



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2023 – 08:22 am GMT

PDB ID : 4AQY
Title : Structure of ribosome-apramycin complexes
Authors : Matt, T.; Ng, C.L.; Lang, K.; Sha, S.H.; Akbergenov, R.; Shcherbakov, D.; Meyer, M.; Duscha, S.; Xie, J.; Dubbaka, S.R.; Perez-Fernandez, D.; Vasella, A.; Ramakrishnan, V.; Schacht, J.; Bottger, E.C.
Deposited on : 2012-04-20
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

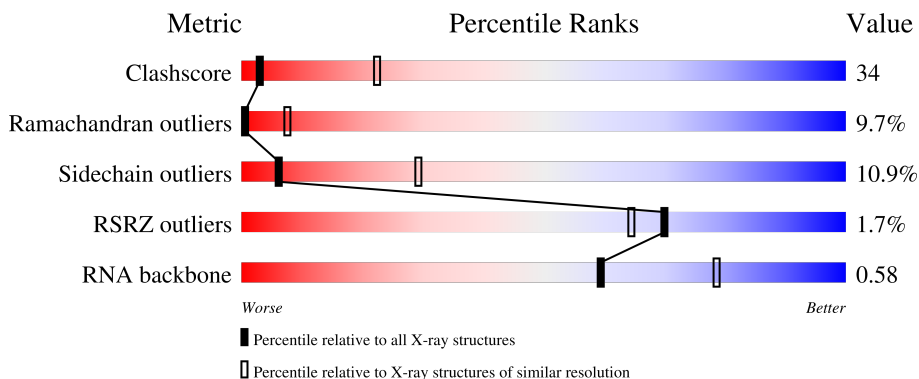
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.






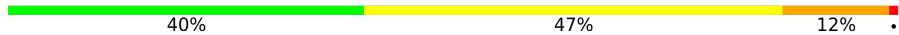
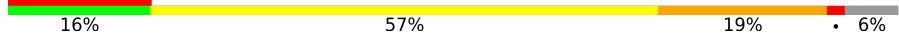
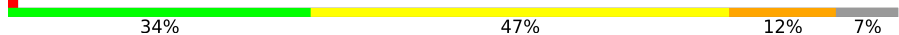
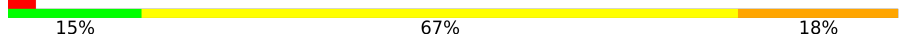
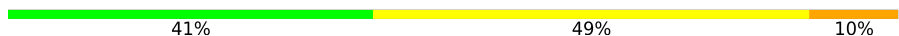




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	 36% 51% 11% 2% 2%
2	B	256	 21% 52% 17% 9% 1%
3	C	239	 20% 47% 17% 14% 2%
4	D	208	 4% 34% 53% 13%

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Mol	Chain	Length	Quality of chain
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	135	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	
22	W	6	
23	Z	15	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2548	-	-	-	X
24	MG	A	2549	-	-	-	X
24	MG	A	2550	-	-	-	X
24	MG	A	2554	-	-	-	X
24	MG	A	2555	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2557	-	-	-	X
24	MG	A	2562	-	-	-	X
24	MG	A	2563	-	-	-	X
24	MG	A	2565	-	-	-	X
24	MG	A	2580	-	-	-	X
24	MG	A	2582	-	-	-	X
24	MG	A	2584	-	-	-	X
24	MG	A	2600	-	-	-	X
24	MG	A	2609	-	-	-	X
24	MG	A	2613	-	-	-	X
24	MG	A	2615	-	-	-	X
24	MG	A	2618	-	-	-	X
24	MG	A	2624	-	-	-	X
24	MG	A	2626	-	-	-	X
24	MG	A	2631	-	-	-	X
24	MG	A	2634	-	-	-	X
24	MG	A	2644	-	-	-	X
24	MG	A	2653	-	-	-	X
24	MG	A	2661	-	-	-	X
24	MG	A	2662	-	-	-	X
24	MG	A	2663	-	-	-	X
24	MG	A	2667	-	-	-	X
24	MG	A	2683	-	-	-	X
24	MG	A	2684	-	-	-	X
24	MG	A	2687	-	-	-	X
24	MG	A	2689	-	-	-	X
24	MG	A	2696	-	-	-	X
24	MG	A	2698	-	-	-	X
24	MG	A	2701	-	-	-	X
24	MG	A	2708	-	-	-	X
24	MG	A	2714	-	-	-	X
24	MG	A	2716	-	-	-	X
24	MG	A	2722	-	-	-	X
24	MG	A	2725	-	-	-	X
24	MG	A	2726	-	-	-	X
24	MG	A	2728	-	-	-	X
24	MG	A	2731	-	-	-	X
24	MG	A	2735	-	-	-	X
24	MG	A	2739	-	-	-	X
24	MG	A	2740	-	-	-	X
24	MG	A	2741	-	-	-	X
24	MG	A	2742	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	2744	-	-	-	X
24	MG	A	2747	-	-	-	X
24	MG	S	1143	-	-	-	X
25	K	A	2670	-	-	-	X
25	K	A	2672	-	-	-	X
25	K	A	2675	-	-	-	X
25	K	A	2680	-	-	-	X
25	K	A	2682	-	-	-	X

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 52514 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 RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1510	32446	14444	6006	10488	1508	0	0	0

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1702	1066	339	290	7	0	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	842	531	155	153	3	0	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	155	1256	781	252	217	6	0	0	0

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	138	1115	705	215	192	3	0	0	0

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	127	1010	639	198	173	0	0	0

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	98	794	499	156	138	1	0	0	0

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	119	884	549	168	164	3	0	0	0

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	125	971	611	196	163	1	0	0	1

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	125	996	617	207	170	2	0	0	0

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	60	491	312	104	71	4	0	0	0

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	88	733	459	147	125	2	0	0	0

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	83	700	443	139	117	1	0	0	0

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	104	856	547	161	146	2	0	0	0

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	R	73	596	380	118	98	0	0	0

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	80	647	414	119	112	2	0	0	0

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	T	99	761	469	162	128	2	0	0	0

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*CP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

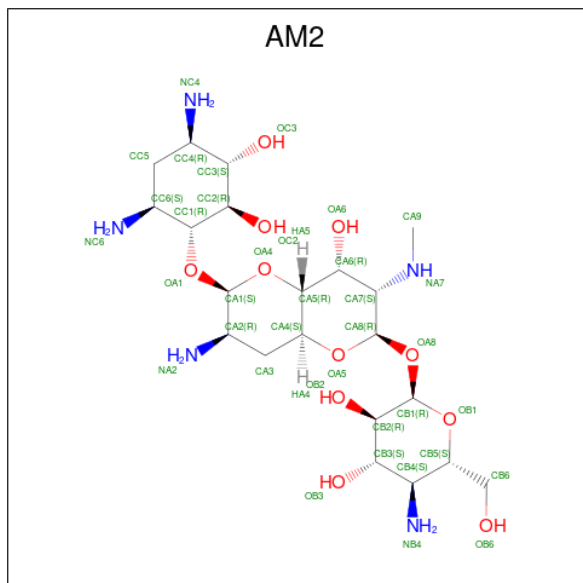
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	190	Total	Mg	0	0
			190	190		
24	D	1	Total	Mg	0	0
			1	1		
24	F	1	Total	Mg	0	0
			1	1		
24	G	2	Total	Mg	0	0
			2	2		
24	H	1	Total	Mg	0	0
			1	1		
24	J	1	Total	Mg	0	0
			1	1		
24	K	1	Total	Mg	0	0
			1	1		
24	L	1	Total	Mg	0	0
			1	1		
24	M	1	Total	Mg	0	0
			1	1		
24	S	1	Total	Mg	0	0
			1	1		
24	W	2	Total	Mg	0	0
			2	2		
24	Z	1	Total	Mg	0	0
			1	1		

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	14	Total K 14 14	0	0
25	V	1	Total K 1 1	0	0

- Molecule 26 is APRAMYCIN (three-letter code: AM2) (formula: C₂₁H₄₁N₅O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C N O 37 21 5 11	0	0
26	A	1	Total C N O 37 21 5 11	0	0
26	A	1	Total C N O 37 21 5 11	0	0
26	A	1	Total C N O 37 21 5 11	0	0
26	A	1	Total C N O 37 21 5 11	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	D	1	Total Zn 1 1	0	0
27	N	1	Total Zn 1 1	0	0

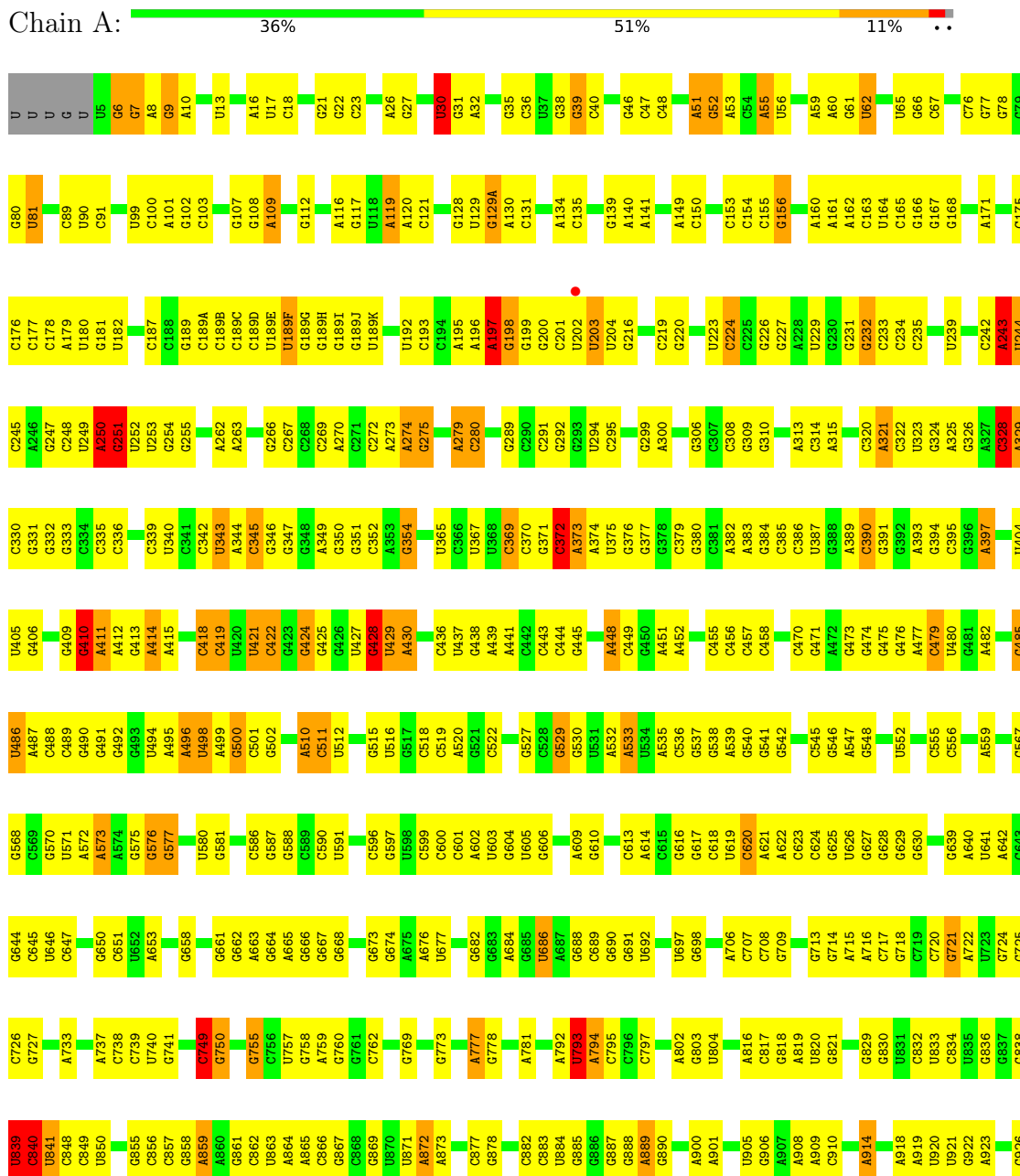
- Molecule 28 is water.

