



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2022 – 02:14 PM EDT

PDB ID : 6MN4
Title : Crystal structure of aminoglycoside acetyltransferase AAC(3)-IVa, H154A mutant, in complex with apramycin
Authors : Stogios, P.J.; Evdokimova, E.; Michalska, K.; Di Leo, R.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2018-10-01
Resolution : 2.80 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 ⓘ symbol.

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

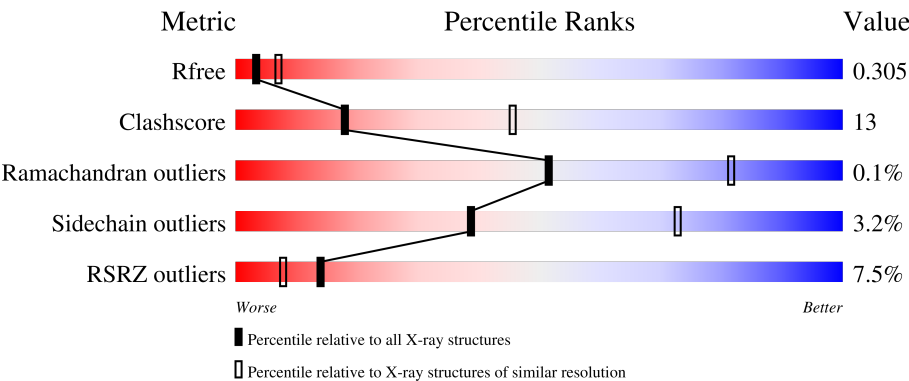
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	260	<div><div>81%18%.</div></div>
1	B	260	<div><div>79%19%..</div></div>
1	C	260	<div><div>75%22%..</div></div>
1	D	260	<div><div>70%28%..</div></div>
1	E	260	<div><div>14%62%36%..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	260	

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
2	AM2	F	301	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12349 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 Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1957	1243	347	359	8			
1	B	258	Total	C	N	O	S	0	0	0
			1961	1246	348	359	8			
1	C	258	Total	C	N	O	S	0	0	0
			1961	1246	348	359	8			
1	D	258	Total	C	N	O	S	0	0	0
			1961	1246	348	359	8			
1	E	258	Total	C	N	O	S	0	0	0
			1954	1240	347	359	8			
1	F	242	Total	C	N	O	S	0	0	0
			1833	1164	325	336	8			

There are 18 discrepancies between the modelled and reference sequences:

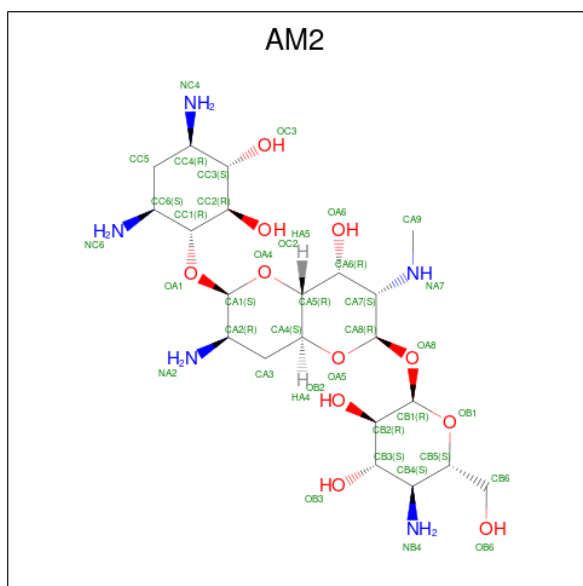
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP Q306W4
A	0	GLY	-	expression tag	UNP Q306W4
A	154	ALA	HIS	engineered mutation	UNP Q306W4
B	-1	GLN	-	expression tag	UNP Q306W4
B	0	GLY	-	expression tag	UNP Q306W4
B	154	ALA	HIS	engineered mutation	UNP Q306W4
C	-1	GLN	-	expression tag	UNP Q306W4
C	0	GLY	-	expression tag	UNP Q306W4
C	154	ALA	HIS	engineered mutation	UNP Q306W4
D	-1	GLN	-	expression tag	UNP Q306W4
D	0	GLY	-	expression tag	UNP Q306W4
D	154	ALA	HIS	engineered mutation	UNP Q306W4
E	-1	GLN	-	expression tag	UNP Q306W4
E	0	GLY	-	expression tag	UNP Q306W4
E	154	ALA	HIS	engineered mutation	UNP Q306W4
F	-1	GLN	-	expression tag	UNP Q306W4
F	0	GLY	-	expression tag	UNP Q306W4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	154	ALA	HIS	engineered mutation	UNP Q306W4

- Molecule 2 is APRAMYCIN (three-letter code: AM2) (formula: $C_{21}H_{41}N_5O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	21	5	11		
2	B	1	Total	C	N	O	0	0
			37	21	5	11		
2	C	1	Total	C	N	O	0	0
			37	21	5	11		
2	D	1	Total	C	N	O	0	0
			37	21	5	11		
2	E	1	Total	C	N	O	0	0
			37	21	5	11		
2	F	1	Total	C	N	O	0	0
			37	21	5	11		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

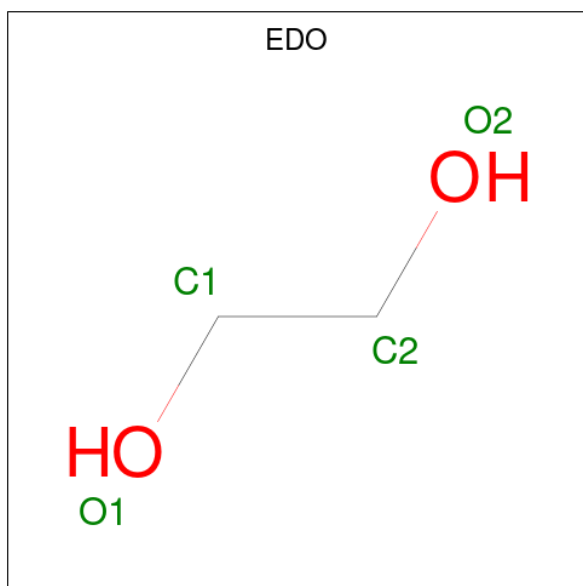
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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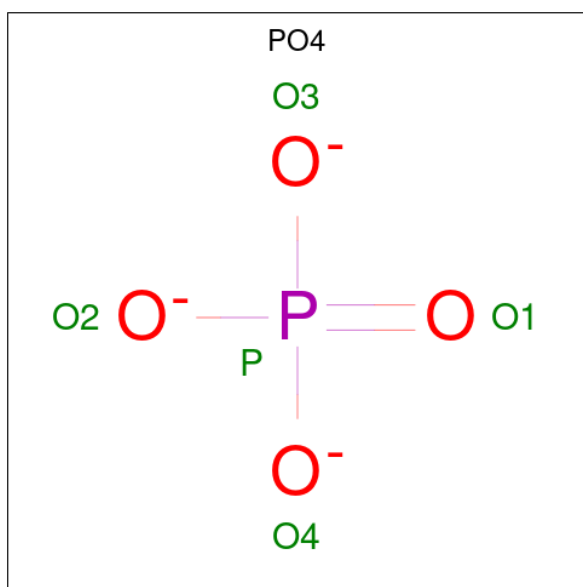
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



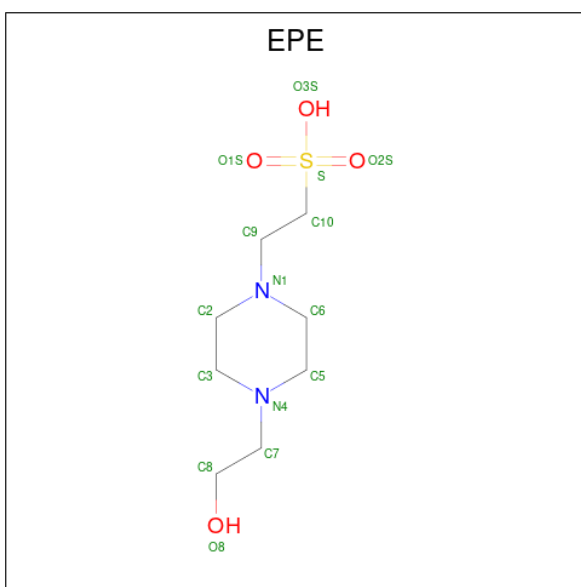
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



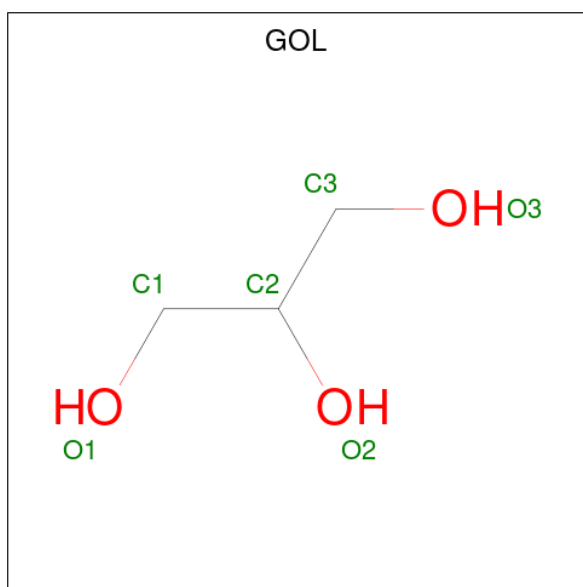
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

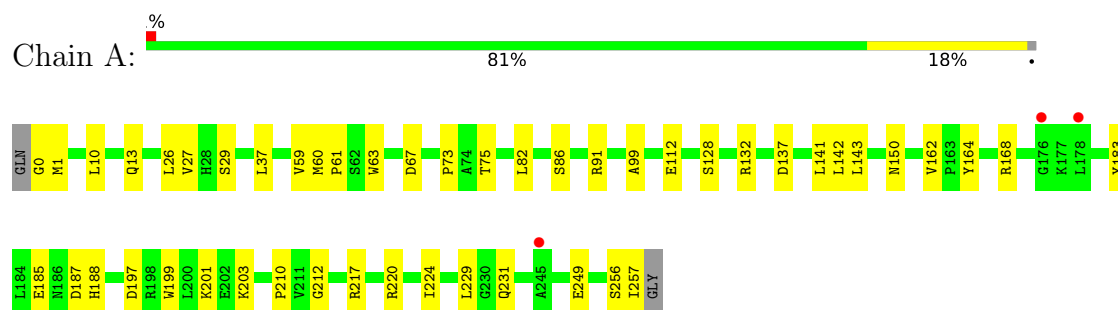
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	77	Total	O	0	0
			77	77		
8	B	100	Total	O	0	0
			100	100		
8	C	49	Total	O	0	1
			50	50		
8	D	49	Total	O	0	0
			49	49		
8	E	36	Total	O	0	0
			36	36		
8	F	28	Total	O	0	0
			28	28		

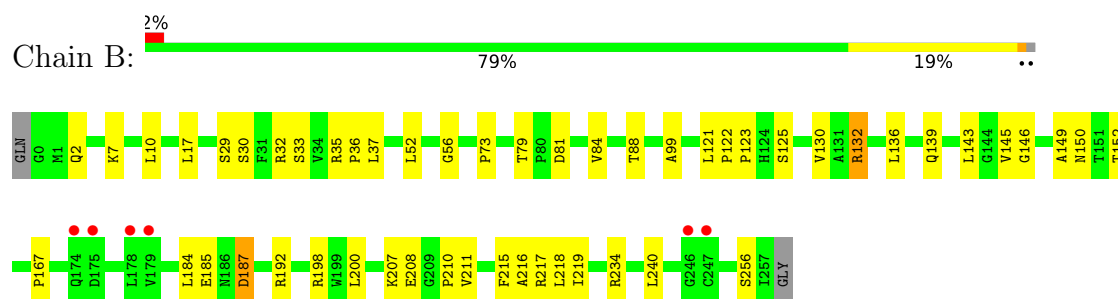
3 Residue-property plots

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.

