



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:52 AM UTC

PDB ID : 7E9A / pdb_00007e9a
Title : Crystal structure of KPC-2 in complex with (S)-2-(1-hydroxy-1,3-dihydrobenzo[c][1,2]oxaborol-3-yl)acrylic acid (4a-(S))
Authors : Li, G.-B.; Yan, Y.-H.
Deposited on : 2021-03-03
Resolution : 2.25 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

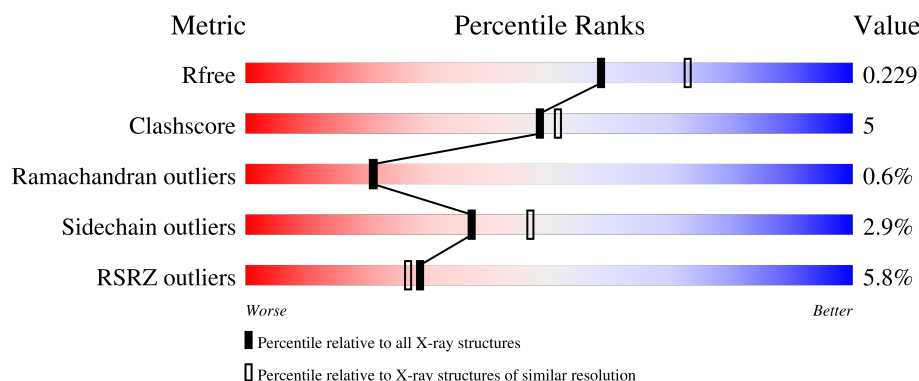
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	265	2% 93% 6%
1	B	265	5% 90% 8% ..
1	C	265	11% 86% 11% ..
1	D	265	5% 88% 12% .

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
5	GOL	A	306	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8391 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.

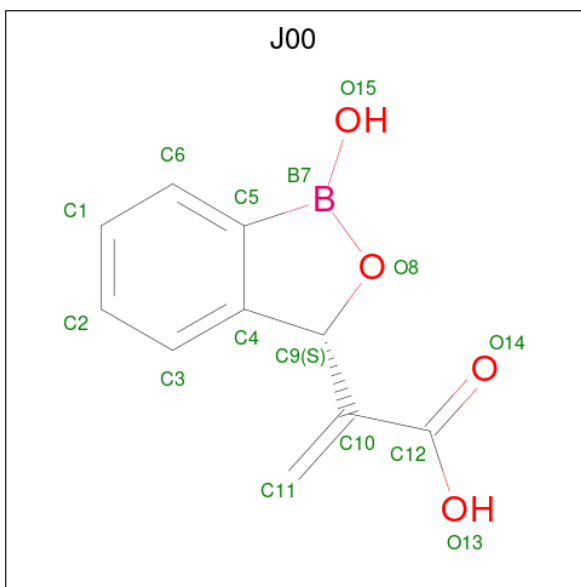
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	1
			1970	1240	346	379	5			
1	B	262	Total	C	N	O	S	0	0	1
			1950	1229	342	374	5			
1	C	265	Total	C	N	O	S	0	0	1
			1970	1240	346	379	5			
1	D	263	Total	C	N	O	S	0	0	1
			1955	1229	344	377	5			

There are 4 discrepancies between the modelled and reference sequences:

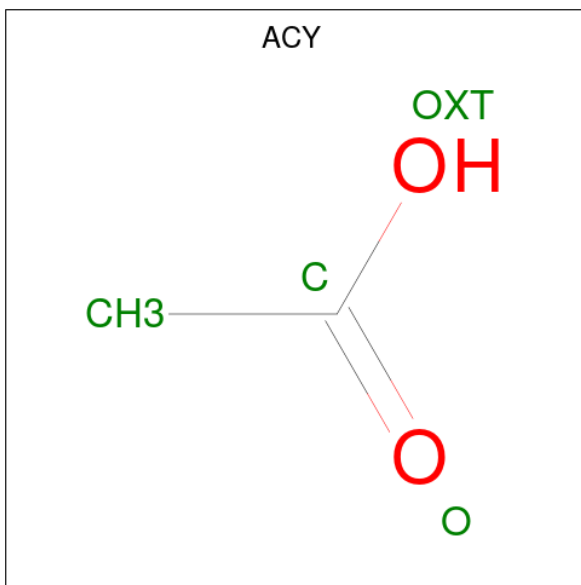
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	SER	-	expression tag	UNP Q93LQ9
B	25	SER	-	expression tag	UNP Q93LQ9
C	25	SER	-	expression tag	UNP Q93LQ9
D	25	SER	-	expression tag	UNP Q93LQ9

- Molecule 2 is 2-[(3S)-1-oxidanyl-3H-2,1-benzoxaborol-3-yl]prop-2-enoic acid (CCD ID: J00) (formula: C₁₀H₉BO₄) (labeled as "Ligand of Interest" by depositor).



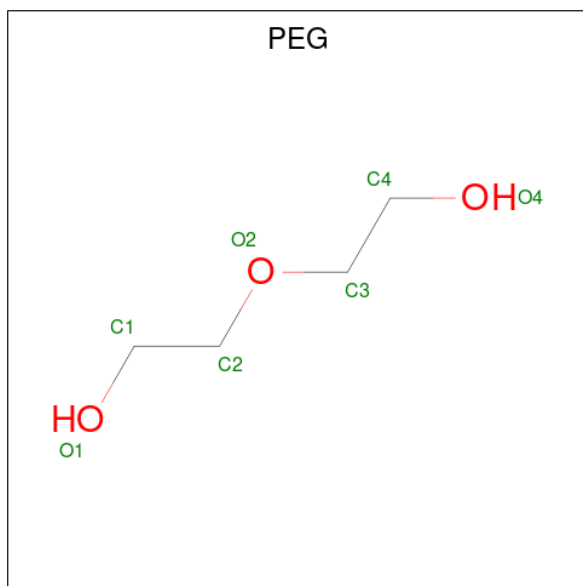
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	B	C	O	0	0
			15	1	10	4		
2	B	1	Total	B	C	O	0	0
			15	1	10	4		
2	C	1	Total	B	C	O	0	0
			15	1	10	4		
2	D	1	Total	B	C	O	0	0
			15	1	10	4		

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



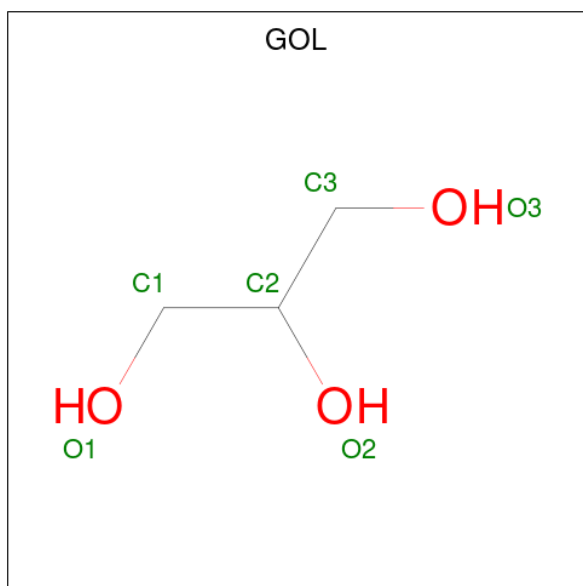
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	115	Total	O	0	0
			115	115		
6	B	92	Total	O	0	0
			92	92		

