Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2025 – 02:08 PM EDT

PDB ID	:	9AW7
Title	:	Yeast 20S proteasome soaked with isolated TMC-95B
Authors	:	Meneghello, R.; Rustiguel, J.K.; Fernandes, A.Z.N.; Trivella, D.B.B.
Deposited on	:	2024-03-05
Resolution	:	2.91 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:

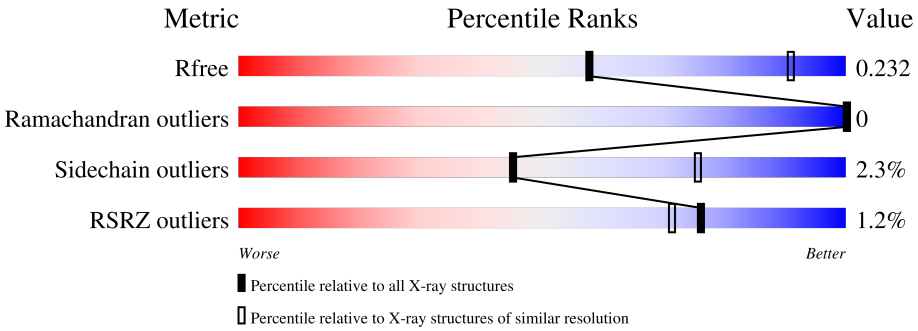
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (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 2.91 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	2797 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	250	2% 99%
1	O	250	2% 97%
2	B	258	2% 92% 6%
2	P	258	3% 93% 5%
3	C	254	4% 95%
3	Q	254	6% 93% 5%

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Mol	Chain	Length	Quality of chain
4	D	260	90% 9%
4	R	260	91% 8%
5	E	234	97%
5	S	234	96%
6	F	287	82% 15%
6	T	287	81% 15%
7	G	252	93% 5%
7	U	252	95%
8	H	232	95%
8	V	232	94%
9	I	205	97%
9	W	205	98%
10	J	198	93% 6%
10	X	198	95%
11	K	212	99%
11	Y	212	99%
12	L	222	98%
12	Z	222	99%
13	M	233	98%
13	a	233	97%
14	N	196	99%
14	b	196	98%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 50383 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 PRE8 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	2	0
			1905	1213	312	377	3			
1	O	248	Total	C	N	O	S	0	2	0
			1892	1204	309	376	3			

- Molecule 2 is a protein called PRE9 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1901	1201	320	377	3			
2	P	244	Total	C	N	O	S	0	0	0
			1900	1200	321	376	3			

- Molecule 3 is a protein called PRE6 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	245	Total	C	N	O	S	0	2	0
			1898	1186	334	374	4			
3	Q	241	Total	C	N	O	S	0	1	0
			1859	1163	329	363	4			

- Molecule 4 is a protein called PUP2 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	236	Total	C	N	O	S	0	1	0
			1821	1141	305	368	7			
4	R	239	Total	C	N	O	S	0	0	0
			1841	1152	311	371	7			

- Molecule 5 is a protein called PRE5 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1767	1111	304	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1769	1114	307	344	4			

- Molecule 6 is a protein called PRE10 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	3	0
			1908	1212	331	360	5			
6	T	244	Total	C	N	O	S	0	3	0
			1911	1214	331	361	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	240	Total	C	N	O	S	0	0	0
			1894	1207	315	364	8			
7	U	242	Total	C	N	O	S	0	0	0
			1917	1218	321	370	8			

- Molecule 8 is a protein called proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	2	0
			1690	1066	293	323	8			
8	V	222	Total	C	N	O	S	0	1	0
			1687	1063	293	323	8			

- Molecule 9 is a protein called PUP3 isoform 1.

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	1	0
			1584	1012	258	306	8			

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	1	0
			1573	1000	267	300	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 endopeptidase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	1	0
			1649	1048	281	313	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called PRE7 isoform 1.

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			

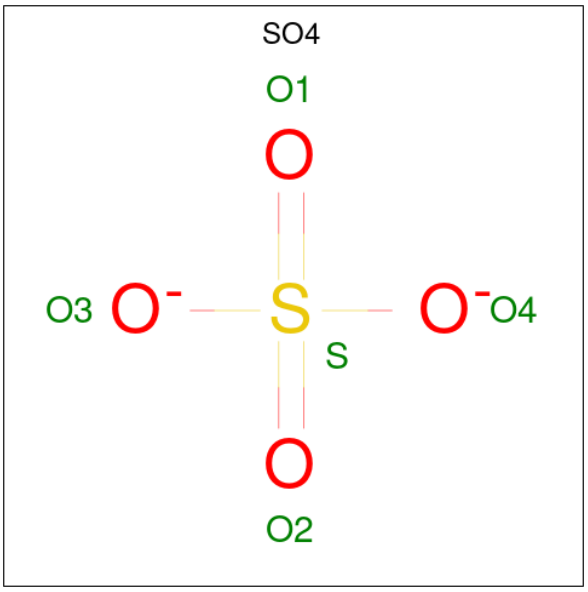
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	1	0
			1829	1157	312	353	7			
13	a	233	Total	C	N	O	S	0	1	0
			1828	1158	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	3	0
			1529	967	251	304	7			
14	b	196	Total	C	N	O	S	0	2	0
			1521	960	250	304	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	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
15	C	1	Total O S 5 4 1	0	0
15	D	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	P	1	Total O S 5 4 1	0	0
15	Q	1	Total O S 5 4 1	0	0
15	R	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
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	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	H	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	J	1	Total O S 5 4 1	0	0
15	J	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	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 10 8 2	0	1
15	L	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	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
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	N	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	V	1	Total O S 5 4 1	0	0
15	X	1	Total O S 5 4 1	0	0
15	X	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	Y	1	Total O S 5 4 1	0	0
15	Y	1	Total O S 10 8 2	0	1
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	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

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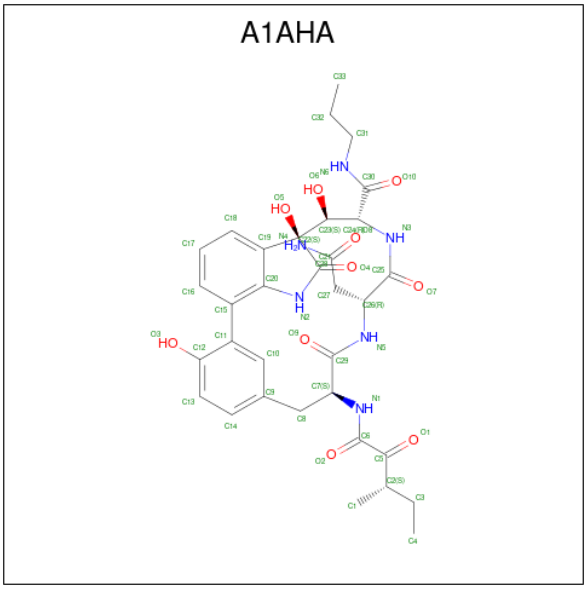
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	a	1	Total O S 5 4 1	0	0
15	b	1	Total O S 5 4 1	0	0
15	b	1	Total O S 10 8 2	0	1
15	b	1	Total O S 5 4 1	0	0

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

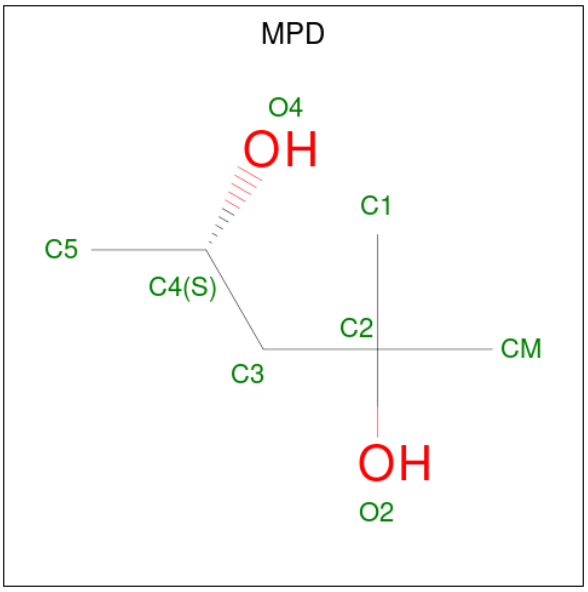
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	2	Total Mg 2 2	0	0
16	U	1	Total Mg 1 1	0	0
16	H	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	K	1	Total Mg 1 1	0	0
16	L	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0
16	X	1	Total Mg 1 1	0	0
16	Y	1	Total Mg 1 1	0	0
16	Z	1	Total Mg 1 1	0	0

- Molecule 17 is TMC-95B (three-letter code: A1AHA) (formula: $C_{33}H_{40}N_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



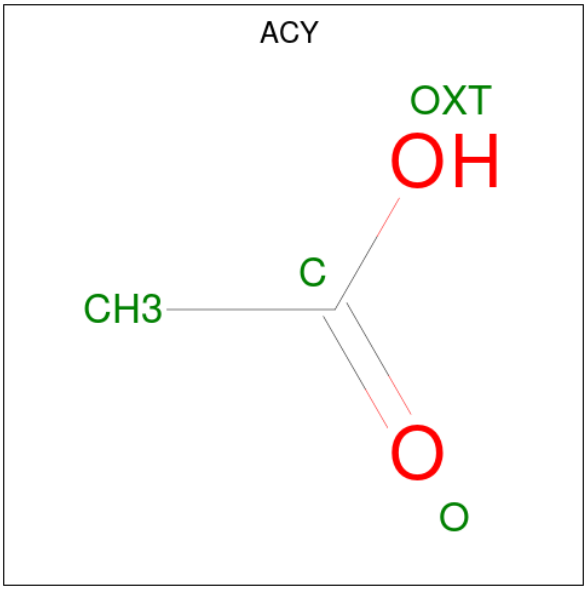
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			49	33	6	10		
17	K	1	Total	C	N	O	0	0
			49	33	6	10		
17	N	1	Total	C	N	O	0	0
			49	33	6	10		
17	V	1	Total	C	N	O	0	0
			49	33	6	10		
17	Y	1	Total	C	N	O	0	0
			49	33	6	10		
17	b	1	Total	C	N	O	0	0
			49	33	6	10		

- Molecule 18 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	1	Total C O 8 6 2	0	0

- Molecule 19 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	V	1	Total C O 4 2 2	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	15	Total O 15 15	0	0
20	B	7	Total O 7 7	0	0
20	C	3	Total O 3 3	0	0
20	D	5	Total O 5 5	0	0
20	E	6	Total O 6 6	0	0
20	F	9	Total O 9 9	0	0
20	G	15	Total O 15 15	0	0
20	O	7	Total O 7 7	0	0
20	P	3	Total O 3 3	0	0
20	Q	6	Total O 6 6	0	0
20	R	1	Total O 1 1	0	0
20	S	4	Total O 4 4	0	0
20	T	6	Total O 6 6	0	0
20	U	6	Total O 6 6	0	0
20	H	16	Total O 16 16	0	0
20	I	11	Total O 11 11	0	0
20	J	15	Total O 15 15	0	0
20	K	9	Total O 9 9	0	0
20	L	11	Total O 11 11	0	0
20	M	12	Total O 12 12	0	0
20	N	14	Total O 14 14	0	0
20	V	17	Total O 17 17	0	0

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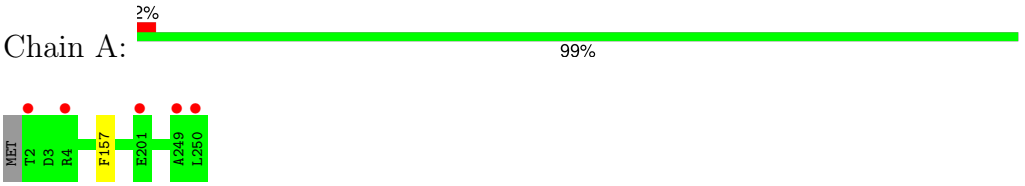
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	W	5	Total O 5 5	0	0
20	X	9	Total O 9 9	0	0
20	Y	7	Total O 7 7	0	0
20	Z	6	Total O 6 6	0	0
20	a	16	Total O 16 16	0	0
20	b	11	Total O 11 11	0	0

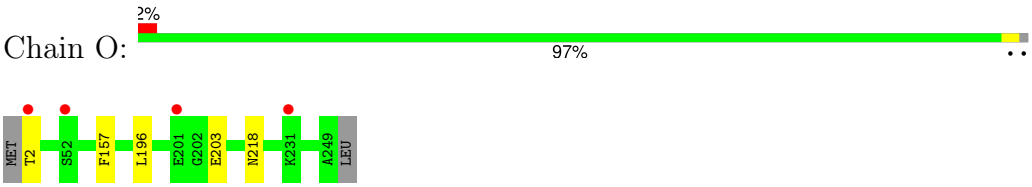
3 Residue-property plots (i)

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.