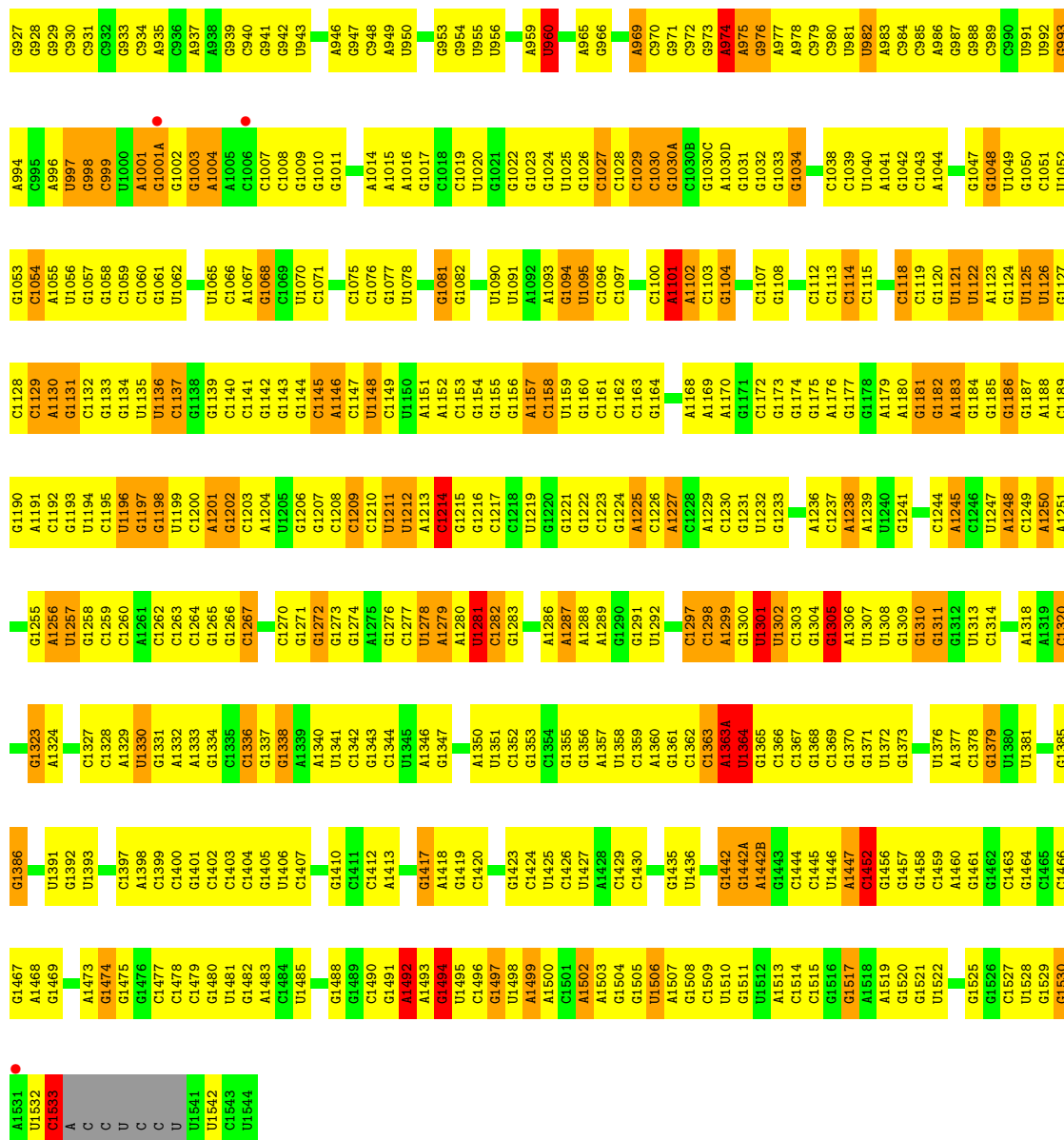
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	O	0	0
			1	1		

3 Residue-property plots

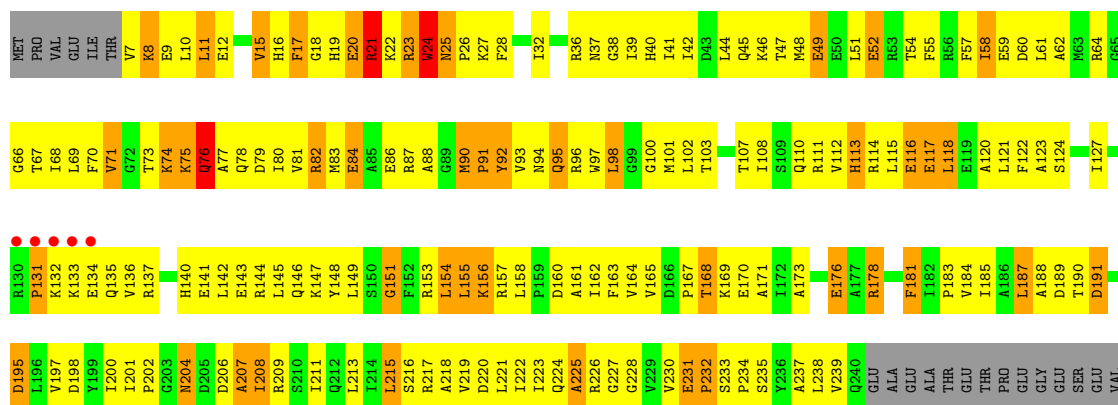
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 16S RIBOSOMAL RNA



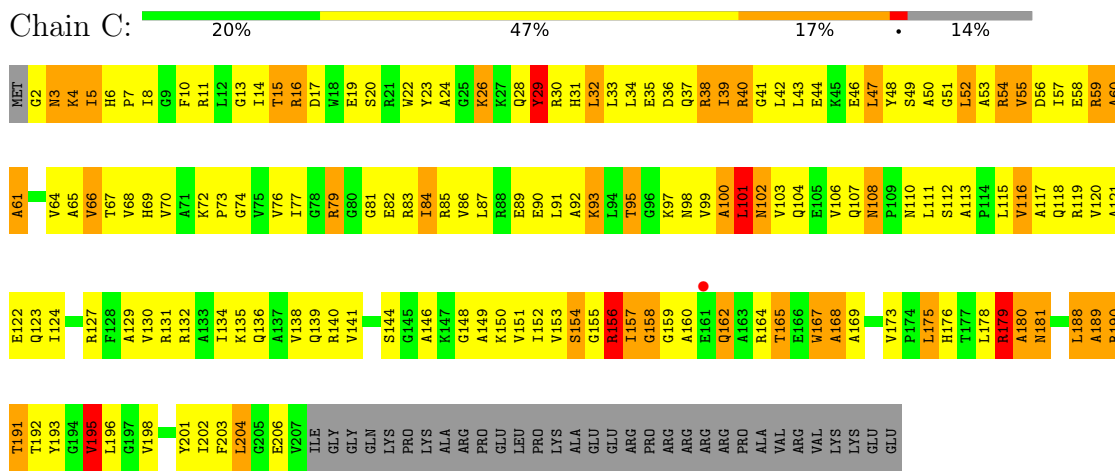


● Molecule 2: 30S RIBOSOMAL PROTEIN S2

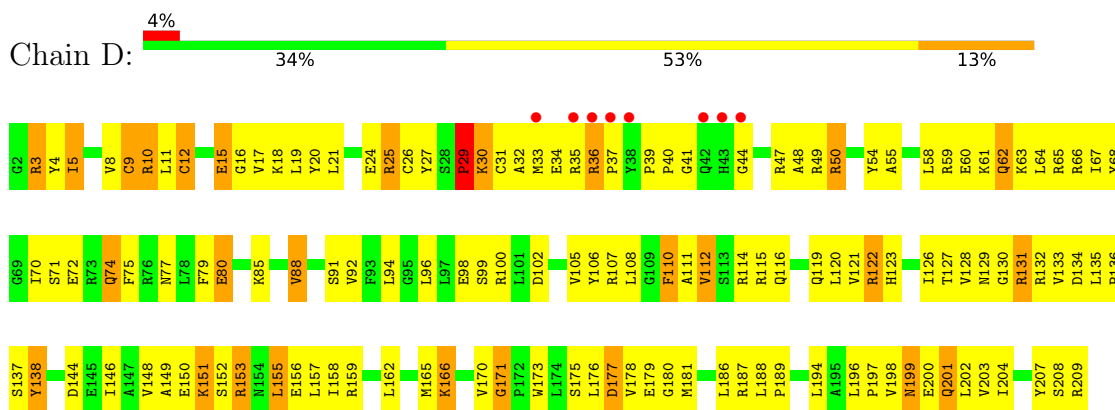


GLU
ALA

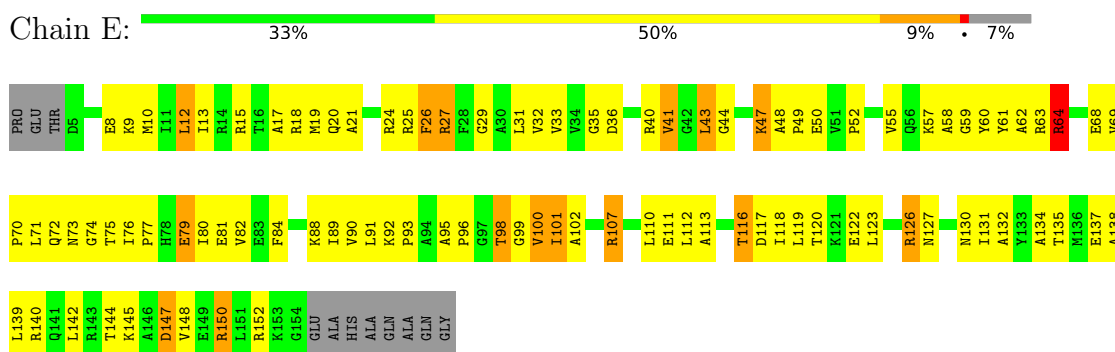
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

