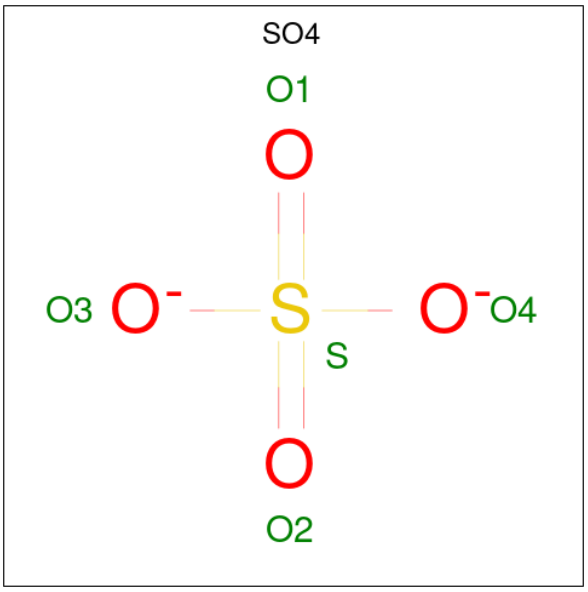
- Molecule 13 is a protein called Proteasome subunit beta type-7.

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		0	0
			5	4	1			
15	C	1	Total	O	S		0	0
			5	4	1			
15	D	1	Total	O	S		0	0
			5	4	1			
15	E	1	Total	O	S		0	0
			5	4	1			
15	E	1	Total	O	S		0	0
			5	4	1			
15	F	1	Total	O	S		0	0
			5	4	1			
15	F	1	Total	O	S		0	0
			5	4	1			
15	F	1	Total	O	S		0	0
			5	4	1			
15	G	1	Total	O	S		0	0
			5	4	1			
15	P	1	Total	O	S		0	0
			5	4	1			
15	Q	1	Total	O	S		0	0
			5	4	1			
15	S	1	Total	O	S		0	0
			5	4	1			
15	S	1	Total	O	S		0	0
			5	4	1			
15	T	1	Total	O	S		0	0
			5	4	1			

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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	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	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	N	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	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	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

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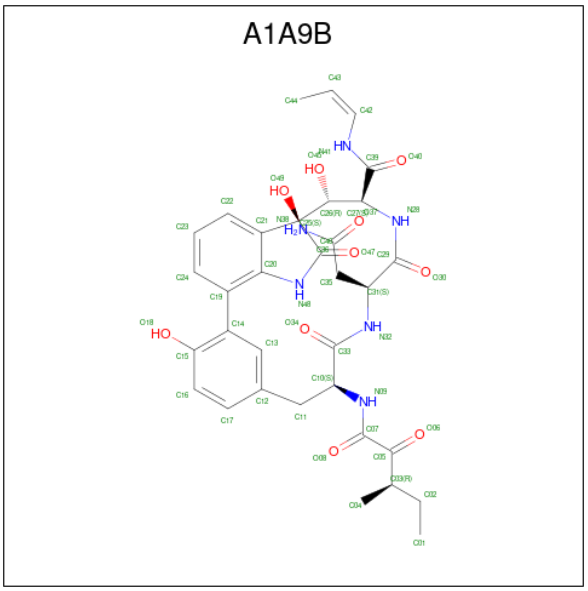
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	H	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	K	1	Total Mg 1 1	0	0
16	L	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0
16	Y	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0

- Molecule 17 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
17	K	1	Total C N O 49 33 6 10	0	0
17	Y	1	Total C N O 49 33 6 10	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	12	Total O 12 12	0	0
18	B	16	Total O 16 16	0	0
18	C	14	Total O 14 14	0	0
18	D	10	Total O 10 10	0	0
18	E	4	Total O 4 4	0	0
18	F	5	Total O 5 5	0	0
18	G	9	Total O 9 9	0	0
18	O	10	Total O 10 10	0	0
18	P	12	Total O 12 12	0	0
18	Q	13	Total O 13 13	0	0

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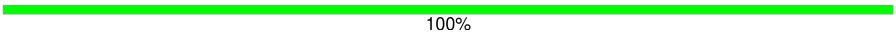
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	R	5	Total O 5 5	0	0
18	S	13	Total O 13 13	0	0
18	T	17	Total O 17 17	0	0
18	U	12	Total O 12 12	0	0
18	H	19	Total O 19 19	0	0
18	I	9	Total O 9 9	0	0
18	J	16	Total O 16 16	0	0
18	K	12	Total O 12 12	0	0
18	L	13	Total O 13 13	0	0
18	M	9	Total O 9 9	0	0
18	N	18	Total O 18 18	0	0
18	V	20	Total O 20 20	0	0
18	W	5	Total O 5 5	0	0
18	X	13	Total O 13 13	0	0
18	Y	12	Total O 12 12	0	0
18	Z	9	Total O 9 9	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.

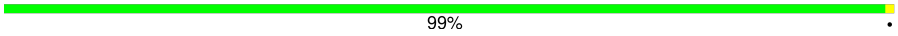
• Molecule 1: Proteasome subunit alpha type-2

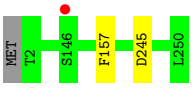
Chain A:



• Molecule 1: Proteasome subunit alpha type-2

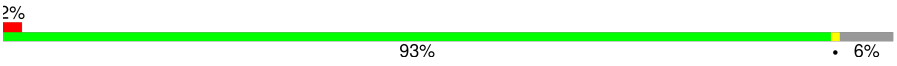
Chain O:

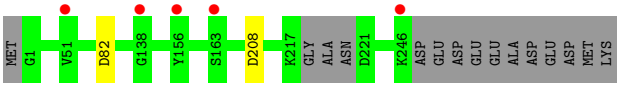




• Molecule 2: Proteasome subunit alpha type-3

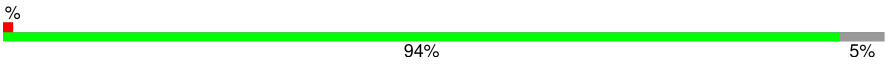
Chain B:

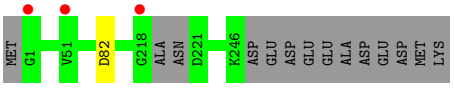




• Molecule 2: Proteasome subunit alpha type-3

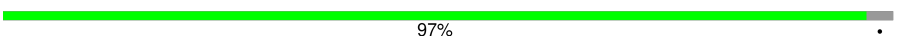
Chain P:

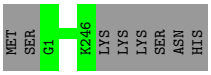




• Molecule 3: Proteasome subunit alpha type-4

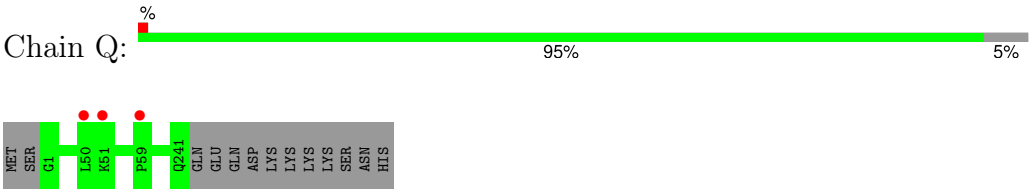
Chain C:





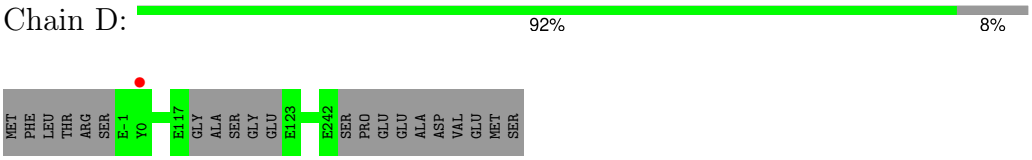
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



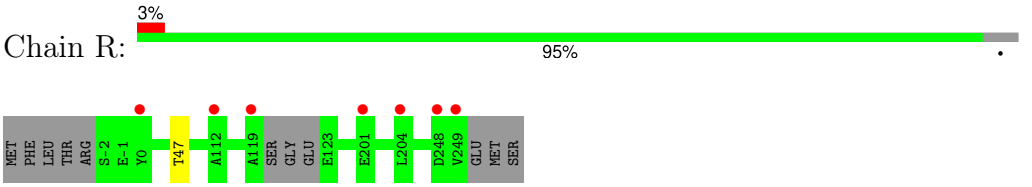
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



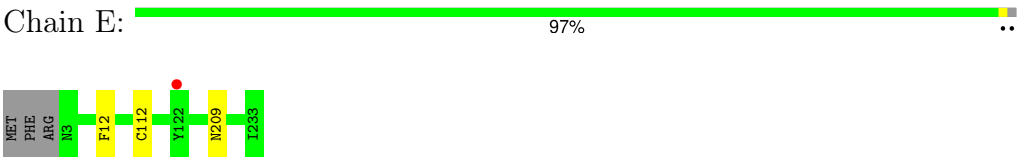
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



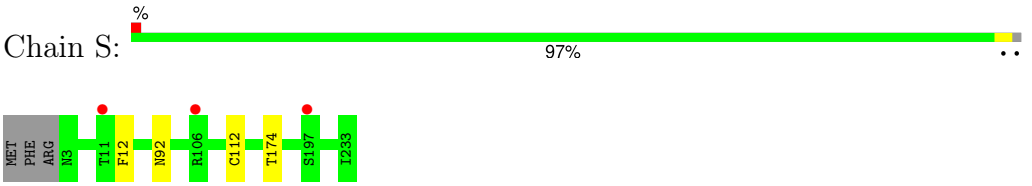
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



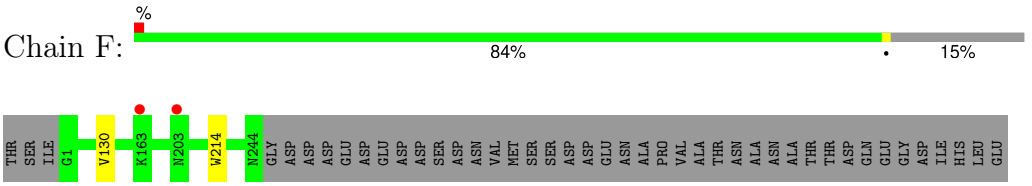
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



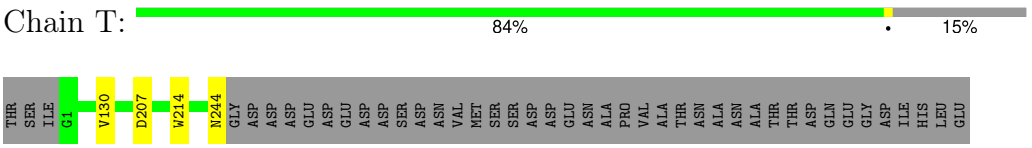
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



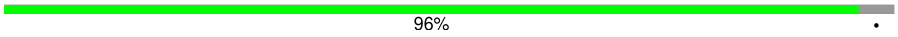
• Molecule 6: Probable proteasome subunit alpha type-7

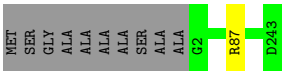
Chain T:



• Molecule 7: Proteasome subunit alpha type-1

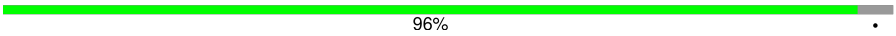
Chain G:

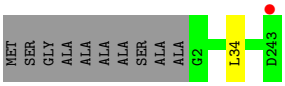




• Molecule 7: Proteasome subunit alpha type-1

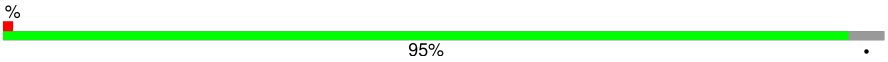
Chain U:

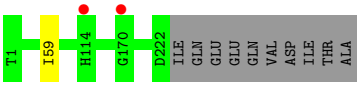




• Molecule 8: Proteasome subunit beta type-2

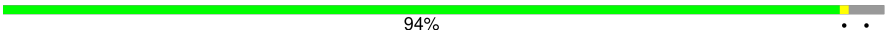
Chain H:





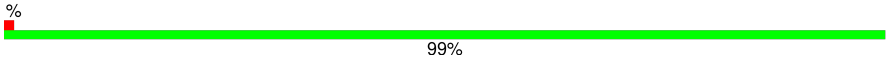
• Molecule 8: Proteasome subunit beta type-2

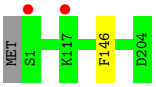
Chain V:



• Molecule 9: Proteasome subunit beta type-3

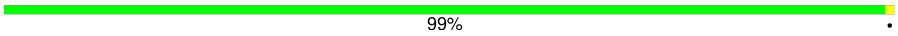
Chain I:

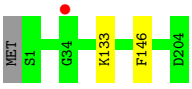




• Molecule 9: Proteasome subunit beta type-3

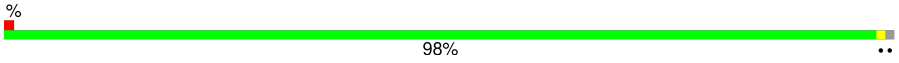
Chain W:





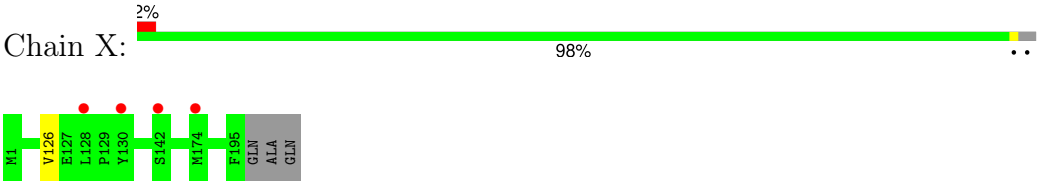
• Molecule 10: Proteasome subunit beta type-4

Chain J:



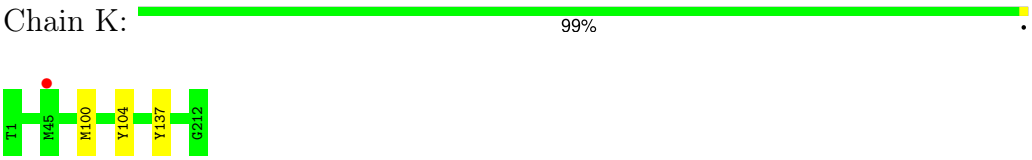
• Molecule 10: Proteasome subunit beta type-4

Chain X:



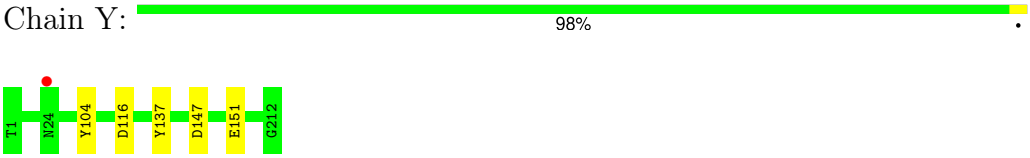
• Molecule 11: Proteasome subunit beta type-5

Chain K:



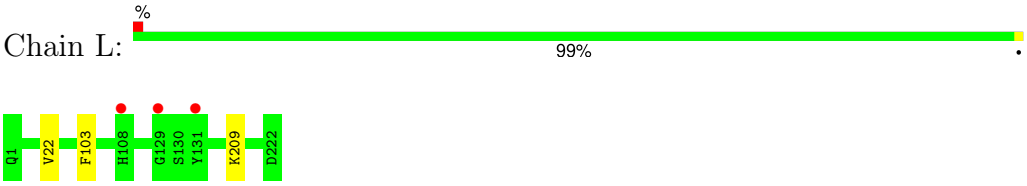
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



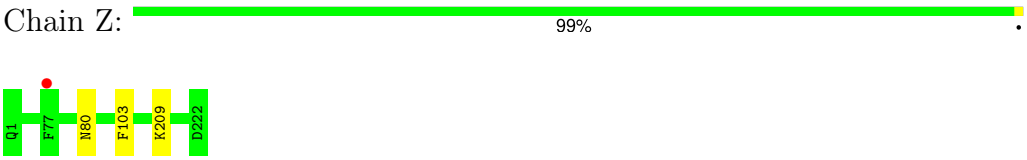
• Molecule 12: Proteasome subunit beta type-6

Chain L:



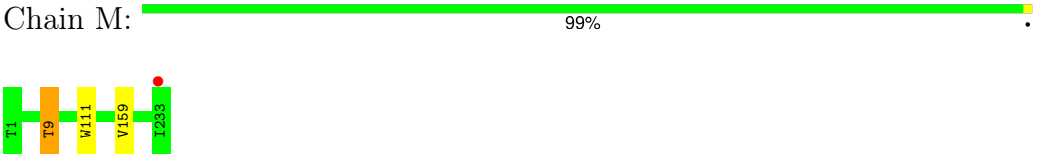
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



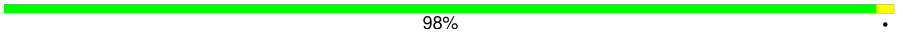
• Molecule 13: Proteasome subunit beta type-7

Chain M:



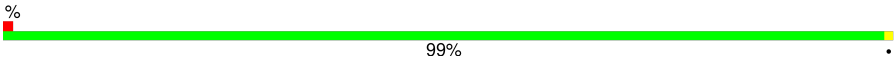
• Molecule 13: Proteasome subunit beta type-7

Chain a:



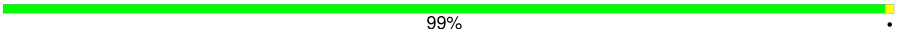
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

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	134.89Å 299.29Å 144.21Å 90.00° 112.78° 90.00°	Depositor
Resolution (Å)	45.74 – 3.44 45.74 – 3.44	Depositor EDS
% Data completeness (in resolution range)	97.4 (45.74-3.44) 85.4 (45.74-3.44)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.21.1.5286	Depositor
R, R_{free}	0.201 , 0.252 0.201 , 0.251	Depositor DCC
R_{free} test set	6758 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 65.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	50274	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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	0.46	0/2632
1	O	0.25	0/1944	0.46	0/2632
2	B	0.24	0/1934	0.48	0/2614
2	P	0.24	0/1938	0.48	0/2619
3	C	0.24	0/1963	0.49	0/2656
3	Q	0.24	0/1919	0.49	0/2598
4	D	0.24	0/1879	0.47	0/2531
4	R	0.24	0/1946	0.47	0/2623
5	E	0.24	0/1800	0.48	0/2433
5	S	0.25	0/1800	0.49	0/2433
6	F	0.25	0/1936	0.46	0/2614
6	T	0.25	0/1936	0.46	0/2614
7	G	0.25	0/1954	0.47	0/2645
7	U	0.25	0/1954	0.47	0/2645
8	H	0.24	0/1715	0.46	0/2326
8	V	0.24	0/1715	0.46	0/2326
9	I	0.25	0/1611	0.47	0/2174
9	W	0.25	0/1611	0.47	0/2174
10	J	0.25	0/1598	0.47	0/2154
10	X	0.25	0/1589	0.47	0/2142
11	K	0.24	0/1681	0.47	0/2274
11	Y	0.24	0/1681	0.47	0/2274
12	L	0.25	0/1795	0.49	0/2420
12	Z	0.25	0/1795	0.49	0/2420
13	M	0.25	0/1855	0.49	0/2514
13	a	0.25	0/1855	0.49	0/2514
14	N	0.24	0/1541	0.46	0/2087
14	b	0.24	0/1541	0.47	0/2087
All	All	0.25	0/50430	0.47	0/68175

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	238 (96%)	9 (4%)	0	100	100
1	O	247/250 (99%)	240 (97%)	7 (3%)	0	100	100
2	B	239/258 (93%)	233 (98%)	6 (2%)	0	100	100
2	P	240/258 (93%)	234 (98%)	6 (2%)	0	100	100
3	C	244/254 (96%)	236 (97%)	8 (3%)	0	100	100
3	Q	239/254 (94%)	232 (97%)	7 (3%)	0	100	100
4	D	235/260 (90%)	229 (97%)	6 (3%)	0	100	100
4	R	245/260 (94%)	235 (96%)	10 (4%)	0	100	100
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
6	F	242/287 (84%)	235 (97%)	7 (3%)	0	100	100
6	T	242/287 (84%)	236 (98%)	6 (2%)	0	100	100
7	G	240/252 (95%)	230 (96%)	10 (4%)	0	100	100
7	U	240/252 (95%)	231 (96%)	9 (4%)	0	100	100
8	H	220/232 (95%)	214 (97%)	6 (3%)	0	100	100
8	V	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	194/198 (98%)	188 (97%)	6 (3%)	0	100	100
10	X	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
12	Z	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	25	58
13	M	231/233 (99%)	220 (95%)	10 (4%)	1 (0%)	30	63
13	a	231/233 (99%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6299/6586 (96%)	6089 (97%)	208 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	9	THR
12	Z	80	ASN