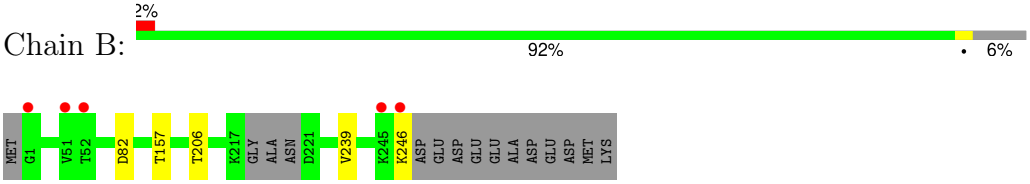
• Molecule 1: PRE8 isoform 1



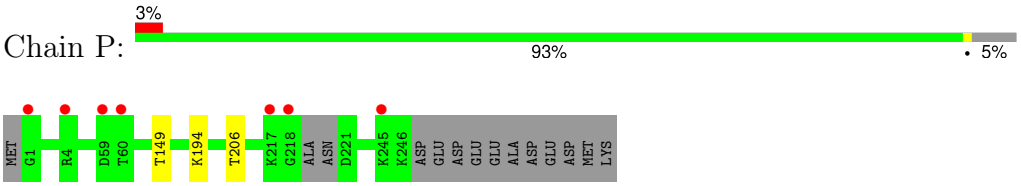
• Molecule 1: PRE8 isoform 1



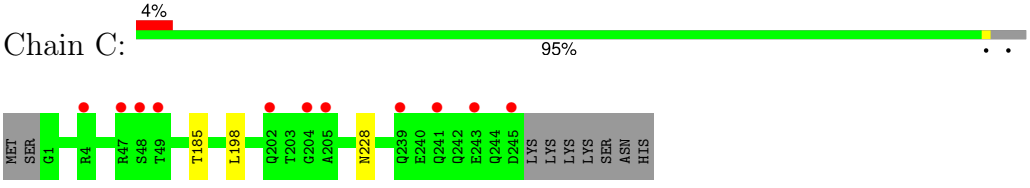
• Molecule 2: PRE9 isoform 1



• Molecule 2: PRE9 isoform 1

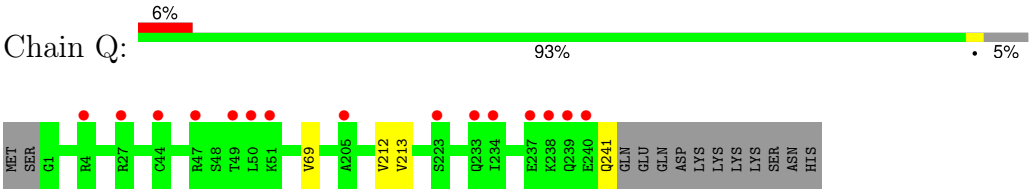


• Molecule 3: PRE6 isoform 1



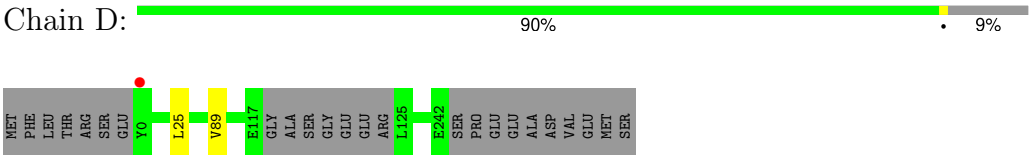
• Molecule 3: PRE6 isoform 1

Chain Q:



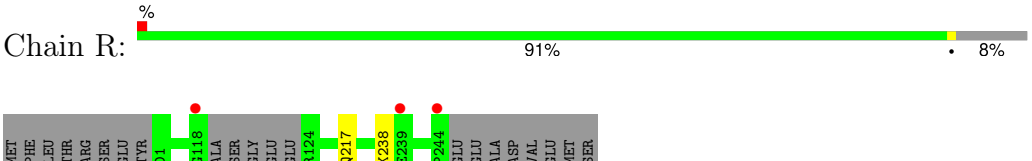
• Molecule 4: PUP2 isoform 1

Chain D:



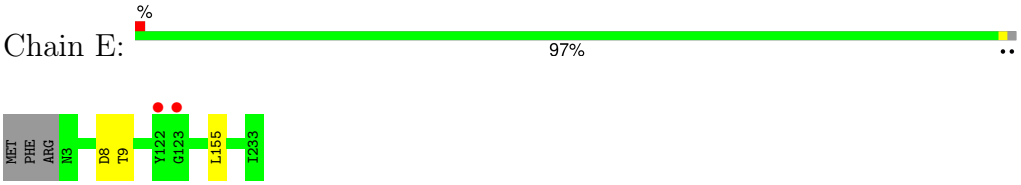
• Molecule 4: PUP2 isoform 1

Chain R:



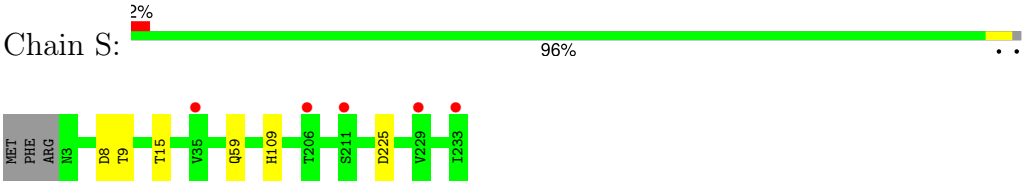
• Molecule 5: PRE5 isoform 1

Chain E:



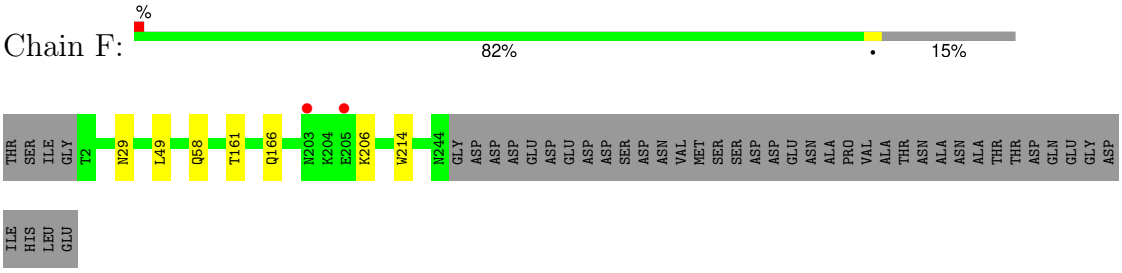
• Molecule 5: PRE5 isoform 1

Chain S:



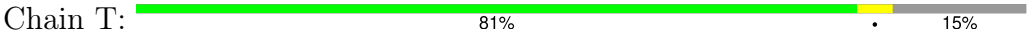
• Molecule 6: PRE10 isoform 1

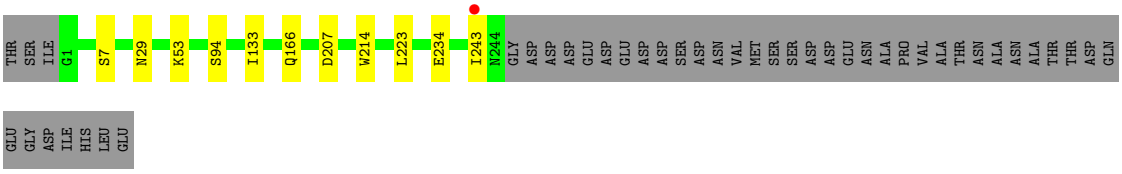
Chain F:



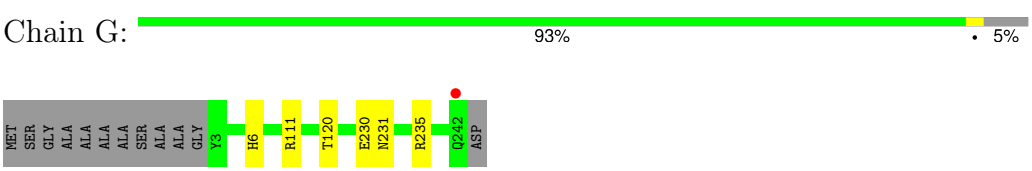
• Molecule 6: PRE10 isoform 1

Chain T:

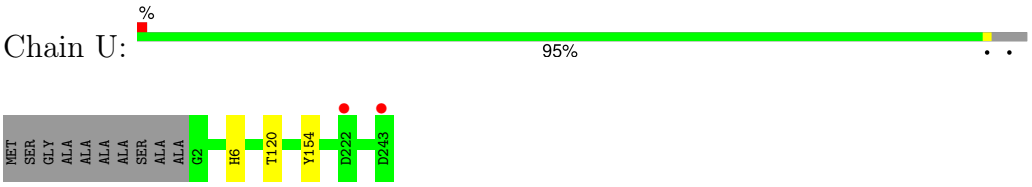




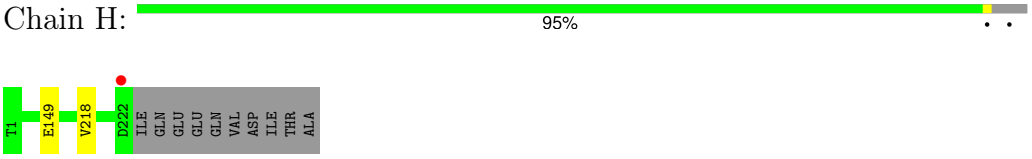
• Molecule 7: Proteasome subunit alpha type-1



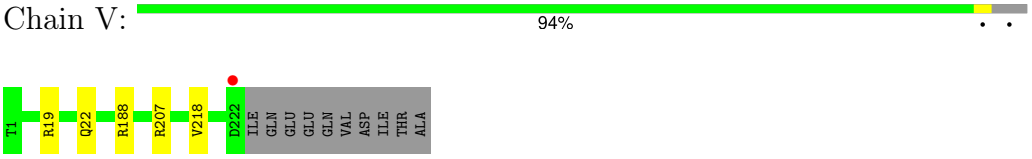
• Molecule 7: Proteasome subunit alpha type-1



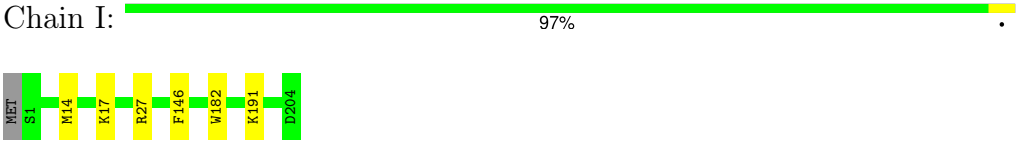
• Molecule 8: proteasome endopeptidase complex



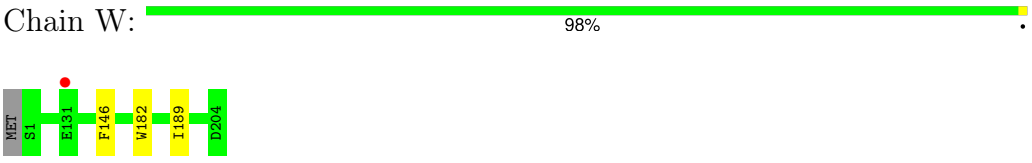
• Molecule 8: proteasome endopeptidase complex



• Molecule 9: PUP3 isoform 1

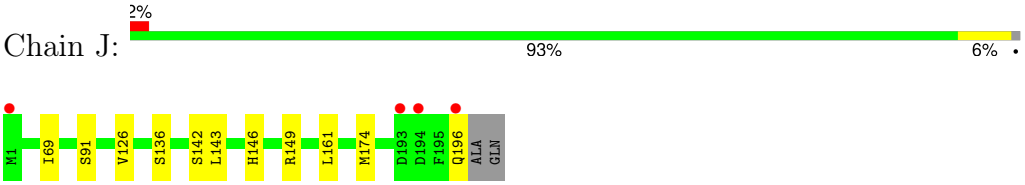


• Molecule 9: PUP3 isoform 1



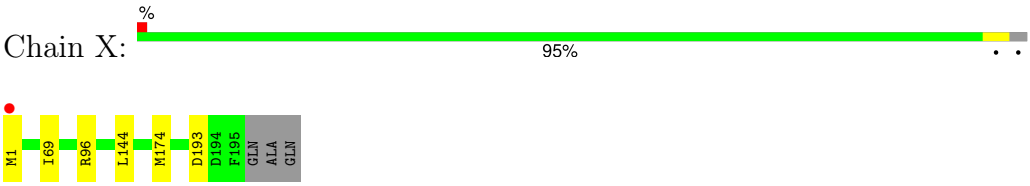
• Molecule 10: Proteasome subunit beta

Chain J:



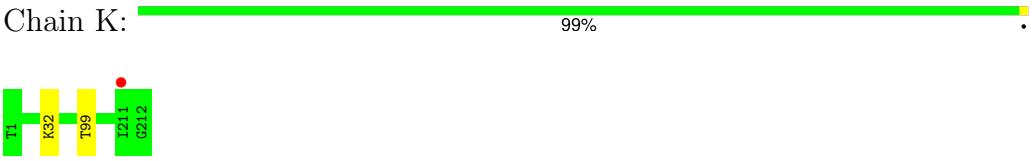
• Molecule 10: Proteasome subunit beta

Chain X:



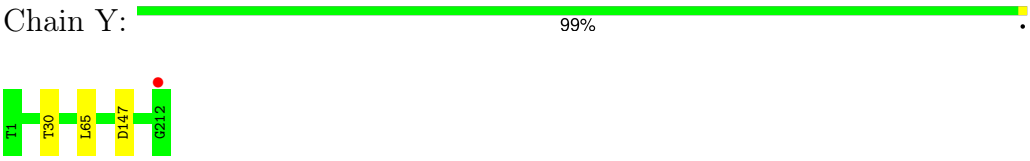
• Molecule 11: proteasome endopeptidase complex

