



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2022 – 10:04 AM EDT

PDB ID : 7UUN  
Title : Crystal structure of aminoglycoside resistance enzyme ApmA H135A mutant, complex with tobramycin and coenzyme A  
Authors : Stogios, P.J.; Evdokimova, E.; Michalska, K.; Di Leo, R.; Bordeleau, E.; Wright, G.D.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2022-04-28  
Resolution : 2.65 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) 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	:	2.31.2
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)	:	2.31.2

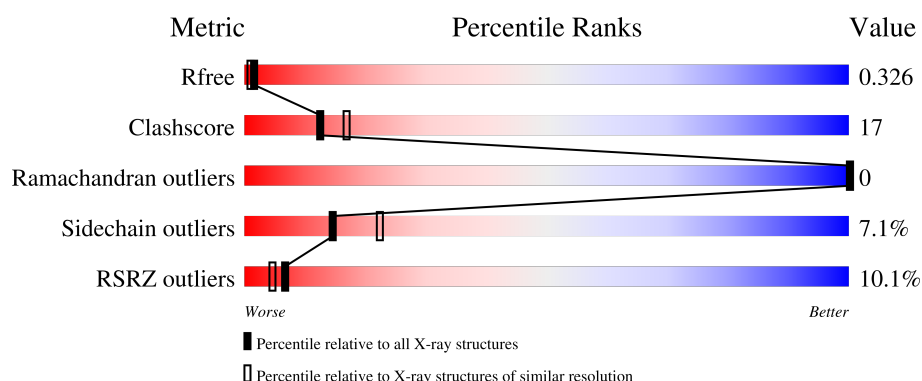
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	276	<div> <div>4%</div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	B	276	<div> <div>5%</div> <div>69%</div> <div>28%</div> <div>..</div> </div>
1	C	276	<div> <div>22%</div> <div>55%</div> <div>40%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6708 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.

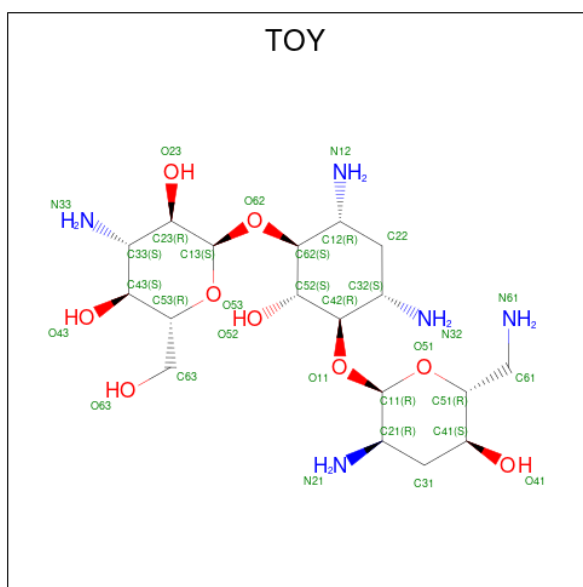
- Molecule 1 is a protein called Aminocyclitol acetyltransferase ApmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2180	1394	365	412	9			
1	B	273	Total	C	N	O	S	0	0	0
			2180	1394	365	412	9			
1	C	272	Total	C	N	O	S	0	0	0
			2176	1392	364	411	9			

There are 9 discrepancies between the modelled and reference sequences:

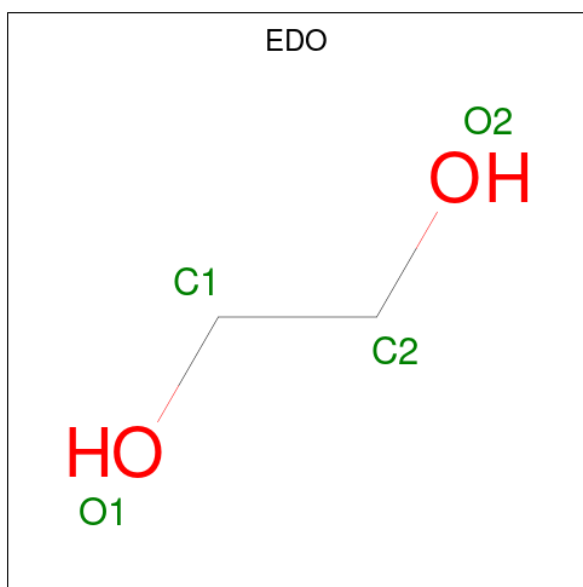
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP A0A1D0AST6
A	0	GLY	-	expression tag	UNP A0A1D0AST6
A	135	ALA	HIS	engineered mutation	UNP A0A1D0AST6
B	-1	GLN	-	expression tag	UNP A0A1D0AST6
B	0	GLY	-	expression tag	UNP A0A1D0AST6
B	135	ALA	HIS	engineered mutation	UNP A0A1D0AST6
C	-1	GLN	-	expression tag	UNP A0A1D0AST6
C	0	GLY	-	expression tag	UNP A0A1D0AST6
C	135	ALA	HIS	engineered mutation	UNP A0A1D0AST6

- Molecule 2 is TOBRAMYCIN (three-letter code: TOY) (formula: C<sub>18</sub>H<sub>37</sub>N<sub>5</sub>O<sub>9</sub>) (labeled as "Ligand of Interest" by depositor).



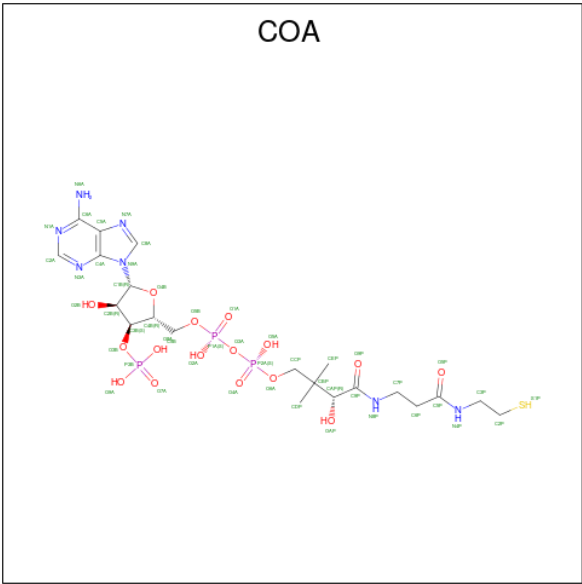
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	18	5	9		
2	B	1	Total	C	N	O	0	0
			32	18	5	9		
2	C	1	Total	C	N	O	0	0
			32	18	5	9		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

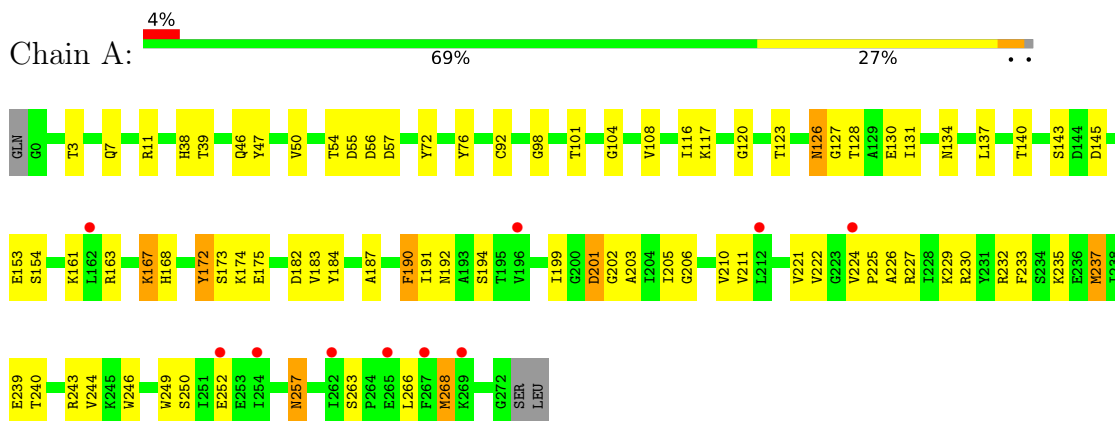
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	9	Total	O	0	0
			9	9		
5	C	2	Total	O	0	0
			2	2		