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%)	208 (100%)	0	100	100
1	O	208/209 (100%)	206 (99%)	2 (1%)	73	84
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%)	218 (100%)	0	100	100
3	Q	213/226 (94%)	213 (100%)	0	100	100
4	D	198/215 (92%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	205/215 (95%)	204 (100%)	1 (0%)	86	92
5	E	190/193 (98%)	187 (98%)	3 (2%)	58	76
5	S	190/193 (98%)	186 (98%)	4 (2%)	48	71
6	F	201/238 (84%)	199 (99%)	2 (1%)	73	84
6	T	201/238 (84%)	197 (98%)	4 (2%)	50	72
7	G	207/210 (99%)	206 (100%)	1 (0%)	86	92
7	U	207/210 (99%)	206 (100%)	1 (0%)	86	92
8	H	181/190 (95%)	180 (99%)	1 (1%)	84	91
8	V	181/190 (95%)	178 (98%)	3 (2%)	56	75
9	I	172/173 (99%)	171 (99%)	1 (1%)	84	91
9	W	172/173 (99%)	170 (99%)	2 (1%)	67	81
10	J	174/175 (99%)	172 (99%)	2 (1%)	70	82
10	X	173/175 (99%)	172 (99%)	1 (1%)	84	91
11	K	169/169 (100%)	166 (98%)	3 (2%)	54	74
11	Y	169/169 (100%)	164 (97%)	5 (3%)	36	63
12	L	185/185 (100%)	182 (98%)	3 (2%)	58	76
12	Z	185/185 (100%)	183 (99%)	2 (1%)	70	82
13	M	199/199 (100%)	196 (98%)	3 (2%)	60	77
13	a	199/199 (100%)	195 (98%)	4 (2%)	50	72
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%)	5284 (99%)	53 (1%)	73	84

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	82	ASP
2	B	208	ASP
5	E	12	PHE
5	E	112	CYS
5	E	209	ASN
6	F	130	VAL
6	F	214	TRP
7	G	87	ARG
1	O	157	PHE

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Mol	Chain	Res	Type
1	O	245	ASP
2	P	82	ASP
4	R	47	THR
5	S	12	PHE
5	S	92	ASN
5	S	112	CYS
5	S	174	THR
6	T	130	VAL
6	T	207	ASP
6	T	214	TRP
6	T	244	ASN
7	U	34	LEU
8	H	59	ILE
9	I	146	PHE
10	J	78	GLN
10	J	126	VAL
11	K	100	MET
11	K	104	TYR
11	K	137	TYR
12	L	22	VAL
12	L	103	PHE
12	L	209	LYS
13	M	9	THR
13	M	111	TRP
13	M	159	VAL
14	N	83	LYS
8	V	38	SER
8	V	188	ARG
8	V	222	ASP
9	W	133	LYS
9	W	146	PHE
10	X	126	VAL
11	Y	104	TYR
11	Y	116	ASP
11	Y	137	TYR
11	Y	147	ASP
11	Y	151	GLU
12	Z	103	PHE
12	Z	209	LYS
13	a	9	THR
13	a	25	ASP
13	a	111	TRP

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Mol	Chain	Res	Type
13	a	159	VAL
14	b	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	37	ASN
11	Y	209	ASN
14	b	141	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 71 ligands modelled in this entry, 8 are monoatomic - leaving 63 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	K	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	305	-	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	0.08	0
15	SO4	W	302	-	4,4,4	0.67	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SO4	Y	305	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	T	304	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	G	301	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	W	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	302	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	E	302	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	Y	306	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	T	303	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	303	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	J	202	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	S	302	-	4,4,4	0.67	0	6,6,6	0.08	0
17	A1A9B	Y	301	-	51,52,52	3.58	18 (35%)	67,76,76	3.30	15 (22%)
15	SO4	D	301	-	4,4,4	0.66	0	6,6,6	0.08	0
15	SO4	F	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Y	303	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	K	305	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Z	305	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	N	201	-	4,4,4	0.66	0	6,6,6	0.07	0
15	SO4	N	202	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	U	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	304	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Z	302	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	b	201	-	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	a	305	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	H	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Z	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	L	302	-	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	0.08	0
15	SO4	M	306	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	b	203	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	Q	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	K	306	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	L	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	Z	304	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	T	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	P	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	J	201	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	301	-	4,4,4	0.66	0	6,6,6	0.08	0
15	SO4	I	302	-	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	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SO4	a	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	V	302	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	K	304	-	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	0.06	0
15	SO4	F	302	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	I	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	M	304	-	4,4,4	0.67	0	6,6,6	0.09	0
17	A1A9B	K	301	-	51,52,52	3.60	18 (35%)	67,76,76	3.46	21 (31%)
15	SO4	S	301	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	a	306	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	F	303	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	H	304	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	a	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	b	202	-	4,4,4	0.67	0	6,6,6	0.08	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