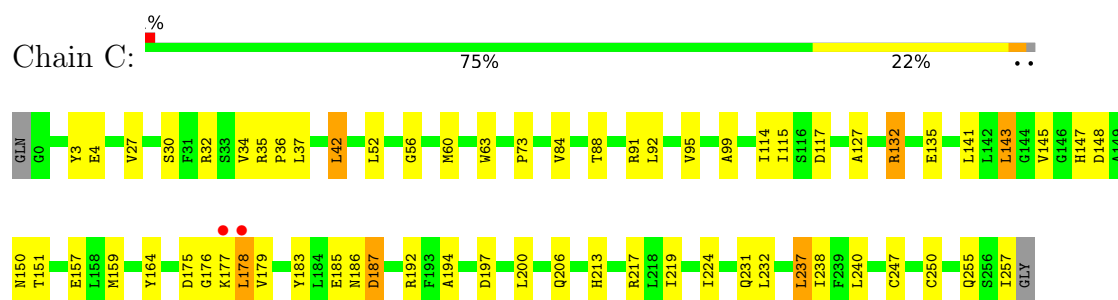
- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa



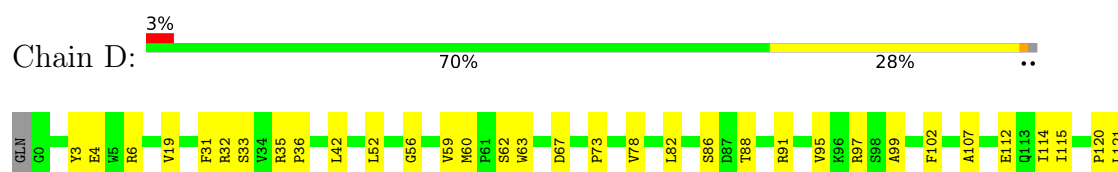
- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa

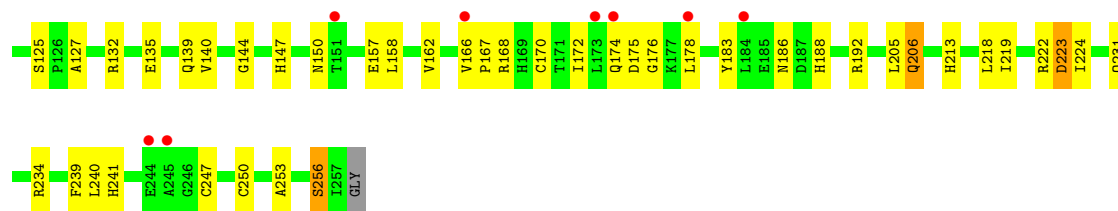


- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa

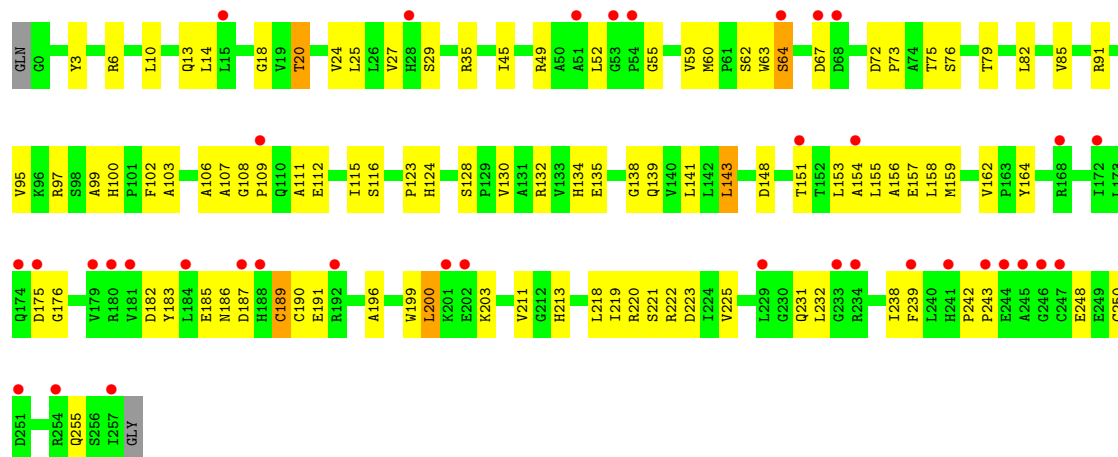


- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa

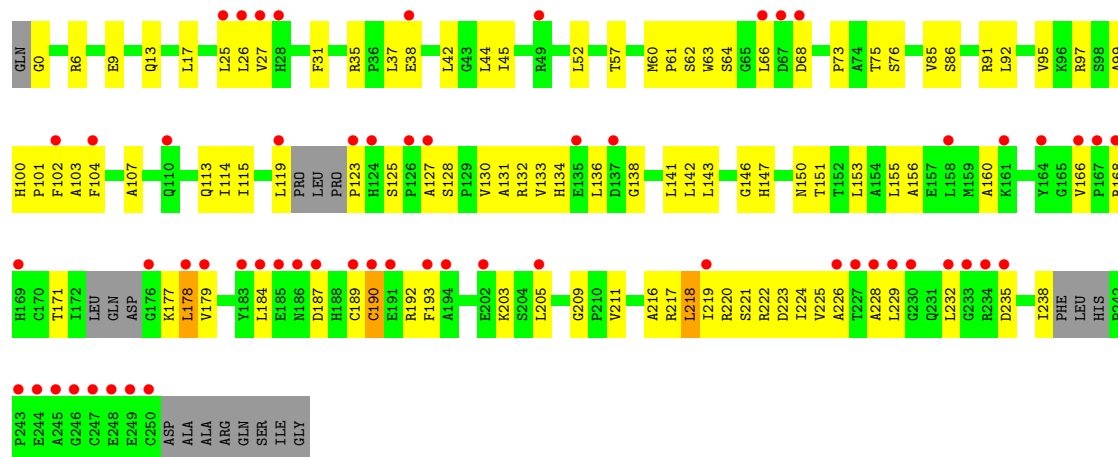




• Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa



• Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.55Å 130.51Å 264.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.33 – 2.80 29.33 – 2.73	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.33-2.80) 76.9 (29.33-2.73)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.07 (at 2.72Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, R_{free}	0.247 , 0.304 0.248 , 0.305	Depositor DCC
R_{free} test set	1984 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12349	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: EDO, EPE, AM2, ZN, GOL, PO4

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	0.28	0/2008	0.46	0/2742
1	B	0.29	0/2012	0.47	0/2746
1	C	0.26	0/2012	0.47	0/2746
1	D	0.31	0/2012	0.49	1/2746 (0.0%)
1	E	0.32	0/2005	0.60	1/2738 (0.0%)
1	F	0.31	0/1877	0.61	0/2554
All	All	0.30	0/11926	0.52	2/16272 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	GLY	N-CA-C	6.27	128.77	113.10
1	E	176	GLY	C-N-CA	-5.33	108.39	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1957	0	1946	30	0
1	B	1961	0	1957	30	0
1	C	1961	0	1957	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1961	0	1958	55	0
1	E	1954	0	1940	73	0
1	F	1833	0	1833	84	0
2	A	37	0	41	1	0
2	B	37	0	41	5	0
2	C	37	0	41	4	0
2	D	37	0	41	2	0
2	E	37	0	41	1	0
2	F	37	0	41	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	24	0	0
4	B	4	0	6	0	0
4	E	4	0	6	0	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
5	C	5	0	0	0	0
5	D	5	0	0	1	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	A	15	0	17	0	0
6	B	15	0	17	3	0
6	C	15	0	17	3	0
6	D	15	0	17	0	0
6	E	15	0	17	1	0
6	F	15	0	17	2	0
7	D	6	0	8	0	0
7	E	6	0	8	0	0
8	A	77	0	0	2	0
8	B	100	0	0	0	0
8	C	50	0	0	0	0
8	D	49	0	0	0	0
8	E	36	0	0	1	0
8	F	28	0	0	2	0
All	All	12349	0	11991	323	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 13.