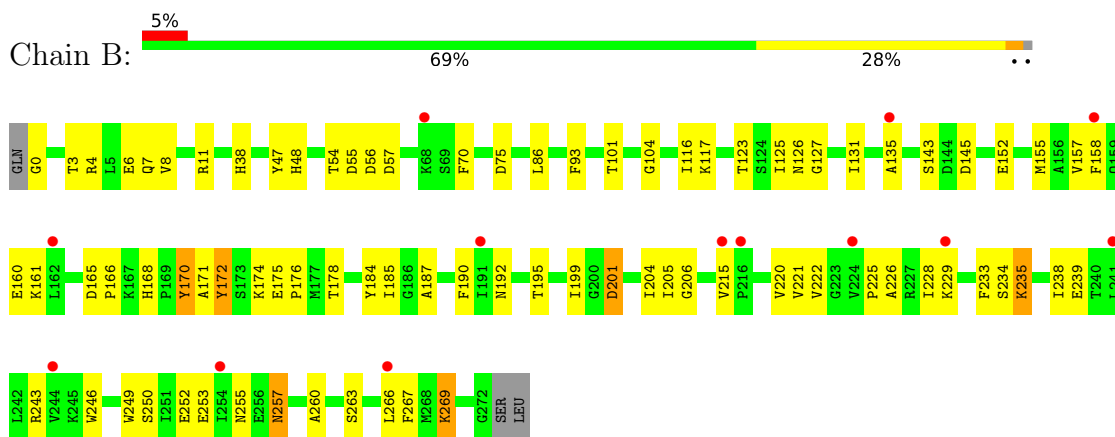
### 3 Residue-property plots [i](#)

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

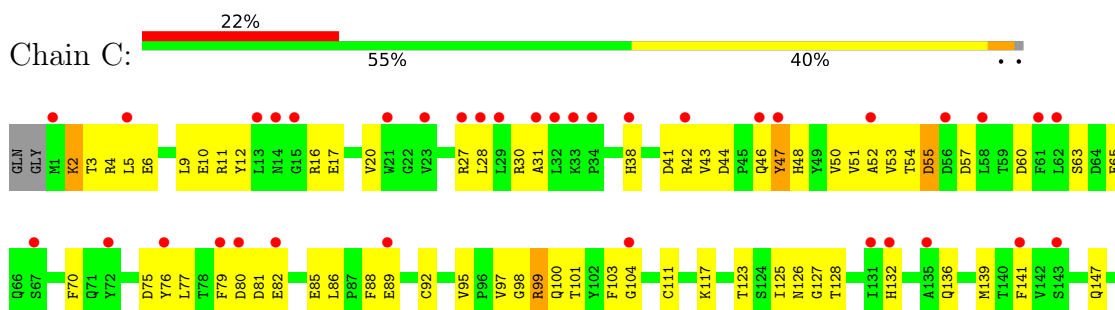
#### • Molecule 1: Aminocyclitol acetyltransferase ApmA

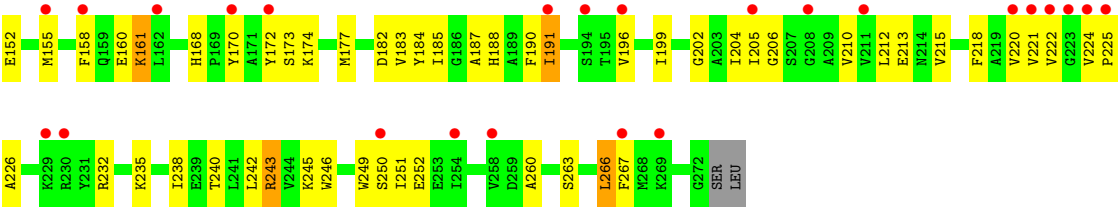


#### • Molecule 1: Aminocyclitol acetyltransferase ApmA



#### • Molecule 1: Aminocyclitol acetyltransferase ApmA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.29Å 108.29Å 87.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.45 – 2.65 29.45 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.45-2.65) 92.8 (29.45-2.64)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.286 , 0.328 0.287 , 0.326	Depositor DCC
$R_{free}$ test set	1639 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.3	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l 0.477 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: COA, TOY, EDO

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	0.32	0/2233	0.55	0/3027
1	B	0.33	0/2233	0.56	0/3027
1	C	0.37	0/2229	0.58	0/3022
All	All	0.34	0/6695	0.57	0/9076

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2180	0	2117	60	0
1	B	2180	0	2117	65	1
1	C	2176	0	2114	104	0
2	A	32	0	37	0	0
2	B	32	0	37	0	0
2	C	32	0	37	0	0
3	A	4	0	6	0	0
4	B	48	0	32	3	1
5	A	13	0	0	0	0
5	B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2	0	0	0	0
All	All	6708	0	6497	222	1

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 17.