Chain K:



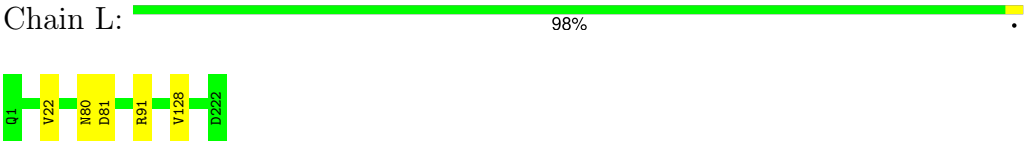
• Molecule 11: proteasome endopeptidase complex

Chain Y:



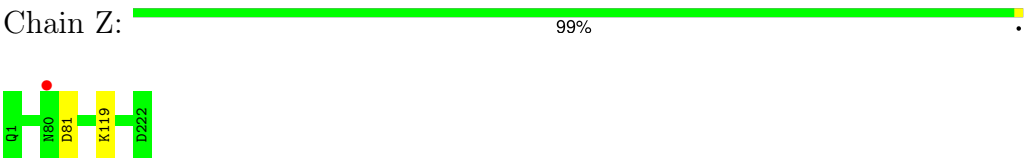
• Molecule 12: PRE7 isoform 1

Chain L:



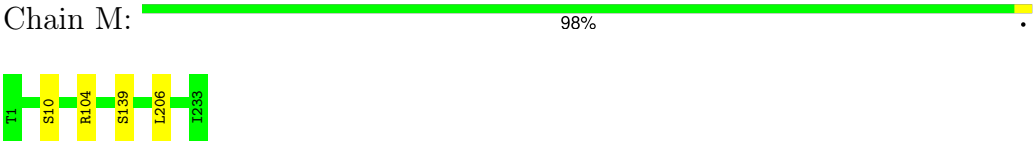
• Molecule 12: PRE7 isoform 1

Chain Z:



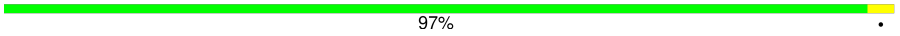
• Molecule 13: Proteasome subunit beta

Chain M:



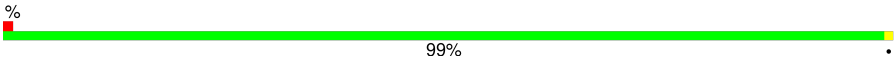
• Molecule 13: Proteasome subunit beta

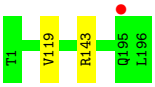
Chain a:



• Molecule 14: Proteasome subunit beta type-1

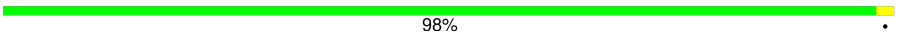
Chain N:





• 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	134.62Å 299.91Å 144.66Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	30.04 – 2.91 30.04 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.04-2.91) 89.0 (30.04-2.91)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.194 , 0.232 0.194 , 0.232	Depositor DCC
R_{free} test set	11353 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	50383	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: A1AHA, ACY, MG, SO4, MPD, CSO

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	0.26	0/1945	0.47	0/2636
1	O	0.26	0/1932	0.47	0/2621
2	B	0.25	0/1930	0.49	0/2610
2	P	0.25	0/1929	0.49	0/2608
3	C	0.26	0/1930	0.51	0/2617
3	Q	0.25	0/1888	0.52	0/2561
4	D	0.24	0/1848	0.48	0/2490
4	R	0.24	0/1866	0.48	0/2514
5	E	0.25	0/1794	0.49	0/2426
5	S	0.25	0/1796	0.49	0/2425
6	F	0.26	0/1954	0.48	0/2639
6	T	0.27	0/1957	0.48	0/2643
7	G	0.26	0/1924	0.48	0/2606
7	U	0.26	0/1947	0.48	0/2634
8	H	0.28	0/1727	0.50	0/2342
8	V	0.25	0/1721	0.48	0/2334
9	I	0.26	0/1611	0.49	0/2174
9	W	0.26	0/1617	0.50	0/2182
10	J	0.26	0/1601	0.49	0/2158
10	X	0.25	0/1589	0.49	0/2142
11	K	0.26	0/1689	0.49	0/2285
11	Y	0.26	0/1681	0.50	0/2274
12	L	0.26	0/1795	0.50	0/2420
12	Z	0.27	0/1795	0.51	0/2420
13	M	0.26	0/1863	0.51	0/2525
13	a	0.26	0/1862	0.51	0/2524
14	N	0.25	0/1564	0.48	0/2119
14	b	0.25	0/1553	0.47	0/2105
All	All	0.26	0/50308	0.49	0/68034

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	249/250 (100%)	245 (98%)	4 (2%)	0	100	100
1	O	248/250 (99%)	244 (98%)	4 (2%)	0	100	100
2	B	239/258 (93%)	232 (97%)	7 (3%)	0	100	100
2	P	240/258 (93%)	235 (98%)	5 (2%)	0	100	100
3	C	245/254 (96%)	237 (97%)	8 (3%)	0	100	100
3	Q	240/254 (94%)	234 (98%)	6 (2%)	0	100	100
4	D	233/260 (90%)	226 (97%)	7 (3%)	0	100	100
4	R	235/260 (90%)	225 (96%)	10 (4%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	244/287 (85%)	238 (98%)	6 (2%)	0	100	100
6	T	245/287 (85%)	238 (97%)	7 (3%)	0	100	100
7	G	237/252 (94%)	229 (97%)	8 (3%)	0	100	100
7	U	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
8	H	222/232 (96%)	217 (98%)	5 (2%)	0	100	100
8	V	221/232 (95%)	218 (99%)	3 (1%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	W	203/205 (99%)	195 (96%)	8 (4%)	0	100	100
10	J	195/198 (98%)	191 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	211/212 (100%)	208 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	232/233 (100%)	222 (96%)	10 (4%)	0	100	100
13	a	232/233 (100%)	224 (97%)	8 (3%)	0	100	100
14	N	197/196 (100%)	192 (98%)	5 (2%)	0	100	100
14	b	196/196 (100%)	191 (97%)	5 (3%)	0	100	100
All	All	6306/6586 (96%)	6135 (97%)	171 (3%)	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	207/209 (99%)	206 (100%)	1 (0%)	86	95
1	O	205/209 (98%)	200 (98%)	5 (2%)	44	74
2	B	203/216 (94%)	198 (98%)	5 (2%)	42	73
2	P	201/216 (93%)	198 (98%)	3 (2%)	60	84
3	C	207/226 (92%)	204 (99%)	3 (1%)	62	85
3	Q	203/226 (90%)	199 (98%)	4 (2%)	50	78
4	D	195/215 (91%)	193 (99%)	2 (1%)	73	90
4	R	197/215 (92%)	195 (99%)	2 (1%)	73	90
5	E	189/193 (98%)	186 (98%)	3 (2%)	58	83
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	204/238 (86%)	197 (97%)	7 (3%)	32	65
6	T	204/238 (86%)	192 (94%)	12 (6%)	16	43
7	G	203/209 (97%)	197 (97%)	6 (3%)	36	69
7	U	206/209 (99%)	203 (98%)	3 (2%)	60	84
8	H	182/190 (96%)	179 (98%)	3 (2%)	58	83
8	V	182/190 (96%)	177 (97%)	5 (3%)	40	72
9	I	172/173 (99%)	166 (96%)	6 (4%)	31	64
9	W	173/173 (100%)	170 (98%)	3 (2%)	56	82
10	J	173/175 (99%)	162 (94%)	11 (6%)	14	40
10	X	173/175 (99%)	167 (96%)	6 (4%)	31	64
11	K	170/169 (101%)	168 (99%)	2 (1%)	67	87
11	Y	169/169 (100%)	166 (98%)	3 (2%)	54	81
12	L	185/185 (100%)	180 (97%)	5 (3%)	40	72
12	Z	185/185 (100%)	183 (99%)	2 (1%)	70	89
13	M	200/199 (100%)	196 (98%)	4 (2%)	50	78
13	a	200/199 (100%)	194 (97%)	6 (3%)	36	69
14	N	165/162 (102%)	162 (98%)	3 (2%)	54	81
14	b	163/162 (101%)	160 (98%)	3 (2%)	54	81
All	All	5306/5518 (96%)	5182 (98%)	124 (2%)	45	75

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	PHE
2	B	82	ASP
2	B	157	THR
2	B	206	THR
2	B	239	VAL
2	B	246	LYS
3	C	185	THR
3	C	198	LEU
3	C	228	ASN
4	D	25	LEU
4	D	89	VAL
5	E	8	ASP
5	E	9	THR

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Mol	Chain	Res	Type
5	E	155	LEU
6	F	29	ASN
6	F	49	LEU
6	F	58	GLN
6	F	161	THR
6	F	166	GLN
6	F	206	LYS
6	F	214	TRP
7	G	6	HIS
7	G	111	ARG
7	G	120	THR
7	G	230	GLU
7	G	231	ASN
7	G	235	ARG
1	O	2	THR
1	O	157	PHE
1	O	196	LEU
1	O	203	GLU
1	O	218	ASN
2	P	149	THR
2	P	194	LYS
2	P	206	THR
3	Q	69	VAL
3	Q	212	VAL
3	Q	213	VAL
3	Q	241	GLN
4	R	217	GLN
4	R	238	LYS
5	S	8	ASP
5	S	9	THR
5	S	15	THR
5	S	59	GLN
5	S	109	HIS
5	S	225	ASP
6	T	7	SER
6	T	29	ASN
6	T	53	LYS
6	T	94	SER
6	T	133	ILE
6	T	166	GLN
6	T	207[A]	ASP
6	T	207[B]	ASP

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Mol	Chain	Res	Type
6	T	214	TRP
6	T	223	LEU
6	T	234	GLU
6	T	243	ILE
7	U	6	HIS
7	U	120	THR
7	U	154	TYR
8	H	149[A]	GLU
8	H	149[B]	GLU
8	H	218	VAL
9	I	14	MET
9	I	17	LYS
9	I	27	ARG
9	I	146	PHE
9	I	182	TRP
9	I	191	LYS
10	J	69	ILE
10	J	91	SER
10	J	126	VAL
10	J	136	SER
10	J	142	SER
10	J	143	LEU
10	J	146	HIS
10	J	149	ARG
10	J	161	LEU
10	J	174	MET
10	J	196	GLN
11	K	32	LYS
11	K	99	THR
12	L	22	VAL
12	L	80	ASN
12	L	81	ASP
12	L	91	ARG
12	L	128	VAL
13	M	10	SER
13	M	104	ARG
13	M	139	SER
13	M	206	LEU
14	N	119[A]	VAL
14	N	119[B]	VAL
14	N	143	ARG
8	V	19	ARG