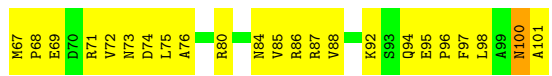


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

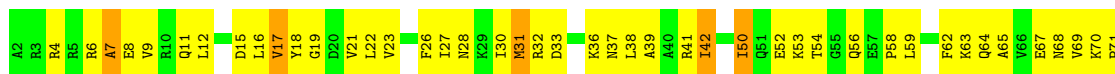


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

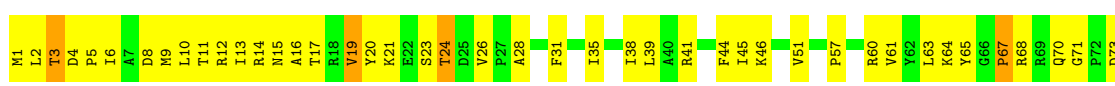




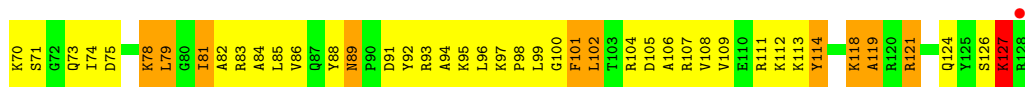
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



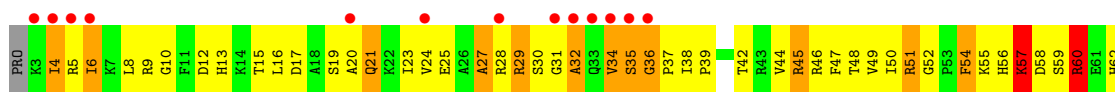
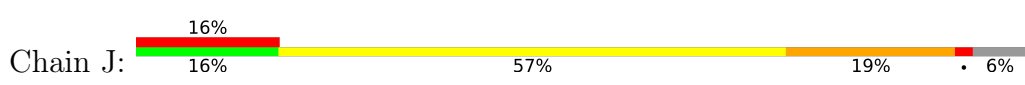
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



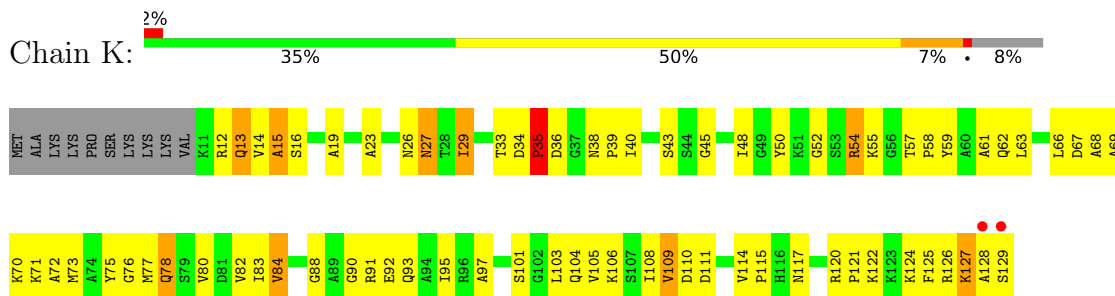
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



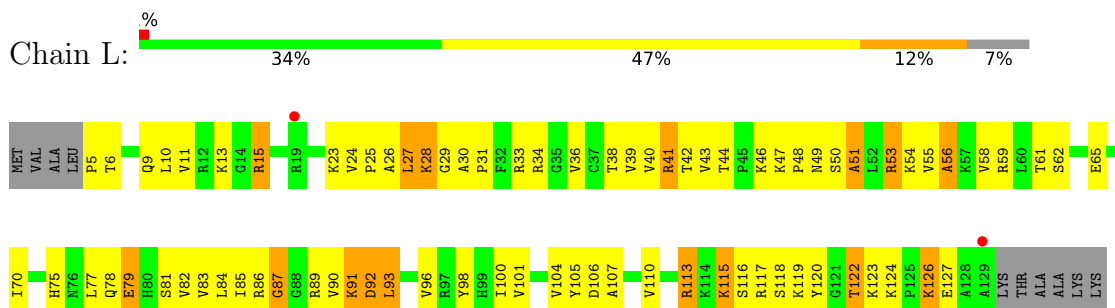
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



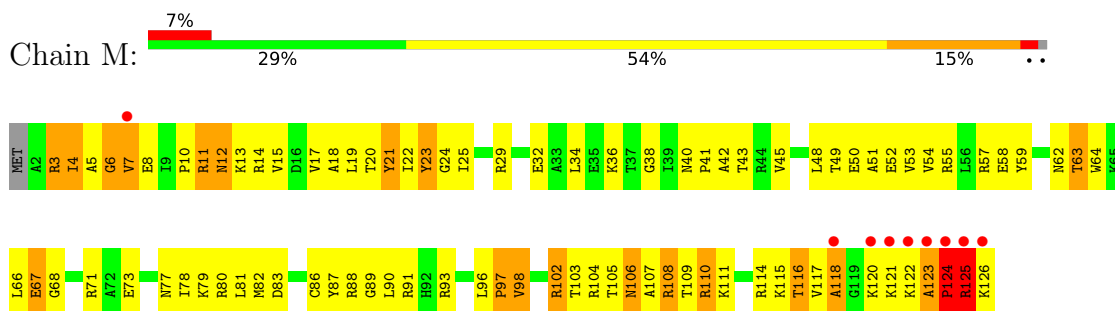
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



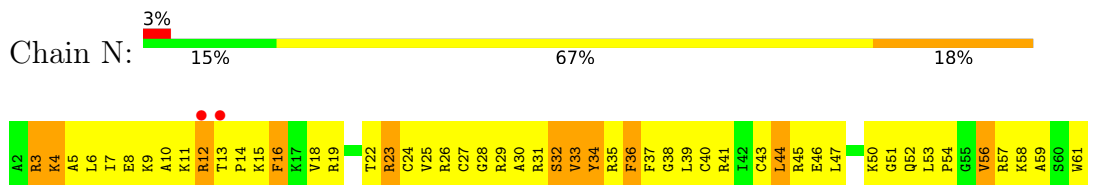
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



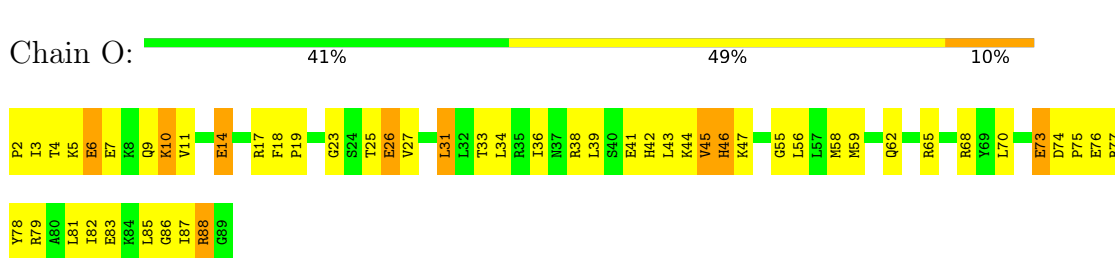
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



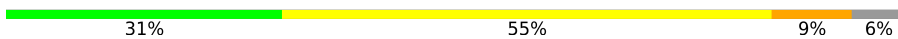
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

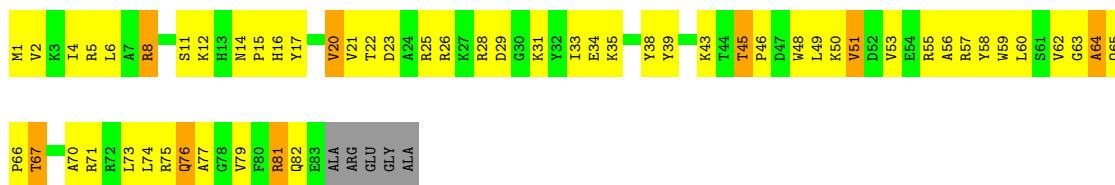


- Molecule 15: 30S RIBOSOMAL PROTEIN S15



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 



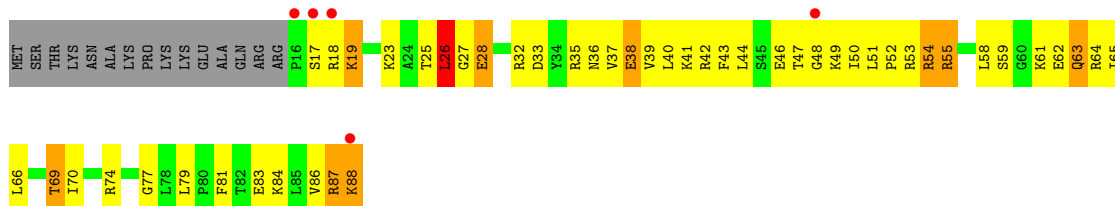
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q: 



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R: 



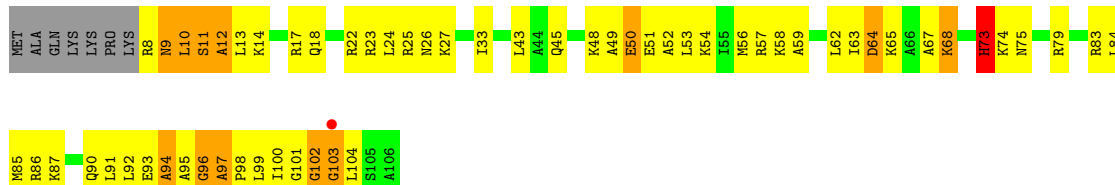
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S: 

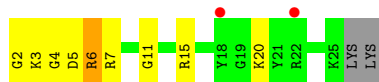


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

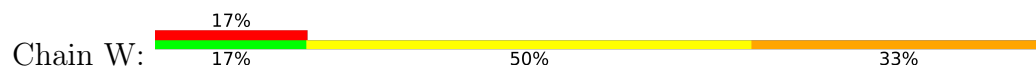
Chain T: 



- Molecule 21: 30S RIBOSOMAL PROTEIN THX



- Molecule 22: 5'-R(*UP*UP*CP*AP*AP*AP)-3'



- Molecule 23: 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.18Å 402.18Å 175.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 39.77 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.50) 99.8 (39.77-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.48Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.193 , 0.235 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	119.8	Xtrriage
Anisotropy	0.253	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 127.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	52514	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: K, ZN, AM2, MG

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	0.51	8/36318 (0.0%)	0.74	31/56682 (0.1%)
2	B	0.37	0/1935	0.68	0/2609
3	C	0.39	0/1636	0.67	0/2205
4	D	0.36	0/1732	0.65	0/2318
5	E	0.43	0/1162	0.74	1/1564 (0.1%)
6	F	0.33	0/855	0.62	0/1154
7	G	0.37	0/1275	0.60	0/1709
8	H	0.42	0/1135	0.75	0/1527
9	I	0.37	0/1028	0.68	0/1378
10	J	0.38	0/807	0.66	0/1085
11	K	0.37	0/899	0.67	0/1213
12	L	0.46	0/987	0.75	0/1322
13	M	0.36	0/1007	0.67	0/1347
14	N	0.42	0/500	0.69	0/664
15	O	0.35	0/744	0.59	0/992
16	P	0.41	0/716	0.71	0/963
17	Q	0.41	0/869	0.71	0/1159
18	R	0.34	0/602	0.62	0/799
19	S	0.35	0/661	0.66	0/890
20	T	0.40	0/763	0.75	1/1006 (0.1%)
21	V	0.48	0/212	0.63	0/277
22	W	2.62	10/137 (7.3%)	0.91	1/211 (0.5%)
23	Z	1.61	1/357 (0.3%)	0.93	1/555 (0.2%)
All	All	0.50	19/56337 (0.0%)	0.72	35/83629 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	8	22
22	W	0	1
23	Z	0	3
All	All	8	26