All (222) 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:C:99:ARG:NH2	1:C:250:SER:HA	1.80	0.95
1:C:101:THR:HG23	1:C:123:THR:HG22	1.48	0.95
1:C:101:THR:CG2	1:C:123:THR:HG22	1.99	0.93
1:C:4:ARG:HH21	1:C:77:LEU:HD11	1.35	0.92
1:B:126:ASN:HD22	1:B:187:ALA:HB2	1.37	0.89
1:C:147:GLN:HE21	1:C:158:PHE:HE2	1.22	0.88
1:C:263:SER:HB3	1:C:266:LEU:HB2	1.57	0.86
1:A:252:GLU:HG3	1:B:47:TYR:OH	1.76	0.85
1:B:225:PRO:HB3	4:B:302:COA:H2A	1.58	0.85
1:C:204:ILE:HD11	1:C:232:ARG:HD3	1.58	0.83
1:A:101:THR:HG22	1:A:123:THR:H	1.44	0.82
1:C:43:VAL:HA	1:C:48:HIS:HD2	1.48	0.79
1:C:251:ILE:HD12	1:C:251:ILE:H	1.47	0.79
1:C:65:GLU:OE1	1:C:65:GLU:N	2.17	0.77
1:B:54:THR:HG23	1:B:57:ASP:H	1.51	0.75
1:C:17:GLU:OE1	1:C:48:HIS:ND1	2.22	0.72
1:C:27:ARG:HA	1:C:30:ARG:HG2	1.72	0.72
1:A:235:LYS:HZ1	1:A:239:GLU:HG3	1.54	0.72
1:A:206:GLY:HA3	1:A:222:VAL:HG12	1.72	0.70
1:B:160:GLU:HB2	1:C:89:GLU:HG3	1.72	0.69
1:C:6:GLU:HA	1:C:9:LEU:HB2	1.75	0.69
1:C:210:VAL:HG13	1:C:224:VAL:HG12	1.74	0.69
1:C:242:LEU:O	1:C:245:LYS:NZ	2.26	0.69
1:C:3:THR:HG22	1:C:6:GLU:HG3	1.74	0.69
1:C:168:HIS:CE1	1:C:174:LYS:HB3	2.29	0.67
1:A:54:THR:HG23	1:A:57:ASP:H	1.58	0.67
1:C:54:THR:HA	1:C:80:ASP:HB2	1.75	0.67
4:B:302:COA:HN8	4:B:302:COA:H131	1.58	0.67
1:C:99:ARG:NH2	1:C:249:TRP:O	2.22	0.67
1:A:257:ASN:N	1:A:257:ASN:HD22	1.92	0.66
1:B:126:ASN:ND2	1:B:187:ALA:HB2	2.09	0.66
1:B:206:GLY:HA3	1:B:222:VAL:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:SER:HB3	1:B:266:LEU:HB2	1.76	0.66
1:C:132:HIS:HB2	1:C:190:PHE:HE1	1.62	0.65
1:C:160:GLU:OE2	1:C:161:LYS:NZ	2.30	0.65
1:C:52:ALA:HB1	1:C:57:ASP:HB3	1.78	0.64
1:B:221:VAL:HG12	1:B:226:ALA:HB1	1.80	0.64
1:B:201:ASP:OD1	1:B:201:ASP:N	2.29	0.64
1:C:168:HIS:CG	1:C:174:LYS:HE3	2.33	0.63
1:C:210:VAL:HG22	1:C:225:PRO:HA	1.80	0.63
1:A:137:LEU:HD13	1:A:167:LYS:HD2	1.80	0.63
1:C:196:VAL:HG22	1:C:213:GLU:C	2.19	0.63
1:C:99:ARG:HH21	1:C:250:SER:HA	1.62	0.63
1:B:116:ILE:HD11	1:B:131:ILE:HD13	1.80	0.62
1:A:104:GLY:HA3	1:A:127:GLY:HA2	1.80	0.62
1:C:185:ILE:HD13	1:C:205:ILE:HD12	1.82	0.62
1:A:168:HIS:CD2	1:A:174:LYS:HE2	2.34	0.62
1:A:257:ASN:N	1:A:257:ASN:ND2	2.47	0.62
1:A:168:HIS:ND1	1:A:172:TYR:O	2.32	0.62
1:C:97:VAL:HG21	1:C:103:PHE:HE1	1.65	0.62
1:C:147:GLN:NE2	1:C:158:PHE:HE2	1.95	0.62
1:C:177:MET:HE1	1:C:191:ILE:HG21	1.81	0.62
1:C:123:THR:OG1	1:C:183:VAL:HB	2.00	0.61
1:A:210:VAL:HG13	1:A:225:PRO:HA	1.82	0.61
1:A:137:LEU:CD1	1:A:167:LYS:HD2	2.31	0.61
1:B:192:ASN:OD1	1:B:195:THR:N	2.33	0.61
1:C:95:VAL:HG21	1:C:111:CYS:SG	2.40	0.60
1:B:185:ILE:HG12	1:B:205:ILE:HD12	1.82	0.60
1:B:160:GLU:HG3	1:B:161:LYS:HD2	1.84	0.60
1:A:237:MET:HA	1:A:268:MET:HE3	1.83	0.60
1:C:43:VAL:HA	1:C:48:HIS:CD2	2.33	0.59
1:B:135:ALA:HA	1:B:170:TYR:CE1	2.37	0.59
1:B:117:LYS:HD2	1:B:178:THR:HG22	1.84	0.58
1:C:4:ARG:NH1	1:C:81:ASP:O	2.36	0.58
1:C:168:HIS:HB3	1:C:174:LYS:HE3	1.86	0.58
1:C:43:VAL:HG22	1:C:70:PHE:HZ	1.68	0.58
1:A:163:ARG:NH1	1:A:172:TYR:OH	2.37	0.57
1:C:43:VAL:HG22	1:C:70:PHE:CZ	2.40	0.57
1:C:204:ILE:HB	1:C:220:VAL:HG22	1.87	0.56
1:C:99:ARG:HH22	1:C:250:SER:HA	1.68	0.56
1:C:199:ILE:HD13	1:C:215:VAL:HG22	1.87	0.56
1:B:221:VAL:CG1	1:B:226:ALA:HB1	2.35	0.56
1:C:53:VAL:HB	1:C:57:ASP:OD2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLY:HA3	1:C:222:VAL:HG12	1.88	0.56
1:B:47:TYR:CD1	1:B:48:HIS:NE2	2.74	0.55
1:C:168:HIS:HE2	1:C:173:SER:C	2.10	0.55
1:C:54:THR:OG1	1:C:55:ASP:N	2.39	0.55
1:C:43:VAL:HG21	1:C:50:VAL:HG22	1.87	0.55
1:C:251:ILE:H	1:C:251:ILE:CD1	2.17	0.55
1:A:190:PHE:CE1	1:A:192:ASN:HA	2.41	0.55
1:C:126:ASN:OD1	1:C:128:THR:N	2.39	0.54
1:C:168:HIS:CB	1:C:174:LYS:HE3	2.37	0.54
1:B:204:ILE:HB	1:B:220:VAL:HG22	1.90	0.53
1:B:257:ASN:N	1:B:257:ASN:ND2	2.56	0.53
1:C:168:HIS:HD2	1:C:172:TYR:O	1.91	0.53
1:C:185:ILE:CD1	1:C:205:ILE:HD12	2.37	0.53
1:A:182:ASP:O	1:A:202:GLY:HA2	2.09	0.53
1:C:57:ASP:O	1:C:60:ASP:HB3	2.08	0.53
1:B:225:PRO:CB	4:B:302:COA:H2A	2.34	0.53
1:A:250:SER:OG	1:A:252:GLU:HB3	2.07	0.52
1:C:187:ALA:O	1:C:188:HIS:HB2	2.06	0.52
1:C:28:LEU:HD22	1:C:53:VAL:HG22	1.90	0.52
1:B:250:SER:OG	1:B:252:GLU:HB2	2.10	0.52
1:A:47:TYR:OH	1:B:255:ASN:HB3	2.09	0.52
1:C:182:ASP:O	1:C:202:GLY:HA2	2.09	0.51
1:A:205:ILE:HD13	1:A:211:VAL:HG21	1.93	0.51
1:B:174:LYS:HG3	1:B:175:GLU:N	2.25	0.51
1:B:260:ALA:O	1:B:267:PHE:HB2	2.10	0.51
1:C:221:VAL:HB	1:C:226:ALA:HB1	1.93	0.51
1:A:98:GLY:O	1:A:101:THR:OG1	2.27	0.51
1:A:174:LYS:HG3	1:A:175:GLU:N	2.24	0.51
1:B:234:SER:O	1:B:238:ILE:HD13	2.11	0.50
1:C:246:TRP:HA	1:C:249:TRP:CE2	2.47	0.50
1:A:250:SER:C	1:A:252:GLU:N	2.66	0.50
1:C:70:PHE:CD2	1:C:75:ASP:HB3	2.47	0.50
1:C:70:PHE:HD2	1:C:75:ASP:HB3	1.77	0.50
1:A:126:ASN:OD1	1:A:187:ALA:HB2	2.12	0.50
1:C:152:GLU:HA	1:C:155:MET:HG3	1.94	0.49
1:C:2:LYS:HB2	1:C:6:GLU:OE2	2.13	0.49
1:C:41:ASP:CG	1:C:42:ARG:H	2.16	0.49
1:B:246:TRP:HA	1:B:249:TRP:CE2	2.47	0.49
1:C:139:MET:HB3	1:C:141:PHE:O	2.12	0.49
1:C:199:ILE:HD12	1:C:205:ILE:HD11	1.93	0.49
1:C:202:GLY:HA3	1:C:218:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:O	1:A:167:LYS:HD3	2.12	0.49
1:B:104:GLY:HA3	1:B:127:GLY:HA2	1.95	0.49
1:A:47:TYR:CE2	1:B:252:GLU:HA	2.48	0.49
1:B:235:LYS:NZ	1:B:239:GLU:HG3	2.28	0.49
1:C:168:HIS:CD2	1:C:172:TYR:O	2.66	0.49
1:C:44:ASP:HB3	1:C:47:TYR:HB2	1.96	0.48
1:A:104:GLY:O	1:A:108:VAL:HG23	2.13	0.48
1:A:252:GLU:HA	1:B:47:TYR:CZ	2.49	0.48
1:A:7:GLN:O	1:A:11:ARG:HG3	2.14	0.48
1:C:177:MET:HE1	1:C:191:ILE:CG2	2.44	0.47
1:C:240:THR:HA	1:C:243:ARG:CG	2.44	0.47
1:A:190:PHE:HE1	1:A:192:ASN:HA	1.78	0.47
1:B:125:ILE:HA	1:B:185:ILE:HB	1.96	0.47
1:C:224:VAL:HG23	1:C:224:VAL:O	2.15	0.47
1:B:3:THR:O	1:B:7:GLN:HG3	2.14	0.47
1:C:199:ILE:HD13	1:C:215:VAL:CG2	2.45	0.47
1:B:152:GLU:HG3	1:C:11:ARG:HH21	1.79	0.47
1:C:170:TYR:HB2	1:C:172:TYR:CD1	2.50	0.47
1:C:4:ARG:N	1:C:82:GLU:OE2	2.44	0.47
1:A:183:VAL:HG13	1:A:203:ALA:O	2.14	0.47
1:B:101:THR:HG23	1:B:123:THR:HB	1.97	0.47
1:C:85:GLU:HB2	1:C:100:GLN:HA	1.97	0.46
1:C:92:CYS:O	1:C:95:VAL:HG22	2.16	0.46
1:C:12:TYR:HE2	1:C:88:PHE:CE1	2.33	0.46
1:B:3:THR:HB	1:B:6:GLU:HB2	1.98	0.46
1:C:20:VAL:HA	1:C:51:VAL:HG13	1.96	0.46
1:A:221:VAL:HB	1:A:226:ALA:HB1	1.97	0.46
1:A:50:VAL:O	1:A:76:TYR:HA	2.15	0.46
1:B:4:ARG:O	1:B:8:VAL:HG23	2.14	0.46
1:B:228:ILE:O	1:B:228:ILE:HD12	2.14	0.46
1:C:210:VAL:CG2	1:C:225:PRO:HA	2.46	0.46
1:A:168:HIS:CD2	1:A:174:LYS:HB3	2.50	0.46
1:B:235:LYS:HZ2	1:B:239:GLU:HG3	1.81	0.46
1:A:224:VAL:HG23	1:A:224:VAL:O	2.16	0.45
1:B:157:VAL:HG21	1:C:250:SER:HB3	1.98	0.45
1:B:257:ASN:N	1:B:257:ASN:HD22	2.13	0.45
1:C:125:ILE:HA	1:C:185:ILE:HB	1.96	0.45
1:B:235:LYS:HA	1:B:238:ILE:HB	1.98	0.45
1:C:199:ILE:CD1	1:C:205:ILE:HD11	2.47	0.45
1:A:101:THR:HG21	1:A:120:GLY:O	2.16	0.45
1:A:229:LYS:HE2	1:A:230:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:H	1:A:194:SER:HB2	1.81	0.45
1:A:190:PHE:CD1	1:A:190:PHE:C	2.89	0.45
1:B:249:TRP:HB3	1:B:253:GLU:HB2	1.99	0.45
1:C:54:THR:H	1:C:57:ASP:HB2	1.82	0.45
1:A:72:TYR:HA	1:A:76:TYR:CZ	2.52	0.45
1:A:199:ILE:CD1	1:A:205:ILE:HD11	2.47	0.45
1:C:70:PHE:HB3	1:C:76:TYR:HD2	1.82	0.45
1:C:136:GLN:HG3	1:C:139:MET:HG2	1.99	0.45
1:C:260:ALA:HB1	1:C:267:PHE:HA	1.99	0.45
1:A:182:ASP:OD2	1:A:232:ARG:NH1	2.47	0.45
1:C:104:GLY:HA3	1:C:127:GLY:HA2	1.99	0.45
1:C:251:ILE:HD12	1:C:251:ILE:N	2.24	0.45
1:C:260:ALA:O	1:C:267:PHE:HB2	2.16	0.45
1:B:70:PHE:CD2	1:B:75:ASP:HB3	2.52	0.44
1:A:172:TYR:C	1:A:173:SER:HG	2.17	0.44
1:A:11:ARG:HE	1:A:11:ARG:HB3	1.49	0.44
1:B:269:LYS:HD3	1:B:269:LYS:HA	1.44	0.44
1:C:210:VAL:HG23	1:C:212:LEU:HD11	1.99	0.44
1:B:233:PHE:HB2	1:B:238:ILE:CD1	2.47	0.44
1:C:89:GLU:OE2	1:C:98:GLY:HA2	2.18	0.44
1:A:233:PHE:HB3	1:A:237:MET:HB2	2.00	0.43
1:C:16:ARG:HH11	1:C:16:ARG:HB2	1.83	0.43
1:B:168:HIS:ND1	1:B:172:TYR:O	2.34	0.43
1:A:246:TRP:HA	1:A:249:TRP:CE2	2.53	0.43
1:C:5:LEU:HD22	1:C:79:PHE:CD1	2.53	0.43
1:C:199:ILE:HA	1:C:215:VAL:HG22	1.99	0.43
1:A:263:SER:HB3	1:A:266:LEU:HB2	1.98	0.43
1:C:86:LEU:HD13	1:C:88:PHE:CZ	2.53	0.43
1:C:92:CYS:HB3	1:C:95:VAL:HG22	1.99	0.43
1:A:72:TYR:HA	1:A:76:TYR:CE2	2.53	0.43
1:B:54:THR:HG23	1:B:57:ASP:N	2.27	0.43
1:C:4:ARG:NH2	1:C:77:LEU:HD11	2.18	0.43
1:C:184:TYR:HB3	1:C:204:ILE:HG23	1.99	0.43
1:B:199:ILE:HD12	1:B:205:ILE:HD11	2.00	0.42
1:B:70:PHE:HD2	1:B:75:ASP:HB3	1.85	0.42
1:A:190:PHE:HD1	1:A:191:ILE:N	2.17	0.42
1:A:199:ILE:HD12	1:A:205:ILE:HD11	2.01	0.42
1:C:204:ILE:CD1	1:C:232:ARG:HD3	2.40	0.42
1:B:117:LYS:HD2	1:B:178:THR:CG2	2.49	0.42
1:C:218:PHE:HD2	1:C:238:ILE:HG23	1.85	0.42
1:C:240:THR:HA	1:C:243:ARG:HE	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ALA:HA	1:B:174:LYS:HE3	2.02	0.42
1:B:239:GLU:O	1:B:243:ARG:HG3	2.20	0.42
1:B:161:LYS:N	1:B:161:LYS:CD	2.83	0.42
1:B:199:ILE:HD13	1:B:215:VAL:HB	2.02	0.42
1:A:101:THR:CG2	1:A:123:THR:H	2.24	0.41
1:B:157:VAL:HG21	1:C:250:SER:CB	2.51	0.41
1:B:235:LYS:O	1:B:235:LYS:HG2	2.20	0.41
1:C:30:ARG:HG3	1:C:31:ALA:N	2.35	0.41
1:B:117:LYS:HB2	1:B:176:PRO:HB2	2.02	0.41
1:A:239:GLU:O	1:A:243:ARG:HG3	2.20	0.41
1:A:116:ILE:HD11	1:A:131:ILE:HD13	2.02	0.41
1:A:201:ASP:OD1	1:A:201:ASP:N	2.52	0.41
1:B:11:ARG:HE	1:B:11:ARG:HB3	1.53	0.41
1:A:128:THR:OG1	1:A:187:ALA:HB1	2.21	0.41
1:C:3:THR:N	1:C:6:GLU:OE2	2.53	0.41
1:A:240:THR:O	1:A:244:VAL:HG23	2.20	0.41
1:B:0:GLY:HA3	1:B:93:PHE:HA	2.03	0.41
1:B:155:MET:HE1	1:B:158:PHE:HD2	1.85	0.41
1:A:126:ASN:HD22	1:A:126:ASN:HA	1.69	0.41
1:A:221:VAL:HA	1:A:227:ARG:O	2.21	0.41
1:A:101:THR:HG22	1:A:123:THR:N	2.24	0.40
1:A:92:CYS:SG	1:A:108:VAL:HG13	2.62	0.40
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.95	0.40
1:B:165:ASP:OD1	1:B:166:PRO:HD2	2.20	0.40
1:B:190:PHE:CE1	1:B:192:ASN:HA	2.57	0.40
1:B:161:LYS:N	1:B:161:LYS:HD3	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:TYR:OH	4:B:302:COA:C7P[3_655]	1.38	0.82