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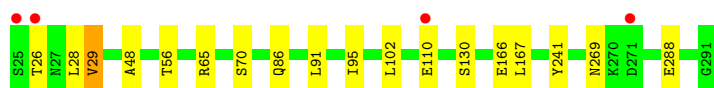
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	54	Total 54	O 54	0	0
6	D	107	Total 107	O 107	0	0

3 Residue-property plots [i](#)

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

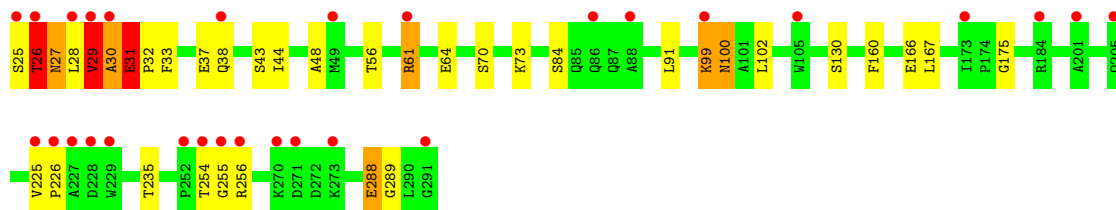
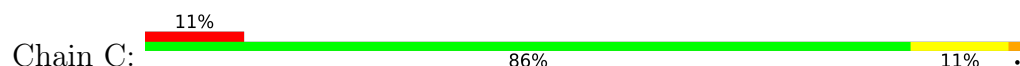
• Molecule 1: Beta-lactamase



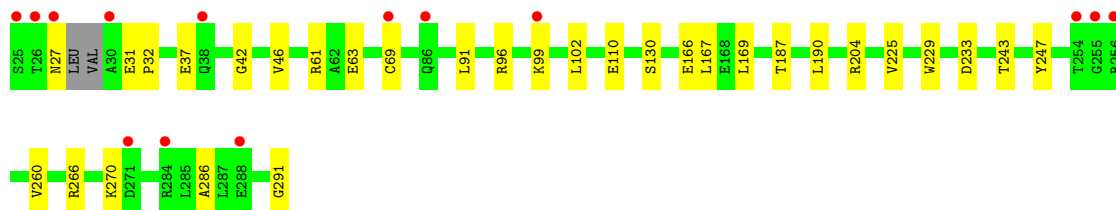
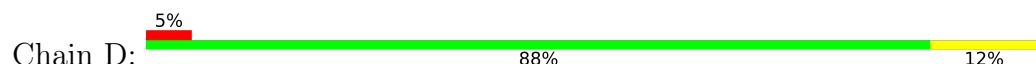
• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.42Å 165.42Å 94.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.43 – 2.25 47.43 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.43-2.25) 95.5 (47.43-2.25)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.180 , 0.221 0.189 , 0.229	Depositor DCC
R_{free} test set	2005 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8391	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, J00, GOL, PEG

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	0.57	0/2010	0.66	0/2740
1	B	0.59	0/1990	0.73	3/2712 (0.1%)
1	C	0.55	0/2010	0.70	4/2740 (0.1%)
1	D	0.57	0/1994	0.66	0/2716
All	All	0.57	0/8004	0.69	7/10908 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	LEU	CA-C-N	7.28	134.80	121.70
1	B	28	LEU	C-N-CA	7.28	134.80	121.70
1	C	26	THR	CA-C-N	7.03	134.35	121.70
1	C	26	THR	C-N-CA	7.03	134.35	121.70
1	C	30	ALA	CA-C-N	6.76	138.29	121.80
1	C	30	ALA	C-N-CA	6.76	138.29	121.80
1	B	29	VAL	N-CA-CB	5.21	120.35	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1970	0	1941	17	0
1	B	1950	0	1926	22	0
1	C	1970	0	1941	38	0
1	D	1955	0	1921	19	0
2	A	15	0	0	2	0
2	B	15	0	0	2	0
2	C	15	0	0	4	0
2	D	15	0	0	0	0
3	A	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
4	A	7	0	10	0	0
4	B	28	0	40	3	0
4	C	28	0	40	4	0
4	D	7	0	10	0	0
5	A	18	0	24	5	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	115	0	0	1	0
6	B	92	0	0	3	0
6	C	54	0	0	1	0
6	D	107	0	0	5	0
All	All	8391	0	7886	87	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 5.

