



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:04 AM UTC

PDB ID : 7K8K / pdb_00007k8k
Title : Beta-lactamase mixed with Sulbactam, 60ms
Authors : Pandey, S.; Schmidt, M.
Deposited on : 2020-09-27
Resolution : 2.70 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

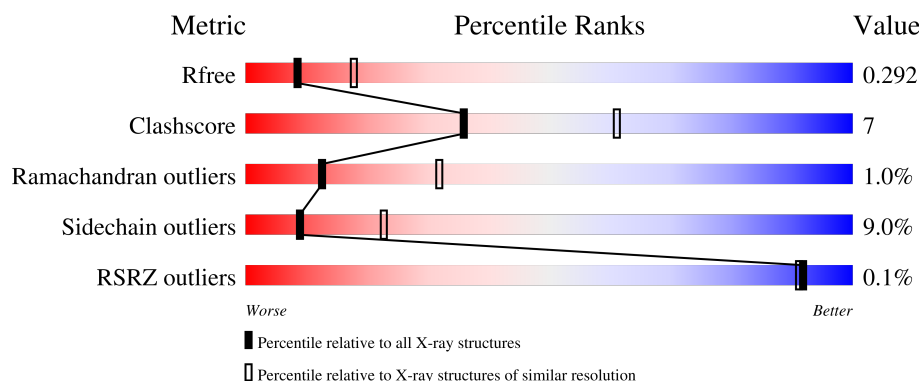
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	267	
1	B	267	
1	C	267	
1	D	267	

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	ORN	C	301	-	-	X	-

2 Entry composition [i](#)

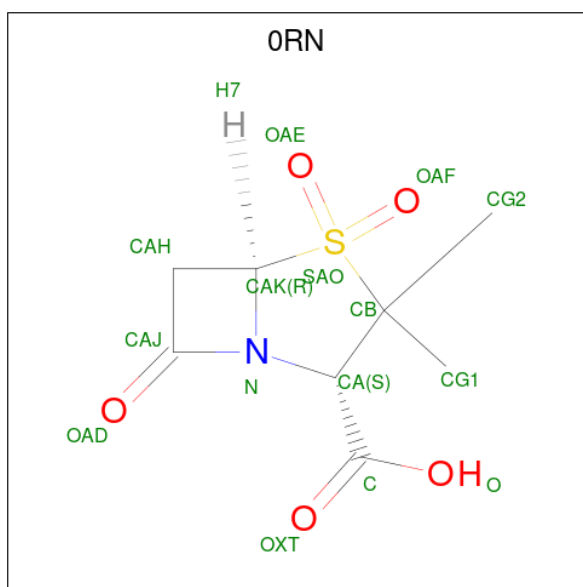
There are 5 unique types of molecules in this entry. The entry contains 8230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

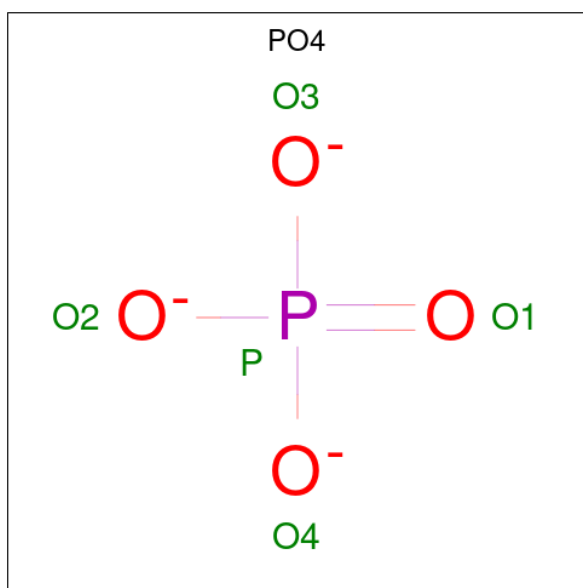
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			1988	1243	352	387	6			
1	B	265	Total	C	N	O	S	0	0	0
			1988	1243	352	387	6			
1	C	265	Total	C	N	O	S	0	0	0
			1988	1243	352	387	6			
1	D	265	Total	C	N	O	S	0	0	0
			1988	1243	352	387	6			

- Molecule 2 is SULBACTAM (CCD ID: 0RN) (formula: C₈H₁₁NO₅S) (labeled as "Ligand of Interest" by depositor).



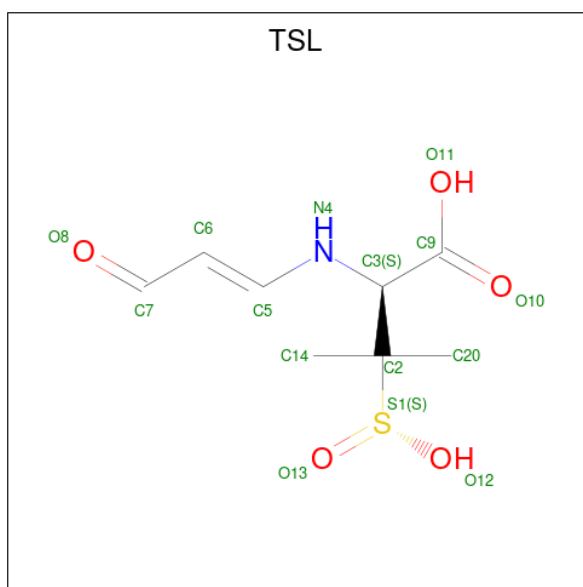
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is TRANS-ENAMINE INTERMEDIATE OF SULBACTAM (CCD ID: TSL) (formula: $C_8H_{13}NO_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

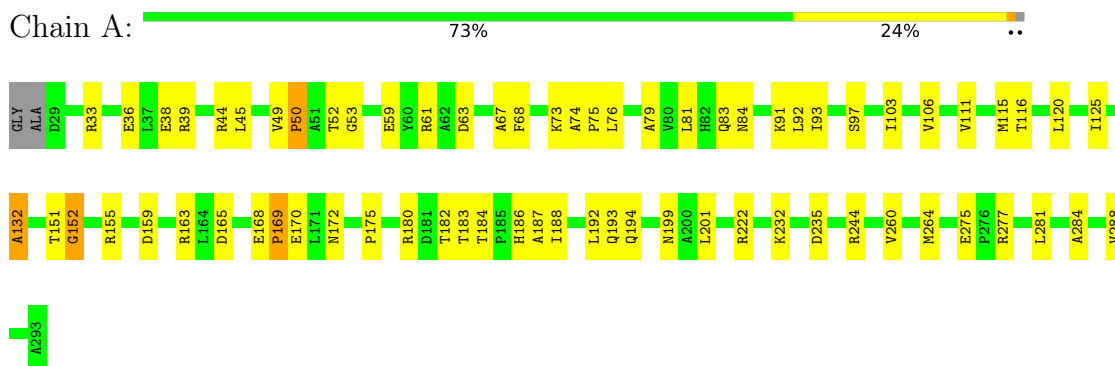
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total	O	0	0
			78	78		
5	B	38	Total	O	0	0
			38	38		
5	C	40	Total	O	0	0
			40	40		
5	D	42	Total	O	0	0
			42	42		