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Mol	Chain	Res	Type
8	V	22	GLN
8	V	188	ARG
8	V	207	ARG
8	V	218	VAL
9	W	146	PHE
9	W	182	TRP
9	W	189	ILE
10	X	1	MET
10	X	69	ILE
10	X	96	ARG
10	X	144	LEU
10	X	174	MET
10	X	193	ASP
11	Y	30	THR
11	Y	65	LEU
11	Y	147	ASP
12	Z	81	ASP
12	Z	119	LYS
13	a	10	SER
13	a	25	ASP
13	a	69	ASP
13	a	104	ARG
13	a	204	THR
13	a	213	GLN
14	b	83	LYS
14	b	143	ARG
14	b	191	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
7	CSO	G	65	7	3,6,7	0.69	0	1,6,8	0.11	0
7	CSO	U	65	7	3,6,7	0.66	0	1,6,8	0.05	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
7	CSO	G	65	7	-	0/1/5/7	-
7	CSO	U	65	7	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 108 ligands modelled in this entry, 12 are monoatomic - leaving 96 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	309	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	J	204	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	Y	304	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	M	307	-	4,4,4	0.67	0	6,6,6	0.12	0
15	SO4	X	203	-	4,4,4	0.66	0	6,6,6	0.16	0
15	SO4	Z	302	-	4,4,4	0.69	0	6,6,6	0.12	0
15	SO4	a	305	-	4,4,4	0.69	0	6,6,6	0.09	0
15	SO4	N	302	-	4,4,4	0.69	0	6,6,6	0.07	0
15	SO4	a	306	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	S	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	a	303	-	4,4,4	0.67	0	6,6,6	0.13	0
18	MPD	K	302	-	7,7,7	0.38	0	9,10,10	0.51	0
15	SO4	B	303	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	b	203[A]	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	E	302	-	4,4,4	0.67	0	6,6,6	0.08	0
17	A1AHA	K	301	-	51,52,52	0.58	1 (1%)	68,76,76	1.42	1 (1%)
15	SO4	a	304	-	4,4,4	0.69	0	6,6,6	0.05	0
17	A1AHA	b	201	-	51,52,52	0.53	1 (1%)	68,76,76	1.33	1 (1%)
15	SO4	b	202	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	T	303	-	4,4,4	0.56	0	6,6,6	0.10	0
15	SO4	M	304	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	N	303	-	4,4,4	0.69	0	6,6,6	0.07	0
15	SO4	B	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	I	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	J	201	-	4,4,4	0.67	0	6,6,6	0.11	0
15	SO4	M	301	-	4,4,4	0.67	0	6,6,6	0.09	0
15	SO4	B	304	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	U	303	-	4,4,4	0.68	0	6,6,6	0.06	0
15	SO4	T	301	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	X	204	-	4,4,4	0.67	0	6,6,6	0.06	0
15	SO4	L	304	-	4,4,4	0.68	0	6,6,6	0.12	0
15	SO4	Z	305	-	4,4,4	0.66	0	6,6,6	0.09	0
15	SO4	Y	308[A]	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	J	203	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	M	303	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	D	301	-	4,4,4	0.69	0	6,6,6	0.07	0
15	SO4	K	310[B]	-	4,4,4	0.68	0	6,6,6	0.16	0
15	SO4	Y	305	-	4,4,4	0.68	0	6,6,6	0.09	0
19	ACY	V	601	-	3,3,3	1.14	0	3,3,3	1.21	0
15	SO4	M	305	-	4,4,4	0.70	0	6,6,6	0.10	0
15	SO4	a	307	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	G	303	-	4,4,4	0.68	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	L	303	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	R	301	-	4,4,4	0.68	0	6,6,6	0.07	0
17	A1AHA	V	602	-	51,52,52	0.52	1 (1%)	68,76,76	1.15	2 (2%)
15	SO4	G	304	-	4,4,4	0.67	0	6,6,6	0.08	0
15	SO4	H	305	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	Z	304	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	Z	307	-	4,4,4	0.58	0	6,6,6	0.55	0
15	SO4	P	301	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	Y	306	-	4,4,4	0.66	0	6,6,6	0.18	0
15	SO4	K	304	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	T	302	-	4,4,4	0.68	0	6,6,6	0.11	0
15	SO4	H	303	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	M	306	-	4,4,4	0.69	0	6,6,6	0.09	0
15	SO4	K	308	-	4,4,4	0.69	0	6,6,6	0.09	0
15	SO4	F	302	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	K	310[A]	-	4,4,4	0.66	0	6,6,6	0.17	0
15	SO4	S	303	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	K	307	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	U	302	-	4,4,4	0.69	0	6,6,6	0.06	0
15	SO4	P	302	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	Y	307	-	4,4,4	0.68	0	6,6,6	0.06	0
17	A1AHA	N	301	-	51,52,52	0.52	1 (1%)	68,76,76	1.65	2 (2%)
15	SO4	X	202	-	4,4,4	0.68	0	6,6,6	0.09	0
15	SO4	Z	303	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	N	304	-	4,4,4	0.83	0	6,6,6	0.30	0
17	A1AHA	H	301	-	51,52,52	0.53	1 (1%)	68,76,76	1.17	3 (4%)
15	SO4	V	604	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	b	204	-	4,4,4	0.67	0	6,6,6	0.11	0
15	SO4	Y	303	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	B	302	-	4,4,4	0.68	0	6,6,6	0.05	0
15	SO4	Q	301	-	4,4,4	0.67	0	6,6,6	0.12	0
15	SO4	H	304	-	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	0.09	0
15	SO4	a	302	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	J	202	-	4,4,4	0.63	0	6,6,6	0.14	0
15	SO4	V	605	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	b	203[B]	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	K	306	-	4,4,4	0.69	0	6,6,6	0.11	0
15	SO4	D	302	-	4,4,4	0.69	0	6,6,6	0.08	0
15	SO4	L	302	-	4,4,4	0.69	0	6,6,6	0.08	0
15	SO4	M	308	-	4,4,4	0.68	0	6,6,6	0.07	0
15	SO4	U	304	-	4,4,4	0.68	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SO4	L	305	-	4,4,4	0.72	0	6,6,6	0.17	0
15	SO4	Z	306	-	4,4,4	0.80	0	6,6,6	0.49	0
15	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.07	0
15	SO4	S	302	-	4,4,4	0.68	0	6,6,6	0.06	0
17	A1AHA	Y	301	-	51,52,52	0.49	1 (1%)	68,76,76	1.43	1 (1%)
15	SO4	E	301	-	4,4,4	0.69	0	6,6,6	0.07	0
15	SO4	K	305	-	4,4,4	0.68	0	6,6,6	0.08	0
15	SO4	F	301	-	4,4,4	0.68	0	6,6,6	0.10	0
15	SO4	a	301	-	4,4,4	0.67	0	6,6,6	0.13	0
15	SO4	H	306	-	4,4,4	0.67	0	6,6,6	0.10	0
15	SO4	Y	308[B]	-	4,4,4	0.69	0	6,6,6	0.10	0
15	SO4	V	606	-	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	A1AHA	b	201	-	-	23/60/76/76	0/3/4/4
18	MPD	K	302	-	-	0/5/5/5	-
17	A1AHA	N	301	-	-	20/60/76/76	0/3/4/4
17	A1AHA	K	301	-	-	28/60/76/76	0/3/4/4
17	A1AHA	H	301	-	-	19/60/76/76	0/3/4/4
17	A1AHA	V	602	-	-	17/60/76/76	0/3/4/4
17	A1AHA	Y	301	-	-	28/60/76/76	0/3/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	A1AHA	C22-C23	-3.50	1.54	1.55
17	b	201	A1AHA	C22-C23	-3.11	1.54	1.55
17	H	301	A1AHA	C22-C23	-3.05	1.54	1.55
17	N	301	A1AHA	C22-C23	-3.01	1.54	1.55
17	V	602	A1AHA	C22-C23	-2.95	1.54	1.55
17	Y	301	A1AHA	C22-C23	-2.72	1.54	1.55

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	301	A1AHA	C22-C23-C24	12.22	122.27	112.78
17	Y	301	A1AHA	C22-C23-C24	10.51	120.94	112.78
17	K	301	A1AHA	C22-C23-C24	10.40	120.85	112.78
17	b	201	A1AHA	C22-C23-C24	9.39	120.07	112.78
17	H	301	A1AHA	C22-C23-C24	7.90	118.91	112.78
17	V	602	A1AHA	C22-C23-C24	7.65	118.72	112.78
17	V	602	A1AHA	C16-C15-C11	2.05	122.89	118.74
17	H	301	A1AHA	C16-C15-C11	2.03	122.85	118.74
17	H	301	A1AHA	C11-C15-C20	-2.00	119.63	124.79
17	N	301	A1AHA	C31-N6-C30	2.00	126.14	122.55

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	301	A1AHA	C21-C22-C23-C24
17	H	301	A1AHA	C21-C22-C23-O6
17	H	301	A1AHA	C19-C22-C23-C24
17	H	301	A1AHA	C19-C22-C23-O6
17	H	301	A1AHA	O5-C22-C23-O6
17	H	301	A1AHA	C23-C24-C30-N6
17	H	301	A1AHA	C23-C24-C30-O10
17	K	301	A1AHA	C5-C6-N1-C7
17	K	301	A1AHA	O2-C6-N1-C7
17	K	301	A1AHA	O1-C5-C6-O2
17	K	301	A1AHA	C21-C22-C23-O6
17	K	301	A1AHA	C19-C22-C23-C24
17	K	301	A1AHA	C19-C22-C23-O6
17	K	301	A1AHA	O5-C22-C23-O6
17	K	301	A1AHA	C23-C24-C30-N6
17	K	301	A1AHA	C23-C24-C30-O10
17	N	301	A1AHA	C12-C11-C15-C20
17	N	301	A1AHA	C19-C22-C23-C24
17	N	301	A1AHA	C19-C22-C23-O6
17	N	301	A1AHA	O5-C22-C23-O6
17	N	301	A1AHA	C23-C24-C30-N6
17	N	301	A1AHA	C23-C24-C30-O10
17	V	602	A1AHA	C21-C22-C23-C24
17	V	602	A1AHA	C21-C22-C23-O6
17	V	602	A1AHA	C19-C22-C23-C24
17	V	602	A1AHA	C19-C22-C23-O6
17	V	602	A1AHA	O5-C22-C23-O6
17	V	602	A1AHA	C23-C24-C30-N6

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Mol	Chain	Res	Type	Atoms
17	V	602	A1AHA	C23-C24-C30-O10
17	Y	301	A1AHA	C5-C6-N1-C7
17	Y	301	A1AHA	O2-C6-N1-C7
17	Y	301	A1AHA	O1-C5-C6-N1
17	Y	301	A1AHA	C21-C22-C23-C24
17	Y	301	A1AHA	C21-C22-C23-O6
17	Y	301	A1AHA	C19-C22-C23-C24
17	Y	301	A1AHA	C19-C22-C23-O6
17	Y	301	A1AHA	O5-C22-C23-O6
17	Y	301	A1AHA	C23-C24-C30-N6
17	Y	301	A1AHA	C23-C24-C30-O10
17	b	201	A1AHA	C19-C22-C23-C24
17	b	201	A1AHA	C19-C22-C23-O6
17	b	201	A1AHA	O5-C22-C23-C24
17	b	201	A1AHA	O5-C22-C23-O6
17	N	301	A1AHA	O7-C25-C26-C27
17	b	201	A1AHA	O7-C25-C26-C27
17	V	602	A1AHA	O7-C25-C26-C27
17	H	301	A1AHA	N3-C25-C26-C27
17	K	301	A1AHA	N3-C25-C26-C27
17	N	301	A1AHA	N3-C25-C26-C27
17	V	602	A1AHA	N3-C25-C26-C27
17	Y	301	A1AHA	N3-C25-C26-C27
17	b	201	A1AHA	N3-C25-C26-C27
17	Y	301	A1AHA	O7-C25-C26-C27
17	H	301	A1AHA	O7-C25-C26-C27
17	K	301	A1AHA	O7-C25-C26-C27
17	b	201	A1AHA	C23-C24-C30-N6
17	b	201	A1AHA	C23-C24-C30-O10
17	H	301	A1AHA	C26-C25-N3-C24
17	N	301	A1AHA	C10-C11-C15-C16
17	N	301	A1AHA	C10-C11-C15-C20
17	Y	301	A1AHA	C26-C25-N3-C24
17	H	301	A1AHA	O7-C25-N3-C24
17	K	301	A1AHA	C10-C11-C15-C20
17	V	602	A1AHA	C26-C25-N3-C24
17	N	301	A1AHA	O9-C29-C7-N1
17	K	301	A1AHA	C10-C11-C15-C16
17	K	301	A1AHA	O9-C29-C7-N1
17	N	301	A1AHA	N5-C29-C7-N1
17	Y	301	A1AHA	C10-C11-C15-C20
17	b	201	A1AHA	C10-C11-C15-C20

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Mol	Chain	Res	Type	Atoms
17	Y	301	A1AHA	O7-C25-N3-C24
17	K	301	A1AHA	C12-C11-C15-C20
17	Y	301	A1AHA	C12-C11-C15-C20
17	K	301	A1AHA	C1-C2-C5-O1
17	Y	301	A1AHA	C1-C2-C5-O1
17	V	602	A1AHA	O7-C25-N3-C24
17	Y	301	A1AHA	C1-C2-C5-C6
17	H	301	A1AHA	O9-C29-C7-N1
17	H	301	A1AHA	C26-C27-C28-N4
17	N	301	A1AHA	C26-C27-C28-N4
17	K	301	A1AHA	N5-C29-C7-N1
17	Y	301	A1AHA	O9-C29-C7-N1
17	Y	301	A1AHA	C2-C5-C6-N1
17	b	201	A1AHA	C27-C26-N5-C29
17	N	301	A1AHA	O9-C29-C7-C8
17	V	602	A1AHA	C27-C26-N5-C29
17	V	602	A1AHA	O9-C29-C7-N1
17	b	201	A1AHA	O9-C29-C7-N1
17	H	301	A1AHA	C26-C27-C28-O8
17	K	301	A1AHA	C26-C27-C28-N4
17	Y	301	A1AHA	C26-C27-C28-N4
17	b	201	A1AHA	C26-C27-C28-N4
17	b	201	A1AHA	C26-C27-C28-O8
17	N	301	A1AHA	C27-C26-N5-C29
17	H	301	A1AHA	N5-C29-C7-N1
17	Y	301	A1AHA	N5-C29-C7-N1
17	N	301	A1AHA	C12-C11-C15-C16
17	N	301	A1AHA	C21-C22-C23-O6
17	Y	301	A1AHA	C10-C11-C15-C16
17	b	201	A1AHA	N5-C29-C7-N1
17	N	301	A1AHA	C26-C27-C28-O8
17	Y	301	A1AHA	C26-C27-C28-O8
17	N	301	A1AHA	N5-C29-C7-C8
17	V	602	A1AHA	N5-C29-C7-N1
17	K	301	A1AHA	C26-C25-N3-C24
17	H	301	A1AHA	C27-C26-N5-C29
17	K	301	A1AHA	O9-C29-C7-C8
17	K	301	A1AHA	C26-C27-C28-O8
17	b	201	A1AHA	C10-C11-C15-C16
17	b	201	A1AHA	C12-C11-C15-C20
17	Y	301	A1AHA	C3-C2-C5-O1
17	K	301	A1AHA	C1-C2-C5-C6

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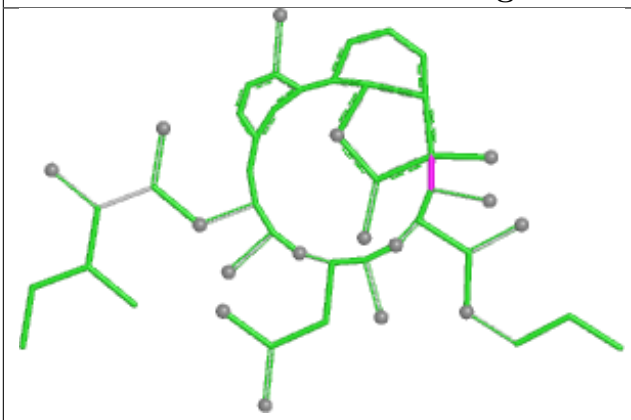
Mol	Chain	Res	Type	Atoms
17	Y	301	A1AHA	C3-C2-C5-C6
17	b	201	A1AHA	C3-C2-C5-C6
17	K	301	A1AHA	C12-C11-C15-C16
17	K	301	A1AHA	C21-C22-C23-C24
17	N	301	A1AHA	C21-C22-C23-C24
17	b	201	A1AHA	C21-C22-C23-C24
17	Y	301	A1AHA	C27-C26-N5-C29
17	K	301	A1AHA	N5-C29-C7-C8
17	K	301	A1AHA	O7-C25-N3-C24
17	H	301	A1AHA	O9-C29-C7-C8
17	b	201	A1AHA	O9-C29-C7-C8
17	H	301	A1AHA	C23-C24-N3-C25
17	Y	301	A1AHA	O9-C29-C7-C8
17	K	301	A1AHA	N6-C31-C32-C33
17	b	201	A1AHA	C26-C25-N3-C24
17	K	301	A1AHA	C27-C26-N5-C29
17	V	602	A1AHA	C23-C24-N3-C25
17	b	201	A1AHA	N3-C24-C30-O10
17	V	602	A1AHA	O9-C29-C7-C8
17	b	201	A1AHA	C23-C24-N3-C25
17	H	301	A1AHA	C12-C11-C15-C20
17	V	602	A1AHA	C12-C11-C15-C20
17	b	201	A1AHA	N3-C24-C30-N6

There are no ring outliers.