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1533	C	N1-C2	15.01	1.55	1.40
1	A	1533	C	C4-C5	13.16	1.53	1.43
22	W	6	A	C5-C4	12.22	1.47	1.38
22	W	6	A	N9-C8	11.21	1.46	1.37
22	W	6	A	C2-N3	10.77	1.43	1.33

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1363(A)	A	C2'-C3'-O3'	9.91	131.30	109.50
1	A	243	A	C2'-C3'-O3'	9.00	129.30	109.50
1	A	1452	C	C2'-C3'-O3'	8.70	128.64	109.50
1	A	410	G	C2'-C3'-O3'	8.31	127.78	109.50
1	A	119	A	C2'-C3'-O3'	7.75	126.55	109.50

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	30	U	C4'
1	A	197	A	C4'
1	A	410	G	C3'
1	A	1181	G	C4'
1	A	1305	G	C3',C4'

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	G	Sidechain
1	A	239	U	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	424	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32446	0	16380	1059	0
2	B	1900	0	1951	285	0
3	C	1612	0	1677	243	0
4	D	1702	0	1762	184	0
5	E	1146	0	1207	115	0
6	F	842	0	857	89	0
7	G	1256	0	1295	94	0
8	H	1115	0	1177	92	0
9	I	1010	0	1043	122	0
10	J	794	0	840	146	0
11	K	884	0	904	92	0
12	L	971	0	1057	97	0
13	M	996	0	1072	107	0
14	N	491	0	529	90	0
15	O	733	0	771	61	0
16	P	700	0	720	68	0
17	Q	856	0	930	69	0
18	R	596	0	668	80	0
19	S	647	0	673	85	0
20	T	761	0	859	70	0
21	V	208	0	221	14	0
22	W	123	0	66	5	0
23	Z	319	0	164	32	0
24	A	190	0	0	0	0
24	D	1	0	0	0	0
24	F	1	0	0	0	0
24	G	2	0	0	0	0
24	H	1	0	0	0	0
24	J	1	0	0	0	0
24	K	1	0	0	0	0
24	L	1	0	0	0	0
24	M	1	0	0	0	0
24	S	1	0	0	0	0
24	W	2	0	0	0	0
24	Z	1	0	0	0	0
25	A	14	0	0	0	0
25	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	185	0	205	9	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
28	A	1	0	0	0	0
All	All	52514	0	37028	3057	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 3057 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:C:C2'	1:A:1114:C:H5'	1.60	1.28
1:A:1147:C:H2'	1:A:1148:U:H5''	1.25	1.12
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.32	1.11
1:A:1271:G:H2'	1:A:1272:G:H5''	1.22	1.11
1:A:972:C:H4'	10:J:57:LYS:HG2	1.30	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	150 (65%)	50 (22%)	32 (14%)	0	3
3	C	204/239 (85%)	123 (60%)	48 (24%)	33 (16%)	0	2
4	D	206/208 (99%)	140 (68%)	45 (22%)	21 (10%)	0	7
5	E	148/161 (92%)	115 (78%)	30 (20%)	3 (2%)	7	39
6	F	99/101 (98%)	74 (75%)	21 (21%)	4 (4%)	3	24
7	G	153/155 (99%)	116 (76%)	28 (18%)	9 (6%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	100 (74%)	27 (20%)	9 (7%)	1	13
9	I	125/128 (98%)	94 (75%)	18 (14%)	13 (10%)	0	7
10	J	96/104 (92%)	61 (64%)	19 (20%)	16 (17%)	0	2
11	K	117/129 (91%)	84 (72%)	25 (21%)	8 (7%)	1	13
12	L	123/135 (91%)	88 (72%)	23 (19%)	12 (10%)	0	7
13	M	123/126 (98%)	79 (64%)	26 (21%)	18 (15%)	0	3
14	N	58/60 (97%)	33 (57%)	14 (24%)	11 (19%)	0	2
15	O	86/88 (98%)	72 (84%)	11 (13%)	3 (4%)	3	27
16	P	81/88 (92%)	60 (74%)	18 (22%)	3 (4%)	3	26
17	Q	102/104 (98%)	82 (80%)	14 (14%)	6 (6%)	1	15
18	R	71/88 (81%)	56 (79%)	9 (13%)	6 (8%)	1	9
19	S	78/92 (85%)	47 (60%)	22 (28%)	9 (12%)	0	6
20	T	97/106 (92%)	71 (73%)	16 (16%)	10 (10%)	0	7
21	V	22/26 (85%)	17 (77%)	3 (14%)	2 (9%)	1	8
All	All	2357/2532 (93%)	1662 (70%)	467 (20%)	228 (10%)	0	7

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	PHE
2	B	24	TRP
2	B	38	GLY
2	B	225	ALA
2	B	232	PRO

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	
2	B	202/220 (92%)	177 (88%)	25 (12%)	4	23
3	C	160/188 (85%)	136 (85%)	24 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	180/180 (100%)	157 (87%)	23 (13%)	4	22
5	E	115/122 (94%)	102 (89%)	13 (11%)	6	27
6	F	90/90 (100%)	84 (93%)	6 (7%)	16	48
7	G	126/126 (100%)	112 (89%)	14 (11%)	6	28
8	H	119/119 (100%)	105 (88%)	14 (12%)	5	25
9	I	98/99 (99%)	89 (91%)	9 (9%)	9	36
10	J	88/91 (97%)	77 (88%)	11 (12%)	4	23
11	K	90/99 (91%)	84 (93%)	6 (7%)	16	48
12	L	104/111 (94%)	94 (90%)	10 (10%)	8	34
13	M	100/101 (99%)	90 (90%)	10 (10%)	7	32
14	N	49/49 (100%)	44 (90%)	5 (10%)	7	32
15	O	79/79 (100%)	73 (92%)	6 (8%)	13	43
16	P	72/74 (97%)	62 (86%)	10 (14%)	3	20
17	Q	96/96 (100%)	84 (88%)	12 (12%)	4	23
18	R	64/77 (83%)	58 (91%)	6 (9%)	8	35
19	S	71/79 (90%)	64 (90%)	7 (10%)	8	33
20	T	76/82 (93%)	70 (92%)	6 (8%)	12	41
21	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1998/2103 (95%)	1781 (89%)	217 (11%)	6	29

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	105	ARG
11	K	93	GLN
18	R	28	GLU
9	I	3	GLN
10	J	21	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	32	ASN
16	P	82	GLN
7	G	68	ASN

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Mol	Chain	Res	Type
16	P	76	GLN
19	S	14	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	250 (16%)	30 (1%)
22	W	5/6 (83%)	1 (20%)	0
23	Z	14/15 (93%)	10 (71%)	3 (21%)
All	All	1527/1543 (98%)	261 (17%)	33 (2%)

5 of 261 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	30	U
1	A	31	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1447	A
1	A	1452	C
23	Z	40	C
1	A	496	A
1	A	485	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 225 ligands modelled in this entry, 220 are monoatomic - leaving 5 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
26	AM2	A	3003	-	40,40,40	0.92	2 (5%)	53,60,60	0.90	1 (1%)
26	AM2	A	3002	-	40,40,40	0.98	2 (5%)	53,60,60	0.87	1 (1%)
26	AM2	A	3005	-	40,40,40	0.92	1 (2%)	53,60,60	0.80	1 (1%)
26	AM2	A	3004	-	40,40,40	0.88	0	53,60,60	0.85	1 (1%)
26	AM2	A	3001	-	40,40,40	0.87	1 (2%)	53,60,60	1.16	2 (3%)

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
26	AM2	A	3003	-	-	1/12/84/84	0/4/4/4
26	AM2	A	3002	-	-	3/12/84/84	0/4/4/4
26	AM2	A	3005	-	-	4/12/84/84	0/4/4/4
26	AM2	A	3004	-	-	2/12/84/84	0/4/4/4
26	AM2	A	3001	-	-	2/12/84/84	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	3002	AM2	OB1-CB1	2.47	1.48	1.41
26	A	3003	AM2	CB5-CB4	2.10	1.56	1.52
26	A	3001	AM2	OB1-CB1	2.06	1.47	1.41
26	A	3005	AM2	OB1-CB1	2.05	1.47	1.41
26	A	3002	AM2	OA4-CA1	2.03	1.47	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	3001	AM2	CA9-NA7-CA7	6.70	124.14	114.38
26	A	3003	AM2	CA9-NA7-CA7	5.19	121.94	114.38
26	A	3004	AM2	CA9-NA7-CA7	4.75	121.30	114.38
26	A	3005	AM2	CA9-NA7-CA7	4.17	120.46	114.38
26	A	3002	AM2	CA9-NA7-CA7	4.04	120.26	114.38