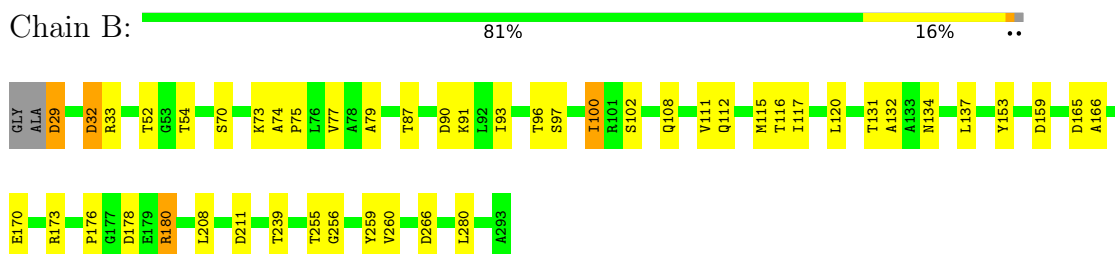
3 Residue-property plots

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: Beta-lactamase



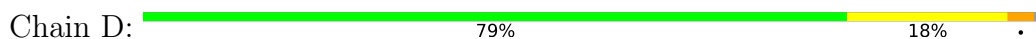
• Molecule 1: Beta-lactamase

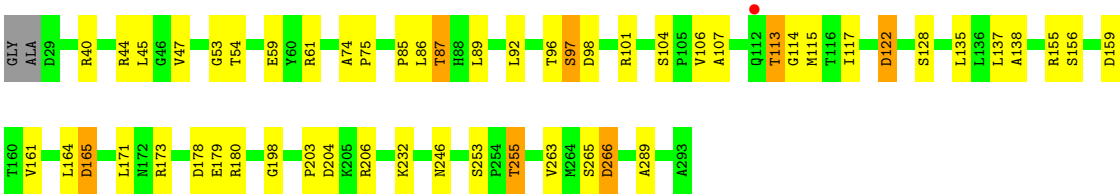


• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.91Å 99.53Å 112.50Å 90.00° 108.44° 90.00°	Depositor
Resolution (Å)	27.47 – 2.70 27.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.1 (27.47-2.70) 82.1 (27.47-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.215 , 0.292 0.220 , 0.292	Depositor DCC
R_{free} test set	1890 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8230	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.96% 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: 0RN, PO4, TSL

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	1.13	1/2027 (0.0%)	1.56	5/2767 (0.2%)
1	B	1.09	0/2027	1.54	5/2767 (0.2%)
1	C	1.13	0/2027	1.59	9/2767 (0.3%)
1	D	1.07	0/2027	1.52	3/2767 (0.1%)
All	All	1.10	1/8108 (0.0%)	1.55	22/11068 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	ALA	C-O	5.53	1.30	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	PRO	N-CA-CB	-6.13	96.82	103.25
1	B	208	LEU	CA-C-N	5.95	128.57	120.54
1	B	208	LEU	C-N-CA	5.95	128.57	120.54
1	C	271	GLY	CA-C-O	-5.89	117.87	122.52
1	A	68	PHE	CA-CB-CG	5.72	119.53	113.80
1	A	175	PRO	N-CA-C	5.71	117.67	110.70
1	C	44	ARG	CB-CA-C	5.63	119.43	110.19
1	A	132	ALA	CA-C-N	5.59	127.71	120.44
1	A	132	ALA	C-N-CA	5.59	127.71	120.44
1	D	122	ASP	CA-CB-CG	5.41	118.01	112.60
1	D	289	ALA	CA-C-N	5.37	125.94	119.98
1	D	289	ALA	C-N-CA	5.37	125.94	119.98
1	C	206	ARG	CA-C-N	5.34	127.87	120.29
1	C	206	ARG	C-N-CA	5.34	127.87	120.29
1	B	90	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	159	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	PRO	N-CA-CB	-5.25	96.83	102.60
1	C	38	GLU	CA-C-N	5.18	127.18	120.44
1	C	38	GLU	C-N-CA	5.18	127.18	120.44
1	C	151	THR	CB-CA-C	5.17	119.38	110.79
1	C	147	THR	CA-CB-OG1	-5.17	101.84	109.60
1	B	32	ASP	CB-CA-C	5.17	119.06	110.90

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	1988	0	1956	40	0
1	B	1988	0	1955	18	0
1	C	1988	0	1956	39	0
1	D	1988	0	1955	19	0
2	A	15	0	10	2	0
2	C	15	0	10	7	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	15	0	11	0	0
4	D	15	0	11	0	0
5	A	78	0	0	5	0
5	B	38	0	0	1	0
5	C	40	0	0	5	0
5	D	42	0	0	1	0
All	All	8230	0	7864	116	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 7.