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	A1A9B	Y	301	-	-	8/59/76/76	0/3/4/4
17	A1A9B	K	301	-	-	22/59/76/76	0/3/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	A1A9B	C25-C21	11.79	1.66	1.51
17	Y	301	A1A9B	C25-C21	11.77	1.66	1.51
17	Y	301	A1A9B	O49-C25	-11.00	1.27	1.42
17	K	301	A1A9B	O49-C25	-10.92	1.27	1.42
17	K	301	A1A9B	C39-N41	10.89	1.49	1.34
17	Y	301	A1A9B	C39-N41	10.79	1.49	1.34
17	K	301	A1A9B	C33-N32	7.52	1.50	1.34
17	Y	301	A1A9B	C33-N32	7.24	1.49	1.34
17	Y	301	A1A9B	C29-N28	7.18	1.49	1.34
17	K	301	A1A9B	C29-N28	7.15	1.49	1.34
17	Y	301	A1A9B	C07-N09	6.68	1.48	1.34
17	K	301	A1A9B	C07-N09	6.64	1.48	1.34
17	K	301	A1A9B	C36-N38	4.38	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	A1A9B	C36-N38	4.37	1.46	1.32
17	Y	301	A1A9B	C46-N48	-4.12	1.30	1.35
17	K	301	A1A9B	C46-N48	-4.11	1.30	1.35
17	Y	301	A1A9B	C20-N48	-3.61	1.31	1.38
17	K	301	A1A9B	C20-N48	-3.52	1.31	1.38
17	K	301	A1A9B	C42-N41	2.81	1.48	1.40
17	Y	301	A1A9B	C42-N41	2.76	1.48	1.40
17	Y	301	A1A9B	C19-C14	2.53	1.55	1.49
17	K	301	A1A9B	O18-C15	2.52	1.41	1.36
17	Y	301	A1A9B	O18-C15	2.50	1.41	1.36
17	K	301	A1A9B	C19-C14	2.36	1.54	1.49
17	K	301	A1A9B	C22-C21	2.29	1.42	1.39
17	Y	301	A1A9B	O08-C07	-2.29	1.19	1.23
17	K	301	A1A9B	O08-C07	-2.26	1.19	1.23
17	K	301	A1A9B	O30-C29	-2.25	1.19	1.23
17	Y	301	A1A9B	O40-C39	-2.23	1.19	1.23
17	Y	301	A1A9B	C22-C21	2.22	1.42	1.39
17	K	301	A1A9B	O40-C39	-2.18	1.19	1.23
17	Y	301	A1A9B	O30-C29	-2.14	1.19	1.23
17	Y	301	A1A9B	O34-C33	-2.13	1.19	1.23
17	K	301	A1A9B	O34-C33	-2.12	1.19	1.23
17	K	301	A1A9B	C11-C12	2.03	1.56	1.51
17	Y	301	A1A9B	C11-C12	2.00	1.56	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	301	A1A9B	C20-N48-C46	22.65	129.66	111.26
17	Y	301	A1A9B	C20-N48-C46	22.54	129.57	111.26
17	K	301	A1A9B	C25-C46-N48	-7.97	98.02	108.21
17	Y	301	A1A9B	C25-C46-N48	-7.72	98.34	108.21
17	Y	301	A1A9B	O47-C46-C25	5.11	131.11	125.22
17	K	301	A1A9B	O47-C46-C25	4.99	130.97	125.22
17	Y	301	A1A9B	C21-C20-N48	-4.54	105.08	110.00
17	K	301	A1A9B	C21-C20-N48	-4.43	105.20	110.00
17	K	301	A1A9B	O47-C46-N48	4.41	130.96	126.28
17	Y	301	A1A9B	O47-C46-N48	4.03	130.55	126.28
17	K	301	A1A9B	C10-C33-N32	3.78	124.68	116.63
17	K	301	A1A9B	C22-C21-C25	3.53	135.75	130.81
17	Y	301	A1A9B	C22-C21-C25	3.37	135.53	130.81
17	K	301	A1A9B	C25-C21-C20	-3.12	104.83	108.47
17	K	301	A1A9B	C14-C19-C20	-3.03	117.00	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	301	A1A9B	C31-C29-N28	2.94	122.89	116.63
17	Y	301	A1A9B	C25-C21-C20	-2.88	105.10	108.47
17	K	301	A1A9B	O34-C33-N32	-2.88	117.81	122.96
17	K	301	A1A9B	C39-C27-N28	2.87	118.13	110.32
17	Y	301	A1A9B	C14-C19-C20	-2.75	117.70	124.79
17	K	301	A1A9B	O40-C39-N41	-2.73	119.66	123.47
17	K	301	A1A9B	C31-N32-C33	-2.64	115.97	121.65
17	Y	301	A1A9B	O40-C39-N41	-2.62	119.81	123.47
17	K	301	A1A9B	C19-C20-N48	2.34	134.69	131.09
17	K	301	A1A9B	C10-N09-C07	-2.34	118.05	122.00
17	Y	301	A1A9B	C31-C35-C36	2.31	116.86	112.21
17	Y	301	A1A9B	C19-C20-N48	2.25	134.54	131.09
17	K	301	A1A9B	C13-C14-C15	2.23	120.25	117.63
17	K	301	A1A9B	C27-C39-N41	2.21	120.70	116.56
17	K	301	A1A9B	C31-C35-C36	2.14	116.51	112.21
17	Y	301	A1A9B	C27-C39-N41	2.06	120.42	116.56
17	K	301	A1A9B	O08-C07-N09	-2.04	119.50	123.09
17	Y	301	A1A9B	C43-C42-N41	-2.03	117.75	123.80
17	Y	301	A1A9B	C31-C29-N28	2.01	120.92	116.63
17	K	301	A1A9B	O30-C29-N28	-2.01	119.36	122.96
17	Y	301	A1A9B	C13-C14-C15	2.00	119.98	117.63

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	301	A1A9B	C21-C25-C26-C27
17	K	301	A1A9B	C01-C02-C03-C05
17	K	301	A1A9B	O06-C05-C07-O08
17	Y	301	A1A9B	O06-C05-C07-O08
17	K	301	A1A9B	C11-C10-C33-O34
17	K	301	A1A9B	C11-C10-C33-N32
17	K	301	A1A9B	C01-C02-C03-C04
17	K	301	A1A9B	N28-C27-C39-O40
17	K	301	A1A9B	C33-C10-C11-C12
17	K	301	A1A9B	N28-C27-C39-N41
17	K	301	A1A9B	N09-C10-C11-C12
17	K	301	A1A9B	N32-C31-C35-C36
17	K	301	A1A9B	C29-C31-C35-C36
17	K	301	A1A9B	O06-C05-C07-N09
17	K	301	A1A9B	C03-C05-C07-O08
17	K	301	A1A9B	C02-C03-C05-O06

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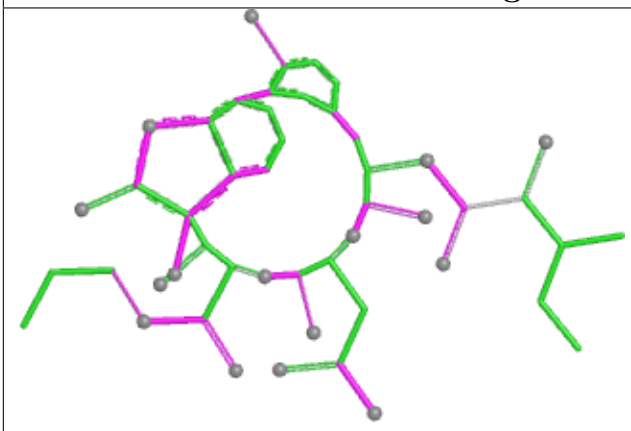
Mol	Chain	Res	Type	Atoms
17	K	301	A1A9B	C02-C03-C05-C07
17	K	301	A1A9B	C03-C05-C07-N09
17	Y	301	A1A9B	O45-C26-C27-C39
17	Y	301	A1A9B	N09-C10-C33-O34
17	Y	301	A1A9B	C33-C10-N09-C07
17	Y	301	A1A9B	N09-C10-C33-N32
17	Y	301	A1A9B	O30-C29-C31-N32
17	K	301	A1A9B	C43-C42-N41-C39
17	Y	301	A1A9B	C43-C42-N41-C39
17	K	301	A1A9B	C26-C27-N28-C29
17	K	301	A1A9B	C15-C14-C19-C20
17	Y	301	A1A9B	C15-C14-C19-C20
17	K	301	A1A9B	C21-C25-C26-O45
17	K	301	A1A9B	O45-C26-C27-C39

There are no ring outliers.

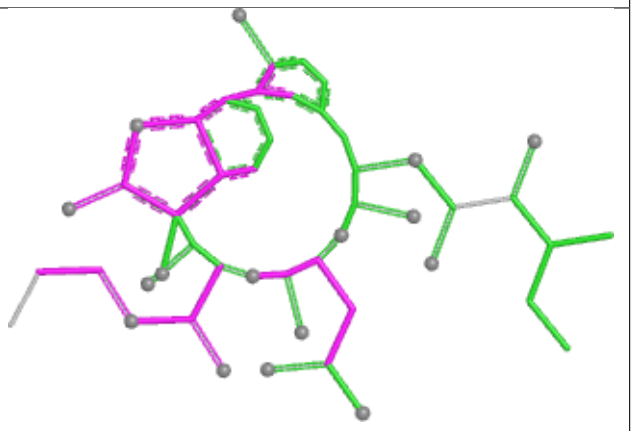
No monomer is involved in short contacts.