All (323) 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:E:29:SER:HA	1:E:143:LEU:HB3	1.67	0.76
1:D:240:LEU:HD11	1:D:253:ALA:HB3	1.65	0.76
1:F:31:PHE:O	1:F:35:ARG:HG2	1.90	0.71
1:E:115:ILE:HD12	1:E:116:SER:N	2.06	0.70
1:F:60:MET:CE	1:F:86:SER:HA	2.24	0.68
1:F:205:LEU:HD13	1:F:223:ASP:OD2	1.93	0.68
1:C:117:ASP:OD2	1:C:132:ARG:NH1	2.27	0.67
1:D:52:LEU:HB3	1:D:56:GLY:HA3	1.77	0.67
1:D:140:VAL:HG11	1:D:224:ILE:HD12	1.78	0.66
1:F:223:ASP:O	1:F:226:ALA:N	2.29	0.66
1:E:27:VAL:HG22	1:E:60:MET:HG2	1.79	0.65
1:F:63:TRP:HA	1:F:103:ALA:H	1.60	0.65
1:D:247:CYS:HB3	1:D:250:CYS:HB2	1.77	0.65
1:D:102:PHE:HD1	1:D:120:PRO:HD2	1.63	0.64
1:D:157:GLU:OE1	1:D:186:ASN:ND2	2.30	0.64
1:E:132:ARG:HA	1:E:135:GLU:HG2	1.79	0.64
1:D:125:SER:HA	1:D:158:LEU:HD22	1.80	0.64
1:B:187:ASP:OD2	2:B:301:AM2:NA2	2.32	0.63
1:E:108:GLY:N	1:E:111:ALA:HB2	2.14	0.63
1:F:141:LEU:HD13	1:F:218:LEU:HG	1.81	0.63
1:F:218:LEU:C	1:F:219:ILE:HD13	2.19	0.62
1:F:219:ILE:HB	1:F:224:ILE:HD11	1.81	0.61
1:C:63:TRP:HH2	1:C:151:THR:HG21	1.65	0.61
1:A:27:VAL:HG22	1:A:60:MET:HG2	1.82	0.61
1:C:187:ASP:CG	2:C:301:AM2:NA2	2.54	0.61
1:B:192:ARG:NH1	1:B:240:LEU:O	2.34	0.61
1:F:235:ASP:HB3	1:F:238:ILE:HB	1.82	0.60
1:F:37:LEU:O	6:F:303:EPE:H102	2.02	0.60
1:D:188:HIS:HB2	1:D:240:LEU:HD21	1.83	0.60
1:B:30:SER:HB2	1:B:145:VAL:HG23	1.84	0.60
1:D:192:ARG:HD3	1:D:239:PHE:C	2.22	0.60
1:E:138:GLY:O	1:E:221:SER:N	2.27	0.59
1:E:232:LEU:HD21	1:E:239:PHE:CE2	2.37	0.59
1:F:136:LEU:HD23	1:F:136:LEU:O	2.02	0.59
1:A:197:ASP:OD1	1:A:217:ARG:NH1	2.35	0.59
1:C:176:GLY:O	1:C:177:LYS:HB2	2.02	0.59
1:F:134:HIS:CD2	1:F:155:LEU:HD11	2.36	0.59
1:B:211:VAL:HG12	1:B:216:ALA:HB2	1.85	0.59
1:F:168:ARG:HH12	2:F:301:AM2:HA32	1.68	0.59
1:E:189:CYS:SG	1:E:190:CYS:N	2.76	0.59
1:F:134:HIS:CE1	1:F:222:ARG:NH1	2.71	0.59
1:F:45:ILE:HD11	1:F:85:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:SER:HB2	1:F:101:PRO:O	2.01	0.58
1:D:205:LEU:HD13	1:D:223:ASP:HB3	1.85	0.58
1:E:156:ALA:HB2	1:E:225:VAL:HG23	1.85	0.58
1:C:73:PRO:HG3	1:C:99:ALA:HA	1.84	0.58
1:E:63:TRP:CZ2	1:E:82:LEU:HD21	2.39	0.58
1:E:159:MET:CE	1:E:225:VAL:HG21	2.34	0.57
1:F:76:SER:O	1:F:97:ARG:NH2	2.37	0.57
1:A:142:LEU:HB2	1:A:217:ARG:HB2	1.85	0.57
1:F:189:CYS:O	1:F:190:CYS:SG	2.61	0.57
1:F:17:LEU:HD23	1:F:209:GLY:HA3	1.87	0.57
1:A:256:SER:O	1:A:257:ILE:HG13	2.05	0.57
1:C:177:LYS:O	1:C:179:VAL:HG23	2.04	0.57
1:E:232:LEU:HD11	1:E:239:PHE:CZ	2.40	0.56
1:E:59:VAL:HG13	1:E:106:ALA:HB2	1.88	0.56
1:C:132:ARG:HA	1:C:135:GLU:HG2	1.86	0.56
1:F:101:PRO:HD2	1:F:119:LEU:HD13	1.88	0.56
1:F:134:HIS:HE1	1:F:222:ARG:NH1	2.03	0.55
1:F:95:VAL:HG13	1:F:107:ALA:HB2	1.89	0.55
1:E:134:HIS:CE1	1:E:222:ARG:HG3	2.41	0.55
1:F:62:SER:O	1:F:103:ALA:HB3	2.07	0.55
1:F:160:ALA:HB3	1:F:232:LEU:HD13	1.87	0.55
1:E:255:GLN:NE2	8:E:401:HOH:O	2.40	0.55
1:F:35:ARG:NH2	6:F:303:EPE:O3S	2.34	0.55
1:D:91:ARG:HD2	1:E:91:ARG:HD2	1.89	0.55
1:B:32:ARG:N	5:B:304:PO4:O4	2.38	0.55
1:F:60:MET:HE1	1:F:86:SER:HA	1.87	0.55
1:C:197:ASP:OD2	1:C:217:ARG:NH1	2.40	0.55
1:D:31:PHE:O	1:D:35:ARG:HG3	2.06	0.55
1:A:201:LYS:NZ	8:A:401:HOH:O	2.40	0.54
1:F:6:ARG:HA	1:F:38:GLU:HG2	1.89	0.54
1:A:137:ASP:OD1	1:A:220:ARG:NH1	2.41	0.54
1:E:232:LEU:HD11	1:E:239:PHE:CE2	2.43	0.54
1:F:146:GLY:HA2	1:F:217:ARG:HH21	1.72	0.54
1:A:168:ARG:NH1	1:A:187:ASP:OD2	2.41	0.54
1:E:157:GLU:OE1	1:E:186:ASN:ND2	2.41	0.54
1:E:220:ARG:O	1:E:223:ASP:N	2.37	0.54
1:E:248:GLU:O	1:E:248:GLU:HG2	2.08	0.54
1:E:139:GLN:HE21	1:E:218:LEU:HD21	1.73	0.53
1:F:42:LEU:HD12	1:F:42:LEU:H	1.72	0.53
1:F:64:SER:O	1:F:66:LEU:HD22	2.09	0.53
1:E:112:GLU:OE1	1:E:112:GLU:N	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:HIS:HB2	1:F:101:PRO:HD2	1.91	0.53
1:F:177:LYS:HG3	1:F:178:LEU:N	2.23	0.53
1:C:92:LEU:O	1:C:95:VAL:HG12	2.09	0.53
1:C:157:GLU:OE1	1:C:164:TYR:OH	2.23	0.53
1:E:107:ALA:C	1:E:111:ALA:HB2	2.29	0.53
1:E:64:SER:O	1:E:79:THR:HB	2.08	0.53
1:F:166:VAL:HG23	1:F:168:ARG:HG2	1.91	0.53
1:B:35:ARG:NH1	6:B:305:EPE:O2S	2.41	0.53
2:B:301:AM2:NC6	2:B:301:AM2:HA1	2.23	0.53
1:C:30:SER:HB2	1:C:145:VAL:HG13	1.91	0.53
1:C:187:ASP:OD2	2:C:301:AM2:HA32	2.09	0.52
1:E:189:CYS:SG	1:E:191:GLU:N	2.78	0.52
1:F:68:ASP:HA	1:F:171:THR:OG1	2.09	0.52
1:A:27:VAL:HG12	1:A:141:LEU:HB3	1.92	0.52
1:D:112:GLU:HA	1:D:115:ILE:HD11	1.90	0.52
1:B:132:ARG:O	1:B:136:LEU:HD12	2.09	0.52
1:C:197:ASP:OD1	1:C:206:GLN:NE2	2.35	0.52
1:F:223:ASP:HA	1:F:226:ALA:HB3	1.91	0.52
1:F:60:MET:HE2	1:F:86:SER:HA	1.91	0.52
1:F:224:ILE:HD12	1:F:224:ILE:H	1.75	0.52
1:F:150:ASN:HB3	1:F:153:LEU:HD12	1.91	0.52
1:F:218:LEU:O	1:F:219:ILE:HD13	2.10	0.52
1:C:127:ALA:HA	1:C:132:ARG:HH11	1.74	0.51
1:E:162:VAL:HG11	1:E:164:TYR:CZ	2.45	0.51
1:F:177:LYS:HE2	1:F:178:LEU:HD23	1.91	0.51
1:C:35:ARG:NH2	6:C:304:EPE:O1S	2.30	0.51
1:E:158:LEU:HD21	1:E:186:ASN:OD1	2.11	0.51
1:C:114:ILE:HG22	1:C:115:ILE:HG23	1.93	0.51
1:D:167:PRO:C	1:D:168:ARG:HG2	2.31	0.51
1:D:62:SER:HG	1:D:97:ARG:HE	1.57	0.51
1:D:256:SER:OG	1:D:256:SER:O	2.26	0.51
1:E:72:ASP:HB3	1:E:75:THR:HB	1.91	0.51
1:E:151:THR:O	1:E:154:ALA:HB3	2.10	0.51
1:F:189:CYS:SG	1:F:190:CYS:N	2.84	0.51
1:D:140:VAL:CG1	1:D:224:ILE:HD12	2.41	0.50
1:E:128:SER:HB3	1:E:130:VAL:HG22	1.92	0.50
1:D:4:GLU:HG2	1:D:36:PRO:HB2	1.92	0.50
1:A:162:VAL:HG11	1:A:164:TYR:CZ	2.47	0.50
1:F:203:LYS:HB3	1:F:205:LEU:CD1	2.42	0.50
1:F:223:ASP:O	1:F:224:ILE:C	2.50	0.50
1:A:112:GLU:OE2	1:A:112:GLU:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:ARG:NH1	1:F:187:ASP:OD2	2.44	0.50
1:A:29:SER:HA	1:A:143:LEU:HB3	1.92	0.49
1:A:75:THR:HG22	1:B:84:VAL:HG11	1.94	0.49
1:E:67:ASP:OD2	1:E:67:ASP:N	2.36	0.49
1:C:200:LEU:HD13	1:C:219:ILE:HG21	1.93	0.49
1:D:231:GLN:OE1	1:D:234:ARG:NH2	2.46	0.49
1:B:79:THR:OG1	1:B:81:ASP:OD2	2.27	0.49
1:B:145:VAL:HG11	1:B:149:ALA:HB3	1.93	0.49
1:B:200:LEU:HD13	1:B:219:ILE:HD13	1.93	0.49
2:D:301:AM2:HA1	2:D:301:AM2:NC6	2.26	0.49
1:F:228:ALA:O	1:F:232:LEU:HG	2.13	0.49
1:B:73:PRO:HG3	1:B:99:ALA:HA	1.94	0.49
1:F:147:HIS:HA	1:F:150:ASN:HB2	1.94	0.49
1:D:168:ARG:NH2	2:D:301:AM2:HA5	2.28	0.49
1:E:183:TYR:CE1	1:E:185:GLU:HB2	2.48	0.48
1:F:57:THR:HG21	1:F:114:ILE:HD11	1.94	0.48
1:C:183:TYR:CE1	1:C:185:GLU:HB2	2.48	0.48
1:D:88:THR:HG23	1:E:91:ARG:HB3	1.95	0.48
1:A:73:PRO:HG3	1:A:99:ALA:HA	1.94	0.48
1:B:32:ARG:HG3	1:B:33:SER:N	2.29	0.48
1:C:141:LEU:HD21	1:C:143:LEU:HD12	1.95	0.48
1:C:183:TYR:HE1	1:C:185:GLU:HB2	1.78	0.48
1:F:64:SER:CB	1:F:101:PRO:O	2.60	0.48
1:C:84:VAL:HG21	1:F:75:THR:HA	1.95	0.48
1:A:203:LYS:NZ	8:A:405:HOH:O	2.46	0.48
1:D:140:VAL:HG11	1:D:224:ILE:CD1	2.42	0.48
1:F:27:VAL:HG22	1:F:60:MET:HG2	1.95	0.48
1:F:153:LEU:HD13	1:F:193:PHE:HB3	1.94	0.48
1:B:208:GLU:HB3	1:B:215:PHE:HE2	1.79	0.48
1:C:127:ALA:HA	1:C:132:ARG:NH1	2.29	0.48
1:E:55:GLY:HA2	1:E:109:PRO:HG2	1.96	0.48
1:E:73:PRO:HG3	1:E:99:ALA:HA	1.96	0.48
1:F:127:ALA:HA	1:F:132:ARG:CZ	2.44	0.48
2:F:301:AM2:HA1	2:F:301:AM2:NC6	2.29	0.48
1:B:52:LEU:HB3	1:B:56:GLY:HA3	1.95	0.48
1:B:123:PRO:HD2	1:B:185:GLU:HG3	1.94	0.48
2:B:301:AM2:HB2	2:B:301:AM2:HA8	1.65	0.47
1:D:206:GLN:HB2	1:D:219:ILE:HG13	1.96	0.47
1:F:0:GLY:N	8:F:404:HOH:O	2.47	0.47
1:F:229:LEU:HA	1:F:232:LEU:HD12	1.97	0.47
1:D:60:MET:CE	1:D:86:SER:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:ARG:HA	1:E:52:LEU:HB2	1.96	0.47
1:C:34:VAL:HG21	1:C:143:LEU:CD2	2.44	0.47
1:D:73:PRO:HG3	1:D:99:ALA:HA	1.96	0.47
1:F:13:GLN:OE1	1:F:211:VAL:HA	2.14	0.47