All (116) 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:B:239:THR:HG22	3:B:302:PO4:O4	1.72	0.89
1:C:100:ILE:HA	1:C:131:THR:HG21	1.64	0.80
1:A:172:ASN:ND2	2:A:301:ORN:H1	1.99	0.77
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.64	0.77
1:C:72:PHE:HE1	1:C:76:LEU:HD22	1.56	0.70
1:C:241:ASP:O	1:C:244:ARG:HG3	1.92	0.70
1:C:169:PRO:HB3	2:C:301:ORN:CG2	2.21	0.70
1:A:163:ARG:HH11	1:A:165:ASP:CG	2.04	0.66
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.78	0.65
1:A:83:GLN:O	1:A:84:ASN:ND2	2.32	0.63
1:C:79:ALA:O	1:C:83:GLN:HG2	1.97	0.62
1:C:169:PRO:HB3	2:C:301:ORN:H2	1.81	0.61
1:B:74:ALA:HB3	1:B:75:PRO:CD	2.32	0.60
1:C:169:PRO:CB	2:C:301:ORN:CG2	2.81	0.59
1:C:169:PRO:CB	2:C:301:ORN:H3	2.34	0.57
1:A:39:ARG:NH2	5:A:404:HOH:O	2.36	0.57
1:D:198:GLY:O	1:D:206:ARG:NH1	2.37	0.57
1:A:120:LEU:CD2	1:A:132:ALA:HA	2.35	0.56
1:D:45:LEU:O	1:D:61:ARG:HD2	2.06	0.55
1:C:74:ALA:HB3	1:C:75:PRO:HD3	1.88	0.55
1:A:45:LEU:O	1:A:61:ARG:HD2	2.06	0.55
1:A:170:GLU:N	1:A:170:GLU:OE1	2.40	0.54
1:D:135:LEU:O	1:D:138:ALA:HB3	2.08	0.54
1:C:206:ARG:HD2	5:C:419:HOH:O	2.08	0.53
1:A:52:THR:HG22	1:A:53:GLY:N	2.24	0.53
1:C:65:ARG:HA	1:C:183:THR:O	2.10	0.52
1:C:155:ARG:NH2	5:C:403:HOH:O	2.42	0.52
1:A:201:LEU:HA	5:A:422:HOH:O	2.10	0.52
1:A:180:ARG:O	1:A:182:THR:HG23	2.10	0.52
1:C:82:HIS:CD2	5:C:414:HOH:O	2.63	0.51
1:C:117:ILE:O	1:C:120:LEU:HB2	2.11	0.51
1:C:68:PHE:O	1:C:71:THR:OG1	2.21	0.51
1:D:165:ASP:N	1:D:165:ASP:OD1	2.44	0.50
1:A:50:PRO:CG	1:A:260:VAL:HB	2.42	0.50
1:B:134:ASN:HA	1:B:137:LEU:HD12	1.93	0.50
1:B:115:MET:HE2	1:B:120:LEU:HD23	1.93	0.50
1:A:222:ARG:HD3	1:A:281:LEU:HD12	1.93	0.49
1:A:33:ARG:HA	1:A:36:GLU:HB3	1.95	0.49
1:C:169:PRO:HB3	2:C:301:ORN:H3	1.92	0.49
1:D:104:SER:HB3	1:D:107:ALA:HB3	1.95	0.49
1:A:83:GLN:C	1:A:84:ASN:ND2	2.70	0.49
1:D:47:VAL:HG22	1:D:263:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:OD1	1:A:186:HIS:ND1	2.46	0.49
1:C:139:ASP:HA	5:C:404:HOH:O	2.13	0.49
1:A:67:ALA:HB3	1:A:244:ARG:HD3	1.94	0.48
1:A:38:GLU:OE1	1:A:44:ARG:HA	2.13	0.48
1:B:29:ASP:HA	1:B:32:ASP:OD2	2.14	0.48
1:B:165:ASP:HB2	1:B:180:ARG:NH2	2.28	0.48
1:D:178:ASP:OD1	1:D:180:ARG:HG3	2.14	0.48
1:C:202:PRO:O	1:C:203:PRO:C	2.58	0.47
1:D:86:LEU:HD22	1:D:204:ASP:OD2	2.13	0.47
1:A:275:GLU:HB3	5:A:441:HOH:O	2.15	0.47
1:D:74:ALA:HB3	1:D:75:PRO:CD	2.45	0.47
1:A:277:ARG:HD2	5:A:441:HOH:O	2.13	0.47
1:D:113:THR:HG22	1:D:114:GLY:O	2.13	0.47
1:D:178:ASP:OD1	1:D:179:GLU:N	2.47	0.47
1:C:151:THR:CG2	1:C:164:LEU:H	2.28	0.47
1:A:97:SER:OG	1:A:111:VAL:HG21	2.15	0.47
1:C:72:PHE:CE1	1:C:76:LEU:HD22	2.44	0.46
1:C:120:LEU:HD22	1:C:132:ALA:HA	1.96	0.46
1:A:284:ALA:O	1:A:288:VAL:HG23	2.16	0.46
1:B:173:ARG:O	1:B:173:ARG:HG2	2.15	0.46
1:A:163:ARG:NH1	1:A:165:ASP:OD1	2.45	0.46
1:A:155:ARG:HD3	1:A:159:ASP:O	2.16	0.46
1:C:169:PRO:HB2	2:C:301:ORN:H3	1.97	0.46
1:C:266:ASP:C	1:C:267:ARG:HG3	2.41	0.46
1:D:85:PRO:C	1:D:87:THR:H	2.24	0.45
1:C:104:SER:OG	1:C:131:THR:HG23	2.16	0.45
1:A:49:VAL:HA	1:A:260:VAL:O	2.16	0.45
1:A:151:THR:O	1:A:152:GLY:C	2.59	0.45
1:B:79:ALA:HB2	1:B:153:TYR:CD2	2.52	0.45
1:A:76:LEU:O	1:A:79:ALA:HB3	2.18	0.44
1:D:266:ASP:C	1:D:266:ASP:OD1	2.60	0.44
1:A:192:LEU:O	1:A:193:GLN:C	2.60	0.44
1:C:292:LEU:O	1:C:293:ALA:C	2.61	0.44
1:A:106:VAL:HG12	1:A:115:MET:HE1	2.00	0.44
1:B:165:ASP:HB3	1:B:180:ARG:CZ	2.48	0.44
1:A:168:GLU:HA	1:A:169:PRO:HA	1.77	0.44
1:D:44:ARG:O	1:D:265:SER:HA	2.18	0.44
1:C:163:ARG:HB3	5:C:403:HOH:O	2.17	0.43
1:C:72:PHE:CD1	1:C:72:PHE:C	2.96	0.43
1:C:103:ILE:HG23	2:C:301:ORN:H4	2.00	0.43
1:C:49:VAL:HA	1:C:260:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:O	1:B:116:THR:HA	2.19	0.43
1:B:176:PRO:HB2	5:B:430:HOH:O	2.19	0.43
1:C:284:ALA:O	1:C:288:VAL:HG23	2.19	0.43
1:A:91:LYS:O	1:A:116:THR:HA	2.17	0.43
1:D:74:ALA:HB3	1:D:75:PRO:HD3	2.01	0.43
1:A:183:THR:OG1	1:A:184:THR:N	2.52	0.42
1:A:50:PRO:HA	5:A:414:HOH:O	2.19	0.42
1:B:93:ILE:HD11	1:B:117:ILE:HD11	2.01	0.42
1:C:151:THR:O	1:C:152:GLY:C	2.63	0.42
1:B:100:ILE:HD12	1:B:108:GLN:HA	2.02	0.42
1:C:214:ALA:HB2	1:C:234:ILE:HG22	2.02	0.41
1:A:73:LYS:NZ	1:A:168:GLU:OE1	2.53	0.41
1:C:111:VAL:HG13	1:C:112:GLN:N	2.36	0.41
1:C:202:PRO:O	1:C:204:ASP:N	2.53	0.41
1:D:87:THR:C	1:D:89:LEU:H	2.28	0.41
1:D:155:ARG:NH1	1:D:159:ASP:O	2.51	0.41
1:C:170:GLU:OE1	1:C:170:GLU:N	2.54	0.41
1:A:93:ILE:HD12	1:A:93:ILE:N	2.36	0.41
1:A:50:PRO:HG2	1:A:260:VAL:HB	2.03	0.41
1:A:74:ALA:HB3	1:A:75:PRO:CD	2.42	0.41
1:A:172:ASN:ND2	2:A:301:ORN:CG2	2.78	0.41
1:D:253:SER:OG	1:D:255:THR:HG23	2.21	0.41
1:C:187:ALA:O	1:C:191:VAL:HG23	2.21	0.41
1:B:70:SER:HB3	1:B:73:LYS:HD2	2.03	0.41
1:D:98:ASP:HB2	5:D:423:HOH:O	2.19	0.41
1:C:96:THR:O	1:C:99:ASP:HB2	2.20	0.40
1:C:200:ALA:O	1:C:201:LEU:HD23	2.21	0.40
1:A:92:LEU:C	1:A:93:ILE:HD12	2.46	0.40
1:B:120:LEU:HD22	1:B:132:ALA:HA	2.03	0.40
1:B:52:THR:HG21	1:B:259:TYR:HE1	1.87	0.40
1:B:74:ALA:CB	1:B:75:PRO:CD	2.99	0.40
1:A:49:VAL:HG13	1:A:260:VAL:O	2.22	0.40
1:C:234:ILE:O	1:C:249:ALA:HB1	2.21	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	263/267 (98%)	235 (89%)	25 (10%)	3 (1%)	11	29
1	B	263/267 (98%)	241 (92%)	20 (8%)	2 (1%)	16	37
1	C	263/267 (98%)	242 (92%)	18 (7%)	3 (1%)	11	29
1	D	263/267 (98%)	229 (87%)	31 (12%)	3 (1%)	11	29
All	All	1052/1068 (98%)	947 (90%)	94 (9%)	11 (1%)	12	32