All (87) 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)
4:B:304:PEG:O1	6:B:401:HOH:O	1.80	0.94
1:C:28:LEU:O	1:C:29:VAL:HB	1.75	0.85
1:D:291:GLY:N	6:D:403:HOH:O	2.21	0.72
1:D:27:ASN:O	6:D:401:HOH:O	2.08	0.69
1:C:27:ASN:ND2	6:C:401:HOH:O	2.25	0.69
1:D:110:GLU:OE1	6:D:402:HOH:O	2.12	0.67
1:C:28:LEU:O	1:C:29:VAL:CB	2.43	0.62
1:D:166:GLU:HB3	1:D:167:LEU:HD12	1.81	0.61
1:B:205:GLN:OE1	4:B:305:PEG:H42	2.02	0.60
1:B:28:LEU:HA	1:B:29:VAL:HB	1.83	0.58
1:C:27:ASN:OD1	1:C:27:ASN:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:OG	2:A:301:J00:O15	2.23	0.57
1:C:31:GLU:H	1:C:32:PRO:CD	2.17	0.57
1:A:28:LEU:H	1:C:29:VAL:HG11	1.70	0.57
1:B:284:ARG:NH1	6:B:403:HOH:O	2.38	0.56
1:A:65:ARG:H	5:A:306:GOL:C1	2.19	0.56
1:C:30:ALA:CB	1:C:33:PHE:HD2	2.20	0.55
1:B:38:GLN:OE1	6:B:402:HOH:O	2.17	0.54
1:C:25:SER:O	1:C:26:THR:HB	2.07	0.54
1:D:31:GLU:N	1:D:32:PRO:CD	2.71	0.54
1:B:28:LEU:HG	1:B:29:VAL:HG12	1.90	0.54
1:B:37:GLU:HG2	1:B:42:GLY:O	2.09	0.53
5:A:306:GOL:H2	1:B:65:ARG:HH21	1.73	0.52
1:A:26:THR:HG22	1:C:28:LEU:HD13	1.90	0.52
1:A:28:LEU:N	1:C:29:VAL:HG11	2.24	0.52
1:C:166:GLU:HB3	1:C:167:LEU:HD12	1.92	0.52
1:A:65:ARG:HB2	5:A:306:GOL:H12	1.91	0.51
1:A:65:ARG:H	5:A:306:GOL:H11	1.76	0.51
1:B:28:LEU:HA	1:B:29:VAL:CB	2.41	0.51
1:C:30:ALA:HB1	1:C:33:PHE:HD2	1.76	0.51
1:B:70:SER:OG	2:B:301:J00:O8	2.29	0.50
1:B:29:VAL:HG13	1:B:30:ALA:N	2.27	0.50
1:C:28:LEU:HD12	1:C:289:GLY:O	2.12	0.50
1:B:70:SER:OG	2:B:301:J00:O15	2.29	0.50
1:D:46:VAL:HG11	1:D:286:ALA:HB2	1.93	0.50
1:A:28:LEU:H	1:C:29:VAL:CG1	2.25	0.50
1:C:31:GLU:N	1:C:32:PRO:CD	2.75	0.50
1:C:43:SER:OG	1:C:61:ARG:NH2	2.45	0.49
1:A:166:GLU:HB3	1:A:167:LEU:HD12	1.95	0.48
1:A:288:GLU:OE1	1:D:270:LYS:NZ	2.46	0.48
1:C:99:LYS:HD3	1:C:102:LEU:HD12	1.95	0.48
1:D:169:LEU:C	1:D:169:LEU:HD12	2.39	0.47
1:B:104:PRO:HB2	1:B:105:TRP:CE3	2.49	0.47
6:A:437:HOH:O	1:C:25:SER:HA	2.14	0.47
1:B:225:VAL:CG1	1:B:229:TRP:HB2	2.45	0.47
1:C:29:VAL:O	1:C:30:ALA:HB2	2.14	0.47
1:D:225:VAL:CG1	1:D:229:TRP:HB2	2.46	0.46
1:B:169:LEU:HD12	1:B:169:LEU:C	2.40	0.46
1:A:70:SER:OG	2:A:301:J00:O8	2.34	0.46
1:C:38:GLN:OE1	1:D:42:GLY:HA2	2.16	0.46
1:C:70:SER:CB	2:C:301:J00:O15	2.64	0.46
1:B:28:LEU:CB	1:B:29:VAL:HG12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ARG:CD	6:D:450:HOH:O	2.64	0.45
1:B:29:VAL:CG1	1:B:30:ALA:N	2.80	0.45
1:C:70:SER:HB3	1:C:73:LYS:HD2	1.98	0.45
1:C:100:ASN:OD1	4:C:303:PEG:C4	2.65	0.44
1:D:187:THR:HG23	1:D:260:VAL:HG12	2.00	0.44
1:B:166:GLU:HB3	1:B:167:LEU:HD12	2.00	0.44
1:C:48:ALA:O	1:C:56:THR:HA	2.18	0.43
1:D:99:LYS:HD2	1:D:102:LEU:HD12	2.01	0.43
1:A:29:VAL:HG22	1:A:29:VAL:O	2.18	0.43
1:C:70:SER:CB	2:C:301:J00:O8	2.67	0.43
1:C:27:ASN:OD1	1:C:27:ASN:O	2.37	0.43
1:B:251:TRP:CD2	4:B:305:PEG:H12	2.54	0.42
1:C:160:PHE:C	1:C:160:PHE:CD1	2.97	0.42
1:D:37:GLU:OE1	1:D:61:ARG:NE	2.45	0.42
1:A:102:LEU:HD13	1:A:110:GLU:HG2	2.02	0.42
1:C:100:ASN:OD1	4:C:303:PEG:H42	2.19	0.42
1:C:100:ASN:ND2	4:C:303:PEG:O1	2.53	0.42
1:C:37:GLU:OE2	1:D:266:ARG:NH1	2.49	0.42
1:D:69:CYS:SG	1:D:243:THR:HG22	2.60	0.42
1:A:65:ARG:H	5:A:306:GOL:H12	1.85	0.42
1:B:184:ARG:HD2	1:B:184:ARG:C	2.44	0.42
1:B:168:GLU:OE2	1:C:288:GLU:OE2	2.39	0.41
1:C:235:THR:OG1	2:C:301:J00:O13	2.36	0.41
1:C:70:SER:HB2	2:C:301:J00:O8	2.19	0.41
1:A:241:TYR:HA	1:A:269:ASN:O	2.21	0.41
1:D:204:ARG:HD3	6:D:450:HOH:O	2.20	0.41
1:B:225:VAL:HG12	1:B:226:PRO:O	2.21	0.41
1:B:76:LEU:HD21	1:B:138:LEU:HB2	2.02	0.41
1:D:190:LEU:HD22	1:D:247:TYR:CD1	2.56	0.41
1:C:226:PRO:HD3	4:C:304:PEG:H12	2.03	0.41
1:C:254:THR:O	1:C:256:ARG:N	2.53	0.41
1:A:29:VAL:HG13	1:C:29:VAL:CG2	2.51	0.41
1:C:44:ILE:O	1:C:61:ARG:HG3	2.20	0.41
1:A:48:ALA:O	1:A:56:THR:HA	2.20	0.40
1:C:175:GLY:N	1:D:63:GLU:HG3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	B	260/265 (98%)	255 (98%)	4 (2%)	1 (0%)	30	31
1	C	263/265 (99%)	251 (95%)	7 (3%)	5 (2%)	6	3
1	D	259/265 (98%)	253 (98%)	6 (2%)	0	100	100
All	All	1045/1060 (99%)	1017 (97%)	22 (2%)	6 (1%)	21	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	VAL
1	C	29	VAL
1	C	100	ASN
1	C	26	THR
1	C	255	GLY
1	C	31	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/200 (99%)	193 (98%)	5 (2%)	42	52
1	B	196/200 (98%)	194 (99%)	2 (1%)	68	77
1	C	198/200 (99%)	186 (94%)	12 (6%)	17	17
1	D	196/200 (98%)	192 (98%)	4 (2%)	48	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	788/800 (98%)	765 (97%)	23 (3%)	37	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	86	GLN
1	A	91	LEU
1	A	95	ILE
1	A	130	SER
1	B	28	LEU
1	B	31	GLU
1	C	26	THR
1	C	27	ASN
1	C	29	VAL
1	C	31	GLU
1	C	61	ARG
1	C	64	GLU
1	C	84	SER
1	C	91	LEU
1	C	99	LYS
1	C	130	SER
1	C	225	VAL
1	C	288	GLU
1	D	91	LEU
1	D	96	ARG
1	D	130	SER
1	D	233	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	B	170	ASN
1	B	206	GLN
1	C	100	ASN
1	D	170	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 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	PEG	C	304	-	6,6,6	0.55	0	5,5,5	0.35	0
4	PEG	B	304	-	6,6,6	0.43	0	5,5,5	0.38	0
3	ACY	C	302	-	3,3,3	1.17	0	3,3,3	0.95	0
4	PEG	B	305	-	6,6,6	0.57	0	5,5,5	0.49	0
5	GOL	C	307	-	5,5,5	0.16	0	5,5,5	0.37	0
4	PEG	C	306	-	6,6,6	0.44	0	5,5,5	0.50	0
5	GOL	A	306	-	5,5,5	0.87	0	5,5,5	2.17	3 (60%)
4	PEG	A	303	-	6,6,6	0.48	0	5,5,5	0.44	0
5	GOL	A	305	-	5,5,5	0.61	0	5,5,5	0.78	0
5	GOL	D	303	-	5,5,5	0.40	0	5,5,5	0.67	0
2	J00	A	301	1	14,16,16	3.18	3 (21%)	16,23,23	3.11	6 (37%)
3	ACY	D	302	-	3,3,3	0.97	0	3,3,3	1.05	0
5	GOL	B	306	-	5,5,5	0.50	0	5,5,5	0.85	0
4	PEG	C	303	-	6,6,6	0.50	0	5,5,5	0.72	0
4	PEG	D	304	-	6,6,6	0.57	0	5,5,5	0.40	0
3	ACY	A	302	-	3,3,3	0.89	0	3,3,3	1.22	0
2	J00	D	301	1	14,16,16	3.28	3 (21%)	16,23,23	2.90	6 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	304	-	5,5,5	0.10	0	5,5,5	0.29	0
2	J00	C	301	1	14,16,16	3.16	3 (21%)	16,23,23	2.91	5 (31%)
4	PEG	C	305	-	6,6,6	0.43	0	5,5,5	0.84	0
4	PEG	B	303	-	6,6,6	0.39	0	5,5,5	0.36	0
2	J00	B	301	1	14,16,16	3.34	4 (28%)	16,23,23	2.93	7 (43%)
4	PEG	B	302	-	6,6,6	0.71	0	5,5,5	1.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	C	304	-	-	0/4/4/4	-
4	PEG	B	304	-	-	2/4/4/4	-
4	PEG	B	305	-	-	2/4/4/4	-
5	GOL	C	307	-	-	3/4/4/4	-
4	PEG	C	306	-	-	3/4/4/4	-
5	GOL	A	306	-	-	0/4/4/4	-
4	PEG	A	303	-	-	4/4/4/4	-
5	GOL	A	305	-	-	3/4/4/4	-
5	GOL	D	303	-	-	3/4/4/4	-
2	J00	A	301	1	-	5/8/20/20	0/2/2/2
5	GOL	B	306	-	-	2/4/4/4	-
4	PEG	C	303	-	-	4/4/4/4	-
4	PEG	D	304	-	-	2/4/4/4	-
2	J00	D	301	1	-	5/8/20/20	0/2/2/2
5	GOL	A	304	-	-	2/4/4/4	-
2	J00	C	301	1	-	7/8/20/20	0/2/2/2
4	PEG	C	305	-	-	3/4/4/4	-
4	PEG	B	303	-	-	2/4/4/4	-
2	J00	B	301	1	-	7/8/20/20	0/2/2/2
4	PEG	B	302	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	J00	C4-C5	-11.14	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	J00	C4-C5	-10.69	1.32	1.40
2	B	301	J00	C4-C5	-10.26	1.33	1.40
2	A	301	J00	C4-C5	-9.69	1.33	1.40
2	B	301	J00	C12-C10	4.28	1.53	1.49
2	A	301	J00	C12-C10	4.18	1.53	1.49
2	A	301	J00	B7-O8	4.15	1.42	1.38
2	B	301	J00	B7-O8	4.11	1.42	1.38
2	D	301	J00	C12-C10	2.97	1.52	1.49
2	D	301	J00	B7-O8	2.89	1.41	1.38
2	C	301	J00	B7-O8	2.53	1.40	1.38
2	C	301	J00	C12-C10	2.20	1.51	1.49
2	B	301	J00	C3-C4	2.06	1.42	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	J00	O15-B7-O8	-8.31	103.92	121.91
2	D	301	J00	O15-B7-O8	-7.25	106.20	121.91
2	B	301	J00	O15-B7-O8	-6.78	107.23	121.91
2	A	301	J00	O15-B7-O8	-6.39	108.07	121.91
2	A	301	J00	O13-C12-C10	6.11	121.45	114.41
2	B	301	J00	O13-C12-C10	6.05	121.39	114.41
2	D	301	J00	O13-C12-C10	5.16	120.36	114.41
2	A	301	J00	C3-C4-C5	-5.01	117.31	121.41
2	C	301	J00	O13-C12-C10	4.74	119.88	114.41
2	B	301	J00	C3-C4-C5	-4.26	117.92	121.41
2	D	301	J00	O8-B7-C5	-4.22	106.15	108.47
2	A	301	J00	O8-B7-C5	-3.86	106.34	108.47
2	C	301	J00	C3-C4-C5	-3.58	118.48	121.41
2	D	301	J00	C3-C4-C5	-3.37	118.66	121.41
2	A	301	J00	C6-C5-C4	3.35	122.23	119.04
2	A	301	J00	O14-C12-C10	-3.29	119.17	122.88
2	B	301	J00	O8-B7-C5	-3.24	106.69	108.47
2	D	301	J00	O14-C12-C10	-2.96	119.54	122.88
2	C	301	J00	C6-C5-C4	2.93	121.83	119.04
2	B	301	J00	O14-C12-C10	-2.84	119.67	122.88
2	D	301	J00	C6-C5-C4	2.77	121.68	119.04
5	A	306	GOL	O1-C1-C2	-2.74	98.04	110.38
2	B	301	J00	C6-C5-C4	2.54	121.45	119.04
2	C	301	J00	O14-C12-C10	-2.52	120.03	122.88
5	A	306	GOL	C3-C2-C1	-2.33	103.26	111.80
5	A	306	GOL	O2-C2-C3	2.12	117.97	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	J00	O13-C12-O14	-2.08	118.94	123.90