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

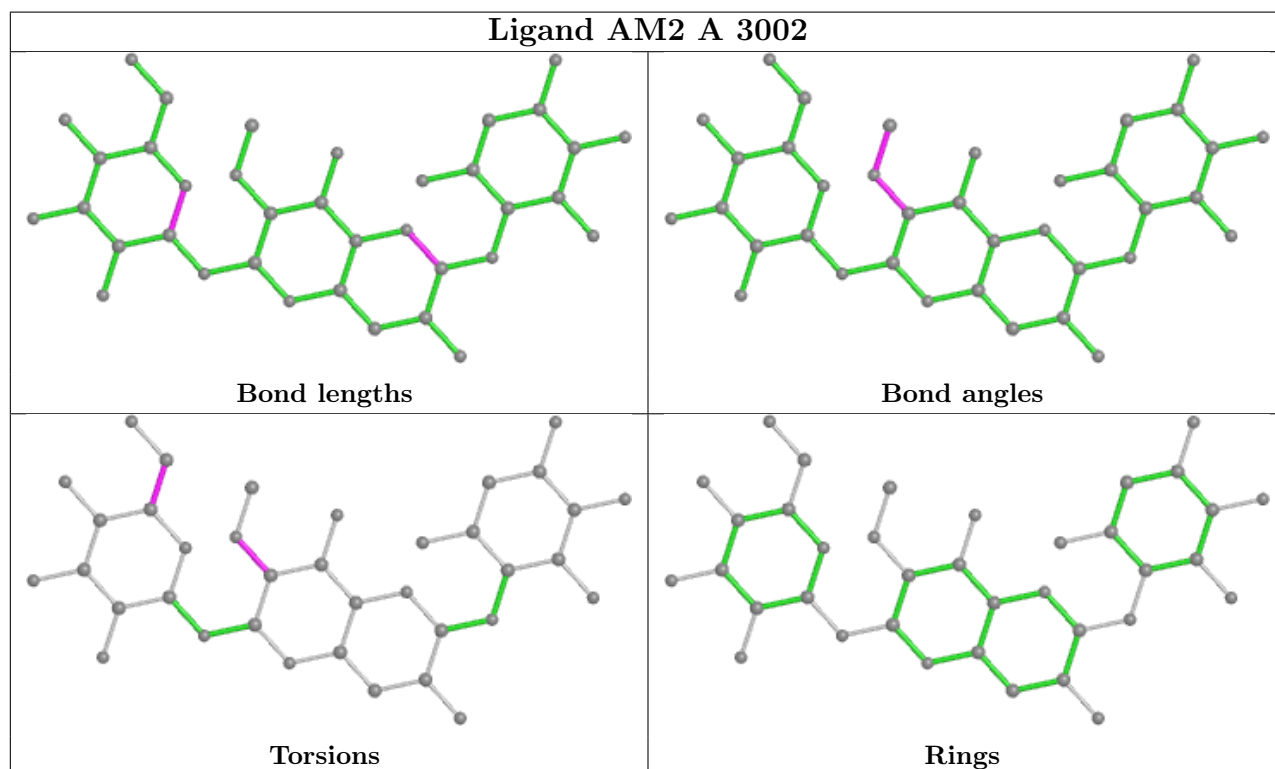
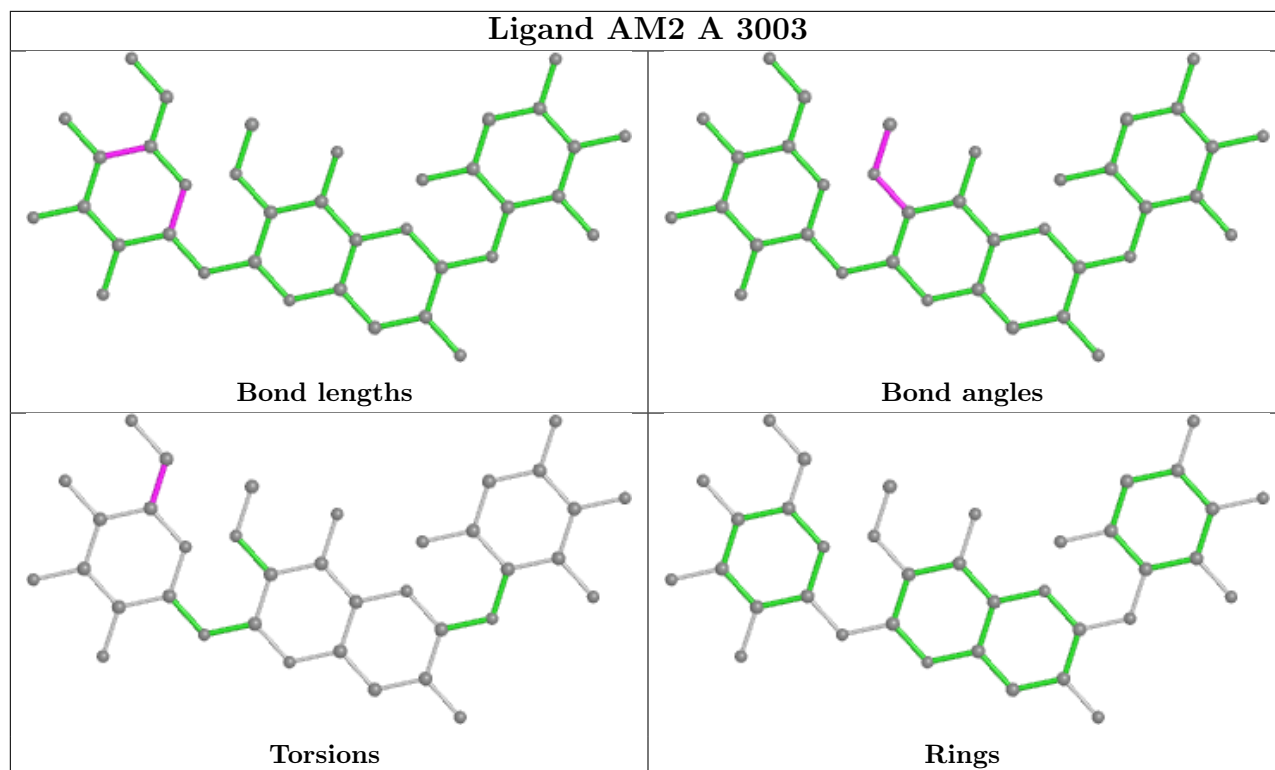
Mol	Chain	Res	Type	Atoms
26	A	3001	AM2	CA8-CA7-NA7-CA9
26	A	3002	AM2	CA8-CA7-NA7-CA9
26	A	3005	AM2	CC6-CC1-OA1-CA1
26	A	3002	AM2	OB1-CB5-CB6-OB6
26	A	3004	AM2	OB1-CB5-CB6-OB6

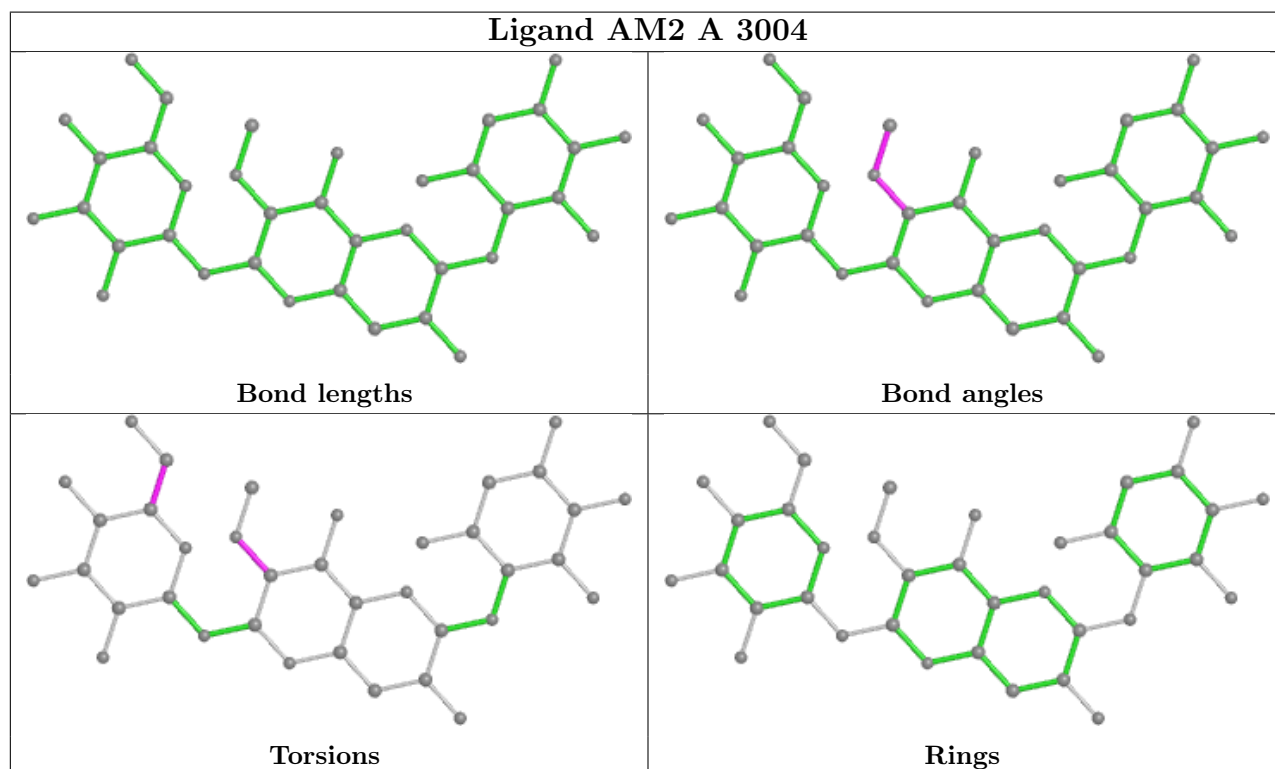
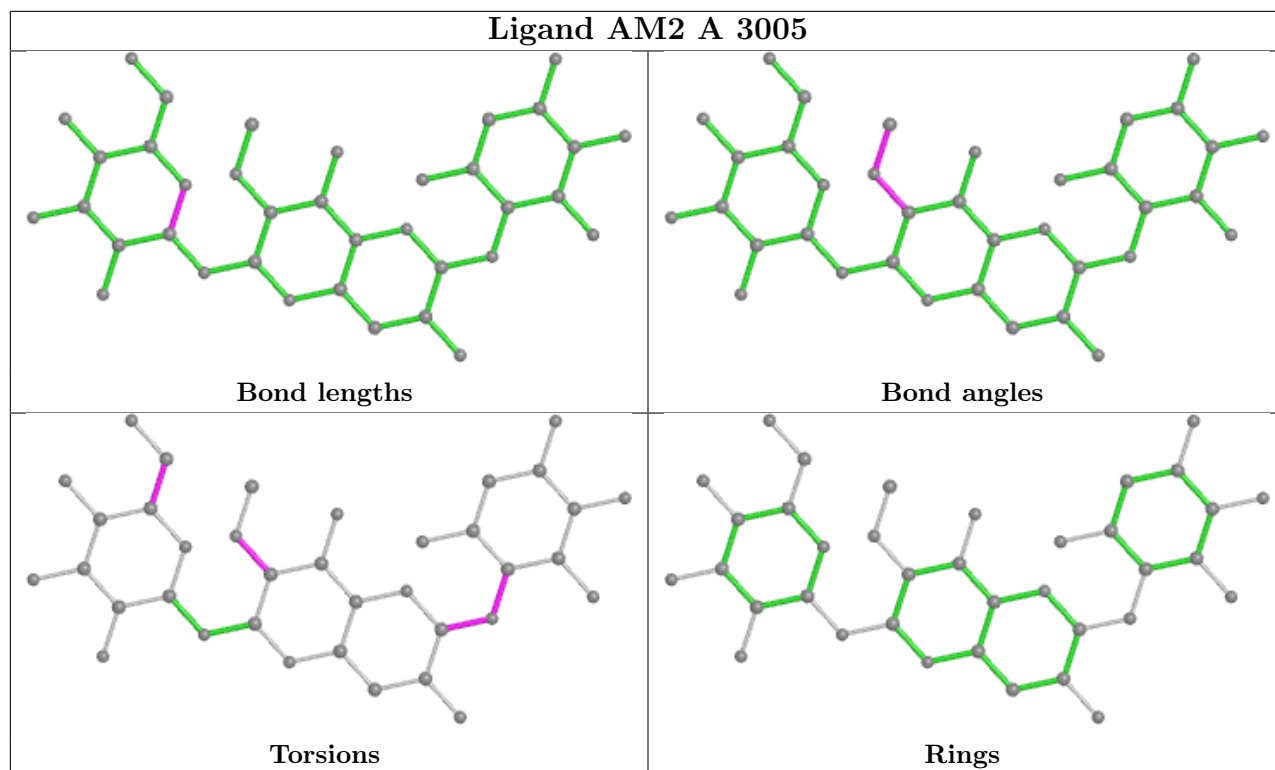
There are no ring outliers.