1:F:26:LEU:HD12	1:F:133:VAL:HG11	1.96	0.47
1:D:192:ARG:HD3	1:D:239:PHE:HA	1.96	0.47
1:A:91:ARG:HB3	1:B:88:THR:HG23	1.95	0.47
1:D:175:ASP:N	1:D:175:ASP:OD1	2.47	0.47
1:E:60:MET:HE1	1:E:85:VAL:HG12	1.97	0.47
6:C:304:EPE:H62	6:C:304:EPE:H102	1.43	0.47
1:B:7:LYS:HA	1:B:10:LEU:HD12	1.96	0.47
1:C:4:GLU:HG2	1:C:36:PRO:HB2	1.96	0.46
1:D:166:VAL:CG2	1:D:253:ALA:HA	2.45	0.46
1:A:13:GLN:OE1	1:A:212:GLY:N	2.40	0.46
1:D:135:GLU:O	1:D:222:ARG:NH2	2.44	0.46
1:F:138:GLY:N	1:F:221:SER:OG	2.47	0.46
1:C:237:LEU:HB2	1:C:240:LEU:HD13	1.97	0.46
1:B:122:PRO:HD2	1:B:125:SER:HB3	1.98	0.46
1:B:29:SER:HA	1:B:143:LEU:HB2	1.98	0.46
1:F:102:PHE:CD2	1:F:123:PRO:HB3	2.51	0.46
2:E:301:AM2:HB1	2:E:301:AM2:HA93	1.98	0.46
1:A:128:SER:O	1:A:132:ARG:HG2	2.15	0.46
1:D:240:LEU:HD23	1:D:240:LEU:HA	1.52	0.45
2:A:301:AM2:NC6	2:A:301:AM2:HA1	2.30	0.45
1:B:37:LEU:O	6:B:305:EPE:H92	2.16	0.45
1:C:36:PRO:HD2	1:C:213:HIS:CD2	2.51	0.45
1:E:76:SER:O	1:E:97:ARG:NH2	2.47	0.45
1:E:196:ALA:O	1:E:200:LEU:HB2	2.16	0.45
1:A:1:MET:H	1:D:33:SER:HB3	1.81	0.45
1:E:25:LEU:HD11	1:E:141:LEU:HB2	1.97	0.45
1:D:3:TYR:O	1:D:213:HIS:NE2	2.41	0.45
1:F:61:PRO:HA	1:F:104:PHE:HA	1.98	0.45
1:C:185:GLU:HG2	1:C:186:ASN:N	2.32	0.45
1:F:44:LEU:HD23	1:F:44:LEU:HA	1.68	0.45
1:A:0:GLY:HA2	1:D:32:ARG:CZ	2.47	0.45
1:B:17:LEU:HD12	1:B:207:LYS:HG3	1.99	0.45
1:C:88:THR:HG23	1:F:91:ARG:HB3	1.99	0.45
1:D:139:GLN:HE21	1:D:218:LEU:HD11	1.82	0.45
1:E:196:ALA:O	1:E:200:LEU:HG	2.16	0.45
1:F:220:ARG:HB3	1:F:223:ASP:HB2	1.98	0.45
1:C:27:VAL:HG22	1:C:141:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:HA	1:C:132:ARG:HD2	1.78	0.45
1:E:143:LEU:CD1	1:E:143:LEU:C	2.85	0.45
2:B:301:AM2:HB2	2:B:301:AM2:HA93	1.99	0.45
1:E:14:LEU:HD13	1:E:211:VAL:HG11	1.99	0.45
1:F:166:VAL:O	1:F:184:LEU:HA	2.17	0.45
1:B:2:GLN:HB2	1:B:36:PRO:HG3	1.99	0.44
1:C:192:ARG:HE	1:C:192:ARG:HB3	1.69	0.44
1:F:178:LEU:O	1:F:179:VAL:HG13	2.17	0.44
1:E:124:HIS:C	1:E:130:VAL:HG21	2.38	0.44
1:F:73:PRO:HG3	1:F:99:ALA:HA	2.00	0.44
1:A:183:TYR:HE1	1:A:185:GLU:HB2	1.82	0.44
1:B:146:GLY:HA2	1:B:217:ARG:NH1	2.32	0.44
1:C:147:HIS:HB2	1:C:194:ALA:HA	1.99	0.44
1:C:150:ASN:HD21	1:C:224:ILE:HD13	1.82	0.44
1:E:185:GLU:HG2	1:E:187:ASP:H	1.83	0.44
1:F:115:ILE:C	1:F:115:ILE:HD12	2.38	0.44
2:F:301:AM2:HB1	2:F:301:AM2:HA93	1.99	0.44
1:E:153:LEU:O	1:E:156:ALA:N	2.50	0.44
1:F:113:GLN:N	8:F:405:HOH:O	2.48	0.44
1:C:148:ASP:OD1	1:C:148:ASP:N	2.50	0.44
1:D:31:PHE:N	5:D:303:PO4:O4	2.48	0.44
1:E:3:TYR:O	1:E:213:HIS:NE2	2.45	0.44
1:A:26:LEU:HA	1:A:59:VAL:O	2.18	0.44
1:E:35:ARG:NH1	6:E:305:EPE:O3S	2.49	0.44
1:E:100:HIS:CE1	1:E:103:ALA:HA	2.52	0.44
1:A:210:PRO:HB3	1:D:3:TYR:CG	2.53	0.44
1:C:32:ARG:HA	1:C:35:ARG:HD2	2.00	0.44
1:E:20:THR:HG22	1:E:139:GLN:OE1	2.17	0.44
1:F:203:LYS:HB3	1:F:205:LEU:HD12	1.99	0.44
1:C:37:LEU:N	6:C:304:EPE:O2S	2.48	0.43
1:E:112:GLU:H	1:E:112:GLU:CD	2.16	0.43
1:A:61:PRO:O	1:A:86:SER:OG	2.35	0.43
1:A:199:TRP:CD2	1:A:231:GLN:HG3	2.53	0.43
1:E:153:LEU:C	1:E:155:LEU:N	2.71	0.43
1:C:255:GLN:C	1:C:257:ILE:H	2.21	0.43
1:D:127:ALA:HA	1:D:132:ARG:NH1	2.33	0.43
1:E:25:LEU:HD12	1:E:139:GLN:O	2.19	0.43
1:B:139:GLN:NE2	1:B:218:LEU:HD21	2.33	0.43
1:C:187:ASP:OD2	2:C:301:AM2:NA2	2.52	0.43
1:D:166:VAL:HG21	1:D:253:ALA:HA	1.99	0.43
1:F:127:ALA:HA	1:F:132:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LYS:HD2	1:B:207:LYS:HA	1.74	0.43
1:D:121:LEU:HD13	1:D:183:TYR:HD1	1.83	0.43
1:E:154:ALA:HA	1:E:157:GLU:OE1	2.19	0.43
1:F:166:VAL:HG21	1:F:187:ASP:OD1	2.19	0.43
1:A:229:LEU:HD23	1:A:229:LEU:HA	1.82	0.43
1:B:210:PRO:HB3	1:C:3:TYR:CD2	2.54	0.43
1:E:10:LEU:O	1:E:13:GLN:N	2.51	0.43
1:D:59:VAL:HG21	1:D:114:ILE:HD13	2.01	0.43
1:C:84:VAL:HG11	1:F:75:THR:HG22	2.01	0.43
1:E:203:LYS:HD2	1:E:203:LYS:HA	1.81	0.43
1:A:63:TRP:CE2	1:A:82:LEU:HD11	2.53	0.42
1:B:167:PRO:HA	1:B:184:LEU:HD23	2.01	0.42
2:B:301:AM2:HA8	2:B:301:AM2:HA93	1.53	0.42
1:E:124:HIS:CA	1:E:130:VAL:HG21	2.49	0.42
1:E:189:CYS:SG	1:E:191:GLU:HB2	2.59	0.42
1:F:128:SER:H	1:F:131:ALA:HB3	1.84	0.42
1:C:63:TRP:CH2	1:C:151:THR:HG21	2.51	0.42
1:E:62:SER:O	1:E:62:SER:OG	2.30	0.42
1:D:19:VAL:HA	1:D:139:GLN:HE22	1.85	0.42
1:E:95:VAL:HA	1:E:107:ALA:HB2	2.01	0.42
1:E:218:LEU:O	1:E:219:ILE:HG13	2.20	0.42
2:C:301:AM2:HB1	2:C:301:AM2:HA93	2.01	0.42
1:C:177:LYS:O	1:C:178:LEU:C	2.58	0.42
1:E:148:ASP:OD1	1:E:148:ASP:N	2.53	0.42
1:E:153:LEU:C	1:E:155:LEU:H	2.22	0.42
1:E:231:GLN:OE1	1:E:238:ILE:HG21	2.19	0.42
1:F:156:ALA:HB2	1:F:225:VAL:HG12	2.02	0.42
1:C:159:MET:H	1:C:159:MET:HG2	1.67	0.42
1:C:185:GLU:OE1	1:C:187:ASP:OD1	2.37	0.42
1:E:102:PHE:CE1	1:E:123:PRO:HG3	2.55	0.42
1:E:199:TRP:CD1	1:E:199:TRP:N	2.86	0.42
1:C:91:ARG:O	1:F:42:LEU:HD21	2.20	0.42
1:C:232:LEU:HD23	1:C:238:ILE:HD12	2.01	0.42
1:B:130:VAL:CG2	1:B:152:THR:HG22	2.49	0.41
1:C:60:MET:HB3	1:C:60:MET:HE2	1.89	0.41
1:D:33:SER:OG	1:D:144:GLY:HA3	2.19	0.41
1:B:121:LEU:HB2	1:B:122:PRO:HD3	2.01	0.41
1:F:27:VAL:HA	1:F:141:LEU:O	2.20	0.41
1:A:188:HIS:HA	1:A:249:GLU:HG2	2.02	0.41
1:C:52:LEU:HB3	1:C:56:GLY:HA3	2.02	0.41
6:B:305:EPE:H81	6:B:305:EPE:H51	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:GLN:CD	1:D:234:ARG:HH21	2.23	0.41
1:D:63:TRP:CZ2	1:D:82:LEU:HD21	2.54	0.41
1:E:115:ILE:HD12	1:E:116:SER:CA	2.50	0.41
1:A:220:ARG:O	1:A:224:ILE:HG13	2.21	0.41
1:C:185:GLU:OE1	1:C:187:ASP:CG	2.59	0.41
1:E:124:HIS:HA	1:E:130:VAL:HG11	2.02	0.41
1:A:67:ASP:OD1	1:A:67:ASP:N	2.40	0.41
1:D:78:VAL:HG13	1:D:82:LEU:HD12	2.02	0.41
1:E:45:ILE:HD13	1:E:45:ILE:HA	1.92	0.41
1:A:10:LEU:HD11	1:A:37:LEU:HD22	2.02	0.41
1:C:247:CYS:HB3	1:C:250:CYS:HB2	2.02	0.41
1:D:172:ILE:CD1	1:D:174:GLN:HG3	2.50	0.41
1:D:192:ARG:HD3	1:D:239:PHE:CA	2.51	0.41
1:D:206:GLN:HB2	1:D:206:GLN:HE21	1.75	0.41
1:F:9:GLU:O	1:F:13:GLN:HG3	2.20	0.41
1:D:125:SER:HA	1:D:158:LEU:CD2	2.51	0.41
1:D:231:GLN:NE2	1:D:234:ARG:HH21	2.19	0.41
1:F:153:LEU:HD13	1:F:193:PHE:CB	2.50	0.41
1:D:67:ASP:OD2	1:D:67:ASP:N	2.41	0.40
1:E:124:HIS:HA	1:E:130:VAL:HG21	2.02	0.40
1:E:124:HIS:ND1	1:E:130:VAL:HG11	2.37	0.40
1:E:242:PRO:HA	1:E:243:PRO:HD3	1.97	0.40
1:F:130:VAL:HG21	1:F:151:THR:HG22	2.03	0.40
1:F:143:LEU:HD21	1:F:211:VAL:HG11	2.03	0.40
1:C:42:LEU:HD23	1:C:42:LEU:HA	1.90	0.40
1:D:95:VAL:HG22	1:D:107:ALA:HB2	2.02	0.40
1:D:147:HIS:HA	1:D:150:ASN:HB2	2.03	0.40
1:D:241:HIS:HB2	1:D:250:CYS:SG	2.61	0.40
1:F:25:LEU:HB2	1:F:52:LEU:HD21	2.04	0.40
1:F:100:HIS:HE1	1:F:102:PHE:O	2.05	0.40
1:D:188:HIS:CB	1:D:240:LEU:HD21	2.50	0.40
1:E:112:GLU:N	1:E:112:GLU:CD	2.74	0.40
1:F:63:TRP:HA	1:F:103:ALA:N	2.34	0.40
1:F:142:LEU:O	1:F:216:ALA:HA	2.21	0.40
1:F:62:SER:N	1:F:103:ALA:O	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	256/260 (98%)	242 (94%)	14 (6%)	0	100	100
1	B	256/260 (98%)	244 (95%)	12 (5%)	0	100	100
1	C	256/260 (98%)	235 (92%)	21 (8%)	0	100	100
1	D	256/260 (98%)	239 (93%)	17 (7%)	0	100	100
1	E	256/260 (98%)	229 (90%)	26 (10%)	1 (0%)	34	66
1	F	234/260 (90%)	210 (90%)	24 (10%)	0	100	100
All	All	1514/1560 (97%)	1399 (92%)	114 (8%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	18	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	207 (100%)	1 (0%)	88	96
1	B	209/210 (100%)	203 (97%)	6 (3%)	42	76
1	C	209/210 (100%)	201 (96%)	8 (4%)	33	67
1	D	209/210 (100%)	201 (96%)	8 (4%)	33	67
1	E	207/210 (99%)	197 (95%)	10 (5%)	25	58
1	F	195/210 (93%)	189 (97%)	6 (3%)	40	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1237/1260 (98%)	1198 (97%)	39 (3%)	39 73