## 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	271/276 (98%)	255 (94%)	16 (6%)	0	100	100
1	B	271/276 (98%)	257 (95%)	14 (5%)	0	100	100
1	C	270/276 (98%)	255 (94%)	15 (6%)	0	100	100
All	All	812/828 (98%)	767 (94%)	45 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	234/237 (99%)	211 (90%)	23 (10%)	8	11
1	B	234/237 (99%)	222 (95%)	12 (5%)	24	37
1	C	234/237 (99%)	219 (94%)	15 (6%)	17	27
All	All	702/711 (99%)	652 (93%)	50 (7%)	14	22

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	38	HIS
1	A	39	THR
1	A	46	GLN
1	A	55	ASP
1	A	56	ASP
1	A	117	LYS
1	A	126	ASN
1	A	130	GLU
1	A	140	THR
1	A	143	SER
1	A	145	ASP
1	A	153	GLU

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Mol	Chain	Res	Type
1	A	154	SER
1	A	161	LYS
1	A	167	LYS
1	A	172	TYR
1	A	184	TYR
1	A	190	PHE
1	A	201	ASP
1	A	237	MET
1	A	257	ASN
1	A	268	MET
1	B	38	HIS
1	B	55	ASP
1	B	56	ASP
1	B	143	SER
1	B	145	ASP
1	B	170	TYR
1	B	172	TYR
1	B	201	ASP
1	B	229	LYS
1	B	235	LYS
1	B	257	ASN
1	B	269	LYS
1	C	2	LYS
1	C	10	GLU
1	C	38	HIS
1	C	46	GLN
1	C	47	TYR
1	C	55	ASP
1	C	63	SER
1	C	99	ARG
1	C	117	LYS
1	C	161	LYS
1	C	191	ILE
1	C	235	LYS
1	C	243	ARG
1	C	252	GLU
1	C	266	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 ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	COA	B	302	-	41,50,50	1.96	11 (26%)	52,75,75	3.43	17 (32%)
2	TOY	A	301	-	34,34,34	1.07	2 (5%)	41,50,50	1.36	4 (9%)
2	TOY	B	301	-	34,34,34	0.98	1 (2%)	41,50,50	1.27	4 (9%)
3	EDO	A	302	-	3,3,3	0.51	0	2,2,2	0.18	0
2	TOY	C	301	-	34,34,34	1.05	2 (5%)	41,50,50	1.29	4 (9%)