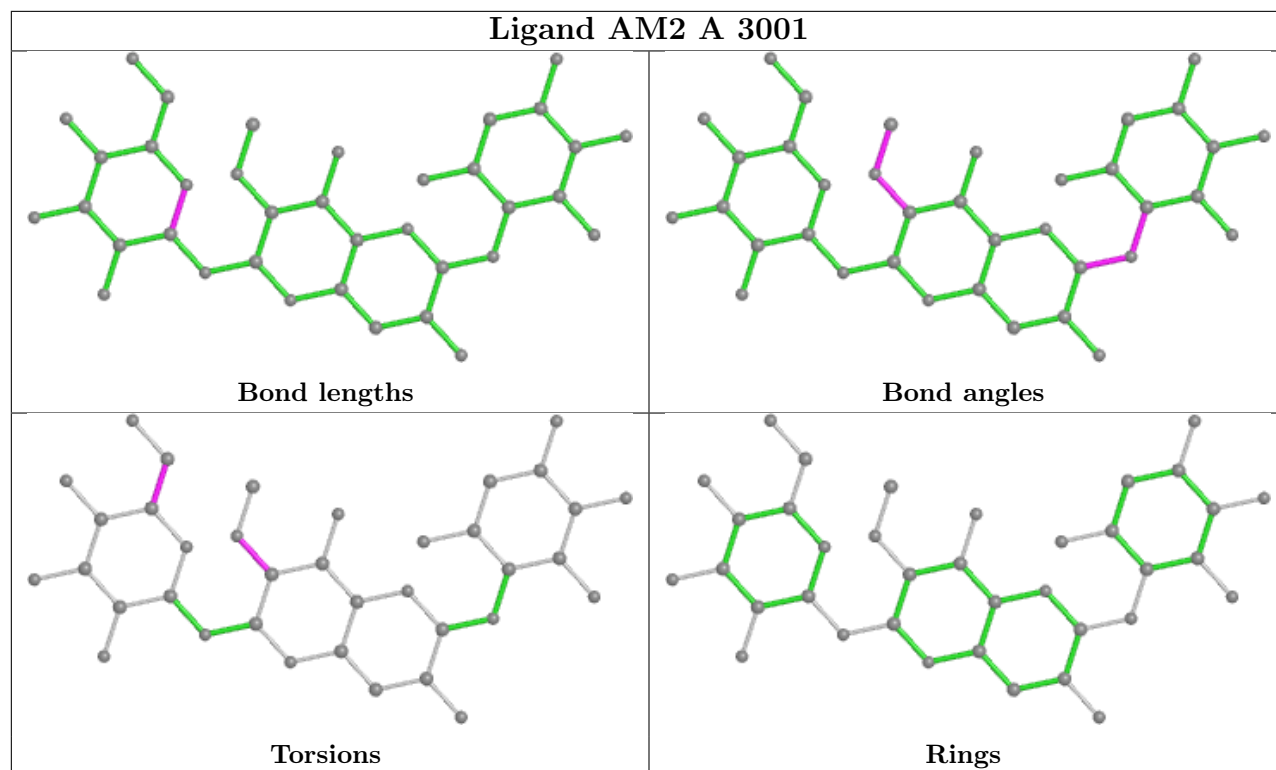
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	3002	AM2	2	0
26	A	3005	AM2	5	0
26	A	3001	AM2	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	1510/1522 (99%)	-0.12	4 (0%) 94 91	82, 115, 181, 202	0
2	B	234/256 (91%)	-0.16	5 (2%) 63 58	84, 153, 190, 202	0
3	C	206/239 (86%)	-0.28	1 (0%) 91 88	86, 139, 185, 202	0
4	D	208/208 (100%)	-0.23	8 (3%) 40 36	90, 133, 184, 202	0
5	E	150/161 (93%)	-0.27	0 100 100	83, 108, 153, 196	0
6	F	101/101 (100%)	-0.35	0 100 100	104, 143, 177, 186	0
7	G	155/155 (100%)	-0.47	1 (0%) 89 86	89, 131, 186, 202	0
8	H	138/138 (100%)	-0.39	0 100 100	76, 105, 141, 163	0
9	I	127/128 (99%)	-0.17	1 (0%) 86 81	89, 144, 178, 202	0
10	J	98/104 (94%)	0.77	17 (17%) 1 1	97, 168, 202, 202	0
11	K	119/129 (92%)	-0.13	2 (1%) 70 64	79, 113, 161, 197	0
12	L	125/135 (92%)	-0.27	2 (1%) 72 66	74, 108, 155, 202	0
13	M	125/126 (99%)	0.23	9 (7%) 15 15	100, 133, 171, 200	0
14	N	60/60 (100%)	0.03	2 (3%) 46 41	93, 136, 178, 198	0
15	O	88/88 (100%)	-0.20	0 100 100	78, 123, 166, 192	0
16	P	83/88 (94%)	-0.38	0 100 100	79, 105, 138, 196	0
17	Q	104/104 (100%)	-0.15	4 (3%) 40 36	78, 106, 161, 202	0
18	R	73/88 (82%)	-0.16	5 (6%) 17 16	93, 130, 184, 196	0
19	S	80/92 (86%)	-0.13	0 100 100	103, 152, 188, 202	0
20	T	99/106 (93%)	-0.27	1 (1%) 82 77	80, 112, 164, 200	0
21	V	24/26 (92%)	0.76	2 (8%) 11 12	82, 126, 160, 173	0
22	W	6/6 (100%)	0.82	1 (16%) 1 2	112, 125, 180, 197	0
23	Z	15/15 (100%)	0.49	1 (6%) 17 16	97, 137, 200, 202	0
All	All	3928/4075 (96%)	-0.15	66 (1%) 70 64	74, 123, 184, 202	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	123	ALA	10.1
10	J	33	GLN	9.7
13	M	124	PRO	8.3
13	M	121	LYS	7.8
11	K	128	ALA	6.8