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	B	132	ARG
1	B	150	ASN
1	B	187	ASP
1	B	198	ARG
1	B	234	ARG
1	B	256	SER
1	C	42	LEU
1	C	132	ARG
1	C	143	LEU
1	C	175	ASP
1	C	178	LEU
1	C	187	ASP
1	C	231	GLN
1	C	237	LEU
1	D	6	ARG
1	D	42	LEU
1	D	162	VAL
1	D	170	CYS
1	D	178	LEU
1	D	206	GLN
1	D	223	ASP
1	D	256	SER
1	E	6	ARG
1	E	20	THR
1	E	24	VAL
1	E	64	SER
1	E	143	LEU
1	E	175	ASP
1	E	182	ASP
1	E	189	CYS
1	E	200	LEU
1	E	250	CYS
1	F	92	LEU
1	F	125	SER
1	F	178	LEU
1	F	190	CYS

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Mol	Chain	Res	Type
1	F	192	ARG
1	F	218	LEU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 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
5	PO4	B	304	-	4,4,4	0.91	0	6,6,6	0.48	0
6	EPE	E	305	-	15,15,15	0.74	1 (6%)	18,20,20	1.81	5 (27%)
2	AM2	B	301	-	40,40,40	1.74	6 (15%)	53,60,60	1.45	10 (18%)
4	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.36	0
5	PO4	F	302	-	4,4,4	0.92	0	6,6,6	0.43	0
2	AM2	D	301	-	40,40,40	1.70	6 (15%)	53,60,60	1.27	5 (9%)
4	EDO	A	306	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	B	303	-	3,3,3	0.48	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	A	307	-	4,4,4	0.89	0	6,6,6	0.48	0
2	AM2	E	301	-	40,40,40	1.69	8 (20%)	53,60,60	1.35	5 (9%)
7	GOL	D	304	-	5,5,5	0.92	0	5,5,5	0.99	0
2	AM2	F	301	-	40,40,40	1.68	7 (17%)	53,60,60	1.40	6 (11%)
6	EPE	A	308	-	15,15,15	0.70	1 (6%)	18,20,20	1.95	6 (33%)
6	EPE	C	304	-	15,15,15	0.78	1 (6%)	18,20,20	1.68	6 (33%)
6	EPE	D	305	-	15,15,15	0.69	1 (6%)	18,20,20	1.81	4 (22%)
7	GOL	E	304	-	5,5,5	0.92	0	5,5,5	1.00	0
5	PO4	C	303	-	4,4,4	0.87	0	6,6,6	0.53	0
6	EPE	B	305	-	15,15,15	0.73	1 (6%)	18,20,20	1.94	5 (27%)
5	PO4	E	303	-	4,4,4	0.90	0	6,6,6	0.44	0
5	PO4	D	303	-	4,4,4	0.92	0	6,6,6	0.46	0
2	AM2	A	301	-	40,40,40	1.67	8 (20%)	53,60,60	1.42	7 (13%)
6	EPE	F	303	-	15,15,15	3.20	1 (6%)	18,20,20	2.27	7 (38%)
4	EDO	A	305	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	A	303	-	3,3,3	0.49	0	2,2,2	0.25	0
4	EDO	E	302	-	3,3,3	0.46	0	2,2,2	0.37	0
2	AM2	C	301	-	40,40,40	1.64	7 (17%)	53,60,60	1.10	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
6	EPE	E	305	-	-	5/9/19/19	0/1/1/1
2	AM2	B	301	-	-	8/12/84/84	0/4/4/4
4	EDO	A	304	-	-	1/1/1/1	-
2	AM2	D	301	-	-	8/12/84/84	0/4/4/4
4	EDO	A	306	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
2	AM2	E	301	-	-	10/12/84/84	0/4/4/4
7	GOL	D	304	-	-	4/4/4/4	-
2	AM2	F	301	-	-	10/12/84/84	0/4/4/4
6	EPE	A	308	-	-	7/9/19/19	0/1/1/1
6	EPE	C	304	-	-	3/9/19/19	0/1/1/1
6	EPE	D	305	-	-	5/9/19/19	0/1/1/1
7	GOL	E	304	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EPE	B	305	-	-	4/9/19/19	0/1/1/1
2	AM2	A	301	-	-	10/12/84/84	0/4/4/4
6	EPE	F	303	-	-	1/9/19/19	0/1/1/1
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	E	302	-	-	0/1/1/1	-
2	AM2	C	301	-	-	9/12/84/84	1/4/4/4

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	303	EPE	C10-S	-12.21	1.60	1.77
2	B	301	AM2	OA4-CA1	4.65	1.53	1.41
2	D	301	AM2	OA4-CA1	4.58	1.53	1.41
2	C	301	AM2	OA4-CA1	4.42	1.53	1.41
2	F	301	AM2	OA4-CA1	4.40	1.53	1.41
2	E	301	AM2	OA4-CA1	4.40	1.53	1.41
2	A	301	AM2	OA4-CA1	4.38	1.53	1.41
2	D	301	AM2	OA4-CA5	3.89	1.50	1.44
2	D	301	AM2	OA5-CA8	3.75	1.51	1.41
2	E	301	AM2	OA4-CA5	3.74	1.49	1.44
2	F	301	AM2	OA5-CA8	3.74	1.51	1.41
2	E	301	AM2	OA5-CA8	3.71	1.51	1.41
2	B	301	AM2	OA5-CA8	3.67	1.51	1.41
2	F	301	AM2	OA4-CA5	3.67	1.49	1.44
2	A	301	AM2	OA4-CA5	3.66	1.49	1.44
2	B	301	AM2	OA4-CA5	3.62	1.49	1.44
2	C	301	AM2	OA5-CA8	3.59	1.51	1.41
2	A	301	AM2	OA5-CA8	3.54	1.50	1.41
2	F	301	AM2	OA5-CA4	3.35	1.52	1.44
2	E	301	AM2	OA5-CA4	3.33	1.52	1.44
2	C	301	AM2	OA4-CA5	3.30	1.49	1.44
2	A	301	AM2	OA5-CA4	3.30	1.52	1.44
2	D	301	AM2	OB1-CB1	3.22	1.50	1.41
2	D	301	AM2	OA5-CA4	3.21	1.52	1.44
2	B	301	AM2	OA5-CA4	3.20	1.52	1.44
2	B	301	AM2	OB1-CB1	3.19	1.50	1.41
2	C	301	AM2	OB1-CB1	3.15	1.49	1.41
2	F	301	AM2	OB1-CB1	3.12	1.49	1.41
2	E	301	AM2	OB1-CB1	3.11	1.49	1.41
2	D	301	AM2	CB3-CB4	-3.10	1.49	1.53
2	A	301	AM2	OB1-CB1	3.07	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	AM2	OA5-CA4	2.96	1.51	1.44
2	E	301	AM2	CB3-CB4	-2.89	1.49	1.53
2	A	301	AM2	CB3-CB4	-2.84	1.50	1.53
2	F	301	AM2	CB3-CB4	-2.82	1.50	1.53
2	C	301	AM2	CB3-CB4	-2.82	1.50	1.53
2	B	301	AM2	CB3-CB4	-2.78	1.50	1.53
6	C	304	EPE	C10-S	2.44	1.81	1.77
6	E	305	EPE	C10-S	2.36	1.80	1.77
6	B	305	EPE	C10-S	2.29	1.80	1.77
6	A	308	EPE	C10-S	2.24	1.80	1.77
2	A	301	AM2	OA8-CA8	-2.18	1.35	1.41
6	D	305	EPE	C10-S	2.16	1.80	1.77
2	A	301	AM2	OA1-CA1	-2.12	1.35	1.41
2	E	301	AM2	OA1-CA1	-2.09	1.35	1.41
2	F	301	AM2	OA8-CA8	-2.06	1.36	1.41
2	E	301	AM2	OA8-CA8	-2.03	1.36	1.41
2	C	301	AM2	OA8-CA8	-2.03	1.36	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	303	EPE	O3S-S-C10	5.45	114.59	105.77
6	A	308	EPE	C5-N4-C3	5.36	120.90	108.83
2	F	301	AM2	CC6-CC5-CC4	4.51	120.44	111.18
2	A	301	AM2	CC6-CC5-CC4	4.49	120.39	111.18
6	D	305	EPE	C5-N4-C3	4.44	118.81	108.83
6	E	305	EPE	C5-N4-C3	4.43	118.80	108.83
6	B	305	EPE	C5-N4-C3	4.30	118.50	108.83
2	E	301	AM2	CC6-CC5-CC4	4.26	119.94	111.18
2	A	301	AM2	CC5-CC4-CC3	4.07	116.18	110.04
6	B	305	EPE	C7-N4-C5	3.85	121.08	111.23
2	F	301	AM2	CC5-CC4-CC3	3.78	115.74	110.04
6	F	303	EPE	O1S-S-C10	3.71	111.38	106.92
2	D	301	AM2	CC6-CC5-CC4	3.58	118.53	111.18
2	B	301	AM2	OA5-CA4-CA5	3.53	117.19	109.75
6	C	304	EPE	O2S-S-C10	3.48	111.11	106.92
6	D	305	EPE	C7-N4-C5	3.47	120.11	111.23
2	E	301	AM2	CC5-CC4-CC3	3.44	115.23	110.04
2	B	301	AM2	CC6-CC5-CC4	3.36	118.09	111.18
6	B	305	EPE	C7-N4-C3	3.24	119.53	111.23
6	E	305	EPE	C7-N4-C3	3.24	119.51	111.23
6	C	304	EPE	C5-N4-C3	3.23	116.09	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	305	EPE	C7-N4-C3	3.22	119.46	111.23
6	E	305	EPE	C7-N4-C5	3.09	119.15	111.23
6	F	303	EPE	C9-N1-C6	-3.03	103.49	111.23
2	D	301	AM2	CC5-CC4-CC3	2.99	114.55	110.04
6	A	308	EPE	C7-N4-C3	2.98	118.85	111.23
2	B	301	AM2	OA1-CC1-CC6	2.93	116.17	109.18
2	B	301	AM2	CC5-CC4-CC3	2.91	114.43	110.04
2	E	301	AM2	CC5-CC6-CC1	2.87	116.79	109.53
2	D	301	AM2	OA4-CA5-CA4	2.87	113.23	108.88
2	B	301	AM2	OA5-CA8-CA7	2.87	116.18	110.58
2	F	301	AM2	CC5-CC6-CC1	2.86	116.76	109.53
6	F	303	EPE	C6-C5-N4	-2.73	105.03	110.64
2	A	301	AM2	CC5-CC6-CC1	2.70	116.37	109.53
6	C	304	EPE	C7-N4-C3	2.70	118.13	111.23
2	A	301	AM2	CA1-OA4-CA5	-2.69	108.73	113.06
6	B	305	EPE	O2S-S-C10	2.64	110.09	106.92
2	F	301	AM2	CA1-OA4-CA5	-2.63	108.83	113.06
2	D	301	AM2	OA1-CC1-CC6	2.62	115.44	109.18
6	A	308	EPE	C7-N4-C5	2.58	117.84	111.23
6	A	308	EPE	O1S-S-C10	2.55	109.98	106.92
6	F	303	EPE	O2S-S-C10	-2.49	103.91	106.92
2	C	301	AM2	CA1-OA4-CA5	-2.49	109.05	113.06
6	A	308	EPE	O3S-S-C10	2.46	109.74	105.77
2	A	301	AM2	OA8-CB1-CB2	2.39	114.30	108.10
2	E	301	AM2	CA1-OA4-CA5	-2.35	109.27	113.06
6	C	304	EPE	C7-N4-C5	2.35	117.24	111.23
6	E	305	EPE	O2S-S-C10	2.33	109.72	106.92
2	D	301	AM2	CC5-CC6-CC1	2.31	115.38	109.53
2	A	301	AM2	OA1-CC1-CC6	2.28	114.61	109.18
6	F	303	EPE	C6-N1-C2	2.27	113.93	108.83
6	F	303	EPE	O2S-S-O1S	-2.26	106.11	113.95
6	A	308	EPE	C5-C6-N1	-2.26	106.01	110.64
2	B	301	AM2	CA8-OA5-CA4	2.22	118.05	113.69
2	F	301	AM2	OA8-CB1-CB2	2.21	113.83	108.10
6	E	305	EPE	O1S-S-C10	2.18	109.54	106.92
2	C	301	AM2	CC5-CC4-CC3	2.17	113.32	110.04
6	C	304	EPE	O3S-S-C10	2.15	109.24	105.77
2	B	301	AM2	OA8-CA8-OA5	-2.12	104.75	110.67
2	F	301	AM2	OA1-CC1-CC6	2.11	114.21	109.18
2	B	301	AM2	CC5-CC6-CC1	2.09	114.82	109.53
2	E	301	AM2	OA1-CC1-CC6	2.08	114.15	109.18
2	B	301	AM2	OA4-CA1-CA2	2.07	114.86	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	304	EPE	C6-N1-C2	2.05	113.45	108.83
6	D	305	EPE	O3S-S-C10	2.05	109.08	105.77
2	A	301	AM2	OA8-CA8-OA5	-2.04	104.96	110.67
6	B	305	EPE	O3S-S-C10	2.04	109.07	105.77
2	B	301	AM2	CA8-CA7-CA6	2.04	116.07	110.06