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	203	PRO
1	D	97	SER
1	A	81	LEU
1	C	269	GLY
1	D	113	THR
1	A	152	GLY
1	B	166	ALA
1	A	50	PRO
1	C	176	PRO
1	D	53	GLY
1	B	256	GLY

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	202/202 (100%)	193 (96%)	9 (4%)	24	52
1	B	202/202 (100%)	182 (90%)	20 (10%)	7	19
1	C	202/202 (100%)	183 (91%)	19 (9%)	8	21
1	D	202/202 (100%)	177 (88%)	25 (12%)	4	11
All	All	808/808 (100%)	735 (91%)	73 (9%)	9	23

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	103	ILE
1	A	125	ILE
1	A	188	ILE
1	A	194	GLN
1	A	199	ASN
1	A	232	LYS
1	A	235	ASP
1	A	264	MET
1	B	29	ASP
1	B	33	ARG
1	B	54	THR
1	B	77	VAL
1	B	87	THR
1	B	96	THR
1	B	97	SER
1	B	100	ILE
1	B	102	SER
1	B	111	VAL
1	B	112	GLN
1	B	131	THR
1	B	170	GLU
1	B	178	ASP
1	B	180	ARG
1	B	211	ASP
1	B	255	THR
1	B	260	VAL
1	B	266	ASP
1	B	280	LEU
1	C	30	LEU
1	C	32	ASP
1	C	44	ARG
1	C	92	LEU

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Mol	Chain	Res	Type
1	C	95	TYR
1	C	96	THR
1	C	98	ASP
1	C	101	ARG
1	C	112	GLN
1	C	113	THR
1	C	116	THR
1	C	176	PRO
1	C	199	ASN
1	C	203	PRO
1	C	208	LEU
1	C	217	THR
1	C	235	ASP
1	C	248	ILE
1	C	291	VAL
1	D	40	ARG
1	D	54	THR
1	D	59	GLU
1	D	87	THR
1	D	92	LEU
1	D	96	THR
1	D	97	SER
1	D	101	ARG
1	D	106	VAL
1	D	115	MET
1	D	117	ILE
1	D	122	ASP
1	D	128	SER
1	D	137	LEU
1	D	156	SER
1	D	161	VAL
1	D	164	LEU
1	D	165	ASP
1	D	171	LEU
1	D	173	ARG
1	D	203	PRO
1	D	232	LYS
1	D	246	ASN
1	D	255	THR
1	D	266	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	193	GLN
1	A	216	ASN
1	B	112	GLN
1	B	194	GLN
1	C	82	HIS
1	C	88	HIS
1	C	109	GLN
1	C	193	GLN
1	C	246	ASN
1	D	88	HIS
1	D	109	GLN
1	D	110	HIS
1	D	112	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
3	PO4	C	302	-	4,4,4	0.81	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ORN	A	301	-	12,16,16	0.87	1 (8%)	17,28,28	1.55	3 (17%)
3	PO4	B	302	-	4,4,4	0.81	0	6,6,6	0.64	0
3	PO4	D	302	-	4,4,4	0.63	0	6,6,6	0.55	0
3	PO4	A	302	-	4,4,4	0.61	0	6,6,6	0.50	0
4	TSL	D	301	1	11,14,14	1.34	1 (9%)	10,19,19	1.26	1 (10%)
4	TSL	B	301	1	11,14,14	1.42	1 (9%)	10,19,19	1.52	1 (10%)
2	ORN	C	301	-	12,16,16	1.18	2 (16%)	17,28,28	1.44	4 (23%)

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	TSL	D	301	1	-	5/17/21/21	-
2	ORN	A	301	-	-	4/4/41/41	0/2/2/2
2	ORN	C	301	-	-	2/4/41/41	0/2/2/2
4	TSL	B	301	1	-	11/17/21/21	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	TSL	C6-C7	-3.53	1.34	1.44
4	B	301	TSL	C6-C7	-3.42	1.35	1.44
2	C	301	ORN	CA-C	2.63	1.56	1.53
2	C	301	ORN	O-C	-2.60	1.22	1.30
2	A	301	ORN	O-C	-2.54	1.22	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	TSL	C6-C5-N4	-3.76	119.02	125.89
2	C	301	ORN	CG1-CB-CG2	-3.72	108.08	111.75
4	D	301	TSL	C6-C5-N4	-3.59	119.33	125.89
2	A	301	ORN	CG2-CB-SAO	3.55	113.93	108.06
2	A	301	ORN	CG1-CB-CG2	-2.98	108.81	111.75
2	A	301	ORN	O-C-CA	2.82	120.58	112.47
2	C	301	ORN	CG2-CB-SAO	2.36	111.96	108.06
2	C	301	ORN	O-C-CA	2.09	118.48	112.47
2	C	301	ORN	CG1-CB-SAO	2.08	111.51	108.06