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	J00	C11-C10-C9-O8
2	B	301	J00	C9-C10-C12-O13
2	B	301	J00	C9-C10-C12-O14
2	B	301	J00	C11-C10-C12-O13
2	B	301	J00	C11-C10-C12-O14
2	C	301	J00	C11-C10-C9-O8
5	A	304	GOL	C1-C2-C3-O3
5	A	305	GOL	O1-C1-C2-C3
5	C	307	GOL	O1-C1-C2-C3
5	D	303	GOL	C1-C2-C3-O3
4	A	303	PEG	O2-C3-C4-O4
4	A	303	PEG	O1-C1-C2-O2
4	B	303	PEG	O2-C3-C4-O4
4	C	306	PEG	O1-C1-C2-O2
5	B	306	GOL	O1-C1-C2-C3
4	B	302	PEG	O1-C1-C2-O2
4	B	304	PEG	O1-C1-C2-O2
4	B	305	PEG	O2-C3-C4-O4
4	C	305	PEG	O1-C1-C2-O2
4	C	305	PEG	O2-C3-C4-O4
5	A	305	GOL	O1-C1-C2-O2
4	B	303	PEG	O1-C1-C2-O2
4	C	303	PEG	O1-C1-C2-O2
4	C	303	PEG	O2-C3-C4-O4
4	A	303	PEG	C1-C2-O2-C3
4	D	304	PEG	O2-C3-C4-O4
5	C	307	GOL	O1-C1-C2-O2
5	D	303	GOL	O1-C1-C2-O2
5	D	303	GOL	O2-C2-C3-O3
4	C	306	PEG	O2-C3-C4-O4
2	A	301	J00	C9-C10-C12-O13
2	A	301	J00	C9-C10-C12-O14
2	A	301	J00	C11-C10-C12-O13
2	A	301	J00	C11-C10-C12-O14
2	C	301	J00	C9-C10-C12-O13
2	C	301	J00	C9-C10-C12-O14

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Mol	Chain	Res	Type	Atoms
2	C	301	J00	C11-C10-C12-O13
2	C	301	J00	C11-C10-C12-O14
2	D	301	J00	C11-C10-C12-O13
4	B	302	PEG	O2-C3-C4-O4
5	A	304	GOL	O2-C2-C3-O3
5	B	306	GOL	O1-C1-C2-O2
5	A	305	GOL	O2-C2-C3-O3
4	C	303	PEG	C1-C2-O2-C3
4	B	305	PEG	C1-C2-O2-C3
4	A	303	PEG	C4-C3-O2-C2
4	C	305	PEG	C1-C2-O2-C3
2	B	301	J00	C12-C10-C9-C4
2	C	301	J00	C12-C10-C9-C4
2	D	301	J00	C9-C10-C12-O13
2	D	301	J00	C9-C10-C12-O14
2	D	301	J00	C11-C10-C12-O14
4	B	304	PEG	C4-C3-O2-C2
4	C	306	PEG	C1-C2-O2-C3
4	C	303	PEG	C4-C3-O2-C2
2	A	301	J00	C11-C10-C9-O8
2	D	301	J00	C11-C10-C9-O8
4	D	304	PEG	C1-C2-O2-C3
5	C	307	GOL	O2-C2-C3-O3
2	B	301	J00	C11-C10-C9-C4
2	C	301	J00	C11-C10-C9-C4