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
4	COA	B	302	-	-	15/44/64/64	0/3/3/3
2	TOY	A	301	-	-	2/12/68/68	0/3/3/3
2	TOY	B	301	-	-	2/12/68/68	0/3/3/3
3	EDO	A	302	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TOY	C	301	-	-	2/12/68/68	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	COA	O9P-C9P	6.63	1.36	1.23
4	B	302	COA	C2A-N3A	4.86	1.39	1.32
4	B	302	COA	C2B-C1B	3.82	1.59	1.53
2	A	301	TOY	C43-C33	-3.19	1.49	1.53
4	B	302	COA	C6A-C5A	-2.61	1.33	1.43
4	B	302	COA	O4B-C4B	2.57	1.50	1.45
4	B	302	COA	C5A-C4A	-2.55	1.34	1.40
2	B	301	TOY	C43-C33	-2.51	1.50	1.53
4	B	302	COA	C3B-C4B	2.48	1.59	1.52
4	B	302	COA	C2A-N1A	2.34	1.38	1.33
4	B	302	COA	C2B-C3B	-2.31	1.47	1.52
4	B	302	COA	C5B-C4B	2.26	1.58	1.51
2	C	301	TOY	C43-C33	-2.22	1.50	1.53
2	A	301	TOY	C52-C42	2.08	1.57	1.52
2	C	301	TOY	O53-C13	2.06	1.47	1.41
4	B	302	COA	P3B-O9A	-2.00	1.47	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	COA	O4B-C4B-C5B	12.89	151.78	109.37
4	B	302	COA	O4B-C1B-C2B	-12.10	89.25	106.93
4	B	302	COA	O4B-C4B-C3B	-8.07	87.57	104.87
4	B	302	COA	C5B-C4B-C3B	-7.70	88.89	114.40
4	B	302	COA	C3B-C2B-C1B	-6.07	86.43	99.89
4	B	302	COA	N3A-C2A-N1A	-5.19	120.57	128.68
2	A	301	TOY	O51-C51-C61	4.51	114.40	106.01
2	B	301	TOY	O51-C51-C61	3.93	113.33	106.01
2	C	301	TOY	O53-C53-C63	3.69	115.62	106.44
2	C	301	TOY	O51-C51-C61	3.64	112.79	106.01
4	B	302	COA	O5B-C5B-C4B	3.42	120.75	108.99
4	B	302	COA	C6P-C7P-N8P	-3.04	105.76	111.90
4	B	302	COA	CAP-C9P-N8P	2.78	122.11	116.58
2	A	301	TOY	C13-O62-C62	-2.76	111.12	117.96
4	B	302	COA	O9P-C9P-CAP	-2.60	113.13	121.06
2	C	301	TOY	C13-O62-C62	-2.55	111.65	117.96
4	B	302	COA	C2B-C3B-C4B	2.54	107.72	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	COA	P2A-O3A-P1A	-2.50	124.25	132.83
2	A	301	TOY	O23-C23-C33	-2.49	105.74	110.22
2	B	301	TOY	C13-O62-C62	-2.36	112.11	117.96
4	B	302	COA	O9A-P3B-O8A	2.32	116.51	107.64
2	B	301	TOY	O53-C53-C63	2.30	112.16	106.44
2	A	301	TOY	O62-C13-O53	-2.28	104.31	110.67
4	B	302	COA	C5A-C6A-N6A	-2.21	116.99	120.35
4	B	302	COA	C7P-N8P-C9P	-2.17	118.72	122.59
2	B	301	TOY	O23-C23-C33	-2.13	106.40	110.22
2	C	301	TOY	O23-C23-C33	-2.12	106.40	110.22
4	B	302	COA	O6A-CCP-CBP	-2.10	107.17	110.55
4	B	302	COA	O6A-P2A-O4A	-2.00	101.25	109.07

There are no chirality outliers.

All (22) torsion outliers are listed below:

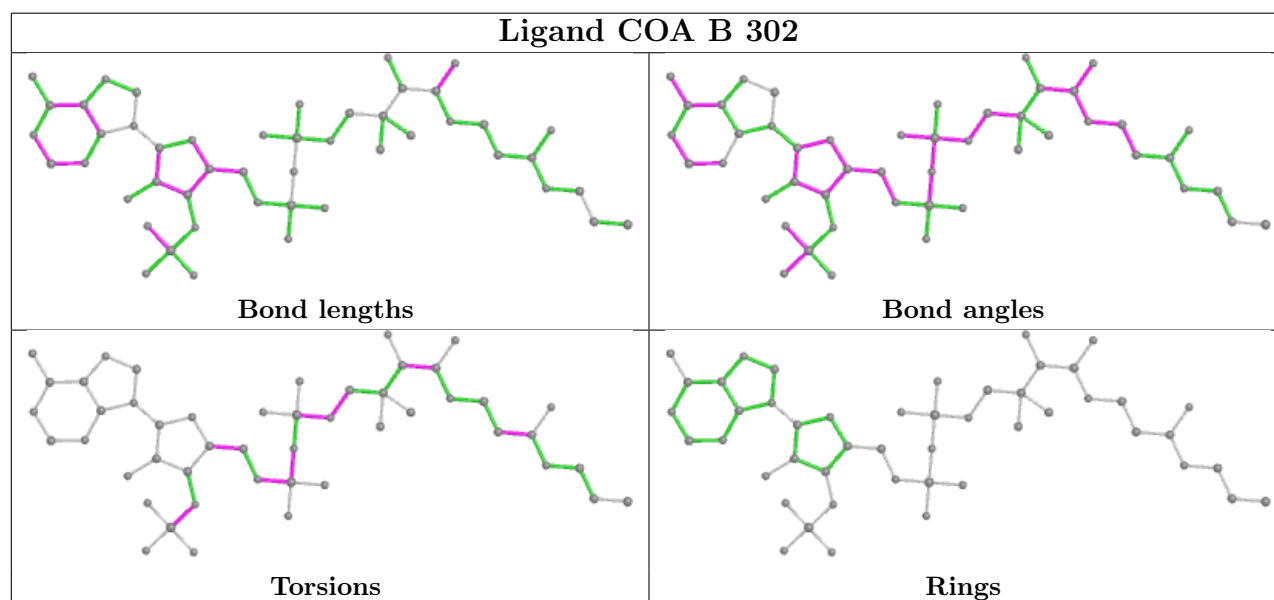
Mol	Chain	Res	Type	Atoms
4	B	302	COA	C5B-O5B-P1A-O1A
4	B	302	COA	CCP-O6A-P2A-O4A
4	B	302	COA	O9P-C9P-CAP-CBP
4	B	302	COA	N8P-C9P-CAP-CBP
4	B	302	COA	O5P-C5P-C6P-C7P
4	B	302	COA	N4P-C5P-C6P-C7P
4	B	302	COA	P2A-O3A-P1A-O1A
2	C	301	TOY	C52-C42-O11-C11
2	B	301	TOY	C52-C42-O11-C11
2	A	301	TOY	C52-C42-O11-C11
4	B	302	COA	C3B-C4B-C5B-O5B
4	B	302	COA	C3B-O3B-P3B-O7A
4	B	302	COA	C5B-O5B-P1A-O3A
4	B	302	COA	CCP-O6A-P2A-O3A
4	B	302	COA	CBP-CCP-O6A-P2A
2	B	301	TOY	O51-C11-O11-C42
4	B	302	COA	C5B-O5B-P1A-O2A
4	B	302	COA	CCP-O6A-P2A-O5A
2	A	301	TOY	O51-C11-O11-C42
2	C	301	TOY	O51-C11-O11-C42
4	B	302	COA	P2A-O3A-P1A-O2A
3	A	302	EDO	O1-C1-C2-O2