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	0RN	OXT-C-CA-CB
2	A	301	0RN	O-C-CA-CB
4	B	301	TSL	C14-C2-S1-O13
4	B	301	TSL	C20-C2-S1-O13
4	B	301	TSL	C14-C2-C3-C9
4	B	301	TSL	C14-C2-C3-N4
4	B	301	TSL	S1-C2-C3-C9
4	B	301	TSL	S1-C2-C3-N4
4	B	301	TSL	C20-C2-C3-C9
4	B	301	TSL	C20-C2-C3-N4
4	B	301	TSL	C6-C5-N4-C3
4	B	301	TSL	N4-C5-C6-C7
4	B	301	TSL	C5-C6-C7-O8
4	D	301	TSL	S1-C2-C3-N4
4	D	301	TSL	C20-C2-C3-N4
4	D	301	TSL	C2-C3-C9-O11
4	D	301	TSL	C5-C6-C7-O8
2	A	301	0RN	OXT-C-CA-N
2	A	301	0RN	O-C-CA-N
2	C	301	0RN	OXT-C-CA-CB
2	C	301	0RN	O-C-CA-CB
4	D	301	TSL	C2-C3-C9-O10

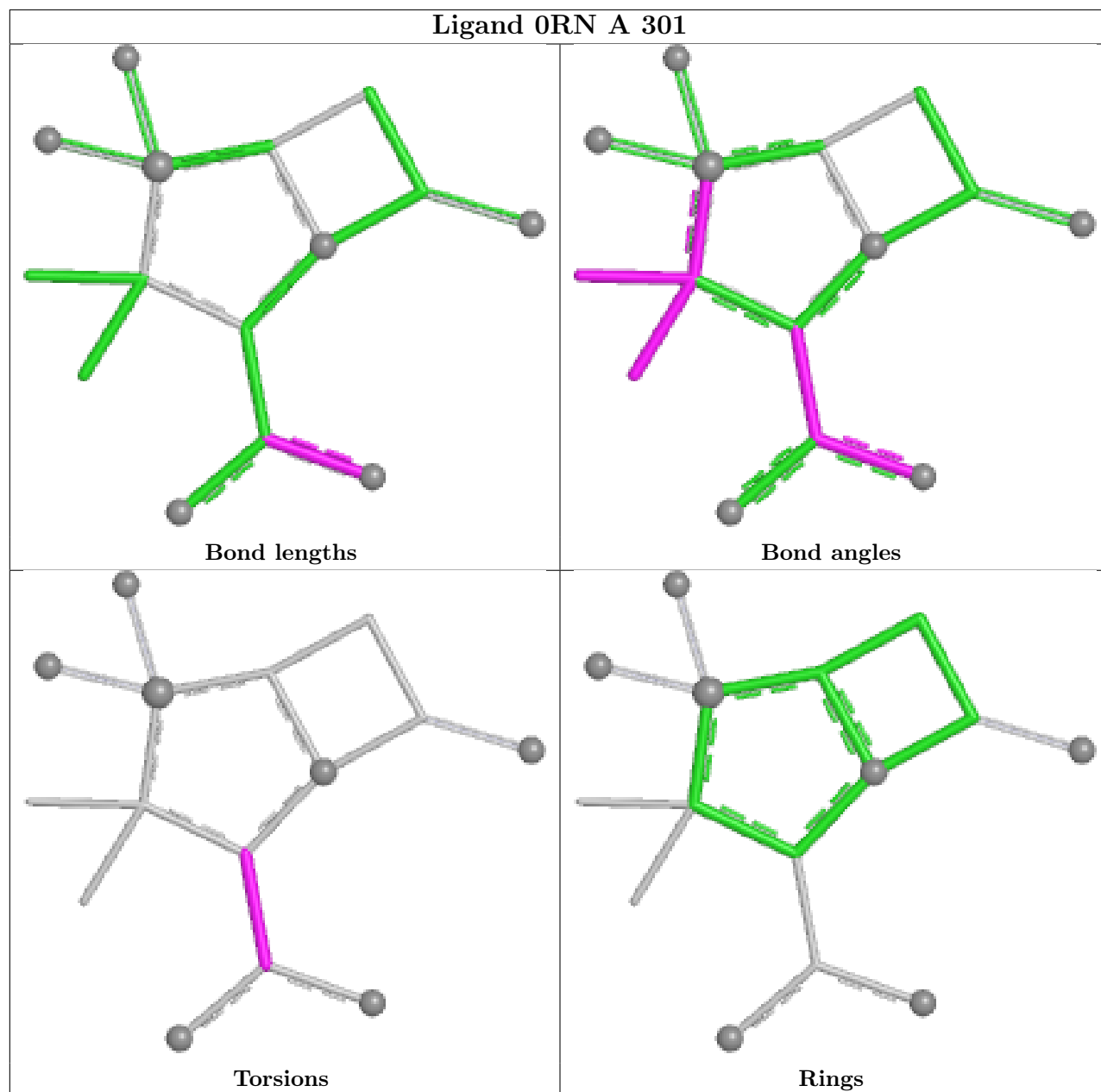
There are no ring outliers.

3 monomers are involved in 10 short contacts:

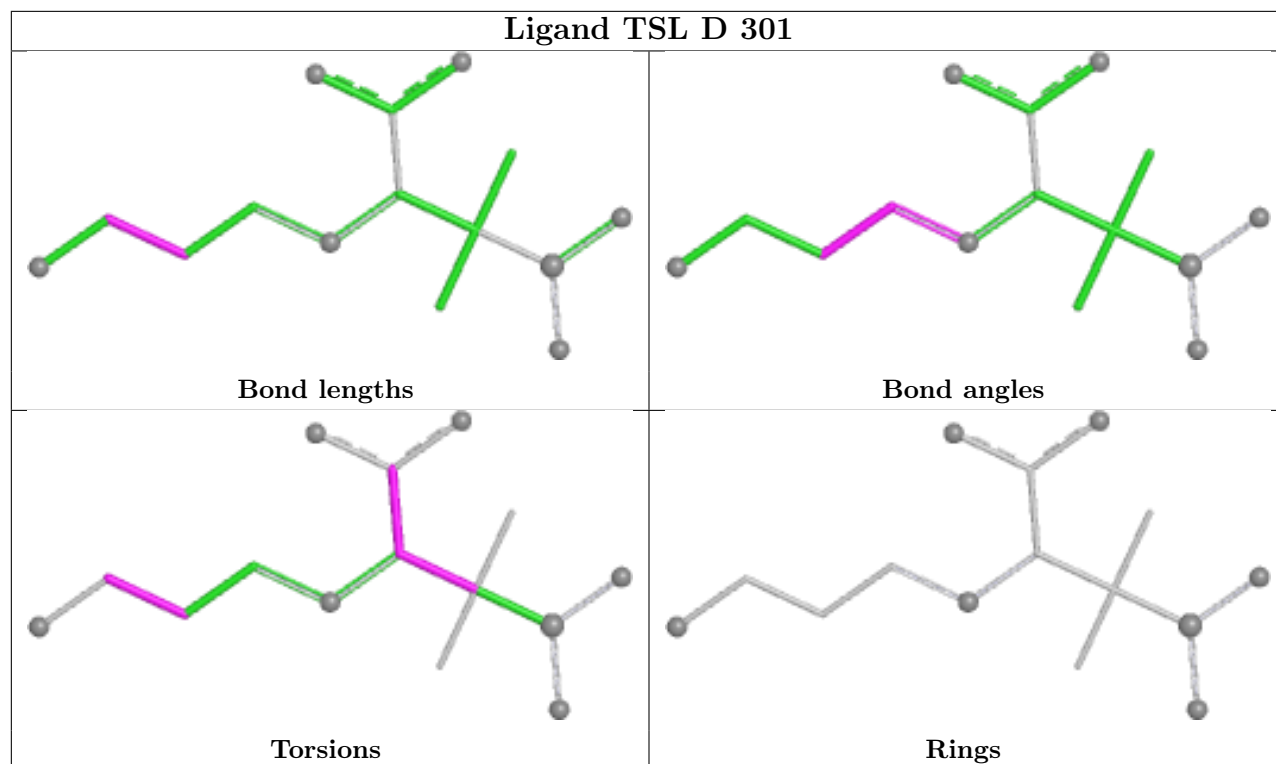
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	0RN	2	0
3	B	302	PO4	1	0
2	C	301	0RN	7	0