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.

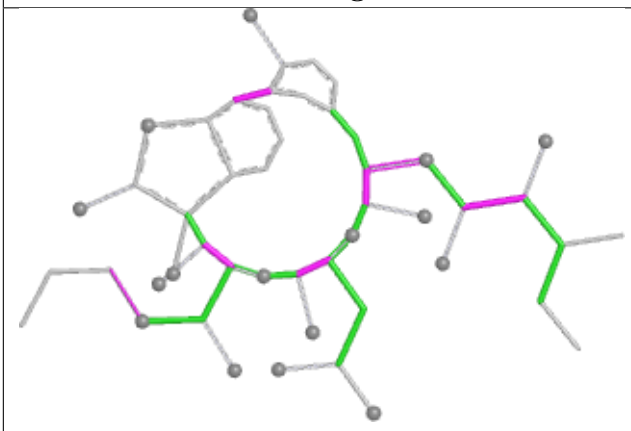
Ligand A1A9B Y 301



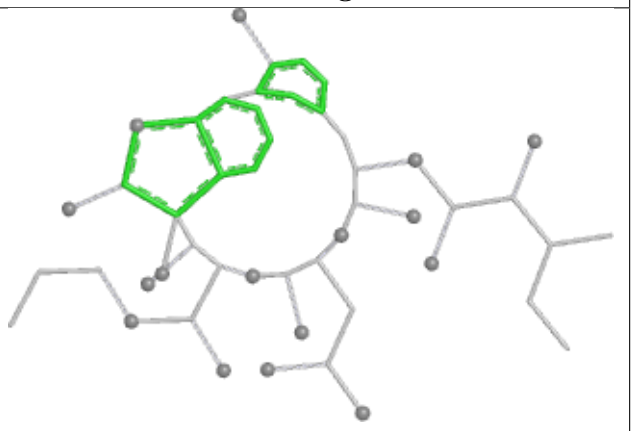
Bond lengths



Bond angles

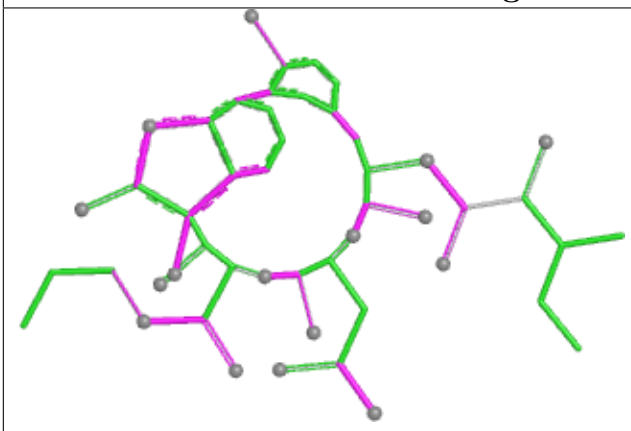


Torsions

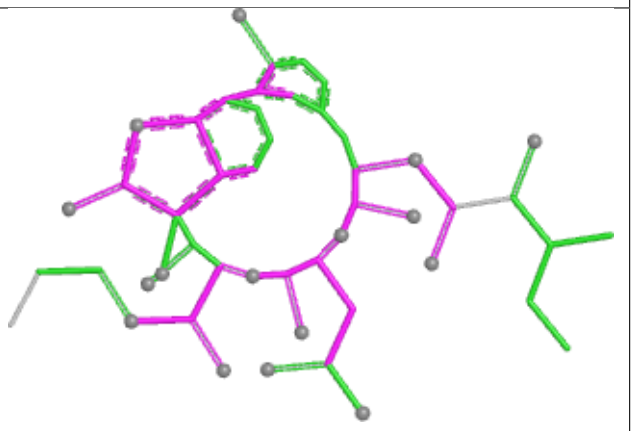


Rings

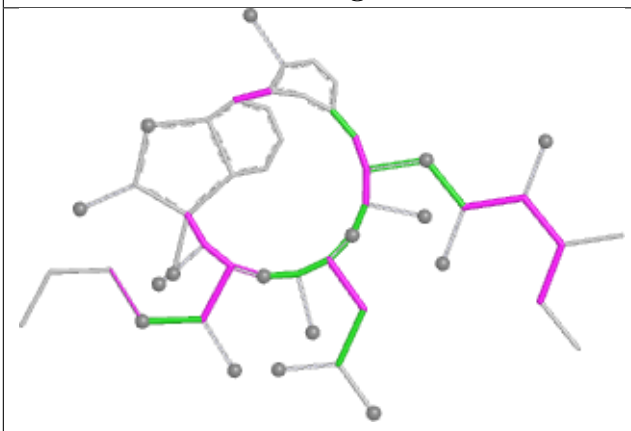
Ligand A1A9B K 301



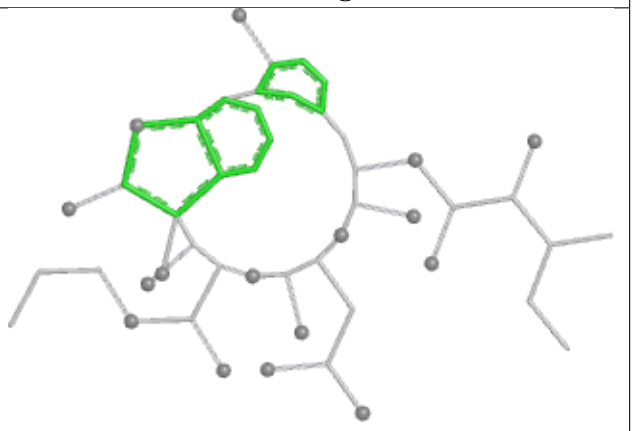
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.04	0 100 100	40, 69, 100, 122	0
1	O	249/250 (99%)	0.17	1 (0%) 89 81	49, 76, 107, 145	0
2	B	243/258 (94%)	0.21	5 (2%) 63 48	47, 73, 117, 145	0
2	P	244/258 (94%)	0.26	3 (1%) 76 61	47, 73, 113, 142	0
3	C	246/254 (96%)	0.16	0 100 100	46, 77, 127, 170	0
3	Q	241/254 (94%)	0.28	3 (1%) 76 61	51, 83, 132, 166	0
4	D	239/260 (91%)	0.17	1 (0%) 89 81	47, 74, 101, 141	0
4	R	249/260 (95%)	0.29	7 (2%) 55 41	54, 81, 130, 167	0
5	E	231/234 (98%)	0.26	1 (0%) 89 81	57, 86, 109, 135	0
5	S	231/234 (98%)	0.31	3 (1%) 74 59	52, 86, 115, 132	0
6	F	244/287 (85%)	0.27	2 (0%) 82 70	48, 75, 110, 147	0
6	T	244/287 (85%)	0.23	0 100 100	47, 72, 109, 128	0
7	G	242/252 (96%)	0.06	0 100 100	44, 67, 92, 157	0
7	U	242/252 (96%)	0.12	1 (0%) 89 81	44, 68, 95, 113	0
8	H	222/232 (95%)	0.11	2 (0%) 81 67	48, 71, 94, 136	0
8	V	222/232 (95%)	0.07	0 100 100	50, 72, 95, 132	0
9	I	204/205 (99%)	0.11	2 (0%) 79 65	47, 71, 94, 108	0
9	W	204/205 (99%)	0.09	1 (0%) 87 78	51, 68, 96, 112	0
10	J	196/198 (98%)	0.07	1 (0%) 87 78	47, 67, 93, 116	0
10	X	195/198 (98%)	0.16	4 (2%) 63 48	49, 67, 91, 125	0
11	K	212/212 (100%)	0.11	1 (0%) 87 78	45, 68, 97, 113	0
11	Y	212/212 (100%)	0.17	1 (0%) 87 78	50, 74, 105, 138	0
12	L	222/222 (100%)	0.18	3 (1%) 73 57	50, 71, 96, 132	0
12	Z	222/222 (100%)	0.13	1 (0%) 87 78	43, 72, 99, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	0.10	1 (0%) 89 81	50, 70, 94, 119	0
13	a	233/233 (100%)	0.07	0 100 100	48, 66, 91, 110	0
14	N	196/196 (100%)	0.09	1 (0%) 87 78	49, 64, 87, 115	0
14	b	196/196 (100%)	0.02	0 100 100	49, 65, 90, 102	0
All	All	6363/6586 (96%)	0.16	45 (0%) 84 72	40, 72, 107, 170	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	248	ASP	4.4
2	P	218	GLY	3.7
2	P	1	GLY	3.6
13	M	233	ILE	3.3
4	R	0	TYR	3.2
6	F	163	LYS	3.2
5	S	11	THR	3.1
4	D	0	TYR	3.0
4	R	249	VAL	2.8
10	X	128	LEU	2.6
4	R	201	GLU	2.6
10	X	142	SER	2.6
2	P	51	VAL	2.6
3	Q	59	PRO	2.5
3	Q	50	LEU	2.5
7	U	243	ASP	2.4
5	S	197	SER	2.4
12	L	129	GLY	2.4
2	B	51	VAL	2.4
11	K	45	MET	2.3
4	R	119	ALA	2.3
12	L	131	TYR	2.3
6	F	203	ASN	2.3
3	Q	51	LYS	2.3
2	B	163	SER	2.3
9	I	117	LYS	2.2
10	X	130	TYR	2.2
4	R	112	ALA	2.2
2	B	138	GLY	2.2
5	E	122	TYR	2.2
2	B	246	LYS	2.2