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	AM2	CB2-CB1-OA8-CA8
2	A	301	AM2	OB1-CB1-OA8-CA8
2	A	301	AM2	CC6-CC1-OA1-CA1
2	B	301	AM2	CA2-CA1-OA1-CC1
2	B	301	AM2	CA8-CA7-NA7-CA9
2	B	301	AM2	CA7-CA8-OA8-CB1
2	B	301	AM2	CB2-CB1-OA8-CA8
2	B	301	AM2	OB1-CB1-OA8-CA8
2	B	301	AM2	CC6-CC1-OA1-CA1
2	C	301	AM2	CA8-CA7-NA7-CA9
2	C	301	AM2	CB2-CB1-OA8-CA8
2	C	301	AM2	OB1-CB1-OA8-CA8
2	C	301	AM2	CC6-CC1-OA1-CA1
2	D	301	AM2	CA8-CA7-NA7-CA9
2	D	301	AM2	CA7-CA8-OA8-CB1
2	D	301	AM2	CB2-CB1-OA8-CA8
2	D	301	AM2	OB1-CB1-OA8-CA8
2	D	301	AM2	CC6-CC1-OA1-CA1
2	E	301	AM2	CA8-CA7-NA7-CA9
2	E	301	AM2	CB2-CB1-OA8-CA8
2	E	301	AM2	OB1-CB1-OA8-CA8
2	E	301	AM2	CC6-CC1-OA1-CA1
2	F	301	AM2	CA8-CA7-NA7-CA9
2	F	301	AM2	CB2-CB1-OA8-CA8
2	F	301	AM2	OB1-CB1-OA8-CA8
2	F	301	AM2	CC6-CC1-OA1-CA1
6	A	308	EPE	C9-C10-S-O2S
6	A	308	EPE	C9-C10-S-O3S
6	B	305	EPE	C8-C7-N4-C5
6	C	304	EPE	C10-C9-N1-C6
6	D	305	EPE	C8-C7-N4-C5
6	D	305	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
6	D	305	EPE	C9-C10-S-O2S
6	D	305	EPE	C9-C10-S-O3S
6	E	305	EPE	C10-C9-N1-C2
6	E	305	EPE	C10-C9-N1-C6
6	E	305	EPE	C9-C10-S-O1S
6	E	305	EPE	C9-C10-S-O2S
6	E	305	EPE	C9-C10-S-O3S
7	D	304	GOL	C1-C2-C3-O3
2	F	301	AM2	OB1-CB5-CB6-OB6
2	A	301	AM2	OB1-CB5-CB6-OB6
2	D	301	AM2	OB1-CB5-CB6-OB6
2	E	301	AM2	OB1-CB5-CB6-OB6
2	F	301	AM2	CB4-CB5-CB6-OB6
2	A	301	AM2	CB4-CB5-CB6-OB6
2	E	301	AM2	CB4-CB5-CB6-OB6
2	D	301	AM2	CB4-CB5-CB6-OB6
2	C	301	AM2	OB1-CB5-CB6-OB6
6	A	308	EPE	N4-C7-C8-O8
6	F	303	EPE	N4-C7-C8-O8
6	C	304	EPE	N4-C7-C8-O8
6	B	305	EPE	N4-C7-C8-O8
6	A	308	EPE	C8-C7-N4-C5
2	A	301	AM2	CA7-CA8-OA8-CB1
2	C	301	AM2	CA7-CA8-OA8-CB1
2	E	301	AM2	CA7-CA8-OA8-CB1
2	F	301	AM2	CA7-CA8-OA8-CB1
6	A	308	EPE	C10-C9-N1-C2
6	A	308	EPE	C10-C9-N1-C6
2	B	301	AM2	OA5-CA8-OA8-CB1
2	D	301	AM2	OA5-CA8-OA8-CB1
2	E	301	AM2	OA5-CA8-OA8-CB1
2	A	301	AM2	OA5-CA8-OA8-CB1
2	F	301	AM2	OA5-CA8-OA8-CB1
7	D	304	GOL	O1-C1-C2-O2
7	D	304	GOL	O2-C2-C3-O3
2	C	301	AM2	CC2-CC1-OA1-CA1
2	F	301	AM2	CC2-CC1-OA1-CA1
6	A	308	EPE	C9-C10-S-O1S
6	D	305	EPE	C9-C10-S-O1S
2	A	301	AM2	CC2-CC1-OA1-CA1
6	C	304	EPE	C8-C7-N4-C3
2	C	301	AM2	CB4-CB5-CB6-OB6

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Mol	Chain	Res	Type	Atoms
2	C	301	AM2	OA5-CA8-OA8-CB1
2	E	301	AM2	CA2-CA1-OA1-CC1
2	F	301	AM2	CA2-CA1-OA1-CC1
6	B	305	EPE	C10-C9-N1-C2
6	B	305	EPE	C10-C9-N1-C6
2	E	301	AM2	CC2-CC1-OA1-CA1
2	A	301	AM2	CA8-CA7-NA7-CA9
7	D	304	GOL	O1-C1-C2-C3
2	B	301	AM2	OB1-CB5-CB6-OB6
4	A	304	EDO	O1-C1-C2-O2
2	A	301	AM2	CA2-CA1-OA1-CC1

All (1) ring outliers are listed below:

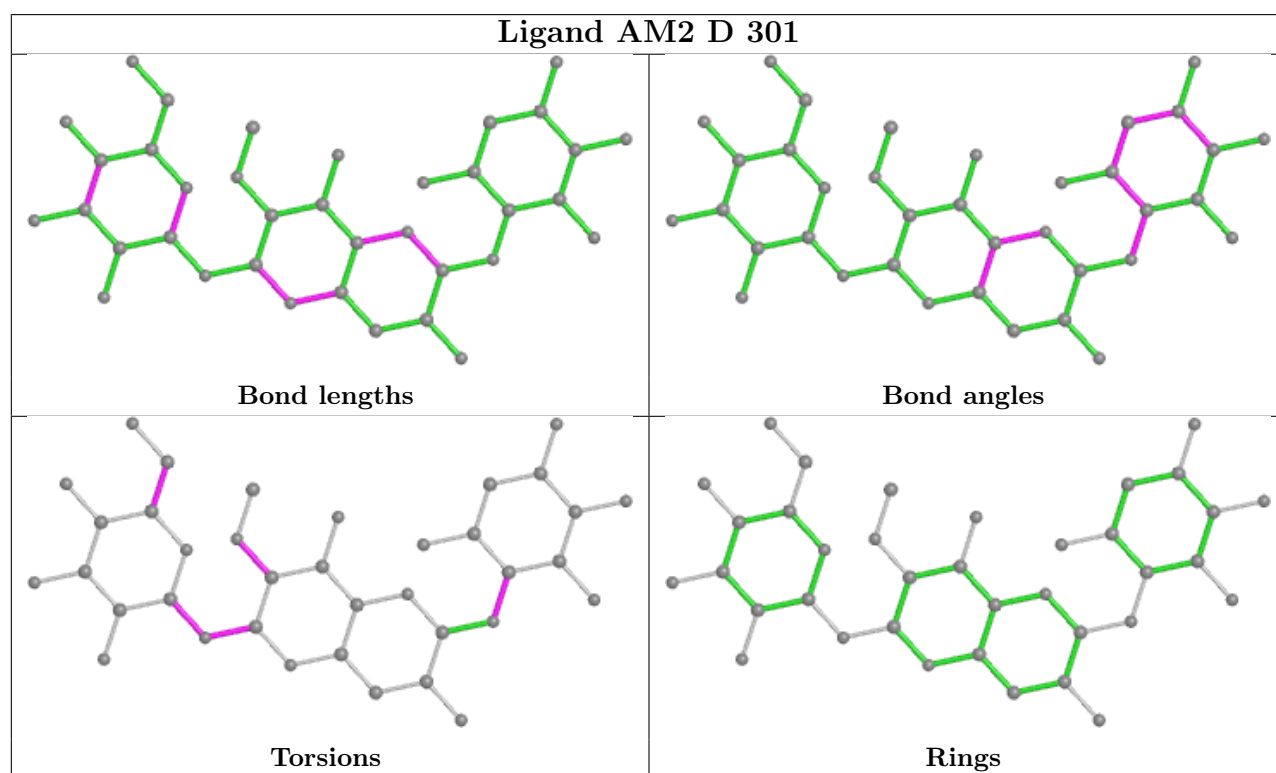
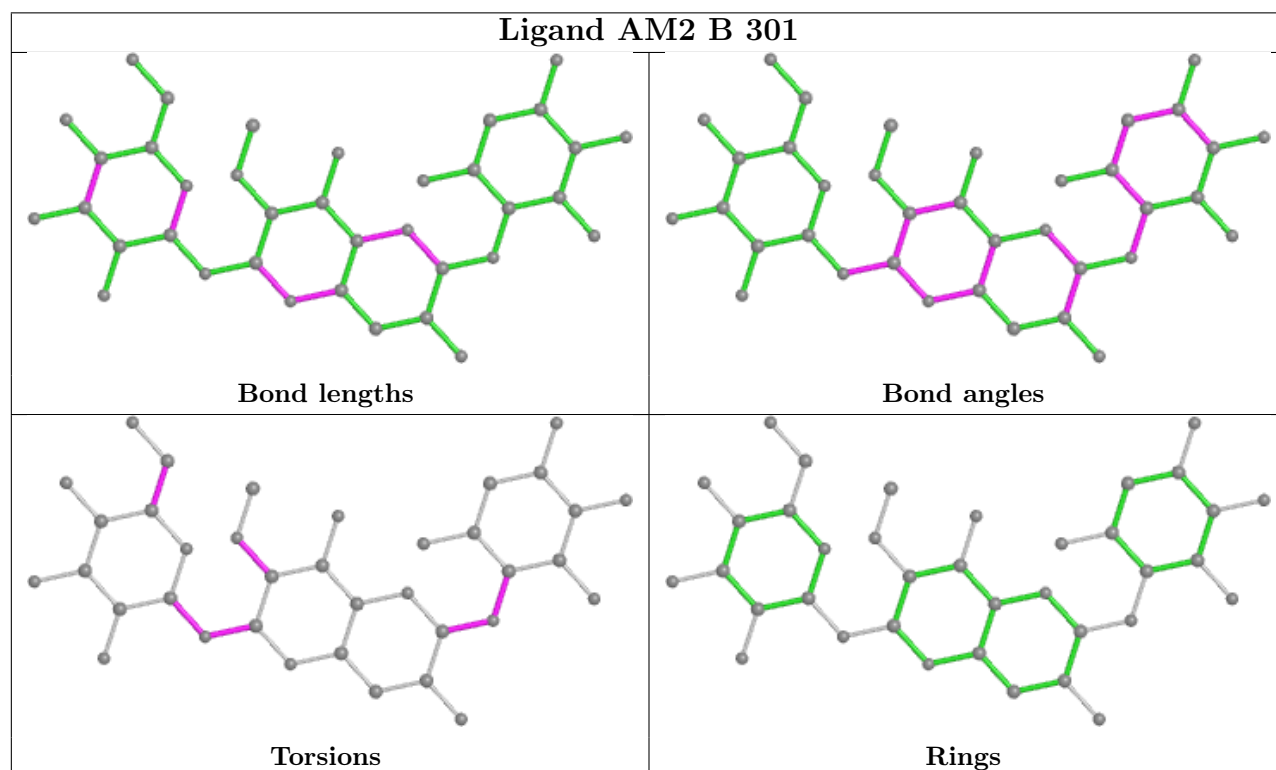
Mol	Chain	Res	Type	Atoms
2	C	301	AM2	CC1-CC2-CC3-CC4-CC5-CC6