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

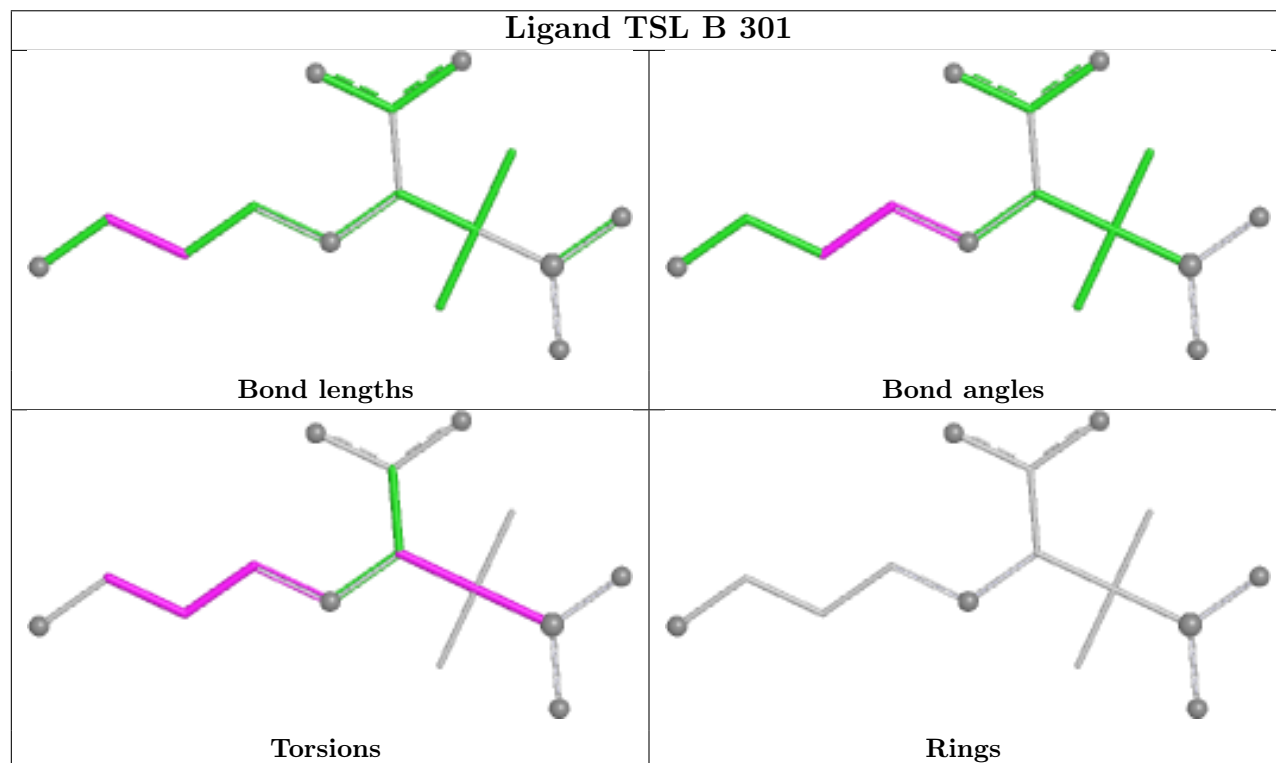
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