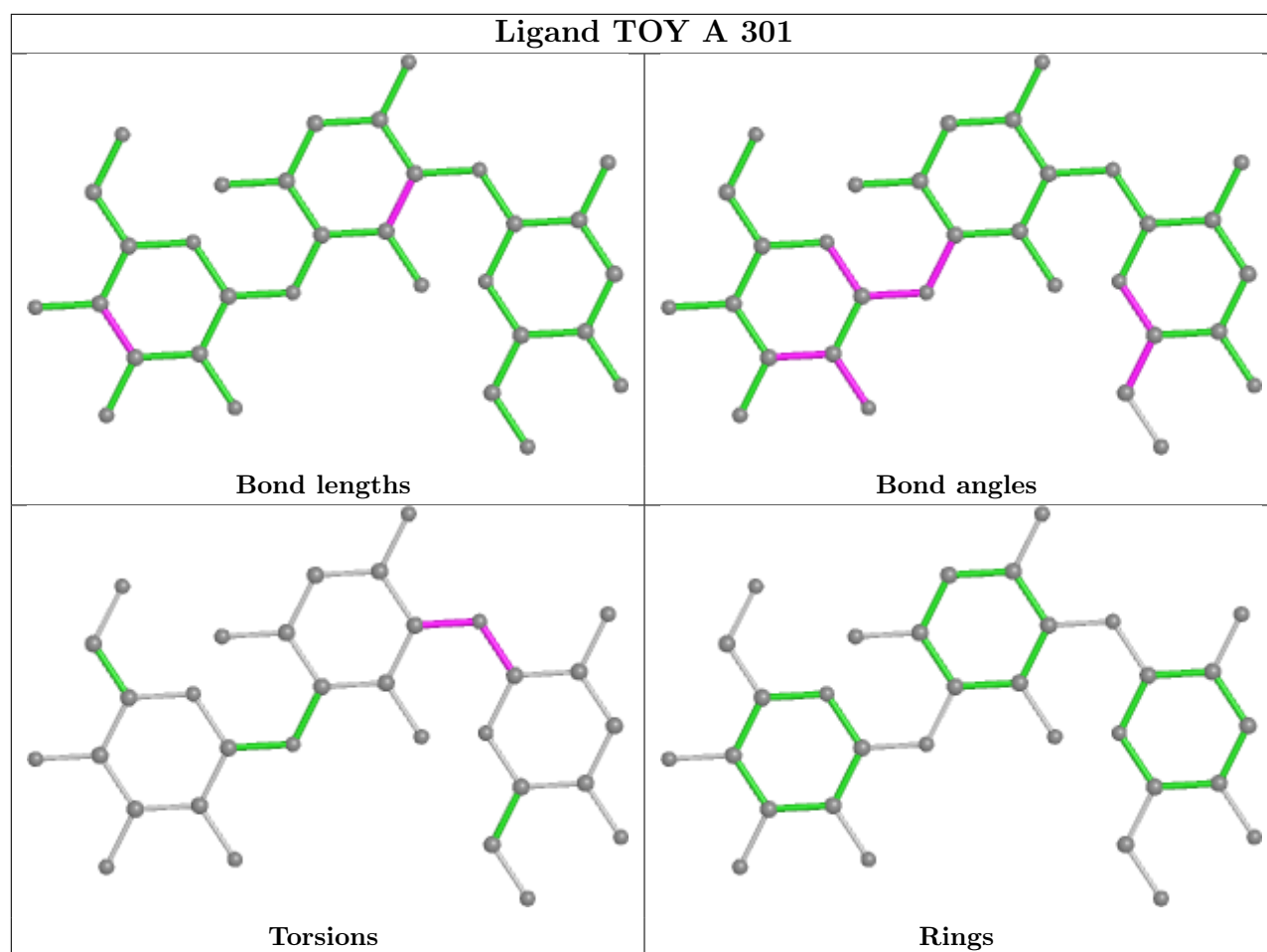
There are no ring outliers.

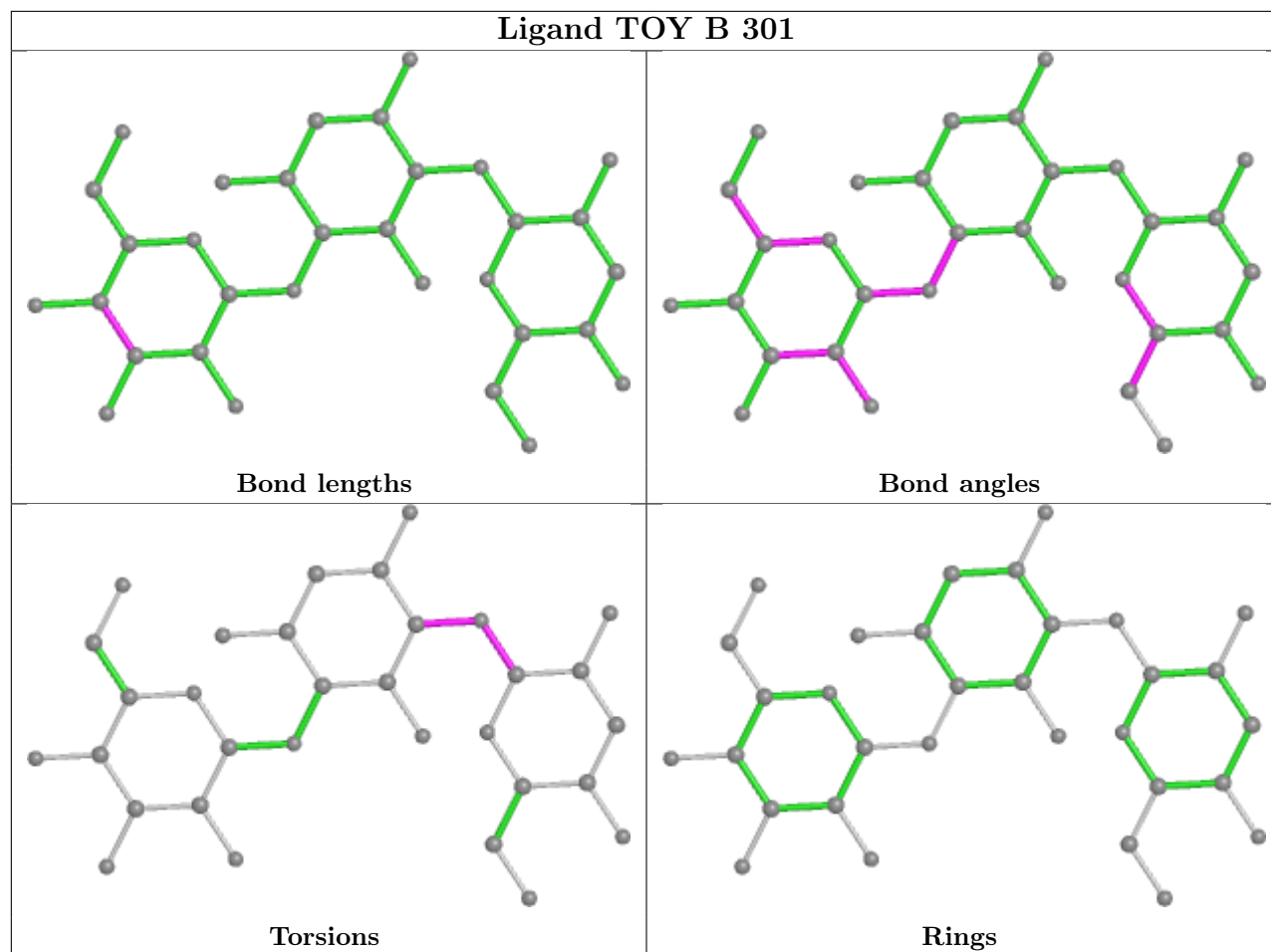
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	COA	3	1