14	N	118	SER	2.2

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Mol	Chain	Res	Type	RSRZ
11	Y	24	ASN	2.2
2	B	156	TYR	2.2
8	H	114	HIS	2.1
9	I	1	SER	2.1
10	J	142	SER	2.1
4	R	204	LEU	2.1
9	W	34	GLY	2.1
12	L	108	HIS	2.1
10	X	174	MET	2.1
5	S	106	ARG	2.1
8	H	170	GLY	2.1
12	Z	77	PHE	2.0
1	O	146	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	K	304	5/5	0.60	0.14	79,88,101,110	5
15	SO4	M	305	5/5	0.69	0.13	95,112,135,144	5
15	SO4	Z	304	5/5	0.71	0.20	75,88,100,114	5
15	SO4	B	301	5/5	0.72	0.17	74,76,118,119	5
15	SO4	b	202	5/5	0.73	0.19	65,67,98,102	5
15	SO4	H	302	5/5	0.77	0.24	80,81,98,106	5
15	SO4	Y	304	5/5	0.79	0.23	61,67,78,80	5
16	MG	L	301	1/1	0.79	0.13	48,48,48,48	0
15	SO4	H	304	5/5	0.80	0.19	70,75,102,103	5
15	SO4	V	303	5/5	0.80	0.15	72,77,101,109	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	Z	302	5/5	0.81	0.23	65,72,87,88	5
15	SO4	J	202	5/5	0.81	0.21	82,83,93,108	5
15	SO4	M	301	5/5	0.83	0.17	75,76,80,86	5
15	SO4	I	303	5/5	0.83	0.15	107,112,140,147	0
15	SO4	a	301	5/5	0.83	0.18	70,72,88,90	5
15	SO4	P	301	5/5	0.83	0.18	91,101,136,145	0
15	SO4	S	301	5/5	0.83	0.20	74,79,105,106	5
15	SO4	D	301	5/5	0.84	0.14	82,85,89,93	5
15	SO4	S	302	5/5	0.84	0.16	73,76,95,99	5
15	SO4	a	303	5/5	0.84	0.30	76,80,98,103	5
15	SO4	T	304	5/5	0.84	0.12	66,68,76,94	5
15	SO4	M	303	5/5	0.84	0.19	64,90,99,103	5
15	SO4	Y	305	5/5	0.85	0.13	58,79,104,106	5
15	SO4	Y	306	5/5	0.85	0.08	80,97,107,113	5
15	SO4	a	306	5/5	0.85	0.12	66,79,103,104	5
15	SO4	Y	303	5/5	0.85	0.17	58,60,83,86	5
15	SO4	T	302	5/5	0.85	0.28	75,81,107,115	5
15	SO4	W	303	5/5	0.86	0.14	76,87,103,105	5
15	SO4	F	303	5/5	0.86	0.15	57,58,93,98	5
16	MG	V	301	1/1	0.86	0.12	71,71,71,71	1
17	A1A9B	Y	301	49/49	0.86	0.14	50,78,96,103	0
15	SO4	C	301	5/5	0.87	0.20	57,63,78,85	5
17	A1A9B	K	301	49/49	0.87	0.18	61,84,98,107	49
15	SO4	W	302	5/5	0.87	0.14	63,73,86,88	5
15	SO4	K	305	5/5	0.88	0.09	55,67,82,96	5
16	MG	Y	302	1/1	0.88	0.10	77,77,77,77	0
16	MG	Z	301	1/1	0.88	0.11	61,61,61,61	0
15	SO4	E	302	5/5	0.88	0.17	67,74,84,89	5
15	SO4	Z	303	5/5	0.88	0.17	76,80,102,106	5
15	SO4	F	302	5/5	0.89	0.15	62,67,86,92	5
15	SO4	U	301	5/5	0.89	0.15	61,80,94,104	5
15	SO4	L	302	5/5	0.89	0.11	77,83,98,114	5
15	SO4	M	306	5/5	0.89	0.19	59,68,75,94	5
15	SO4	b	201	5/5	0.90	0.13	39,48,53,55	5
15	SO4	N	202	5/5	0.90	0.20	61,68,84,98	5
15	SO4	V	302	5/5	0.90	0.25	69,71,84,91	5
15	SO4	Z	305	5/5	0.90	0.18	69,79,95,109	5
15	SO4	H	303	5/5	0.90	0.12	70,72,89,92	5
15	SO4	a	302	5/5	0.90	0.15	68,83,104,104	5
15	SO4	G	301	5/5	0.90	0.22	56,71,90,102	5
15	SO4	M	302	5/5	0.90	0.22	61,72,86,95	5
15	SO4	E	301	5/5	0.91	0.13	85,86,123,129	5