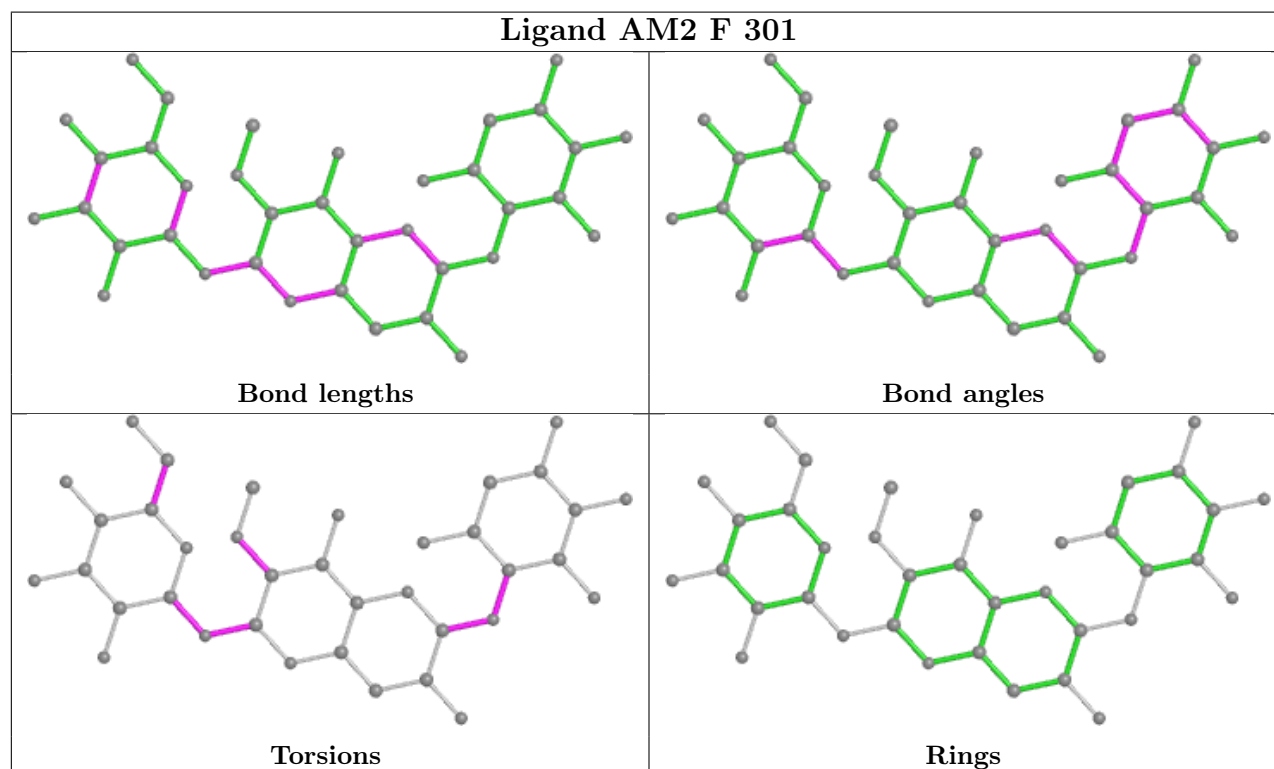
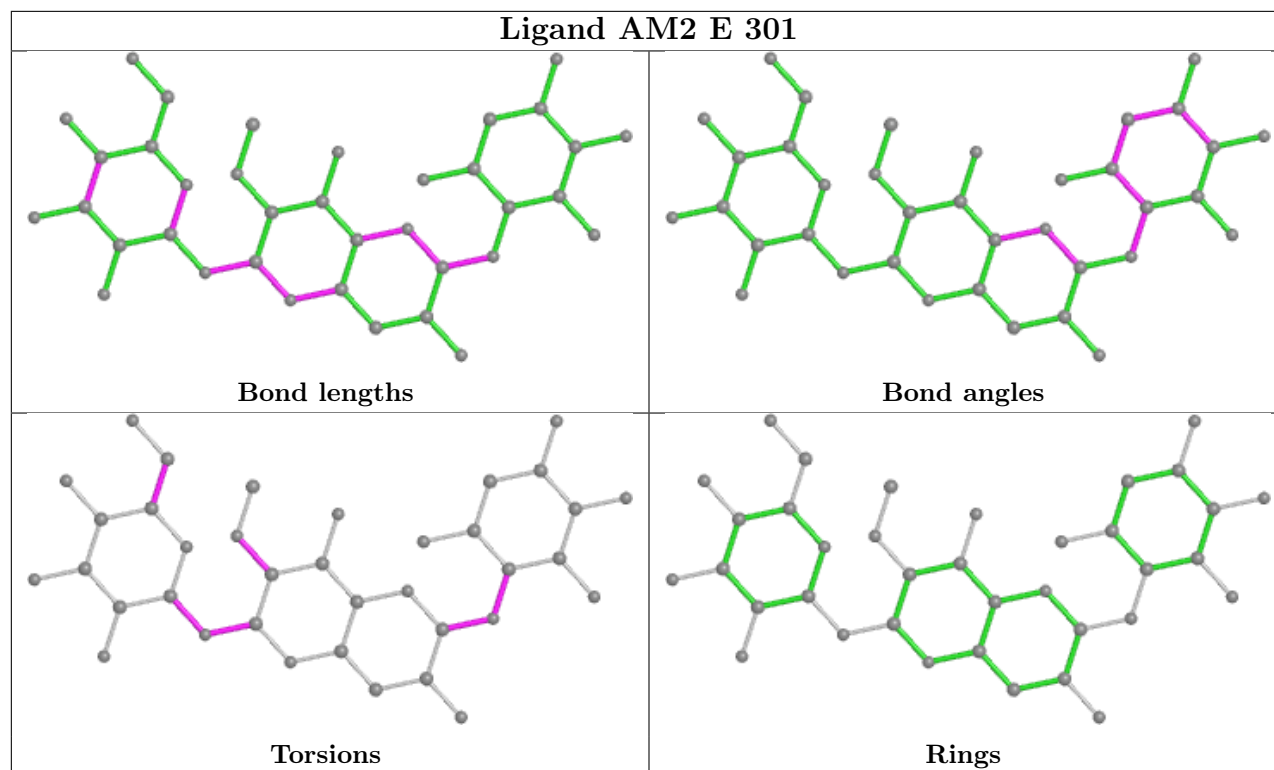
12 monomers are involved in 27 short contacts:

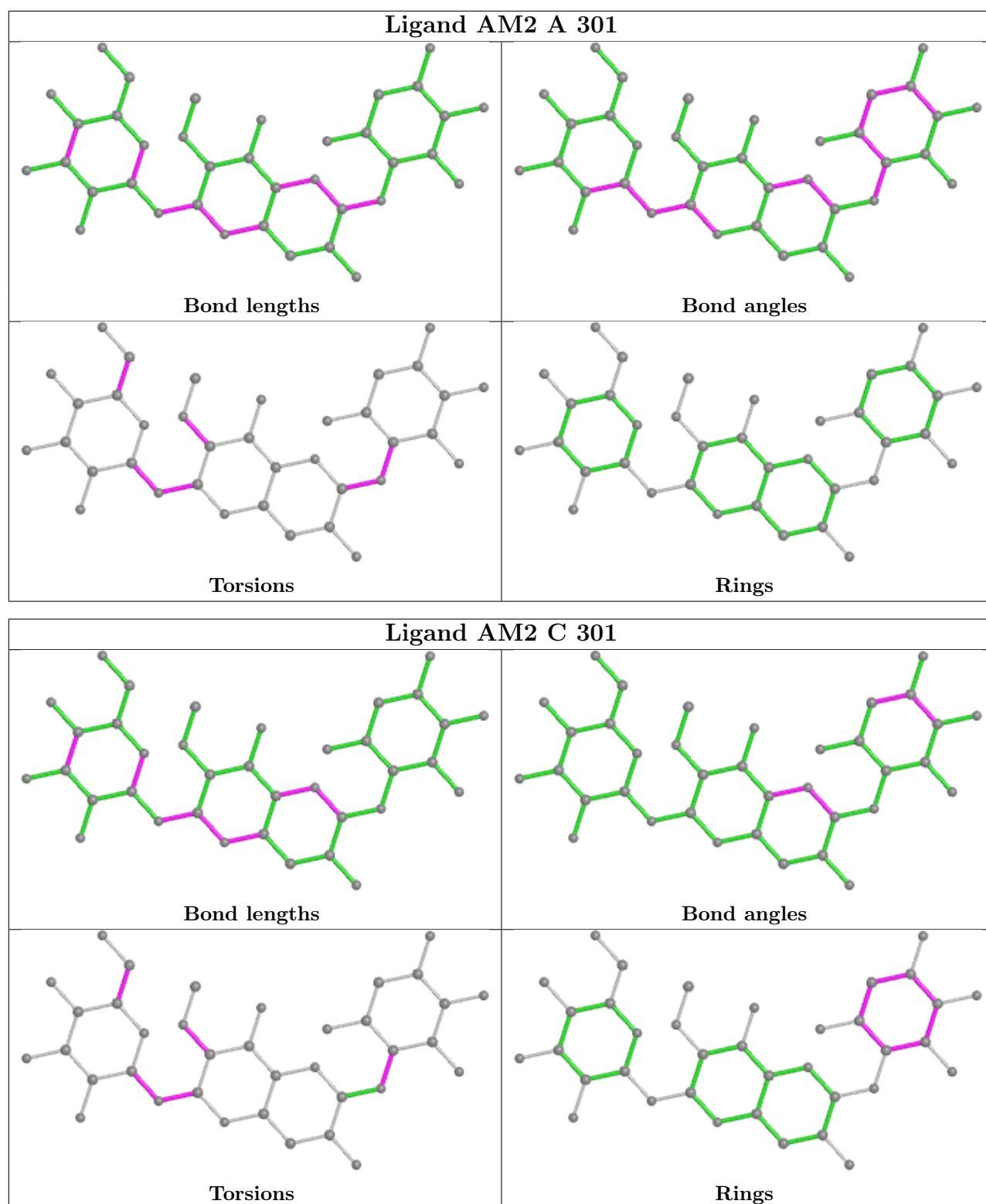
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	PO4	1	0
6	E	305	EPE	1	0
2	B	301	AM2	5	0
2	D	301	AM2	2	0
2	E	301	AM2	1	0
2	F	301	AM2	3	0
6	C	304	EPE	3	0
6	B	305	EPE	3	0
5	D	303	PO4	1	0
2	A	301	AM2	1	0
6	F	303	EPE	2	0
2	C	301	AM2	4	0

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

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, 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	258/260 (99%)	-0.41	3 (1%) 79 73	38, 55, 93, 144	0
1	B	258/260 (99%)	-0.20	6 (2%) 60 51	32, 57, 107, 145	0
1	C	258/260 (99%)	-0.16	2 (0%) 86 81	42, 72, 117, 156	0
1	D	258/260 (99%)	-0.09	8 (3%) 49 39	45, 77, 133, 165	0
1	E	258/260 (99%)	0.71	37 (14%) 2 1	62, 131, 186, 234	0
1	F	242/260 (93%)	1.24	59 (24%) 0 0	60, 163, 235, 280	0
All	All	1532/1560 (98%)	0.17	115 (7%) 14 8	32, 81, 190, 280	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	233	GLY	10.3
1	E	245	ALA	6.6
1	F	68	ASP	6.5
1	F	227	THR	6.1
1	E	181	VAL	6.1
1	F	245	ALA	6.1
1	F	178	LEU	5.8
1	F	187	ASP	5.6
1	F	190	CYS	5.6
1	F	189	CYS	5.5
1	E	244	GLU	5.4
1	F	247	CYS	5.1
1	F	119	LEU	4.9
1	F	244	GLU	4.8
1	E	246	GLY	4.2
1	F	185	GLU	4.1
1	F	27	VAL	4.1
1	F	166	VAL	4.0
1	F	176	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	183	TYR	4.0
1	F	194	ALA	3.8
1	E	229	LEU	3.8
1	B	174	GLN	3.7
1	F	67	ASP	3.7
1	F	248	GLU	3.7
1	F	184	LEU	3.7
1	F	179	VAL	3.6
1	F	124	HIS	3.6
1	F	164	TYR	3.5
1	E	151	THR	3.4
1	F	249	GLU	3.4
1	F	169	HIS	3.4
1	F	167	PRO	3.3
1	F	191	GLU	3.3
1	F	243	PRO	3.3
1	E	174	GLN	3.2
1	E	179	VAL	3.2
1	F	234	ARG	3.2
1	E	241	HIS	3.2
1	F	219	ILE	3.1
1	B	246	GLY	3.1
1	E	109	PRO	3.1
1	D	166	VAL	3.1
1	E	192	ARG	3.1
1	E	180	ARG	3.1
1	E	187	ASP	3.0
1	F	235	ASP	3.0
1	E	154	ALA	3.0
1	E	202	GLU	3.0
1	F	230	GLY	2.9
1	E	247	CYS	2.9
1	E	234	ARG	2.9
1	B	175	ASP	2.9
1	B	179	VAL	2.9
1	F	102	PHE	2.8
1	F	28	HIS	2.8
1	F	229	LEU	2.8
1	F	127	ALA	2.8
1	E	67	ASP	2.8
1	E	68	ASP	2.8
1	E	188	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	66	LEU	2.7
1	F	104	PHE	2.7
1	D	184	LEU	2.7
1	F	137	ASP	2.7
1	E	184	LEU	2.7
1	B	247	CYS	2.7
1	F	228	ALA	2.7
1	E	54	PRO	2.6
1	E	254	ARG	2.6
1	E	201	LYS	2.6
1	E	175	ASP	2.6
1	F	26	LEU	2.5
1	F	161	LYS	2.5
1	F	250	CYS	2.5
1	D	174	GLN	2.5
1	F	226	ALA	2.5
1	F	123	PRO	2.5
1	C	178	LEU	2.5
1	A	178	LEU	2.5
1	B	178	LEU	2.4
1	E	15	LEU	2.4
1	F	232	LEU	2.4
1	E	251	ASP	2.4
1	D	151	THR	2.4
1	F	135	GLU	2.4
1	E	28	HIS	2.4
1	F	110	GLN	2.3
1	F	202	GLU	2.3
1	F	126	PRO	2.3
1	E	53	GLY	2.3
1	D	173	LEU	2.2
1	F	25	LEU	2.2
1	E	172	ILE	2.2
1	F	168	ARG	2.2
1	F	186	ASN	2.2
1	E	239	PHE	2.2
1	E	64	SER	2.2
1	F	246	GLY	2.1
1	D	244	GLU	2.1
1	F	49	ARG	2.1
1	E	233	GLY	2.1
1	D	178	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	205	LEU	2.1
1	D	245	ALA	2.1
1	E	257	ILE	2.1
1	E	243	PRO	2.1
1	F	193	PHE	2.1
1	F	158	LEU	2.1
1	C	177	LYS	2.1
1	A	245	ALA	2.0
1	F	38	GLU	2.0
1	E	168	ARG	2.0
1	A	176	GLY	2.0
1	E	51	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AM2	F	301	37/37	0.31	0.52	124,150,165,166	37
2	AM2	D	301	37/37	0.70	0.32	103,128,140,143	0
2	AM2	C	301	37/37	0.71	0.27	110,119,124,132	0
2	AM2	E	301	37/37	0.73	0.32	128,139,145,151	0
7	GOL	D	304	6/6	0.74	0.25	101,103,104,105	0
7	GOL	E	304	6/6	0.77	0.25	109,111,114,115	0
4	EDO	A	306	4/4	0.79	0.29	100,101,101,102	0
3	ZN	D	302	1/1	0.83	0.09	99,99,99,99	0
4	EDO	E	302	4/4	0.84	0.26	79,83,88,89	0
2	AM2	A	301	37/37	0.84	0.24	87,101,118,119	0
2	AM2	B	301	37/37	0.84	0.24	71,99,110,114	0