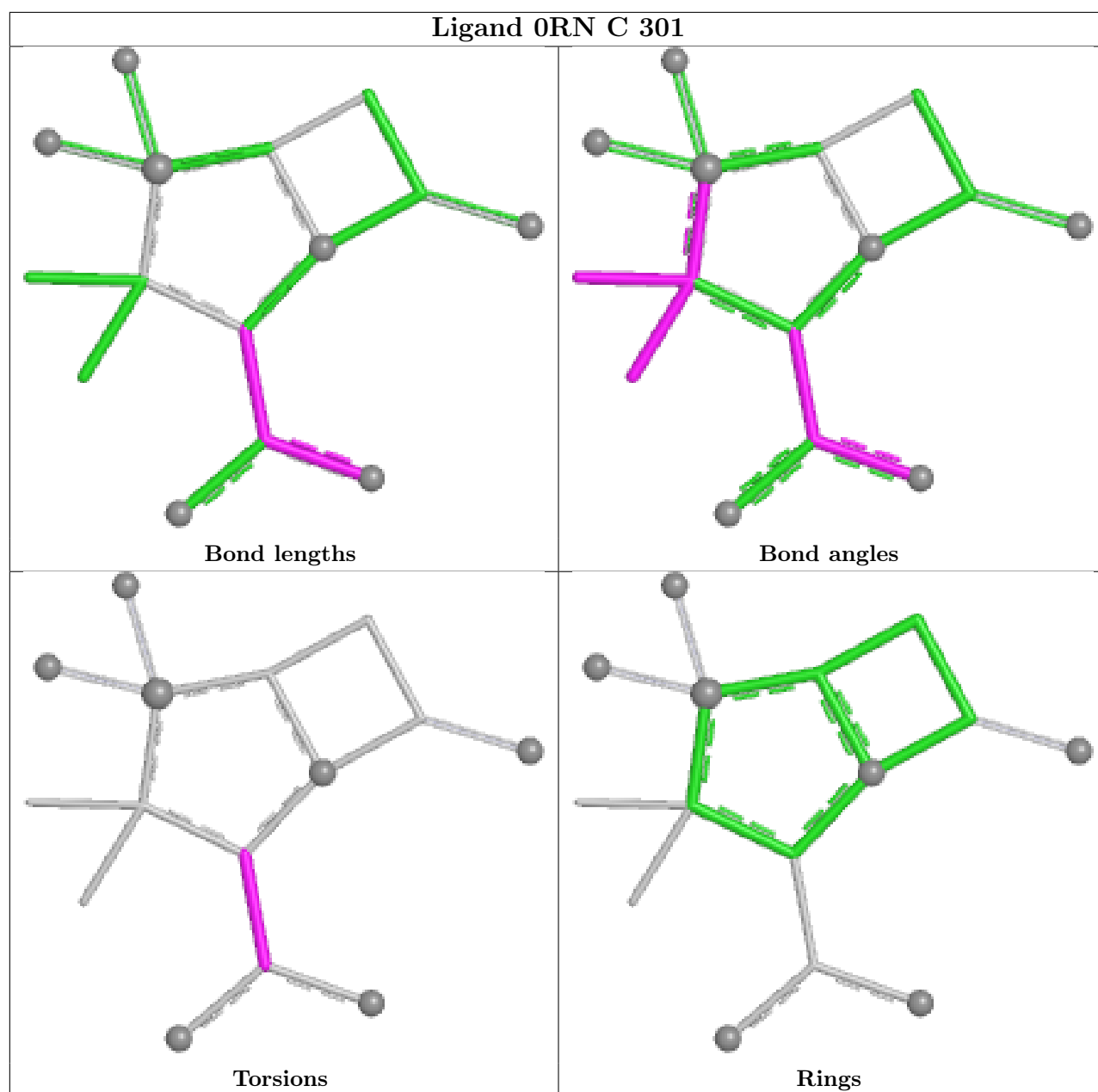


Ligand TSL D 301



Ligand TSL B 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	265/267 (99%)	-0.28	0	100	100	20, 37, 66, 84	0
1	B	265/267 (99%)	-0.32	0	100	100	26, 40, 78, 97	0
1	C	265/267 (99%)	-0.18	0	100	100	21, 41, 70, 100	0
1	D	265/267 (99%)	-0.29	1 (0%)	88	87	19, 41, 73, 100	0
All	All	1060/1068 (99%)	-0.27	1 (0%)	92	91	19, 40, 72, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	GLN	2.6

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(Å ²)	Q<0.9
2	ORN	C	301	15/15	0.73	0.30	110,144,180,181	0

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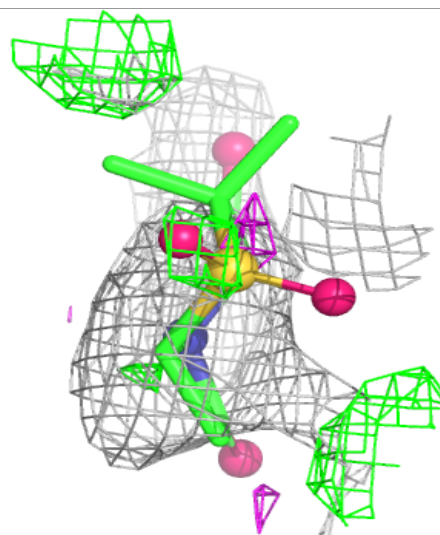
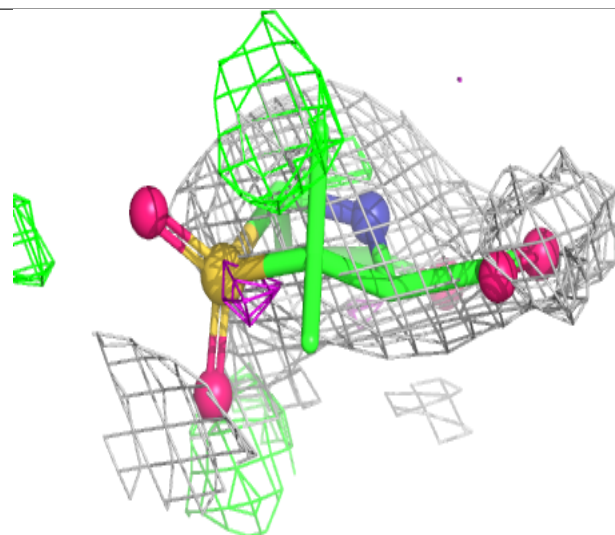
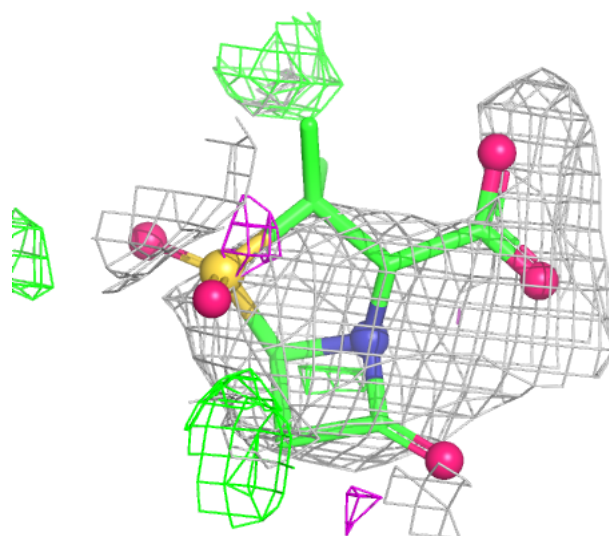
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TSL	B	301	15/15	0.80	0.22	63,109,143,163	0
2	ORN	A	301	15/15	0.88	0.20	116,139,158,160	0
4	TSL	D	301	15/15	0.89	0.17	59,108,124,125	0
3	PO4	D	302	5/5	0.97	0.07	45,48,50,52	0
3	PO4	C	302	5/5	0.98	0.05	46,47,48,48	0
3	PO4	B	302	5/5	0.98	0.08	40,42,46,47	0
3	PO4	A	302	5/5	0.99	0.06	35,37,38,41	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.