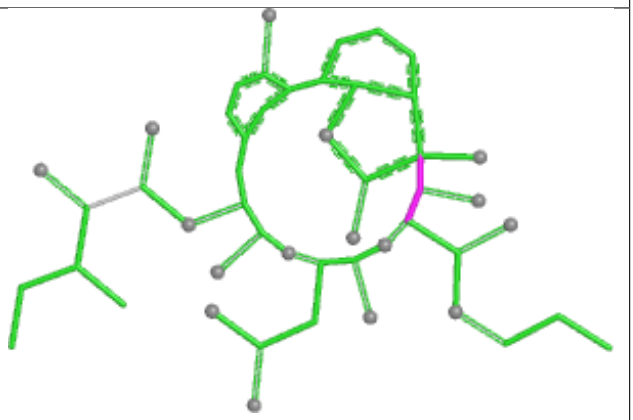
No monomer is involved in short contacts.

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.

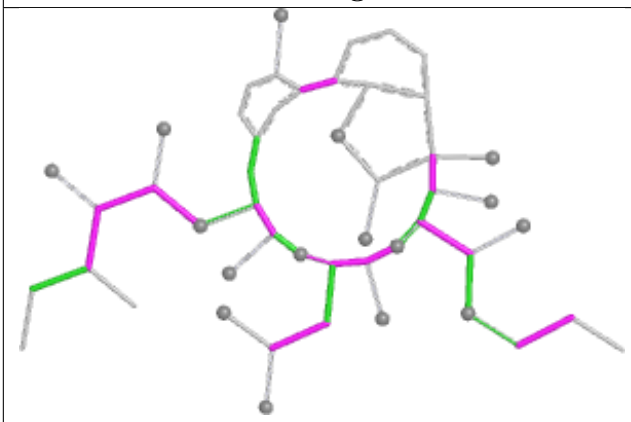
Ligand A1AHA K 301



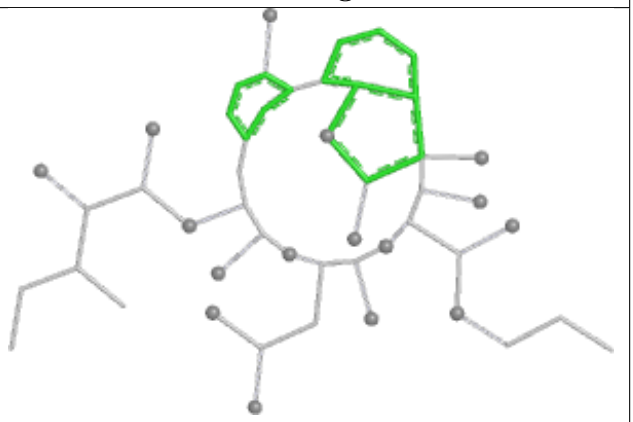
Bond lengths



Bond angles

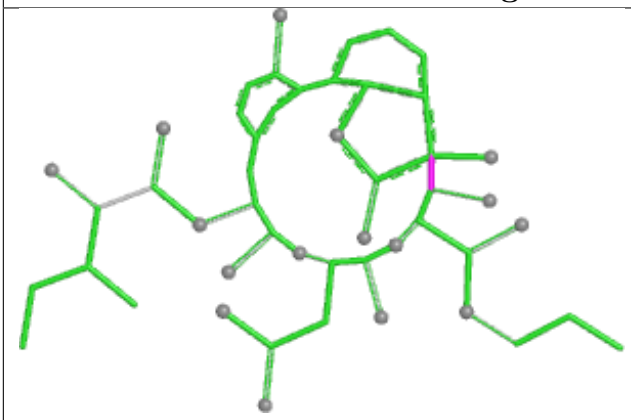


Torsions

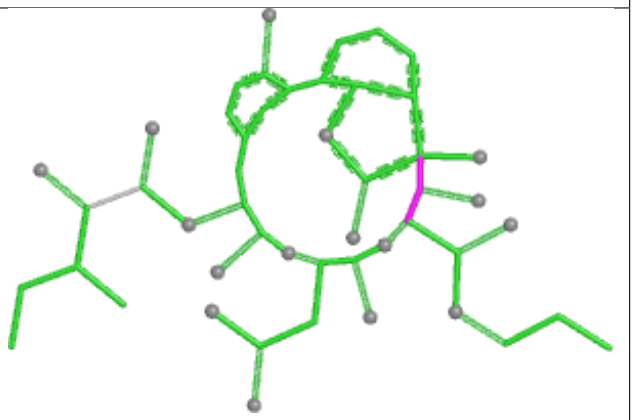


Rings

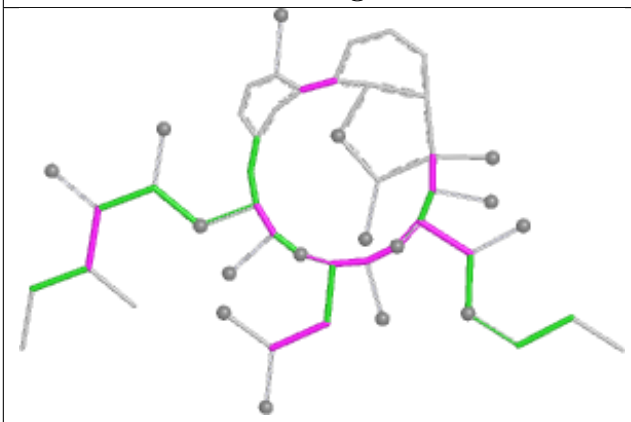
Ligand A1AHA b 201



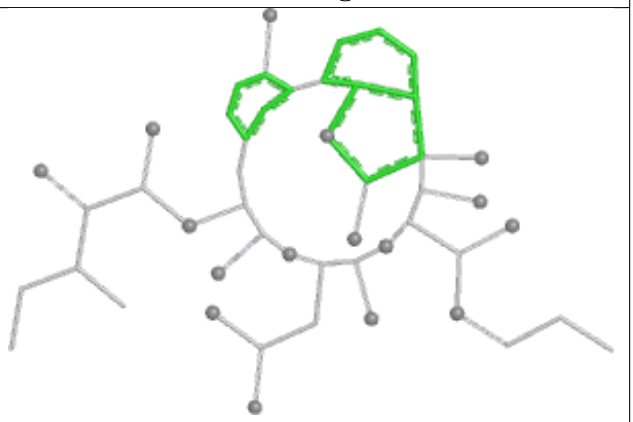
Bond lengths



Bond angles

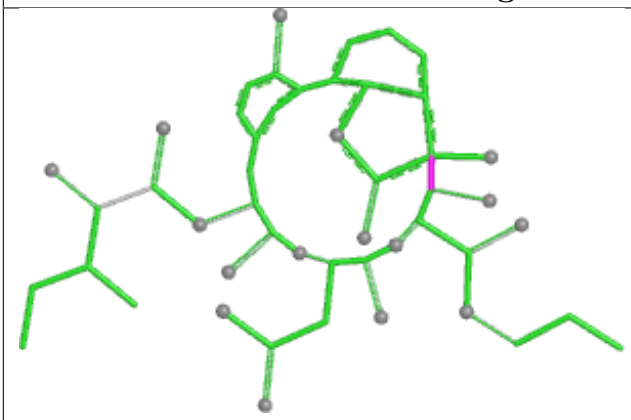


Torsions

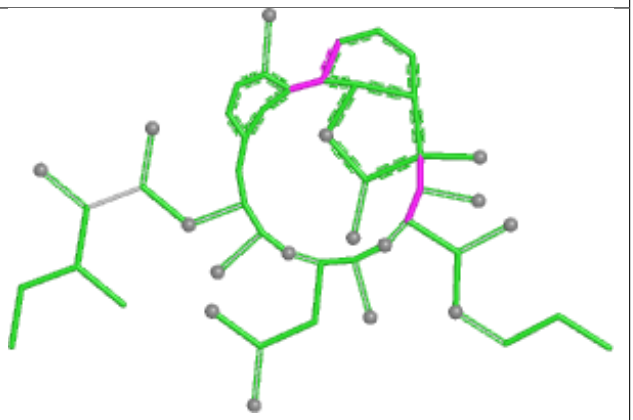


Rings

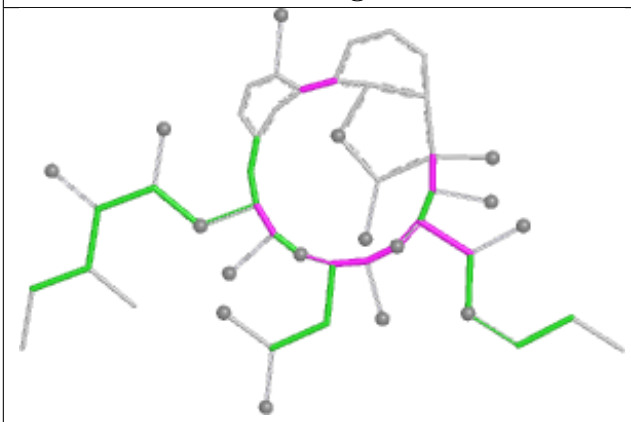
Ligand A1AHA V 602



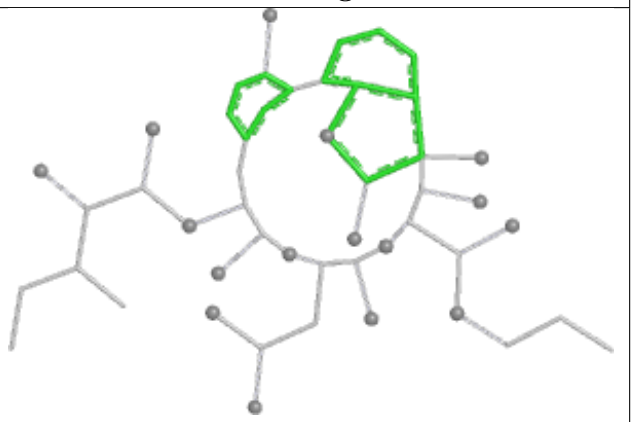
Bond lengths



Bond angles

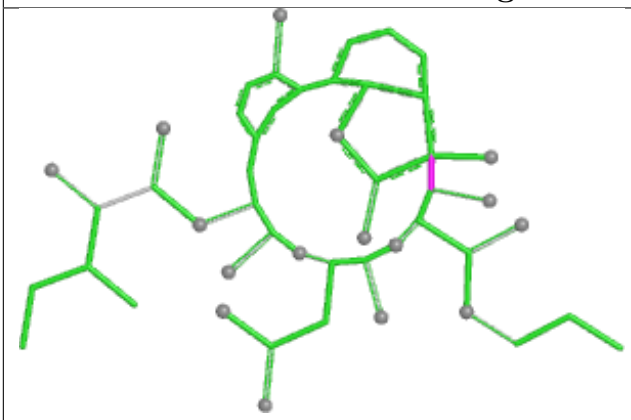


Torsions

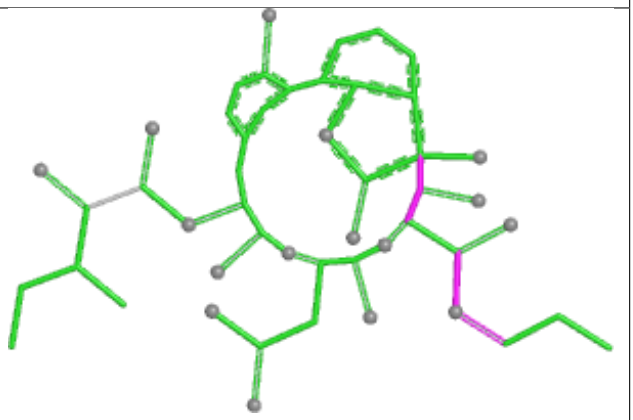


Rings

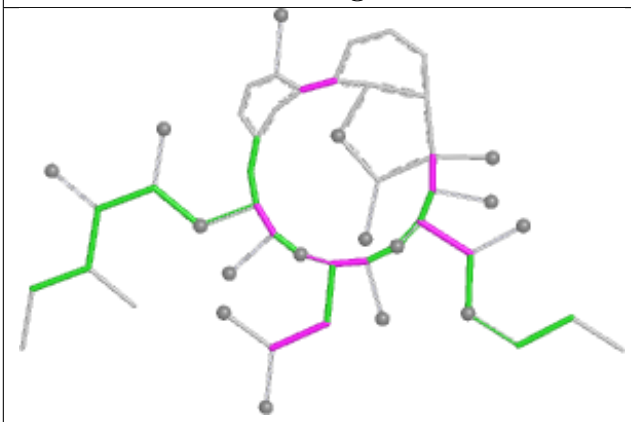
Ligand A1AHA N 301



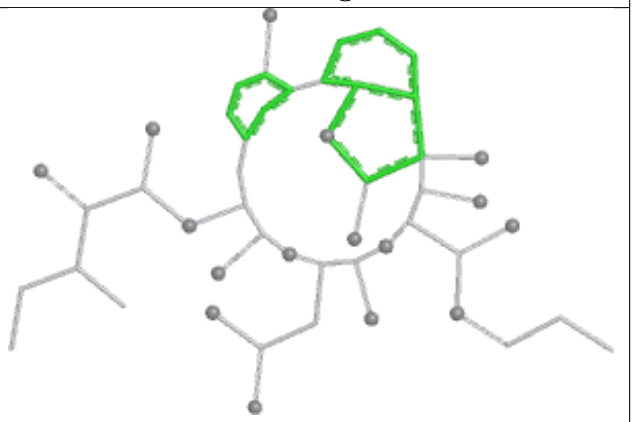
Bond lengths



Bond angles

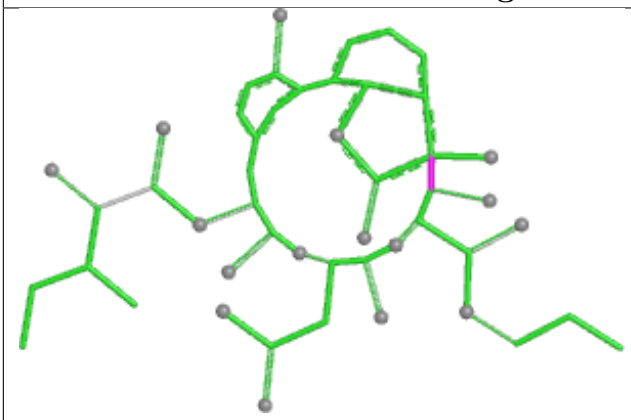


Torsions

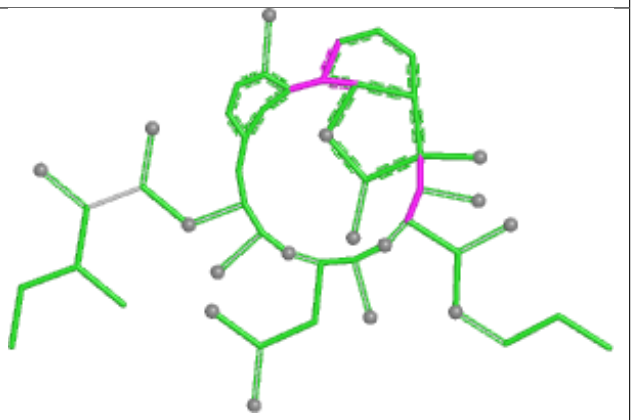


Rings

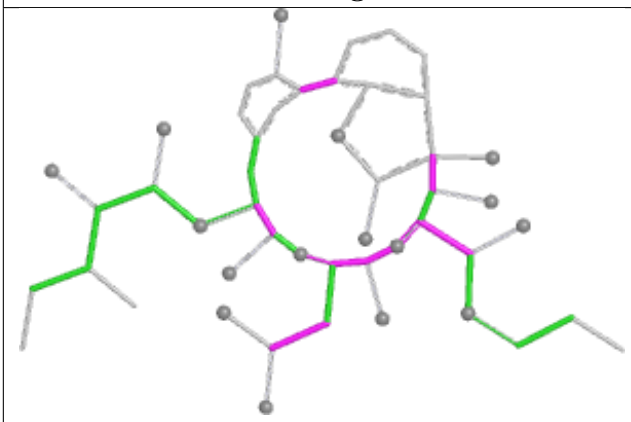
Ligand A1AHA H 301



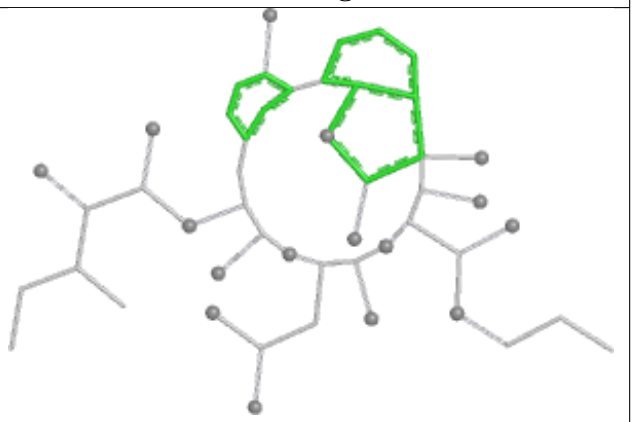
Bond lengths



Bond angles

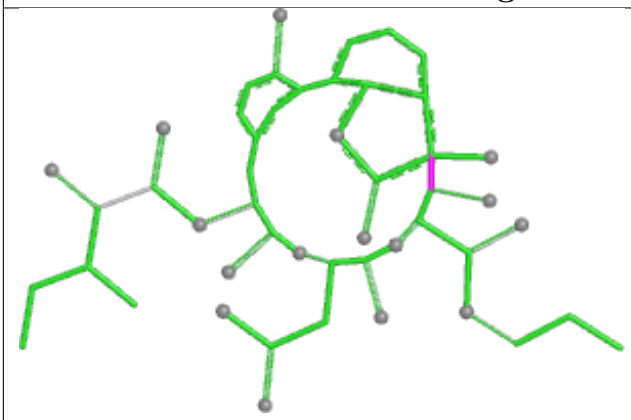


Torsions

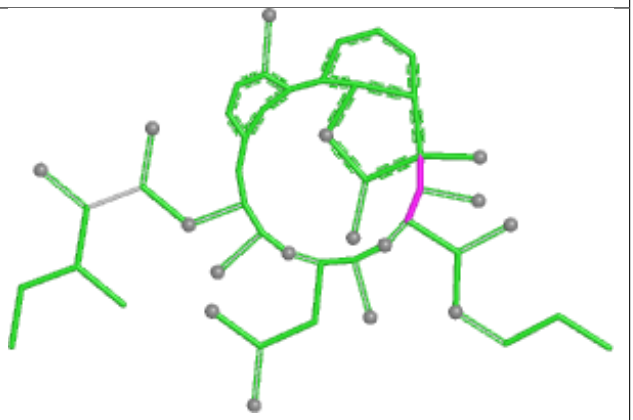


Rings

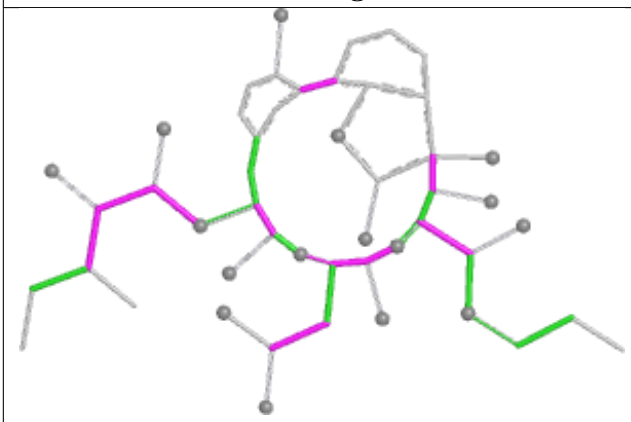
Ligand A1AHA Y 301



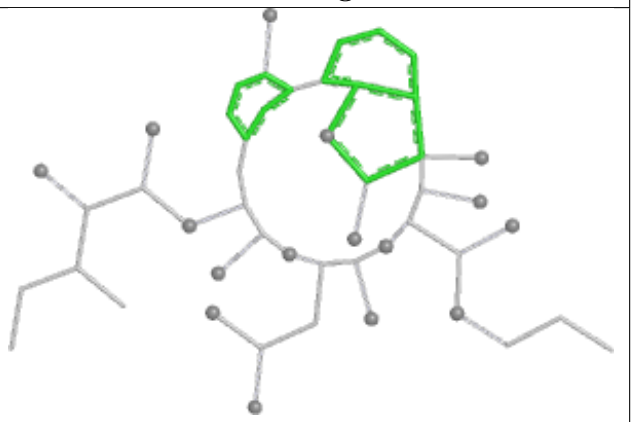
Bond lengths



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%)	-0.13	5 (2%)	64	58	21, 48, 75, 98	2 (0%)
1	O	248/250 (99%)	0.03	4 (1%)	70	65	22, 52, 79, 95	2 (0%)
2	B	243/258 (94%)	0.08	5 (2%)	63	57	34, 51, 84, 106	0
2	P	244/258 (94%)	0.09	7 (2%)	54	48	35, 50, 87, 112	0
3	C	245/254 (96%)	0.23	11 (4%)	39	33	28, 53, 98, 123	3 (1%)
3	Q	241/254 (94%)	0.41	15 (6%)	28	24	28, 56, 106, 135	1 (0%)
4	D	236/260 (90%)	-0.02	1 (0%)	89	87	36, 51, 74, 111	1 (0%)
4	R	239/260 (91%)	0.20	3 (1%)	74	69	40, 56, 79, 103	0
5	E	231/234 (98%)	0.24	2 (0%)	81	76	40, 59, 82, 97	1 (0%)
5	S	231/234 (98%)	0.35	5 (2%)	62	56	40, 60, 83, 98	0
6	F	243/287 (84%)	0.11	2 (0%)	82	78	33, 52, 81, 92	4 (1%)
6	T	244/287 (85%)	0.10	1 (0%)	89	87	31, 51, 79, 96	3 (1%)
7	G	239/252 (94%)	-0.09	1 (0%)	89	87	34, 47, 73, 100	0
7	U	241/252 (95%)	-0.08	2 (0%)	82	78	29, 47, 67, 88	0
8	H	222/232 (95%)	-0.13	1 (0%)	87	84	28, 46, 61, 111	2 (0%)