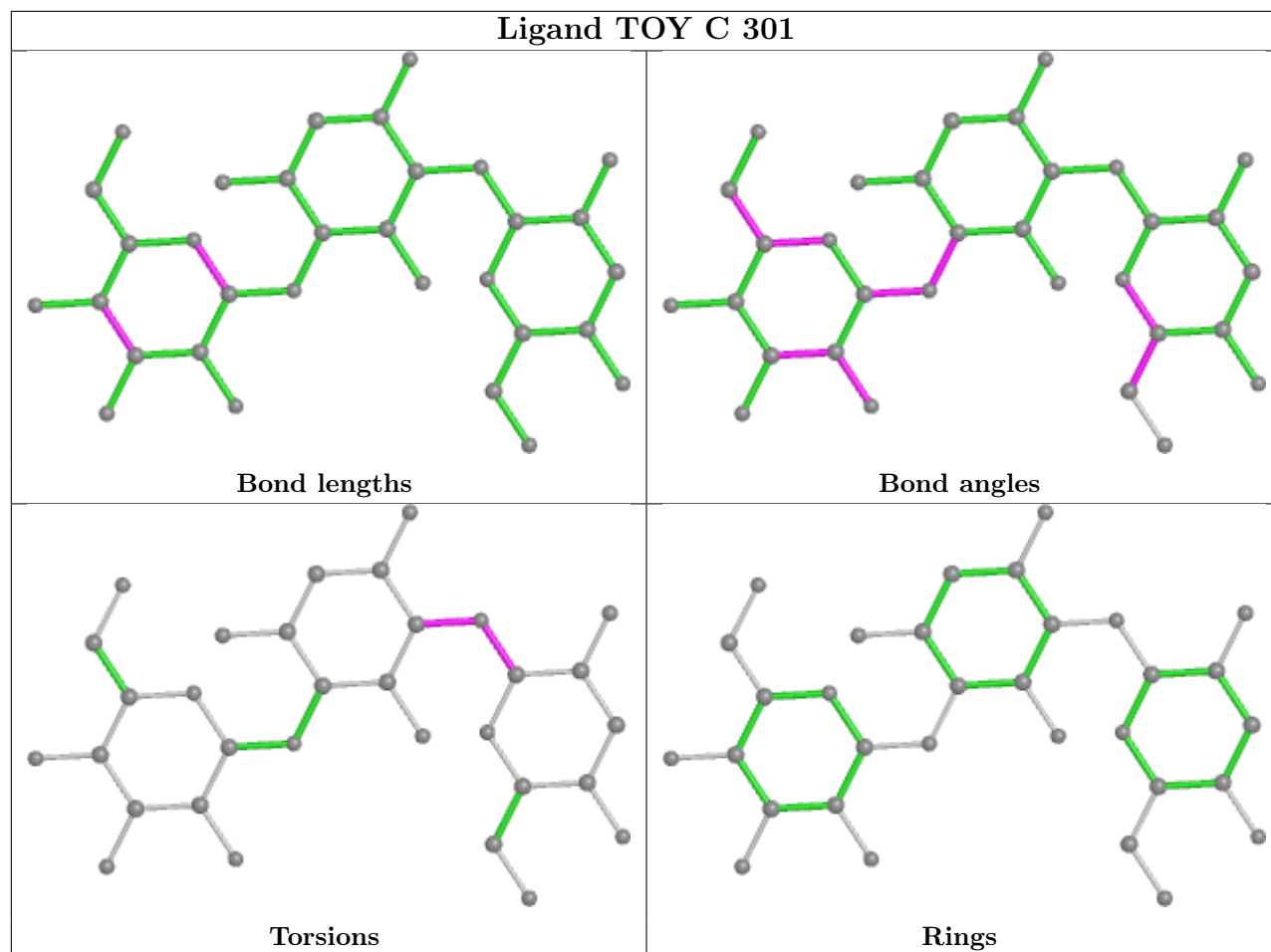
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/276 (98%)	0.17	10 (3%) 41 38	39, 91, 137, 185	0
1	B	273/276 (98%)	0.18	13 (4%) 30 27	39, 92, 137, 173	0
1	C	272/276 (98%)	1.17	60 (22%) 0 0	114, 154, 223, 291	0
All	All	818/828 (98%)	0.50	83 (10%) 7 4	39, 114, 195, 291	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	VAL	10.3
1	C	32	LEU	9.7
1	C	172	TYR	6.0
1	C	33	LYS	5.9
1	C	220	VAL	5.8
1	C	269	LYS	5.8
1	C	230	ARG	5.7
1	C	58	LEU	5.6
1	B	224	VAL	5.3
1	C	135	ALA	4.9
1	C	72	TYR	4.7
1	C	38	HIS	4.5
1	C	229	LYS	4.5
1	C	80	ASP	4.5
1	C	222	VAL	4.0
1	C	162	LEU	3.8
1	B	266	LEU	3.6
1	C	225	PRO	3.5
1	C	208	GLY	3.5
1	C	254	ILE	3.4
1	C	205	ILE	3.4
1	B	191	ILE	3.3
1	C	191	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	211	VAL	3.2
1	C	131	ILE	3.2
1	C	155	MET	3.2
1	B	162	LEU	3.2
1	C	79	PHE	3.2
1	C	223	GLY	3.2
1	C	42	ARG	3.1
1	C	23	VAL	3.1
1	A	224	VAL	3.1
1	C	194	SER	3.0
1	C	132	HIS	3.0
1	A	267	PHE	3.0
1	C	267	PHE	2.9
1	C	1	MET	2.9
1	A	196	VAL	2.8
1	C	196	VAL	2.7
1	C	141	PHE	2.7
1	C	89	GLU	2.7
1	B	215	VAL	2.6
1	B	68	LYS	2.6
1	C	47	TYR	2.6
1	B	254	ILE	2.6
1	C	15	GLY	2.5
1	C	104	GLY	2.5
1	C	76	TYR	2.5
1	C	52	ALA	2.5
1	C	34	PRO	2.4
1	A	254	ILE	2.4
1	B	244	VAL	2.4
1	B	216	PRO	2.4
1	A	212	LEU	2.4
1	C	46	GLN	2.4
1	C	62	LEU	2.3
1	B	229	LYS	2.3
1	C	14	ASN	2.3
1	C	29	LEU	2.3
1	B	135	ALA	2.3
1	C	13	LEU	2.3
1	A	262	ILE	2.3
1	C	221	VAL	2.3
1	C	21	TRP	2.2
1	C	250	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLU	2.2
1	C	56	ASP	2.2
1	C	67	SER	2.2
1	B	241	LEU	2.2
1	C	158	PHE	2.2
1	C	31	ALA	2.2
1	A	265	GLU	2.1
1	C	27	ARG	2.1
1	C	5	LEU	2.1
1	C	61	PHE	2.1
1	B	158	PHE	2.1
1	A	162	LEU	2.1
1	C	28	LEU	2.1
1	C	258	VAL	2.1
1	C	82	GLU	2.1
1	C	170	TYR	2.1
1	C	143	SER	2.0
1	A	269	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

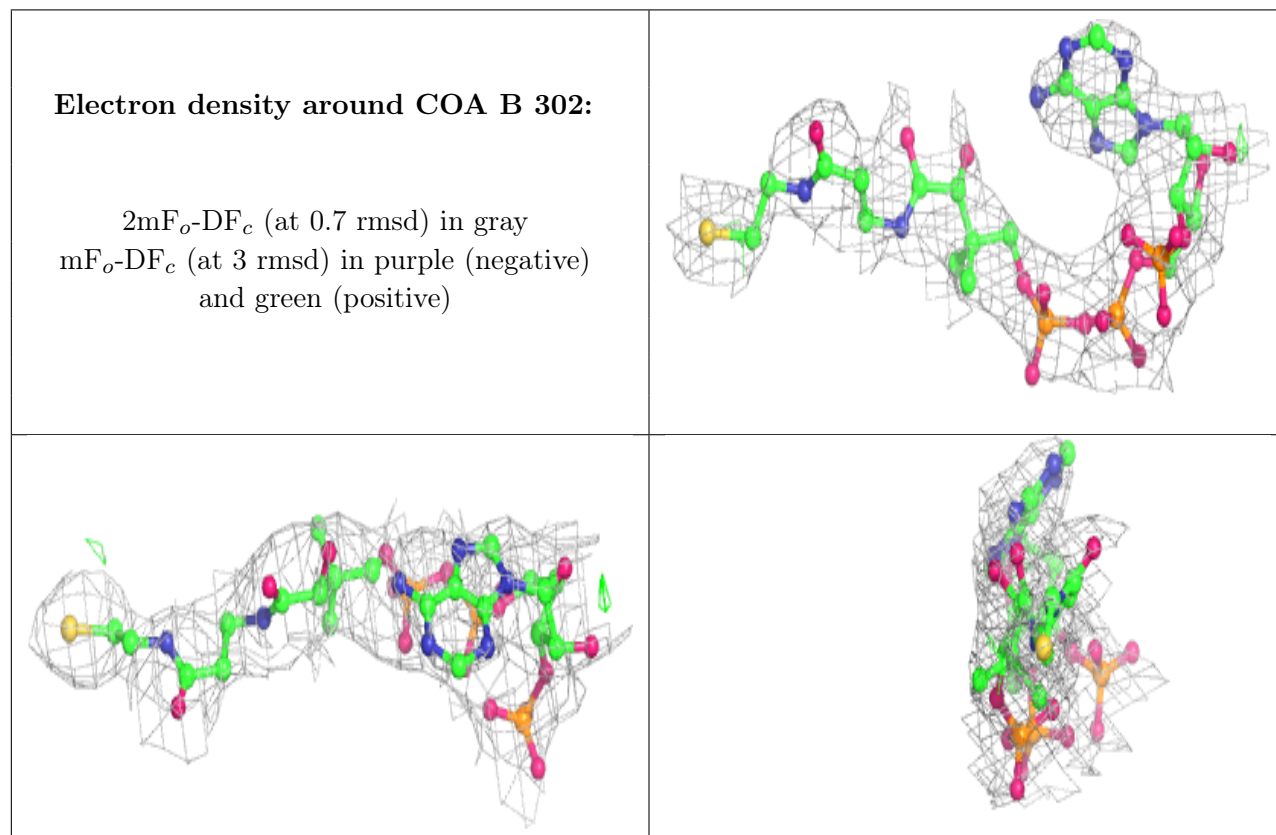
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