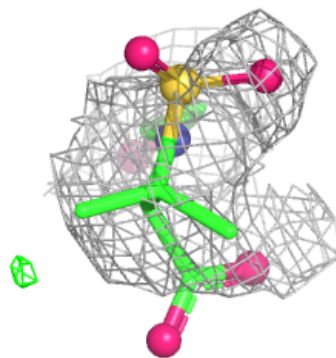
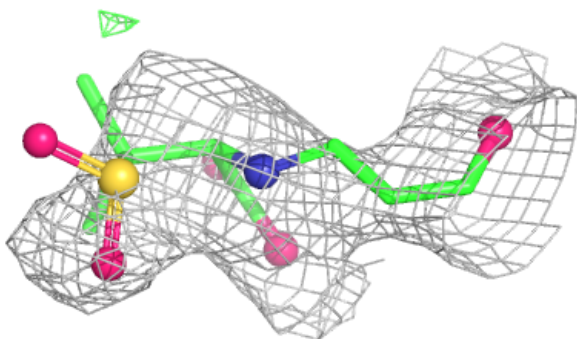
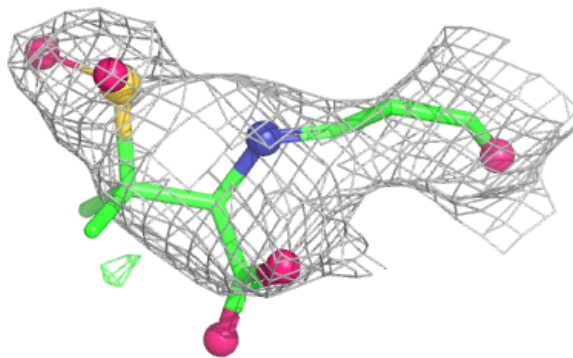
Electron density around ORN C 301:

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



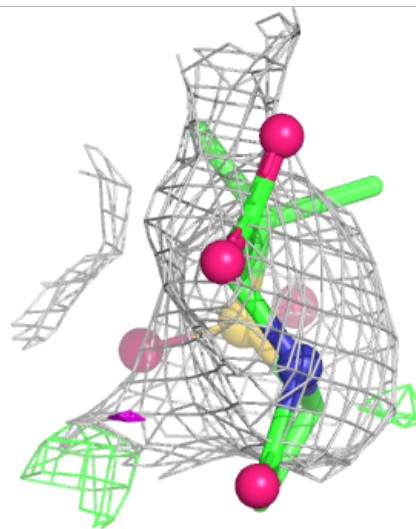
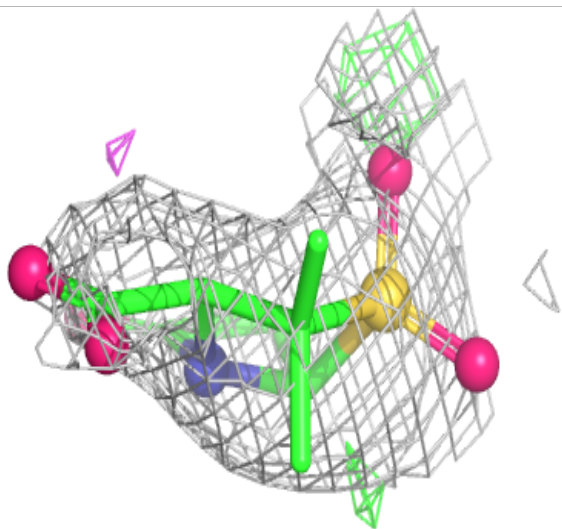
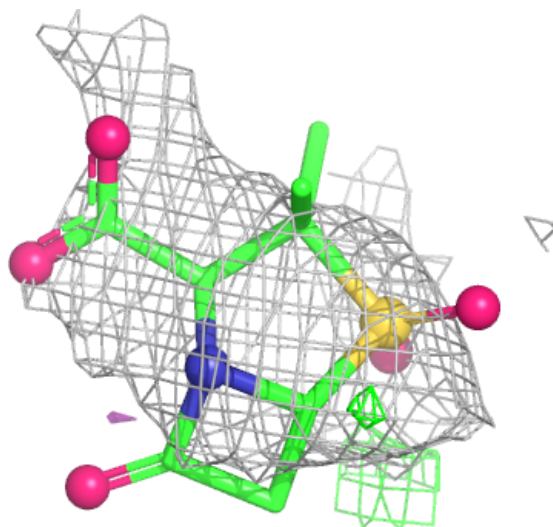
Electron density around TSL B 301:

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



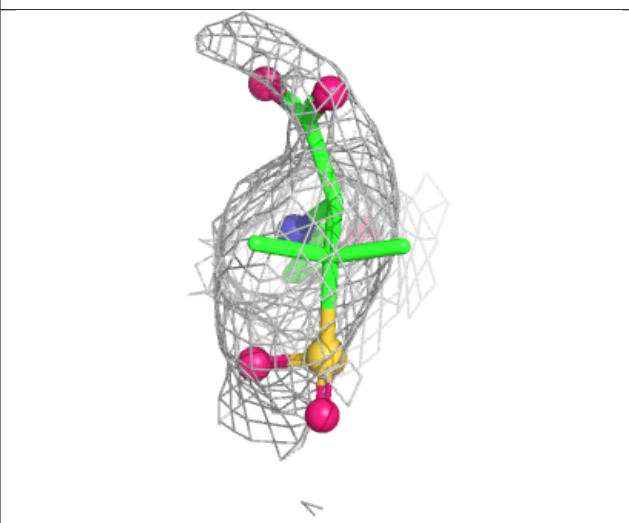
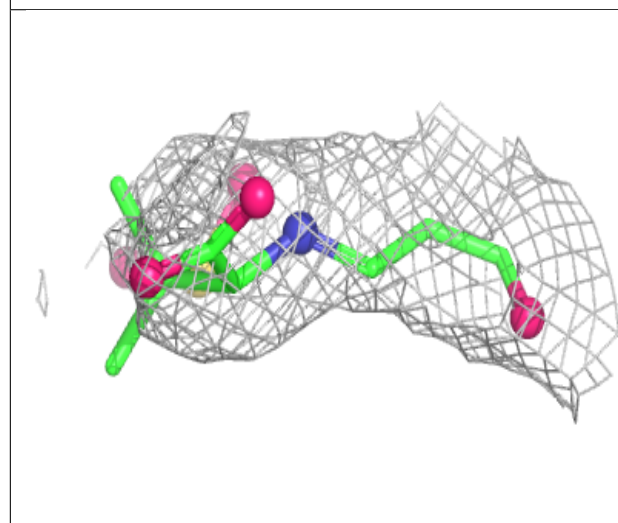
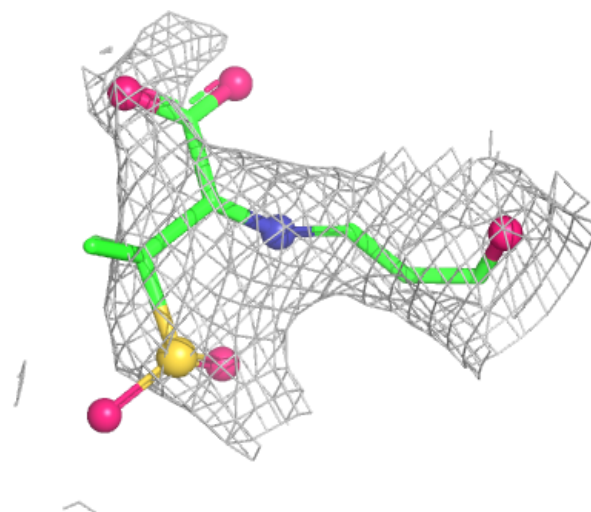
Electron density around ORN A 301:

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



Electron density around TSL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.