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	2550	1/1	0.03	0.85	105,105,105,105	0
24	MG	A	2596	1/1	0.20	0.37	105,105,105,105	0
24	MG	A	2618	1/1	0.21	0.48	97,97,97,97	0
24	MG	A	2721	1/1	0.23	0.15	174,174,174,174	1
25	K	A	2680	1/1	0.26	0.82	180,180,180,180	0
24	MG	A	2557	1/1	0.27	0.55	110,110,110,110	0
24	MG	A	2613	1/1	0.31	0.51	89,89,89,89	0
24	MG	A	2554	1/1	0.34	1.30	134,134,134,134	0
25	K	A	2672	1/1	0.36	0.57	159,159,159,159	0
24	MG	A	2684	1/1	0.37	0.71	88,88,88,88	0
24	MG	A	2548	1/1	0.40	1.58	114,114,114,114	0
24	MG	A	2549	1/1	0.40	0.51	103,103,103,103	0
24	MG	A	2600	1/1	0.42	0.70	93,93,93,93	0
24	MG	A	2601	1/1	0.43	0.39	105,105,105,105	0
24	MG	A	2555	1/1	0.44	0.59	129,129,129,129	0
24	MG	A	2631	1/1	0.47	0.62	96,96,96,96	0
24	MG	A	2701	1/1	0.47	0.82	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	K	A	2679	1/1	0.47	0.30	126,126,126,126	0
24	MG	A	2716	1/1	0.47	0.85	122,122,122,122	0
24	MG	A	2715	1/1	0.48	0.39	113,113,113,113	0
24	MG	A	2661	1/1	0.50	0.51	107,107,107,107	0
25	K	A	2675	1/1	0.50	1.02	143,143,143,143	0
24	MG	A	2552	1/1	0.56	0.27	84,84,84,84	0
24	MG	A	2687	1/1	0.57	0.72	114,114,114,114	0
24	MG	A	2626	1/1	0.57	1.64	102,102,102,102	0
24	MG	A	2634	1/1	0.57	0.42	86,86,86,86	0
25	K	A	2671	1/1	0.58	0.34	117,117,117,117	0
25	K	A	2681	1/1	0.58	0.18	140,140,140,140	0
24	MG	A	2708	1/1	0.60	0.59	105,105,105,105	0
25	K	A	2670	1/1	0.60	0.55	147,147,147,147	0
24	MG	A	2696	1/1	0.61	0.69	92,92,92,92	0
24	MG	A	2735	1/1	0.62	0.54	98,98,98,98	1
24	MG	A	2563	1/1	0.63	0.87	87,87,87,87	0
24	MG	A	2584	1/1	0.65	0.41	108,108,108,108	0
24	MG	A	2663	1/1	0.65	0.57	88,88,88,88	0
24	MG	A	2722	1/1	0.66	0.72	93,93,93,93	0
24	MG	A	2580	1/1	0.66	0.87	76,76,76,76	0
24	MG	A	2689	1/1	0.66	1.22	101,101,101,101	0
24	MG	S	1143	1/1	0.67	0.68	115,115,115,115	0
25	K	A	2676	1/1	0.67	0.29	142,142,142,142	0
24	MG	A	2667	1/1	0.67	0.69	92,92,92,92	0
24	MG	A	2725	1/1	0.67	0.59	101,101,101,101	0
24	MG	A	2611	1/1	0.67	0.27	98,98,98,98	0
24	MG	A	2615	1/1	0.68	0.64	91,91,91,91	0
24	MG	A	2740	1/1	0.68	1.05	92,92,92,92	0
25	K	A	2678	1/1	0.68	0.29	131,131,131,131	0
24	MG	A	2562	1/1	0.69	0.40	108,108,108,108	0
24	MG	A	2565	1/1	0.69	0.44	77,77,77,77	0
24	MG	A	2741	1/1	0.71	0.64	105,105,105,105	0
24	MG	A	2744	1/1	0.71	0.61	90,90,90,90	0
24	MG	A	2714	1/1	0.72	0.59	92,92,92,92	0
24	MG	A	2609	1/1	0.72	0.66	94,94,94,94	0
24	MG	A	2698	1/1	0.72	0.79	115,115,115,115	0
24	MG	A	2621	1/1	0.72	0.39	105,105,105,105	0
24	MG	A	2683	1/1	0.72	0.59	116,116,116,116	0
24	MG	A	2662	1/1	0.73	0.68	109,109,109,109	0
25	K	A	2682	1/1	0.73	0.42	147,147,147,147	0
24	MG	A	2747	1/1	0.74	1.23	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	MG	A	2639	1/1	0.74	0.37	129,129,129,129	0
24	MG	A	2728	1/1	0.74	0.58	108,108,108,108	0
24	MG	A	2624	1/1	0.75	0.45	89,89,89,89	0
24	MG	A	2731	1/1	0.75	1.29	88,88,88,88	0
24	MG	A	2644	1/1	0.77	0.58	121,121,121,121	0
24	MG	A	2695	1/1	0.77	0.38	98,98,98,98	0
24	MG	A	2653	1/1	0.77	0.42	98,98,98,98	0
24	MG	H	1139	1/1	0.77	0.33	100,100,100,100	0
24	MG	A	2582	1/1	0.77	0.56	85,85,85,85	0
24	MG	A	2742	1/1	0.78	2.29	106,106,106,106	0
24	MG	A	2739	1/1	0.79	0.48	101,101,101,101	0
24	MG	A	2726	1/1	0.79	1.68	106,106,106,106	0
25	K	A	2674	1/1	0.80	0.19	133,133,133,133	0
24	MG	A	2641	1/1	0.80	0.28	98,98,98,98	0
24	MG	A	2629	1/1	0.80	0.72	78,78,78,78	0
24	MG	A	2688	1/1	0.80	2.29	109,109,109,109	0
24	MG	A	2553	1/1	0.81	0.40	69,69,69,69	0
24	MG	A	2569	1/1	0.81	0.92	83,83,83,83	0
24	MG	A	2589	1/1	0.81	0.15	93,93,93,93	0
24	MG	A	2593	1/1	0.81	0.20	112,112,112,112	0
24	MG	A	2617	1/1	0.81	0.97	72,72,72,72	0
24	MG	A	2575	1/1	0.81	0.61	108,108,108,108	0
24	MG	A	2576	1/1	0.81	0.31	83,83,83,83	0
24	MG	A	2651	1/1	0.81	0.27	78,78,78,78	0
24	MG	A	2724	1/1	0.81	1.35	95,95,95,95	0
24	MG	A	2551	1/1	0.81	0.28	121,121,121,121	0
24	MG	A	2625	1/1	0.81	1.07	81,81,81,81	0
25	K	A	2800	1/1	0.81	0.19	153,153,153,153	1
24	MG	A	2711	1/1	0.82	1.08	103,103,103,103	0
24	MG	A	2633	1/1	0.82	0.22	87,87,87,87	0
24	MG	A	2666	1/1	0.82	0.35	87,87,87,87	0
24	MG	A	2697	1/1	0.82	0.26	92,92,92,92	0
24	MG	A	2648	1/1	0.83	0.30	89,89,89,89	0
25	K	A	2673	1/1	0.83	0.57	126,126,126,126	0
24	MG	A	2577	1/1	0.83	0.60	94,94,94,94	0
24	MG	A	2743	1/1	0.83	1.72	121,121,121,121	0
24	MG	A	2590	1/1	0.83	0.92	76,76,76,76	0
24	MG	A	2566	1/1	0.83	0.40	91,91,91,91	0
24	MG	F	1102	1/1	0.83	0.15	128,128,128,128	0
24	MG	A	2630	1/1	0.83	0.21	99,99,99,99	0
24	MG	A	2720	1/1	0.83	1.42	128,128,128,128	0
24	MG	A	2699	1/1	0.83	0.29	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	2608	1/1	0.83	0.23	106,106,106,106	0
24	MG	A	2581	1/1	0.84	0.45	69,69,69,69	0
24	MG	A	2692	1/1	0.84	0.30	69,69,69,69	0
24	MG	A	2604	1/1	0.84	0.38	89,89,89,89	0
24	MG	A	2745	1/1	0.84	0.64	101,101,101,101	0
24	MG	A	2700	1/1	0.84	0.52	115,115,115,115	0
24	MG	A	2660	1/1	0.84	0.17	128,128,128,128	0
24	MG	A	2719	1/1	0.84	1.21	96,96,96,96	0
24	MG	A	2594	1/1	0.85	0.41	100,100,100,100	0
24	MG	A	2664	1/1	0.85	0.58	97,97,97,97	0
24	MG	A	2558	1/1	0.85	1.70	74,74,74,74	0
24	MG	A	2646	1/1	0.85	0.26	96,96,96,96	0
24	MG	A	2606	1/1	0.86	0.39	83,83,83,83	0
24	MG	A	2636	1/1	0.86	0.20	92,92,92,92	0
24	MG	A	2598	1/1	0.86	0.56	60,60,60,60	0
24	MG	A	2658	1/1	0.86	0.14	121,121,121,121	0
24	MG	G	1158	1/1	0.86	0.35	112,112,112,112	1
24	MG	A	2603	1/1	0.87	0.72	135,135,135,135	0
24	MG	A	2713	1/1	0.87	0.43	104,104,104,104	0
24	MG	A	2619	1/1	0.87	0.71	82,82,82,82	0
24	MG	A	2642	1/1	0.87	0.47	101,101,101,101	0
24	MG	W	1008	1/1	0.87	0.52	157,157,157,157	1
24	MG	A	2597	1/1	0.87	0.21	80,80,80,80	0
24	MG	A	2717	1/1	0.87	0.29	99,99,99,99	0
24	MG	A	2559	1/1	0.87	0.34	81,81,81,81	0
24	MG	A	2710	1/1	0.87	0.33	99,99,99,99	0
24	MG	A	2723	1/1	0.88	1.24	79,79,79,79	0
24	MG	A	2595	1/1	0.88	0.94	112,112,112,112	0
24	MG	A	2622	1/1	0.88	0.31	73,73,73,73	0
24	MG	A	2614	1/1	0.88	0.18	83,83,83,83	0
24	MG	A	2637	1/1	0.88	0.21	110,110,110,110	0
24	MG	A	2605	1/1	0.88	0.24	79,79,79,79	0
24	MG	A	2632	1/1	0.88	0.44	89,89,89,89	0
24	MG	A	2703	1/1	0.88	0.83	101,101,101,101	0
24	MG	A	2705	1/1	0.88	0.26	104,104,104,104	0
24	MG	A	2665	1/1	0.88	0.33	89,89,89,89	0
24	MG	A	2654	1/1	0.88	0.48	112,112,112,112	1
24	MG	A	2655	1/1	0.89	0.33	76,76,76,76	0
24	MG	A	2561	1/1	0.89	0.61	66,66,66,66	0
25	K	V	1026	1/1	0.89	0.36	132,132,132,132	0
24	MG	A	2702	1/1	0.90	0.55	94,94,94,94	0
24	MG	A	2712	1/1	0.90	0.26	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	2571	1/1	0.90	0.33	49,49,49,49	0
24	MG	A	2732	1/1	0.90	0.22	88,88,88,88	1
24	MG	A	2612	1/1	0.90	0.64	92,92,92,92	0
24	MG	A	2706	1/1	0.90	0.37	87,87,87,87	0
24	MG	A	2568	1/1	0.90	0.27	91,91,91,91	0
24	MG	A	2638	1/1	0.90	0.16	79,79,79,79	0
24	MG	A	2647	1/1	0.91	0.17	60,60,60,60	0
24	MG	A	2691	1/1	0.91	0.61	94,94,94,94	0
24	MG	A	2729	1/1	0.91	0.22	96,96,96,96	1
24	MG	A	2628	1/1	0.91	0.27	95,95,95,95	0
24	MG	A	2650	1/1	0.91	0.24	72,72,72,72	0
24	MG	A	2734	1/1	0.91	1.82	113,113,113,113	0
24	MG	A	2746	1/1	0.91	0.58	85,85,85,85	0
24	MG	A	2545	1/1	0.91	0.28	122,122,122,122	0
24	MG	A	2583	1/1	0.91	0.72	83,83,83,83	0
24	MG	A	2694	1/1	0.92	0.31	88,88,88,88	0
24	MG	A	2709	1/1	0.92	0.36	79,79,79,79	0
24	MG	A	2560	1/1	0.92	0.37	46,46,46,46	0
24	MG	A	2546	1/1	0.92	0.20	100,100,100,100	0
24	MG	A	2656	1/1	0.93	0.31	90,90,90,90	0
24	MG	A	2564	1/1	0.93	0.37	57,57,57,57	0
24	MG	L	1129	1/1	0.93	0.24	59,59,59,59	0
24	MG	A	2635	1/1	0.93	0.19	95,95,95,95	0
24	MG	A	2727	1/1	0.93	0.98	107,107,107,107	0
24	MG	A	2652	1/1	0.93	0.20	70,70,70,70	0
25	K	A	2677	1/1	0.93	0.33	117,117,117,117	0
26	AM2	A	3001	37/37	0.93	0.20	103,105,119,121	0
26	AM2	A	3002	37/37	0.93	0.42	116,119,127,128	0
26	AM2	A	3003	37/37	0.93	0.22	110,114,122,124	0
24	MG	A	2730	1/1	0.94	1.11	70,70,70,70	0
24	MG	A	2623	1/1	0.94	0.57	56,56,56,56	0
24	MG	A	2693	1/1	0.94	0.35	89,89,89,89	0
24	MG	A	2733	1/1	0.94	0.84	93,93,93,93	0
24	MG	A	2587	1/1	0.94	1.02	129,129,129,129	0
24	MG	A	2579	1/1	0.94	0.48	94,94,94,94	0
24	MG	A	2736	1/1	0.94	0.74	103,103,103,103	0
24	MG	A	2573	1/1	0.94	0.11	72,72,72,72	0
26	AM2	A	3004	37/37	0.94	0.25	130,133,141,143	0
26	AM2	A	3005	37/37	0.94	0.23	126,131,135,136	0
24	MG	G	1157	1/1	0.95	0.13	134,134,134,134	1
24	MG	A	2659	1/1	0.95	0.28	80,80,80,80	0
24	MG	A	2685	1/1	0.95	0.36	23,23,23,23	0