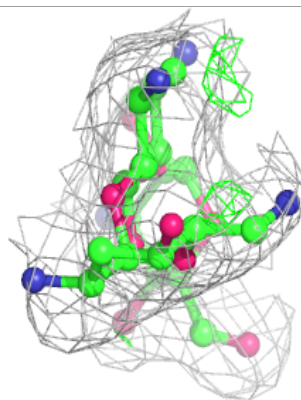
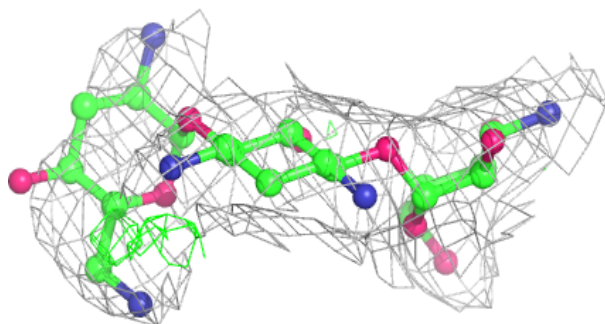
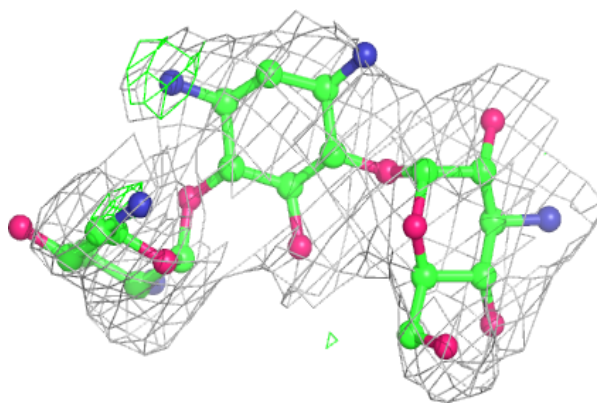
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	COA	B	302	48/48	0.83	0.20	98,153,186,192	0
2	TOY	C	301	32/32	0.84	0.16	89,124,136,139	0
2	TOY	A	301	32/32	0.93	0.15	45,77,84,92	0
2	TOY	B	301	32/32	0.93	0.15	45,72,87,88	0
3	EDO	A	302	4/4	0.95	0.14	46,54,62,64	0

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.

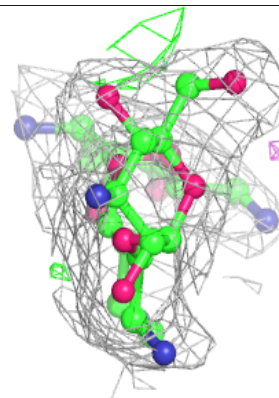
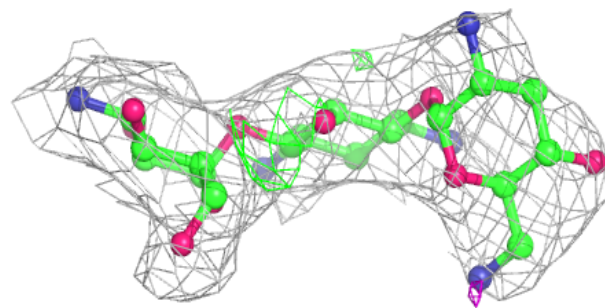
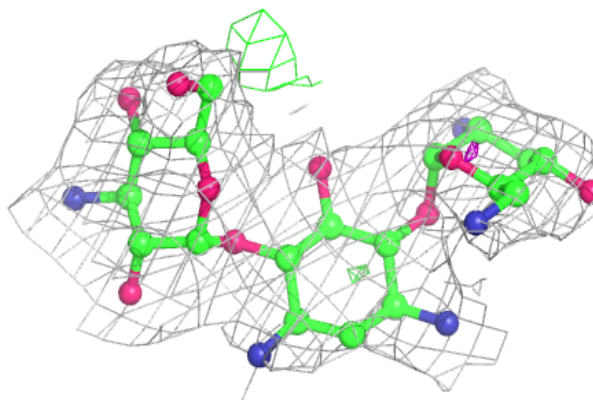


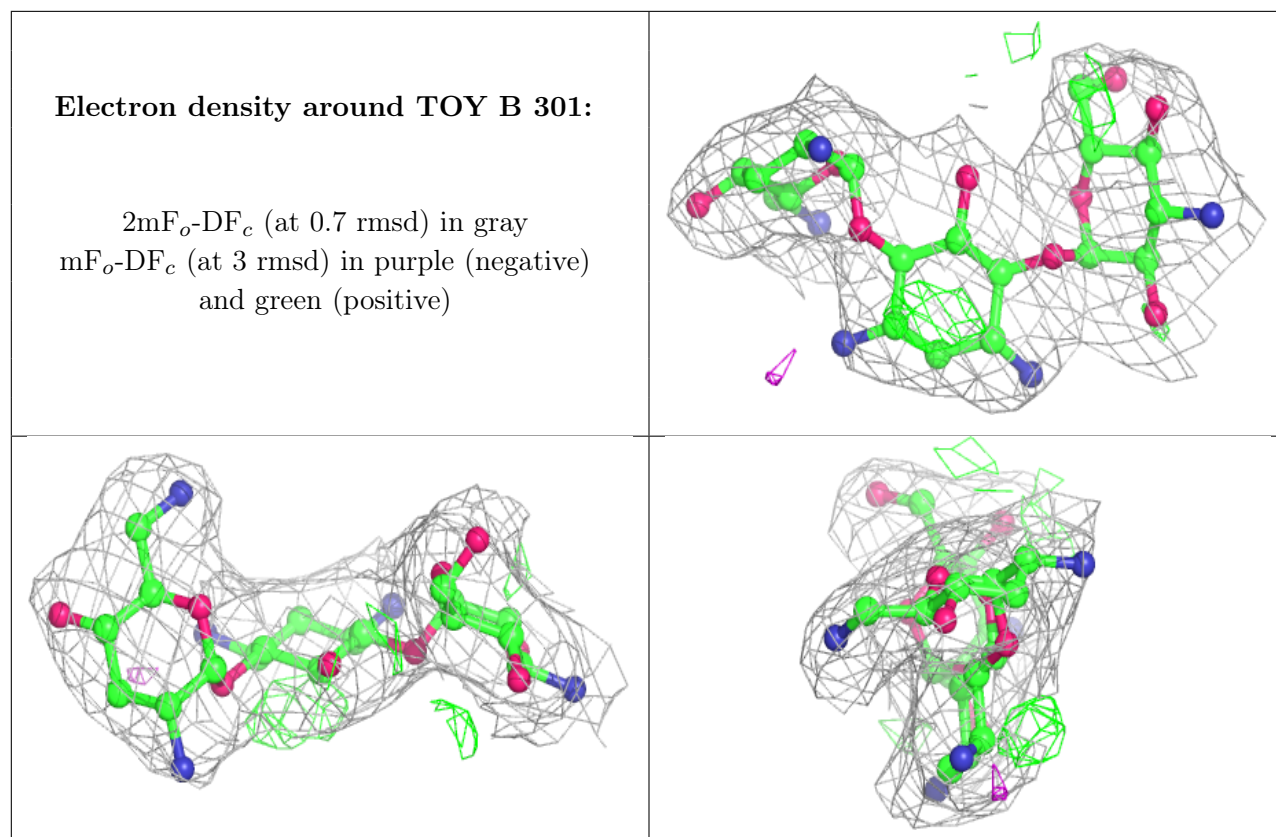
**Electron density around TOY C 301:**

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

**Electron density around TOY 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.