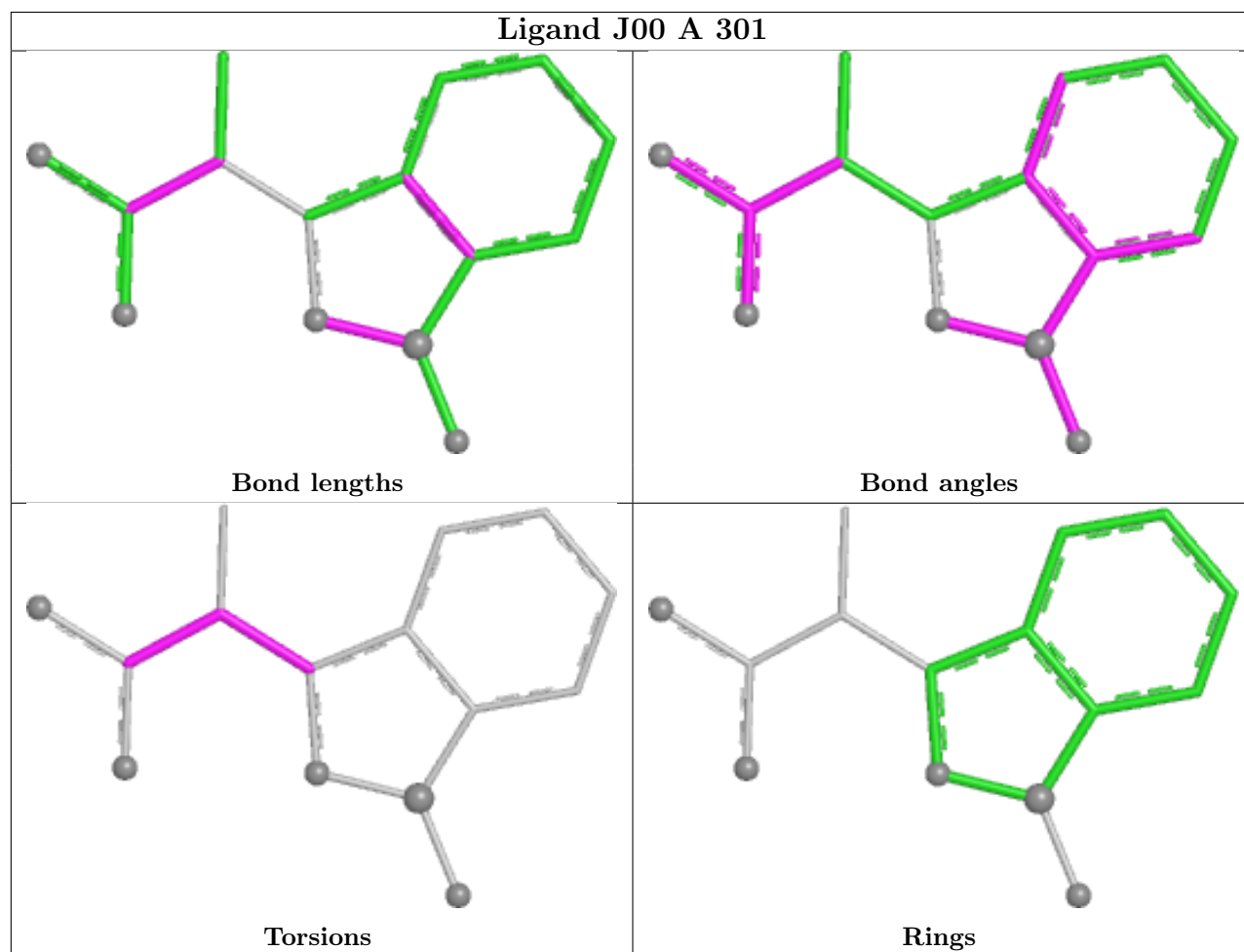
There are no ring outliers.

8 monomers are involved in 20 short contacts:

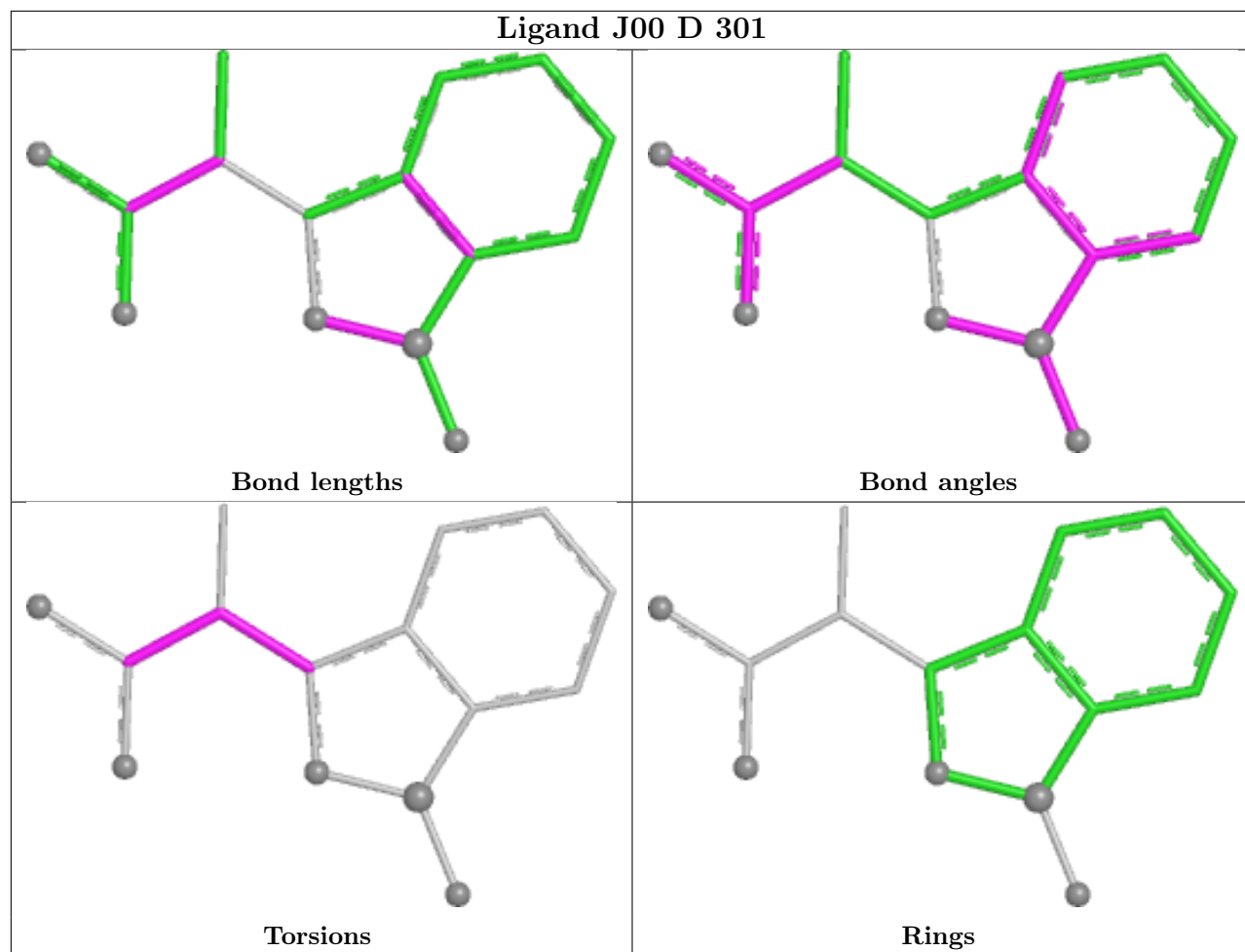
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	304	PEG	1	0
4	B	304	PEG	1	0
4	B	305	PEG	2	0
5	A	306	GOL	5	0
2	A	301	J00	2	0
4	C	303	PEG	3	0
2	C	301	J00	4	0
2	B	301	J00	2	0