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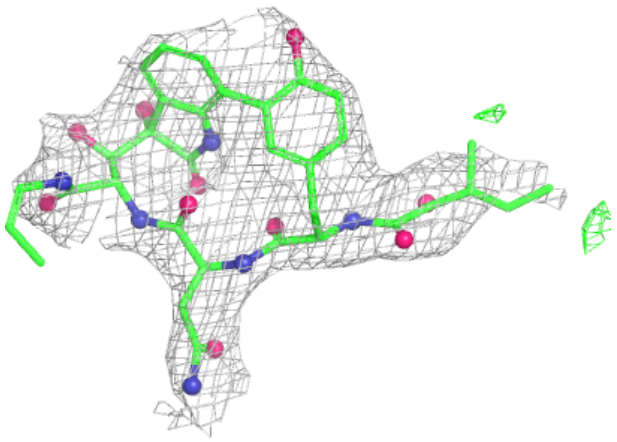
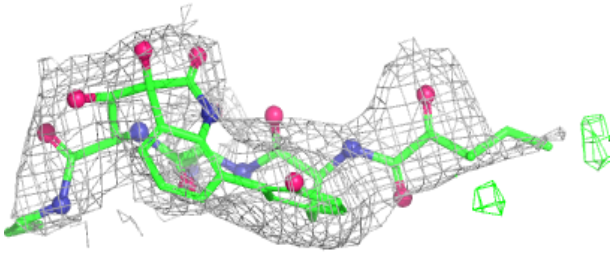
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	K	303	5/5	0.91	0.17	60,71,87,98	5
16	MG	H	301	1/1	0.91	0.09	74,74,74,74	0
15	SO4	F	301	5/5	0.91	0.28	51,63,83,91	5
15	SO4	M	304	5/5	0.91	0.13	58,59,75,76	5
16	MG	W	301	1/1	0.91	0.15	50,50,50,50	0
15	SO4	I	302	5/5	0.91	0.11	64,74,85,95	5
15	SO4	K	306	5/5	0.91	0.12	70,72,84,101	5
15	SO4	N	201	5/5	0.91	0.17	62,63,70,70	5
15	SO4	Q	301	5/5	0.91	0.11	75,78,97,99	5
15	SO4	T	303	5/5	0.92	0.15	57,94,101,102	5
15	SO4	L	303	5/5	0.92	0.20	79,82,90,103	5
15	SO4	b	203	5/5	0.92	0.14	52,66,74,74	5
15	SO4	a	305	5/5	0.92	0.13	63,68,72,77	5
16	MG	I	301	1/1	0.92	0.19	49,49,49,49	0
15	SO4	X	201	5/5	0.92	0.17	57,69,93,103	5
15	SO4	J	201	5/5	0.93	0.17	66,71,84,92	5
15	SO4	T	301	5/5	0.93	0.15	58,92,98,111	5
16	MG	K	302	1/1	0.94	0.09	75,75,75,75	0
15	SO4	a	304	5/5	0.94	0.09	57,65,86,92	5

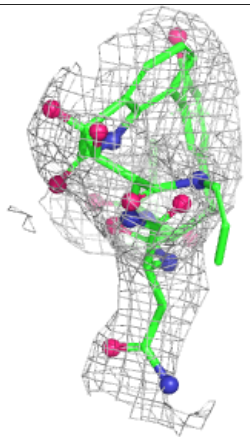
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1A9B 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)

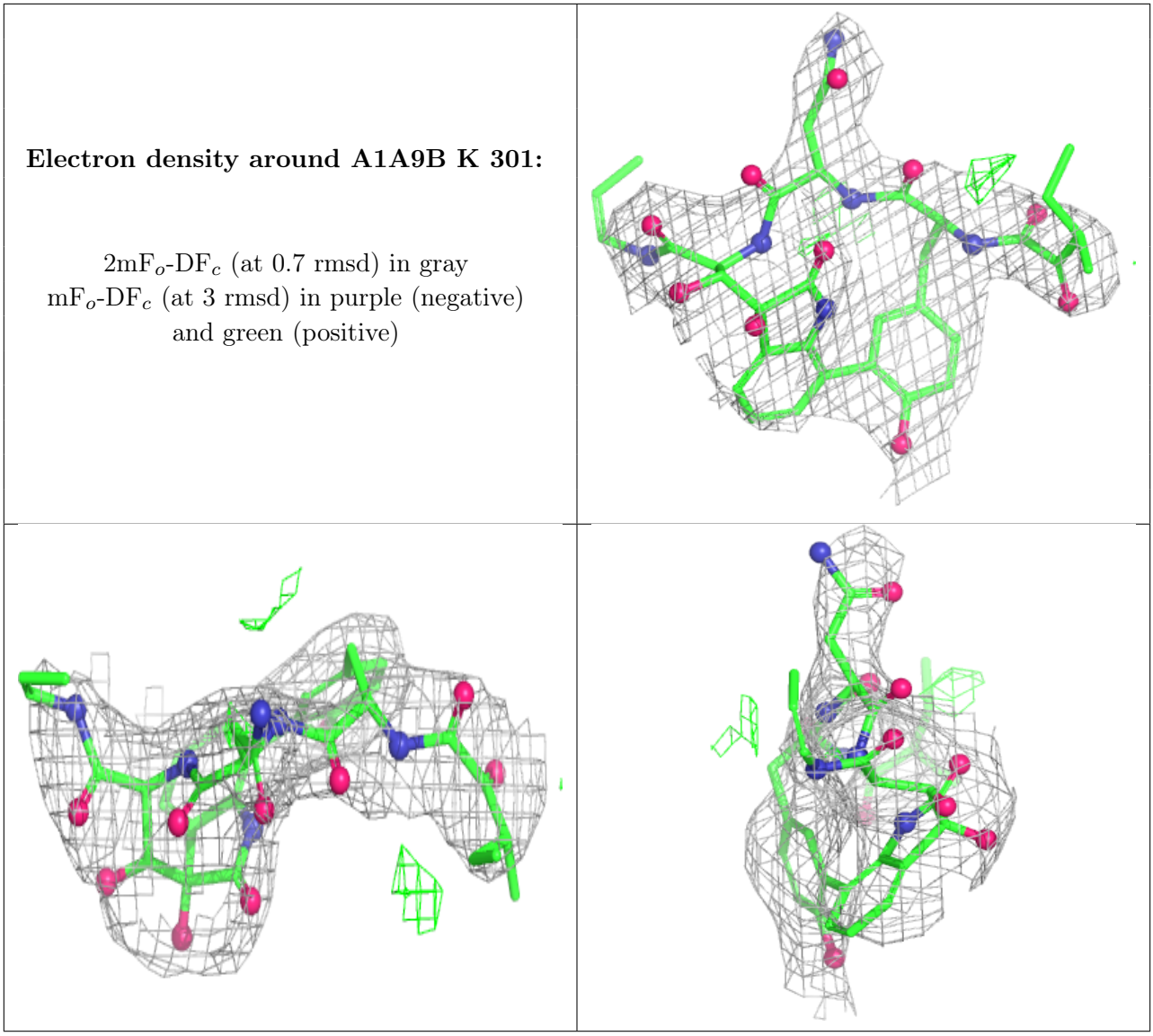






Electron density around A1A9B K 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.