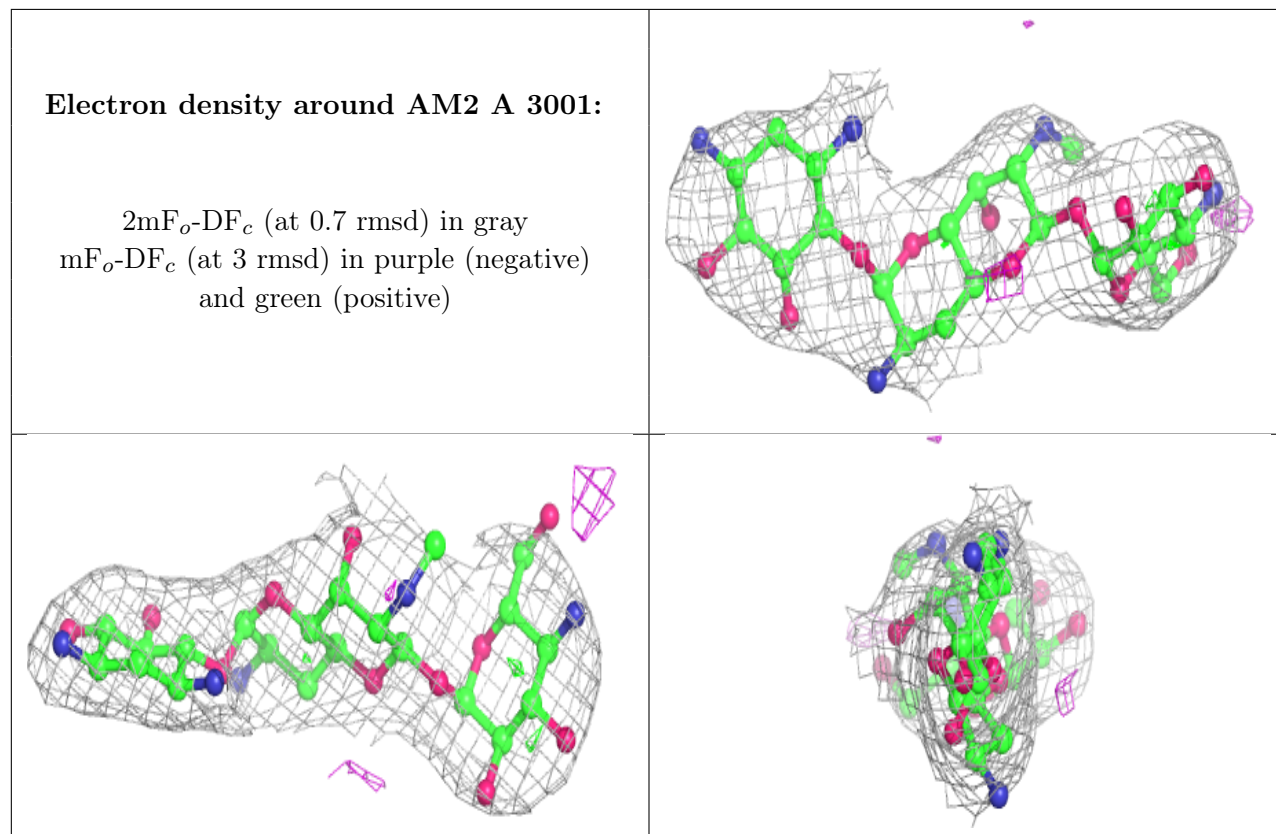
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	J	1101	1/1	0.95	0.21	68,68,68,68	0
24	MG	A	2627	1/1	0.95	0.32	75,75,75,75	0
24	MG	A	2570	1/1	0.95	0.55	97,97,97,97	0
24	MG	A	2602	1/1	0.95	0.39	81,81,81,81	0
24	MG	A	2643	1/1	0.95	0.36	92,92,92,92	0
24	MG	A	2718	1/1	0.95	0.58	60,60,60,60	0
24	MG	A	2572	1/1	0.96	0.36	89,89,89,89	0
24	MG	A	2585	1/1	0.96	0.97	78,78,78,78	0
24	MG	A	2738	1/1	0.96	1.17	94,94,94,94	0
24	MG	A	2599	1/1	0.96	0.18	58,58,58,58	0
24	MG	A	2645	1/1	0.96	0.46	78,78,78,78	0
24	MG	D	1211	1/1	0.96	0.20	82,82,82,82	0
24	MG	Z	1043	1/1	0.96	0.16	123,123,123,123	0
24	MG	A	2567	1/1	0.96	0.29	69,69,69,69	0
24	MG	A	2690	1/1	0.96	0.14	56,56,56,56	0
24	MG	A	2737	1/1	0.97	0.69	61,61,61,61	0
24	MG	W	1007	1/1	0.97	0.06	81,81,81,81	0
24	MG	A	2574	1/1	0.97	0.20	2,2,2,2	0
24	MG	A	2686	1/1	0.97	0.27	140,140,140,140	0
24	MG	A	2620	1/1	0.97	0.09	89,89,89,89	1
24	MG	A	2704	1/1	0.97	0.36	94,94,94,94	0
24	MG	K	1130	1/1	0.97	0.12	69,69,69,69	0
24	MG	A	2657	1/1	0.97	0.09	132,132,132,132	0
24	MG	A	2707	1/1	0.98	0.22	78,78,78,78	0
24	MG	A	2610	1/1	0.98	0.81	75,75,75,75	0
24	MG	A	2586	1/1	0.98	0.34	58,58,58,58	0
24	MG	A	2607	1/1	0.98	0.33	69,69,69,69	0
24	MG	A	2556	1/1	0.98	0.20	114,114,114,114	1
24	MG	A	2588	1/1	0.98	0.44	71,71,71,71	0
24	MG	A	2668	1/1	0.98	0.20	97,97,97,97	0
24	MG	M	1127	1/1	0.98	0.24	104,104,104,104	0
24	MG	A	2640	1/1	0.99	0.13	74,74,74,74	0
24	MG	A	2591	1/1	0.99	0.35	74,74,74,74	0
24	MG	A	2592	1/1	0.99	0.20	78,78,78,78	0
24	MG	A	2547	1/1	0.99	0.27	125,125,125,125	0
24	MG	A	2649	1/1	0.99	0.22	65,65,65,65	0
24	MG	A	2578	1/1	0.99	0.52	66,66,66,66	0
24	MG	A	2669	1/1	0.99	0.05	114,114,114,114	0
27	ZN	N	1062	1/1	0.99	0.22	172,172,172,172	0
27	ZN	D	1210	1/1	1.00	0.22	138,138,138,138	0
24	MG	A	2616	1/1	1.00	0.26	57,57,57,57	0

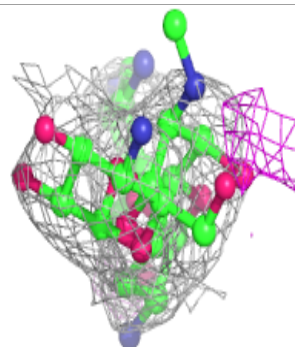
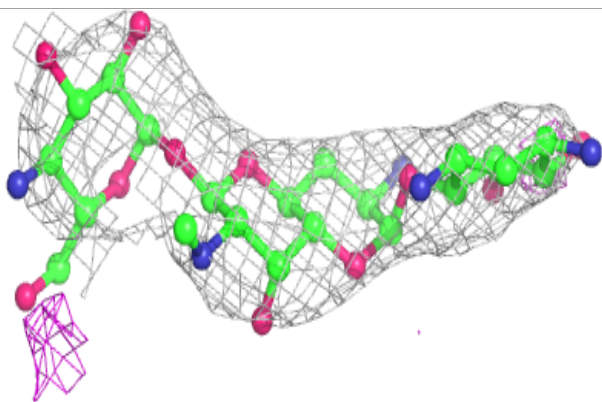
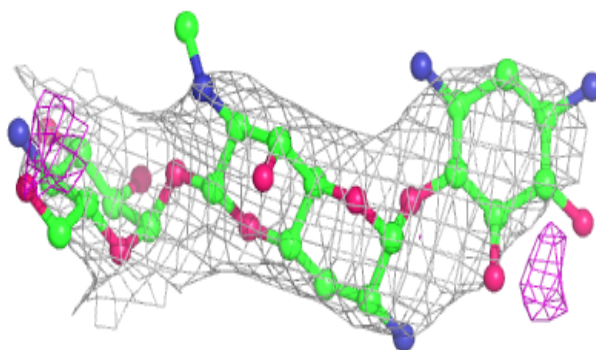
The following is a graphical depiction of the model fit to experimental electron density of all

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.

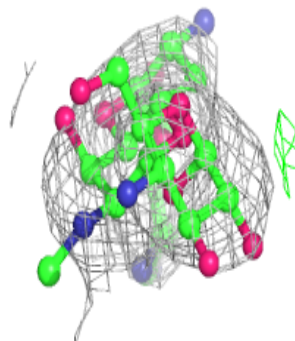
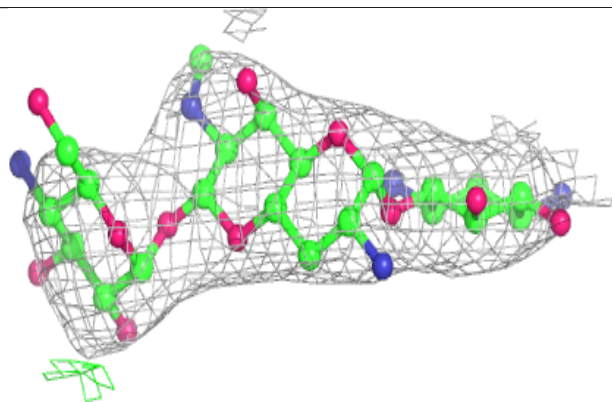


Electron density around AM2 A 3002:

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

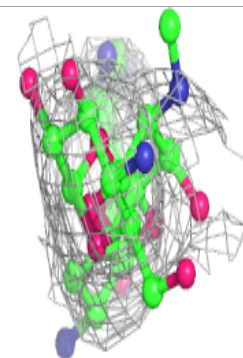
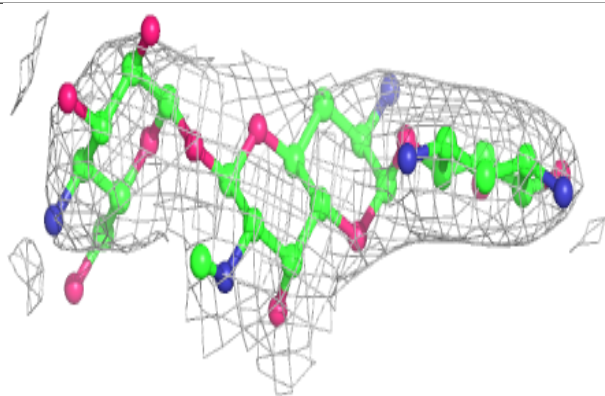
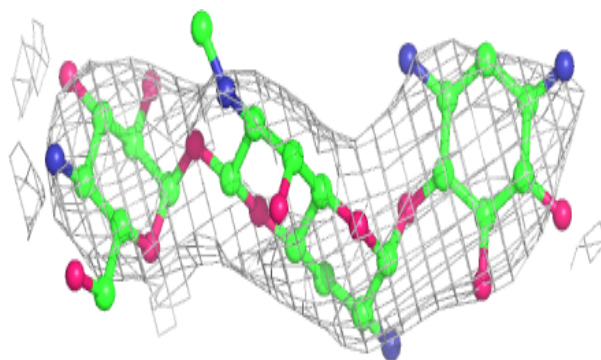
**Electron density around AM2 A 3003:**

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

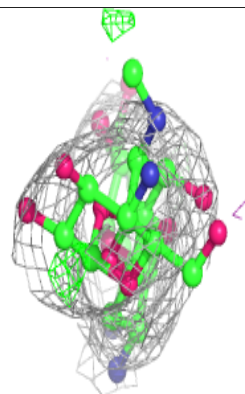
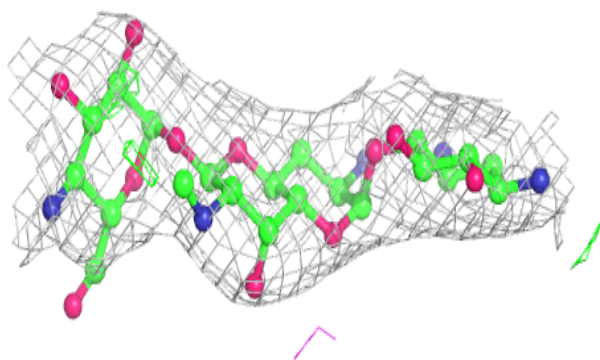
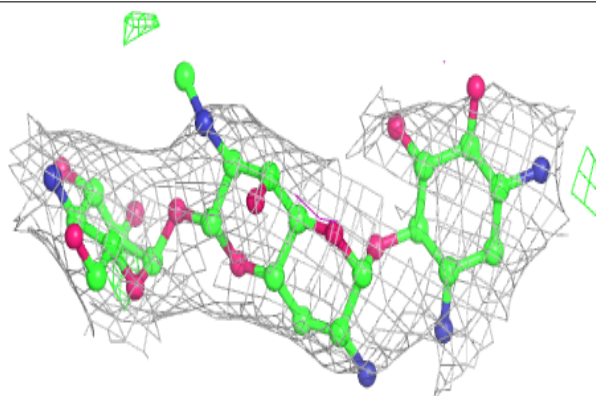


Electron density around AM2 A 3004:

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

**Electron density around AM2 A 3005:**

$2mF_o-DF_c$ (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.