8	V	222/232 (95%)	-0.14	1 (0%)	87	84	30, 47, 62, 128	2 (0%)
9	I	204/205 (99%)	-0.26	0	100	100	31, 45, 64, 82	0
9	W	204/205 (99%)	-0.22	1 (0%)	87	84	28, 44, 66, 85	1 (0%)
10	J	196/198 (98%)	-0.20	4 (2%)	64	58	26, 44, 63, 91	1 (0%)
10	X	195/198 (98%)	-0.24	1 (0%)	87	84	31, 45, 60, 102	0
11	K	212/212 (100%)	-0.15	1 (0%)	87	84	26, 44, 66, 78	1 (0%)
11	Y	212/212 (100%)	-0.07	1 (0%)	87	84	35, 47, 70, 87	0
12	L	222/222 (100%)	-0.18	0	100	100	33, 46, 63, 83	1 (0%)
12	Z	222/222 (100%)	-0.15	1 (0%)	87	84	35, 47, 70, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	-0.19	0 100 100	29, 45, 63, 72	1 (0%)
13	a	233/233 (100%)	-0.24	0 100 100	30, 44, 59, 71	1 (0%)
14	N	196/196 (100%)	-0.18	1 (0%) 87 84	23, 42, 59, 81	3 (1%)
14	b	196/196 (100%)	-0.22	0 100 100	26, 42, 61, 82	2 (1%)
All	All	6343/6586 (96%)	-0.03	76 (1%) 76 71	21, 48, 78, 135	32 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	222	ASP	5.1
3	C	49	THR	5.1
7	G	242	GLN	5.0
1	O	201	GLU	4.7
1	O	52	SER	4.3
4	D	0	TYR	4.1
3	C	243	GLU	4.0
8	V	222	ASP	4.0
3	Q	239	GLN	3.7
2	P	59	ASP	3.6
3	C	48	SER	3.6
3	Q	51	LYS	3.6
6	T	243	ILE	3.6
2	P	218	GLY	3.6
10	J	1	MET	3.6
1	A	201	GLU	3.5
3	Q	50	LEU	3.4
5	E	122	TYR	3.4
3	Q	237	GLU	3.4
14	N	195	GLN	3.4
10	J	194	ASP	3.3
1	O	2	THR	3.3
6	F	205	GLU	3.2
10	J	196	GLN	3.2
6	F	203	ASN	3.1
10	J	193	ASP	3.1
4	R	239	GLU	3.1
3	Q	233	GLN	3.1
3	Q	240	GLU	2.9
5	E	123	GLY	2.9
4	R	118	GLY	2.8
4	R	244	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	1	GLY	2.8
2	P	60	THR	2.8
3	Q	234	ILE	2.8
3	C	202	GLN	2.7
11	Y	212	GLY	2.7
3	C	47	ARG	2.7
5	S	229	VAL	2.7
7	U	243	ASP	2.7
3	C	241	GLN	2.7
1	A	249	ALA	2.6
2	B	51	VAL	2.6
3	C	205	ALA	2.6
2	B	1	GLY	2.6
12	Z	80	ASN	2.6
1	A	2	THR	2.6
1	A	250	LEU	2.6
3	C	245	ASP	2.6
3	Q	27	ARG	2.5
1	O	231	LYS	2.4
3	C	4[A]	ARG	2.4
3	C	204	GLY	2.3
2	P	245	LYS	2.3
3	Q	49	THR	2.3
3	Q	47	ARG	2.3
3	Q	205	ALA	2.3
3	C	239	GLN	2.2
5	S	35	VAL	2.2
11	K	211	ILE	2.2
5	S	211	SER	2.2
5	S	206	THR	2.2
3	Q	44	CYS	2.2
7	U	222	ASP	2.2
2	B	52	THR	2.1
2	B	246	LYS	2.1
5	S	233	ILE	2.1
9	W	131	GLU	2.1
3	Q	223	SER	2.1
2	P	4	ARG	2.1
10	X	1	MET	2.1
2	P	217	LYS	2.1
3	Q	238	LYS	2.1
1	A	4	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	245	LYS	2.0
3	Q	4[A]	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
7	CSO	U	65	7/8	0.93	0.11	44,46,59,62	0
7	CSO	G	65	7/8	0.95	0.08	39,43,50,57	0