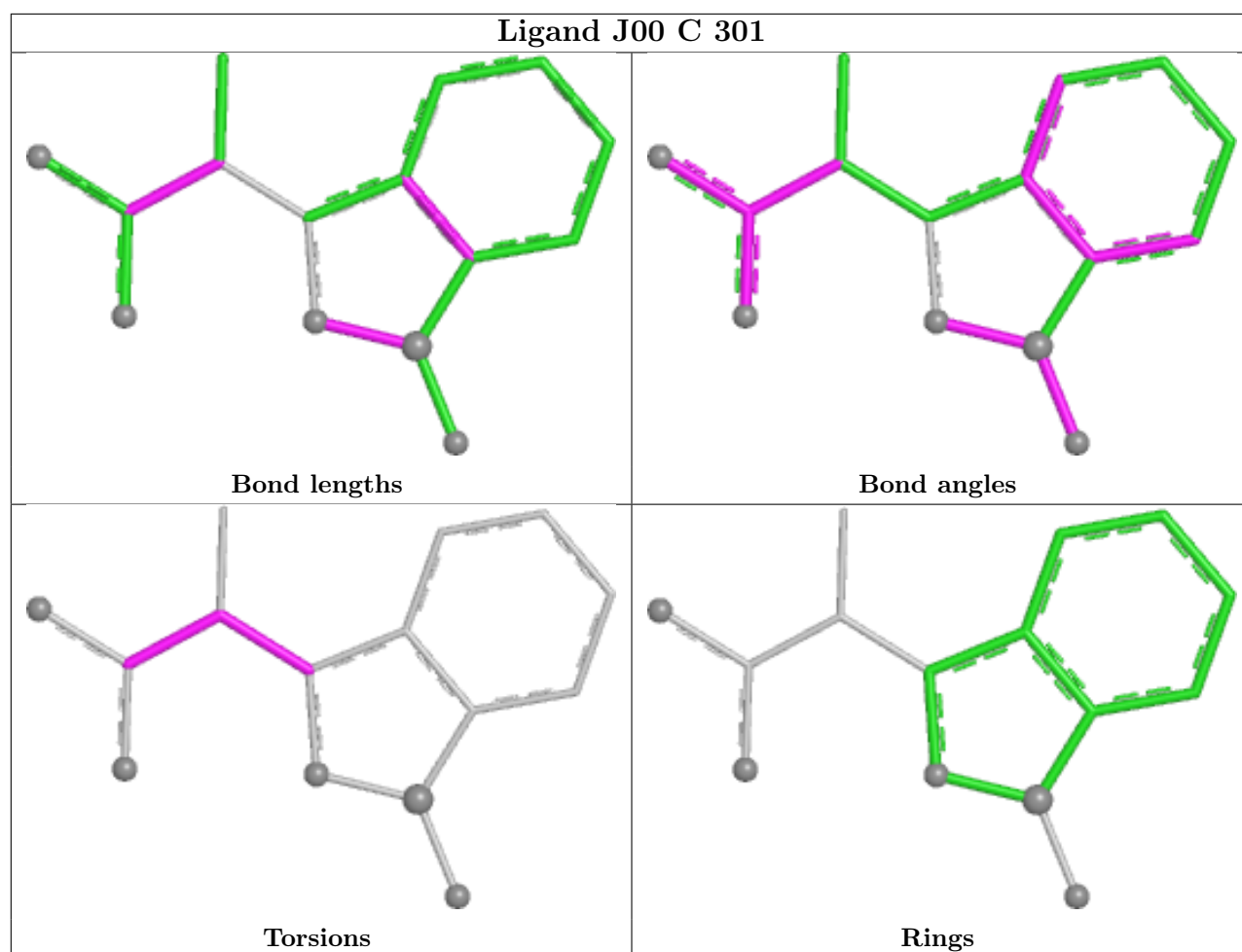
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

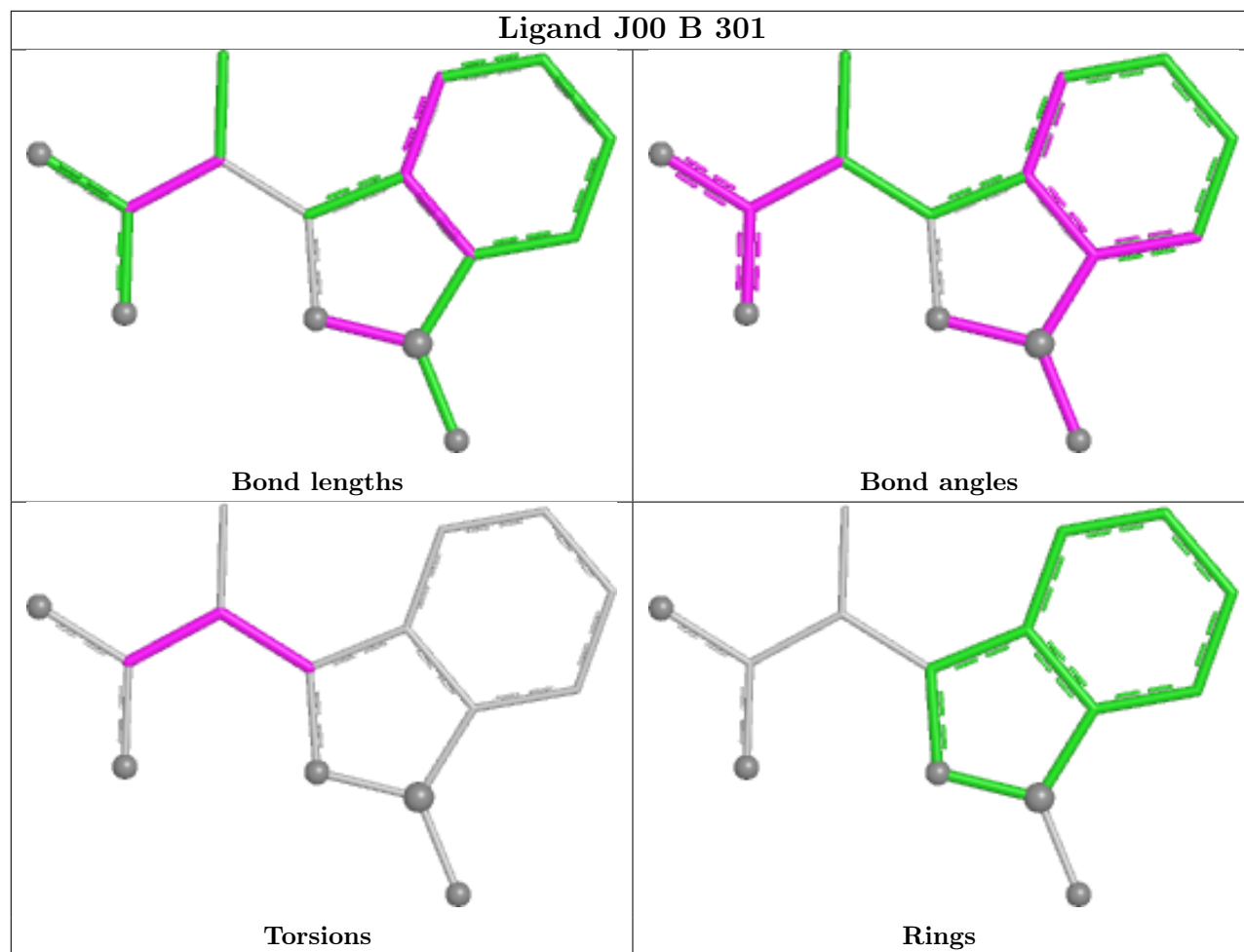
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand J00 D 301