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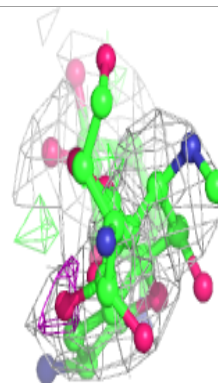
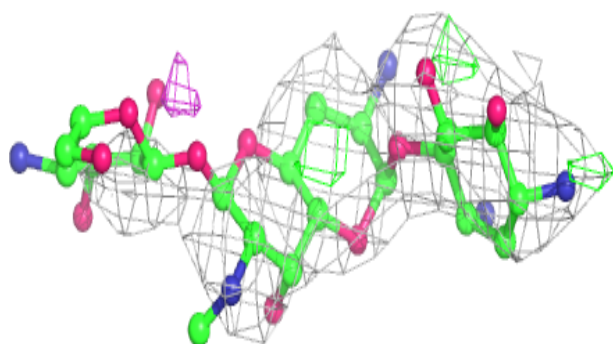
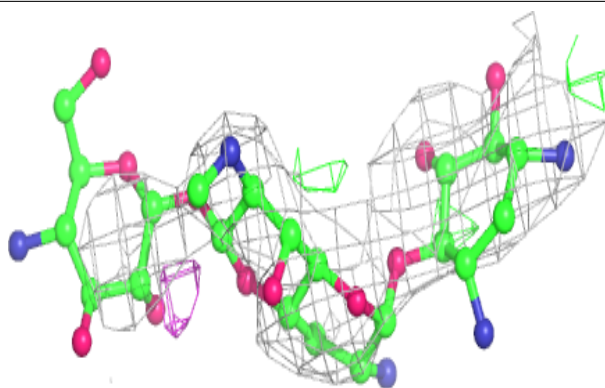
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	305	4/4	0.88	0.36	82,83,85,85	0
4	EDO	B	303	4/4	0.89	0.20	67,70,73,73	0
6	EPE	F	303	15/15	0.91	0.21	83,102,112,112	0
6	EPE	E	305	15/15	0.92	0.20	75,87,99,99	0
3	ZN	B	302	1/1	0.92	0.15	122,122,122,122	0
4	EDO	A	303	4/4	0.93	0.34	64,65,67,69	0
5	PO4	B	304	5/5	0.93	0.13	79,83,84,86	0
3	ZN	A	302	1/1	0.93	0.14	106,106,106,106	0
5	PO4	C	303	5/5	0.94	0.12	70,79,81,82	0
6	EPE	D	305	15/15	0.94	0.24	60,89,102,104	0
5	PO4	E	303	5/5	0.95	0.10	89,92,92,93	0
6	EPE	A	308	15/15	0.95	0.20	60,70,91,93	0
6	EPE	B	305	15/15	0.95	0.24	53,77,111,114	0
5	PO4	D	303	5/5	0.95	0.14	77,78,87,88	0
4	EDO	A	304	4/4	0.96	0.19	52,57,59,64	0
6	EPE	C	304	15/15	0.97	0.17	54,77,83,83	0
5	PO4	A	307	5/5	0.97	0.14	75,78,80,81	0
5	PO4	F	302	5/5	0.97	0.12	85,87,88,91	0
3	ZN	C	302	1/1	0.98	0.05	105,105,105,105	0

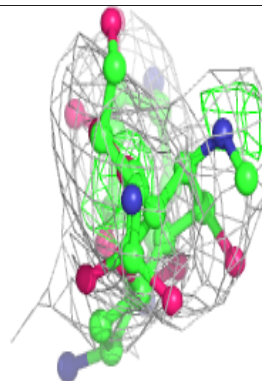
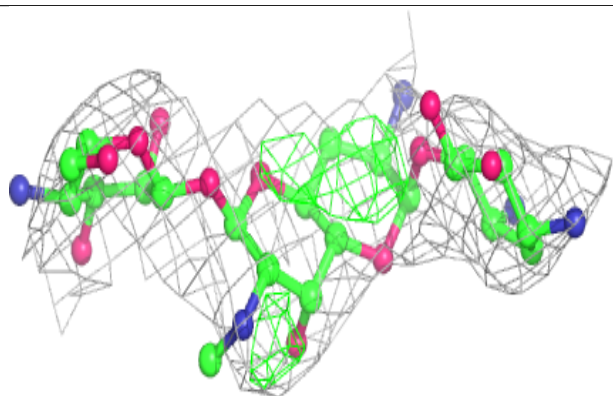
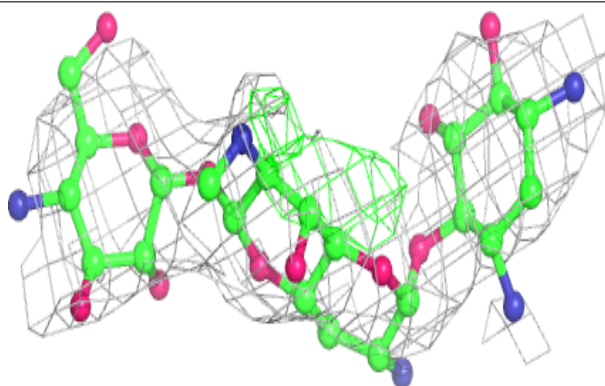
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AM2 F 301:

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

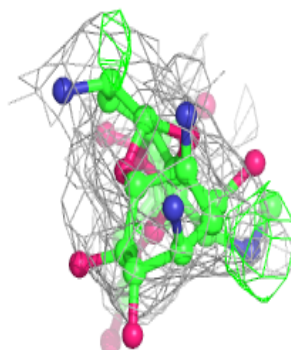
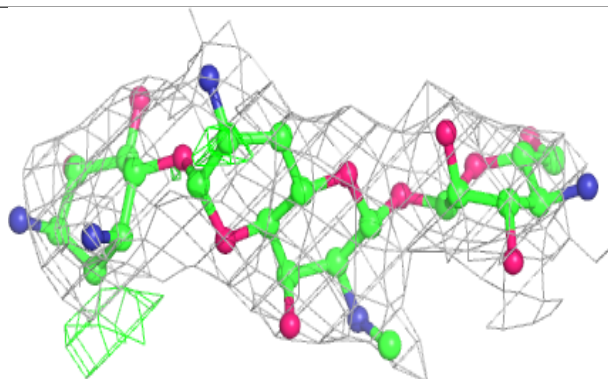
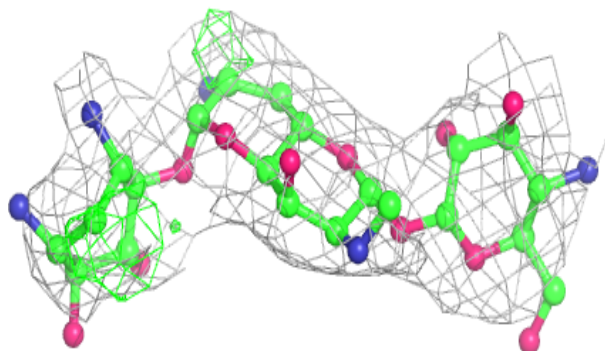
**Electron density around AM2 D 301:**

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

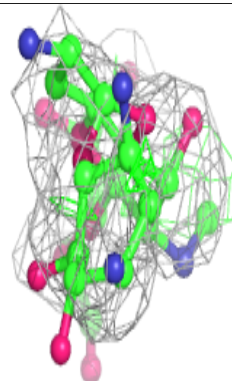
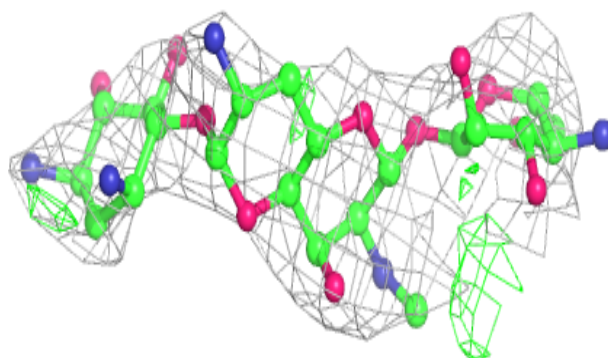
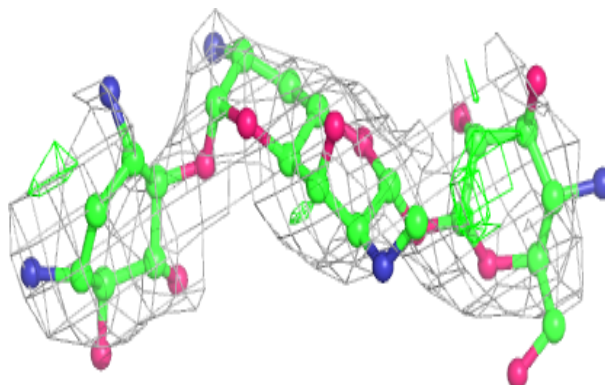


Electron density around AM2 C 301:

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

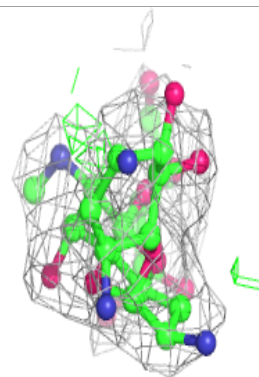
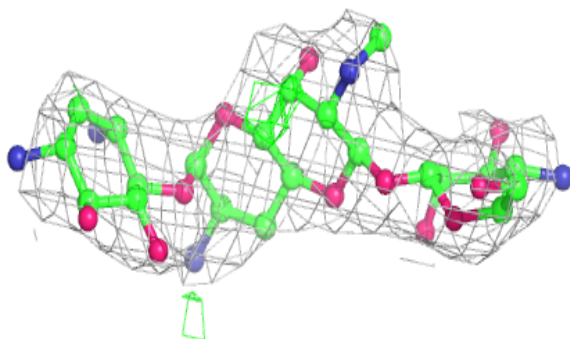
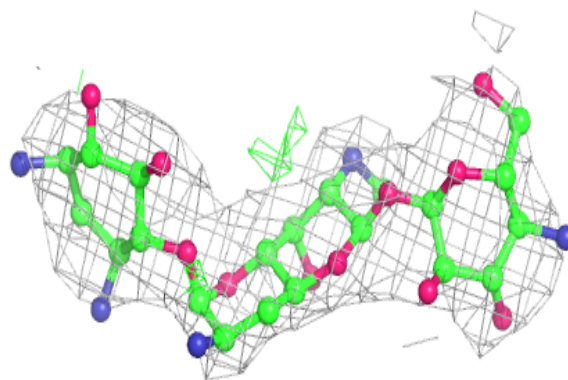
**Electron density around AM2 E 301:**

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

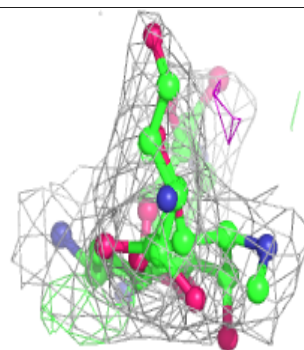
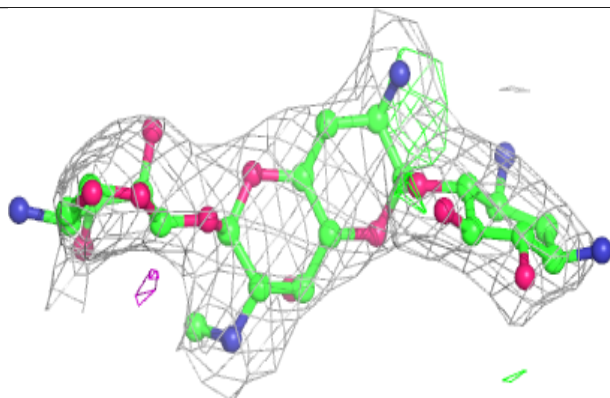
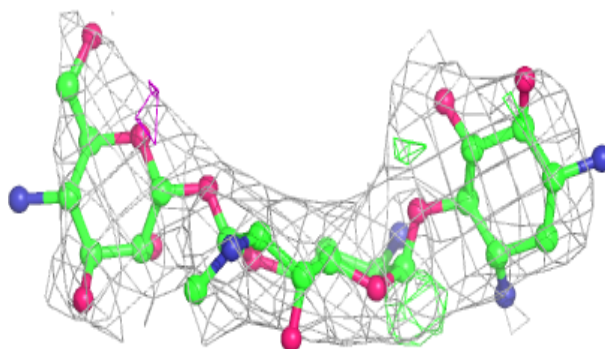


Electron density around AM2 A 301:

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

**Electron density around AM2 B 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.