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	a	307	5/5	0.65	0.23	76,77,81,103	5
15	SO4	H	306	5/5	0.72	0.24	73,75,90,95	5
15	SO4	Y	305	5/5	0.73	0.21	76,97,127,132	0
19	ACY	V	601	4/4	0.75	0.23	46,61,62,69	0
15	SO4	J	204	5/5	0.76	0.22	54,59,67,87	5
15	SO4	Z	306	5/5	0.78	0.21	72,76,86,181	0
15	SO4	T	301	5/5	0.79	0.23	58,61,82,84	5
15	SO4	M	305	5/5	0.79	0.15	77,85,88,117	0
15	SO4	Z	302	5/5	0.80	0.17	48,53,77,89	5
15	SO4	U	303	5/5	0.80	0.16	48,50,64,70	5
15	SO4	a	302	5/5	0.81	0.15	57,66,69,77	5
15	SO4	T	303	5/5	0.82	0.23	31,44,49,69	5
15	SO4	Z	307	5/5	0.82	0.21	39,41,56,66	5
15	SO4	Y	303	5/5	0.82	0.26	86,98,104,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	B	304	5/5	0.82	0.14	60,74,78,92	5
15	SO4	M	303	5/5	0.82	0.14	69,72,82,90	5
16	MG	Z	301	1/1	0.83	0.16	55,55,55,55	0
15	SO4	N	304	5/5	0.83	0.23	40,47,52,67	5
15	SO4	H	303	5/5	0.84	0.16	51,53,63,80	5
15	SO4	N	303	5/5	0.84	0.17	60,69,69,86	5
15	SO4	K	310[A]	5/5	0.84	0.22	37,37,49,53	5
15	SO4	K	310[B]	5/5	0.84	0.22	43,47,53,65	5
15	SO4	L	304	5/5	0.84	0.15	46,51,61,71	5
15	SO4	I	302	5/5	0.84	0.15	49,67,89,91	5
15	SO4	T	302	5/5	0.85	0.23	76,81,101,111	0
15	SO4	F	302	5/5	0.85	0.17	51,57,72,82	5
15	SO4	a	305	5/5	0.85	0.18	73,78,101,109	0
16	MG	Y	302	1/1	0.86	0.10	59,59,59,59	0
15	SO4	b	203[A]	5/5	0.86	0.25	39,43,47,53	5
18	MPD	K	302	8/8	0.86	0.17	43,49,60,61	0
15	SO4	b	203[B]	5/5	0.86	0.25	41,47,60,68	5
15	SO4	M	308	5/5	0.87	0.11	66,71,85,93	5
15	SO4	Z	303	5/5	0.87	0.23	98,102,111,127	0
15	SO4	Z	305	5/5	0.87	0.13	57,62,66,69	5
16	MG	I	301	1/1	0.87	0.15	53,53,53,53	0
15	SO4	H	304	5/5	0.87	0.18	51,54,69,80	5
15	SO4	L	305	5/5	0.87	0.19	53,59,80,111	0
15	SO4	S	303	5/5	0.87	0.15	66,72,85,91	5
15	SO4	G	303	5/5	0.87	0.18	46,50,61,74	5
15	SO4	N	302	5/5	0.88	0.15	53,60,64,84	5
16	MG	W	301	1/1	0.88	0.14	50,50,50,50	0
15	SO4	K	305	5/5	0.88	0.19	79,91,114,123	0
15	SO4	K	304	5/5	0.88	0.17	69,76,88,92	5
15	SO4	b	204	5/5	0.88	0.14	52,54,61,71	5
16	MG	H	302	1/1	0.88	0.11	49,49,49,49	0
15	SO4	Y	304	5/5	0.89	0.15	50,51,81,83	5
15	SO4	K	308	5/5	0.89	0.16	67,69,81,89	5
15	SO4	Y	307	5/5	0.89	0.12	48,49,57,59	5
15	SO4	G	304	5/5	0.89	0.14	44,49,60,62	5
15	SO4	M	302	5/5	0.89	0.15	47,50,61,62	5
15	SO4	P	301	5/5	0.89	0.15	43,48,57,67	5
15	SO4	L	302	5/5	0.89	0.13	53,64,75,101	5
15	SO4	a	301	5/5	0.90	0.13	56,65,71,84	5
15	SO4	K	309	5/5	0.90	0.16	59,64,64,77	5
16	MG	L	301	1/1	0.90	0.14	55,55,55,55	0
15	SO4	V	605	5/5	0.90	0.14	50,53,58,76	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	0.90	0.22	85,86,89,107	0
15	SO4	K	307	5/5	0.90	0.17	69,78,90,116	0
15	SO4	B	303	5/5	0.90	0.15	47,48,61,69	5
15	SO4	Y	306	5/5	0.90	0.20	39,40,51,54	5
15	SO4	Y	308[B]	5/5	0.91	0.12	37,44,49,57	5
15	SO4	S	302	5/5	0.91	0.12	63,65,70,84	5
15	SO4	M	304	5/5	0.91	0.19	64,65,92,92	0
15	SO4	V	606	5/5	0.91	0.21	41,48,55,55	5
15	SO4	L	303	5/5	0.91	0.13	52,58,63,71	5
15	SO4	M	307	5/5	0.91	0.15	45,47,58,61	5
15	SO4	R	301	5/5	0.91	0.13	54,63,74,81	5
15	SO4	K	306	5/5	0.91	0.14	51,72,80,97	0
15	SO4	a	303	5/5	0.91	0.17	49,49,53,63	5
17	A1AHA	H	301	49/49	0.91	0.12	42,53,68,72	49
17	A1AHA	V	602	49/49	0.91	0.12	36,52,65,71	49
15	SO4	H	305	5/5	0.91	0.18	42,47,49,55	5
15	SO4	Y	308[A]	5/5	0.91	0.12	34,38,49,52	5
15	SO4	E	302	5/5	0.92	0.19	41,46,51,55	5
15	SO4	V	604	5/5	0.92	0.13	46,52,62,71	5
16	MG	K	303	1/1	0.92	0.10	46,46,46,46	0
15	SO4	M	306	5/5	0.92	0.14	40,40,48,65	5
15	SO4	M	301	5/5	0.92	0.15	43,47,52,56	5
15	SO4	a	304	5/5	0.92	0.14	61,66,87,99	0
15	SO4	X	204	5/5	0.92	0.14	46,50,57,63	5
15	SO4	D	302	5/5	0.92	0.24	82,84,90,112	0
17	A1AHA	N	301	49/49	0.92	0.10	26,39,52,57	0
15	SO4	Z	304	5/5	0.92	0.15	42,50,61,63	5
15	SO4	Q	301	5/5	0.92	0.11	48,50,67,69	5
15	SO4	J	203	5/5	0.92	0.12	49,53,63,69	5
15	SO4	B	302	5/5	0.93	0.15	41,44,59,59	5
15	SO4	J	201	5/5	0.93	0.11	46,48,58,70	5
15	SO4	C	301	5/5	0.93	0.14	42,44,52,53	5
17	A1AHA	Y	301	49/49	0.93	0.10	35,42,52,65	0
17	A1AHA	b	201	49/49	0.93	0.10	23,36,55,63	0
15	SO4	B	301	5/5	0.93	0.10	41,51,66,67	5
15	SO4	P	302	5/5	0.93	0.14	47,47,63,68	5
17	A1AHA	K	301	49/49	0.94	0.10	34,45,62,73	0
15	SO4	b	202	5/5	0.94	0.12	37,38,48,53	5
15	SO4	S	301	5/5	0.94	0.15	45,46,59,69	5
15	SO4	U	304	5/5	0.94	0.13	52,62,72,76	5
15	SO4	E	301	5/5	0.94	0.14	43,47,52,66	5
15	SO4	a	306	5/5	0.94	0.12	36,44,51,64	5

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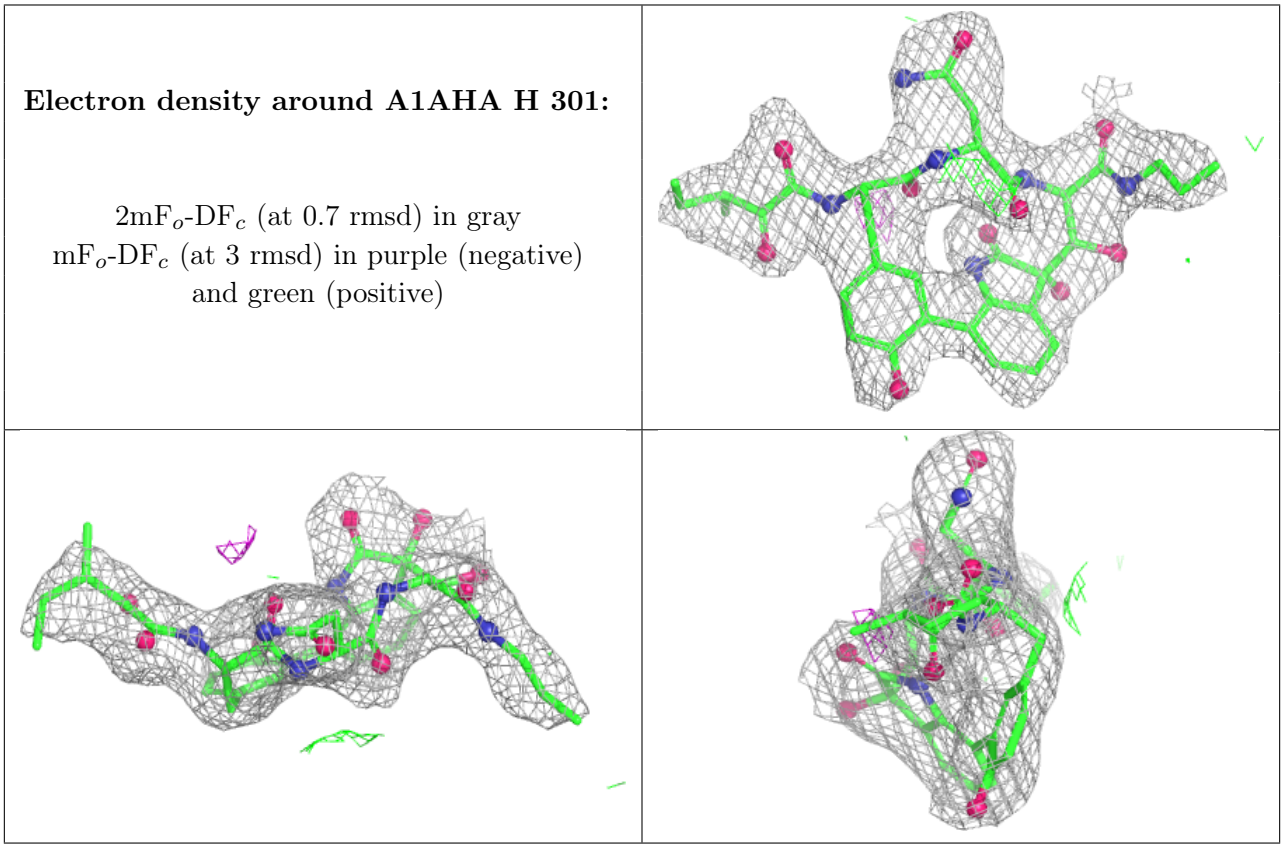
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	SO4	U	302	5/5	0.94	0.13	39,49,57,70	5
15	SO4	D	301	5/5	0.95	0.11	51,52,56,70	5
16	MG	X	201	1/1	0.95	0.26	43,43,43,43	0
15	SO4	X	202	5/5	0.96	0.10	44,49,58,72	5
16	MG	V	603	1/1	0.96	0.06	49,49,49,49	1
16	MG	G	302	1/1	0.97	0.07	39,39,39,39	0
15	SO4	X	203	5/5	0.97	0.11	33,35,37,38	5
15	SO4	J	202	5/5	0.97	0.13	42,42,44,48	5
16	MG	U	301	1/1	0.98	0.08	25,25,25,25	0
16	MG	G	301	1/1	0.98	0.04	23,23,23,23	0