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, 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	265/265 (100%)	-0.34	4 (1%) 72 73	18, 27, 49, 78	0
1	B	262/265 (98%)	-0.25	14 (5%) 32 30	17, 25, 59, 102	0
1	C	265/265 (100%)	0.47	29 (10%) 10 10	24, 39, 77, 118	0
1	D	263/265 (99%)	-0.09	14 (5%) 32 30	20, 28, 60, 143	0
All	All	1055/1060 (99%)	-0.05	61 (5%) 29 27	17, 29, 66, 143	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	25	SER	9.4
1	D	26	THR	7.9
1	B	29	VAL	7.1
1	D	27	ASN	6.2
1	D	254	THR	5.9
1	B	291	GLY	5.8
1	C	26	THR	5.3
1	C	227	ALA	4.9
1	C	254	THR	4.7
1	C	226	PRO	4.3
1	D	30	ALA	4.3
1	D	69	CYS	4.1
1	B	254	THR	4.1
1	C	229	TRP	4.1
1	A	25	SER	4.1
1	C	25	SER	4.0
1	B	28	LEU	3.8
1	C	49	MET	3.7
1	D	86	GLN	3.7
1	A	271	ASP	3.7
1	D	255	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	29	VAL	3.6
1	C	271	ASP	3.5
1	C	252	PRO	3.4
1	C	201	ALA	3.4
1	D	38	GLN	3.3
1	D	288	GLU	3.1
1	B	100	ASN	3.1
1	C	228	ASP	3.0
1	B	99	LYS	3.0
1	C	30	ALA	3.0
1	C	184	ARG	3.0
1	C	273	LYS	3.0
1	C	255	GLY	3.0
1	C	291	GLY	2.9
1	C	86	GLN	2.9
1	B	255	GLY	2.8
1	A	26	THR	2.8
1	C	173	ILE	2.8
1	C	105	TRP	2.7
1	C	256	ARG	2.7
1	D	256	ARG	2.7
1	B	38	GLN	2.6
1	C	88	ALA	2.6
1	B	111	LYS	2.6
1	C	225	VAL	2.6
1	B	31	GLU	2.5
1	B	86	GLN	2.4
1	C	38	GLN	2.4
1	C	28	LEU	2.4
1	C	61	ARG	2.4
1	D	284	ARG	2.3
1	B	290	LEU	2.3
1	C	99	LYS	2.2
1	C	270	LYS	2.2
1	B	289	GLY	2.2
1	D	271	ASP	2.1
1	D	99	LYS	2.1
1	A	110	GLU	2.1
1	B	256	ARG	2.1
1	C	205	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

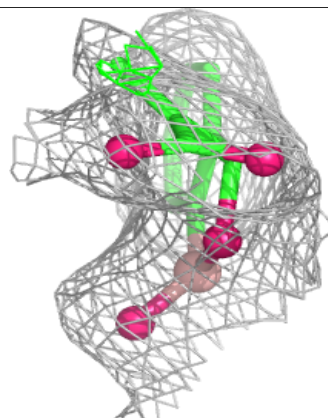
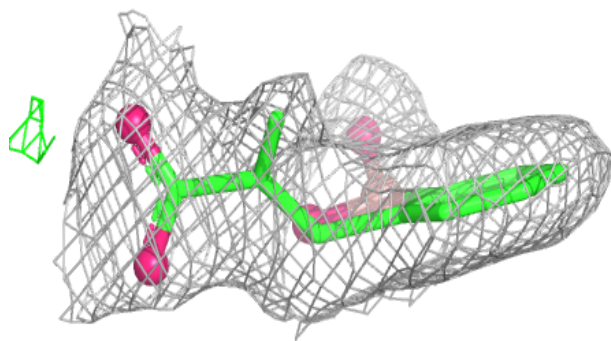
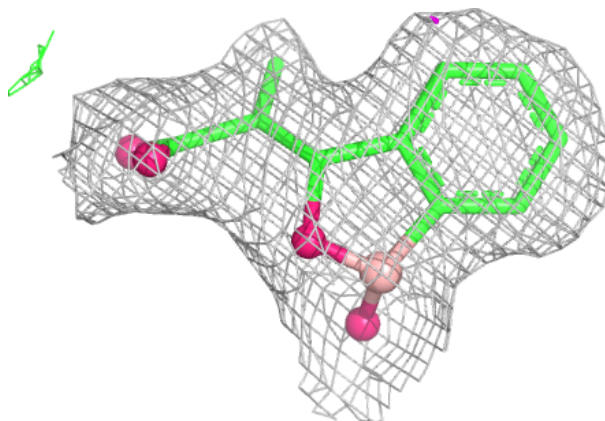
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	D	304	7/7	0.73	0.19	37,45,47,48	0
5	GOL	A	305	6/6	0.80	0.18	37,45,54,54	0
4	PEG	A	303	7/7	0.81	0.15	39,41,46,49	0
4	PEG	B	305	7/7	0.81	0.15	31,38,54,56	0
5	GOL	C	307	6/6	0.86	0.14	39,43,49,62	0
3	ACY	D	302	4/4	0.87	0.17	27,35,39,40	0
4	PEG	B	304	7/7	0.87	0.14	42,44,49,49	0
5	GOL	A	304	6/6	0.88	0.11	31,37,39,54	0
4	PEG	C	304	7/7	0.88	0.11	43,44,49,49	0
4	PEG	C	303	7/7	0.88	0.13	39,42,48,50	0
4	PEG	C	305	7/7	0.89	0.11	41,45,49,58	0
4	PEG	C	306	7/7	0.89	0.12	40,43,45,46	0
4	PEG	B	303	7/7	0.89	0.11	26,27,33,45	0
4	PEG	B	302	7/7	0.90	0.12	24,28,35,44	0
5	GOL	D	303	6/6	0.90	0.10	30,32,41,57	0
5	GOL	A	306	6/6	0.91	0.13	18,38,40,56	0
3	ACY	C	302	4/4	0.92	0.15	18,25,30,34	0
3	ACY	A	302	4/4	0.93	0.21	24,29,33,38	0
5	GOL	B	306	6/6	0.93	0.09	30,34,36,45	0
2	J00	C	301	15/15	0.94	0.09	32,35,39,39	0
2	J00	A	301	15/15	0.95	0.08	26,28,34,56	0
2	J00	D	301	15/15	0.96	0.06	20,27,31,33	0
2	J00	B	301	15/15	0.96	0.06	23,28,31,32	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.

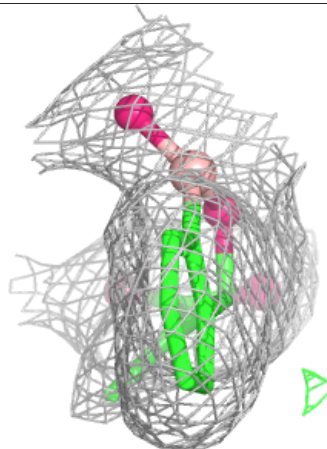
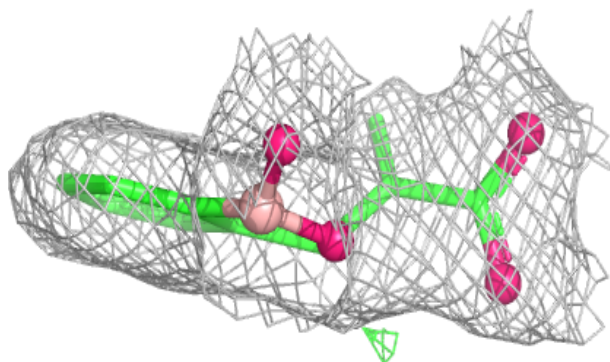
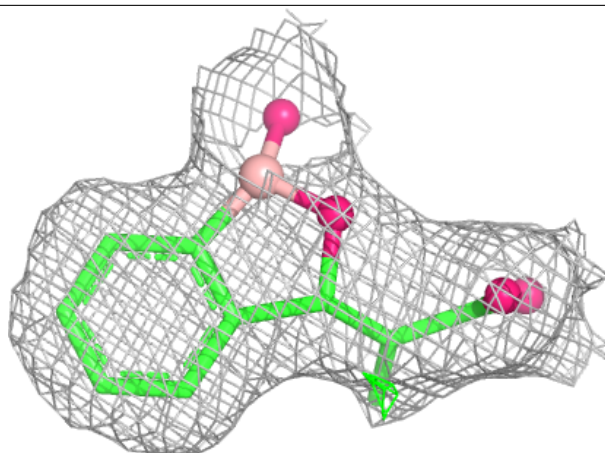
Electron density around J00 C 301:

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



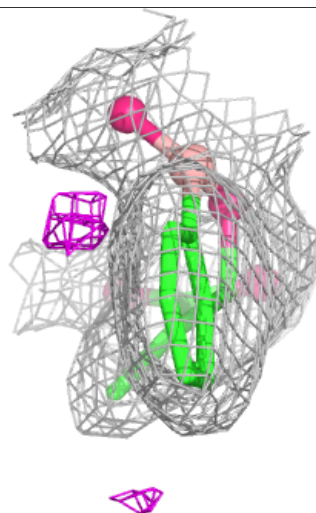
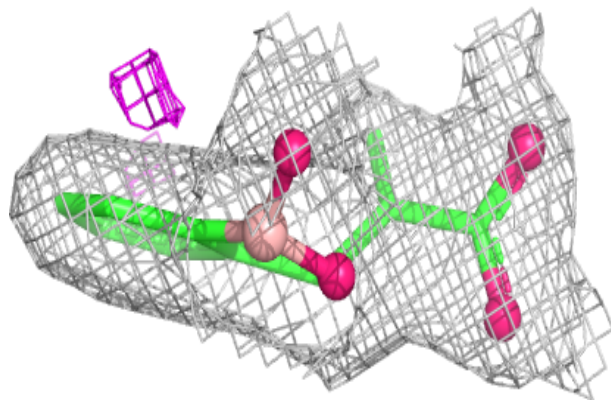
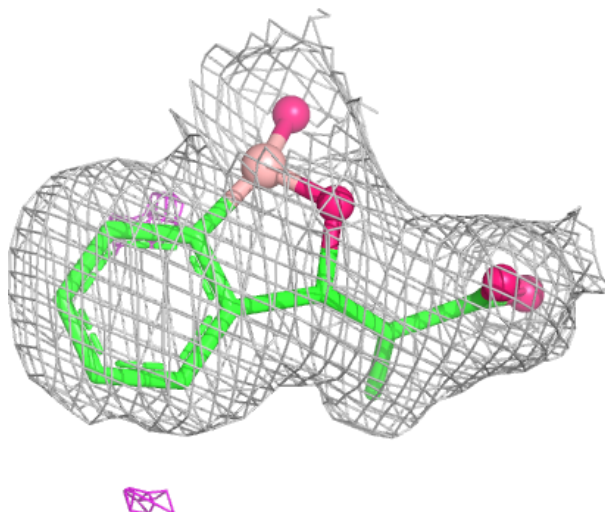
Electron density around J00 A 301:

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



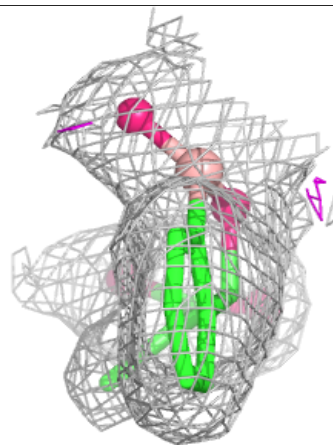
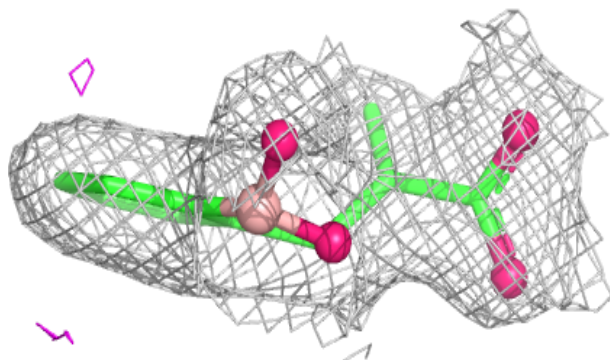
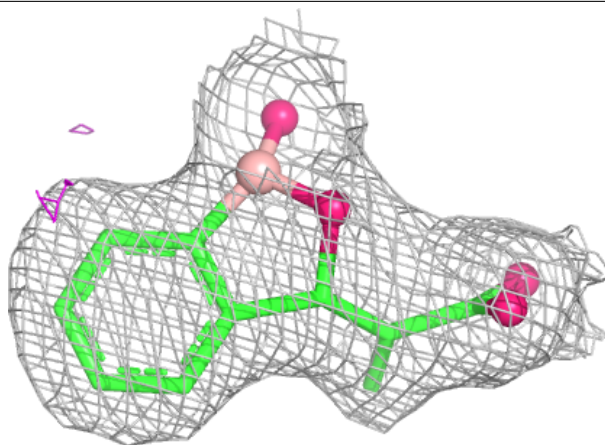
Electron density around J00 D 301:

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



Electron density around J00 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.