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

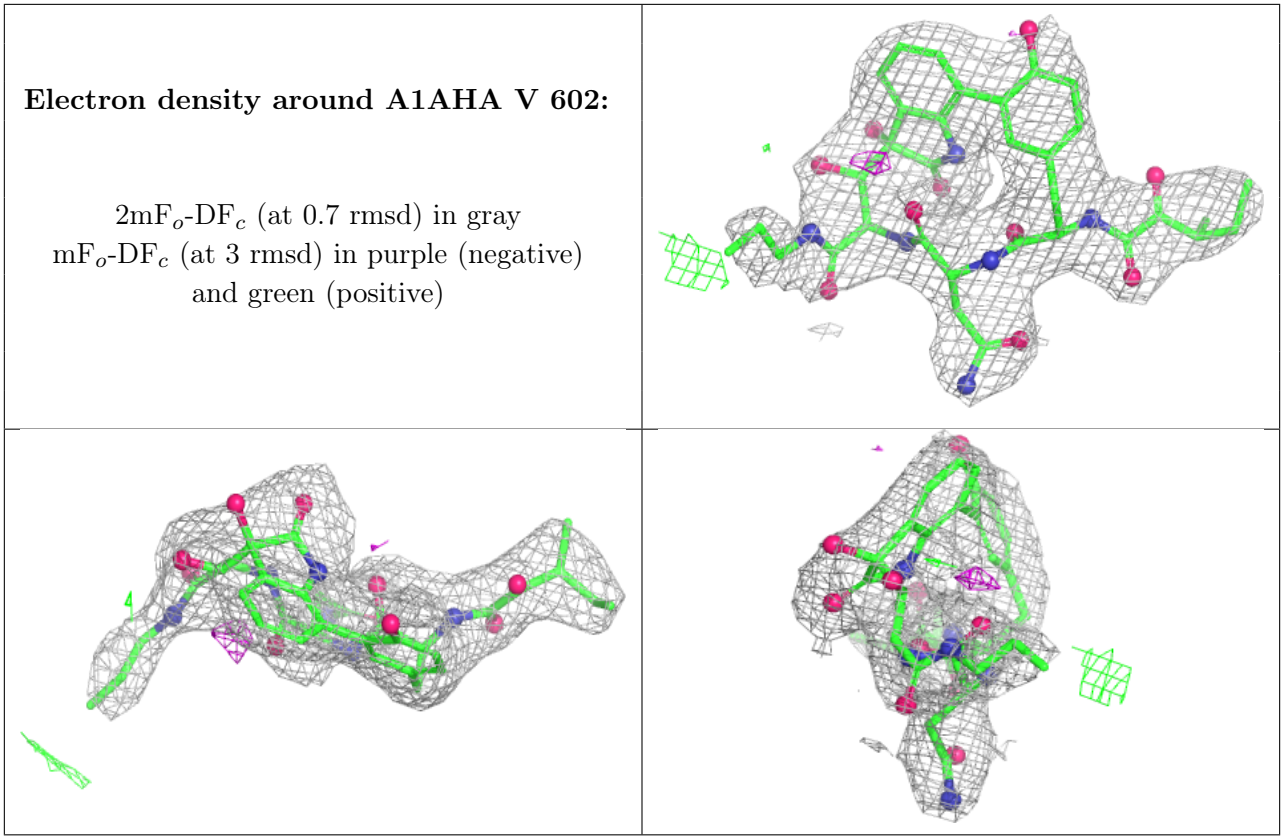
Electron density around A1AHA H 301:

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



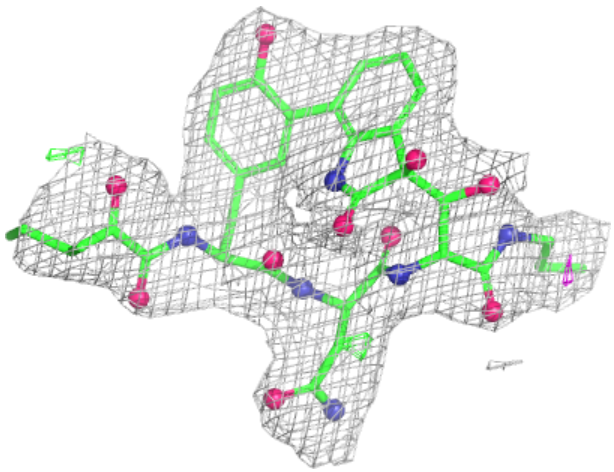
Electron density around A1AHA V 602:

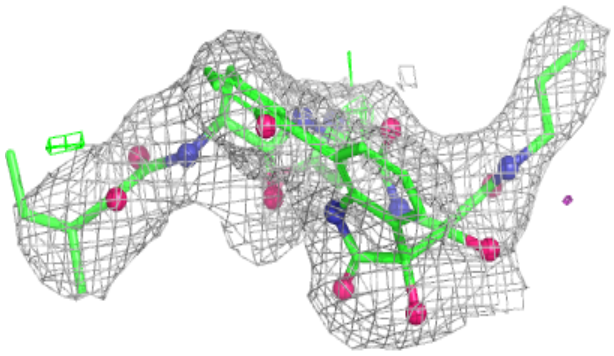
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

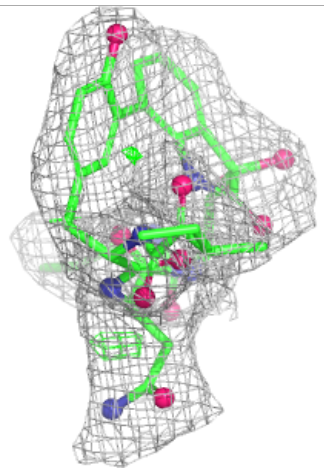


Electron density around A1AHA N 301:

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

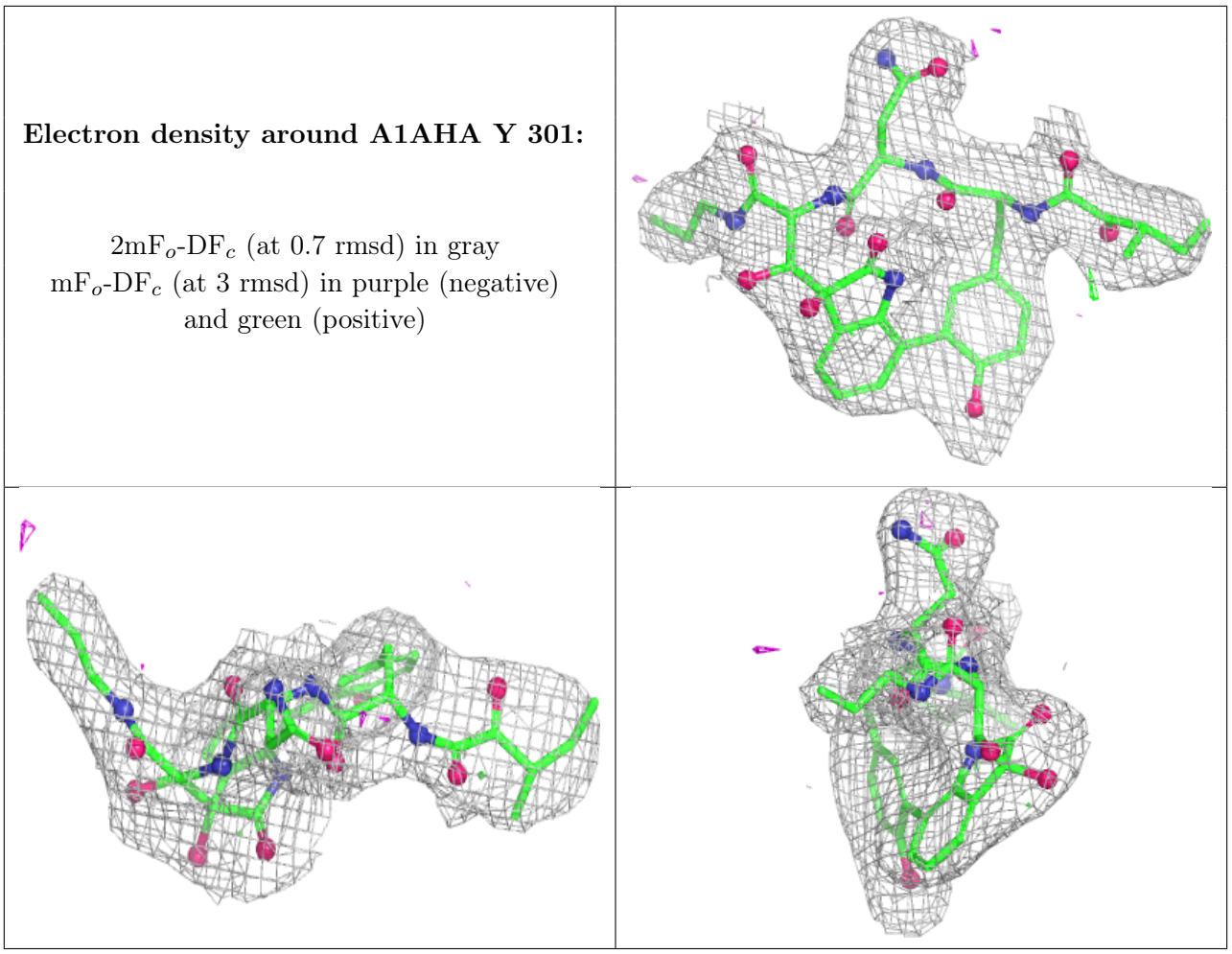






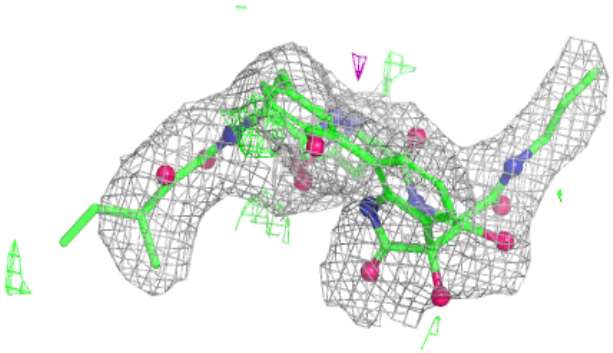
Electron density around A1AHA Y 301:

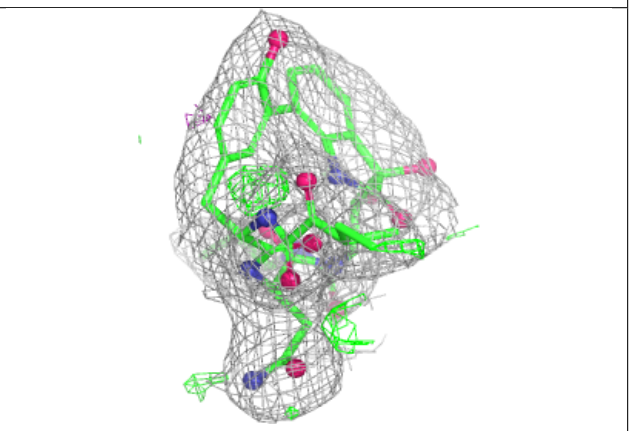
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1AHA b 201:

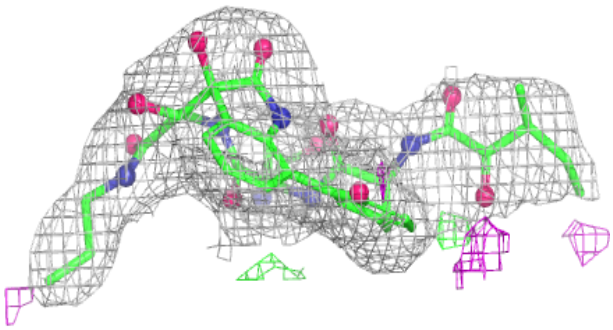
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

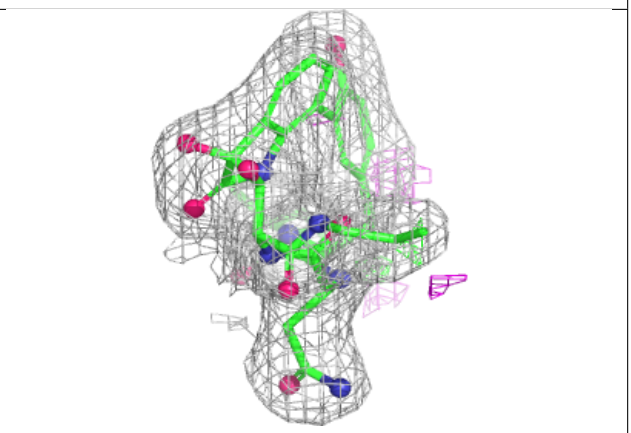




Electron density around A1AHA K 301:

$2mF_o$-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.