



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:12 pm BST

PDB ID : 6JN3
Title : Serine Beta-Lactamase KPC-2 in Complex with Dual MBL/SBL Inhibitor MS05
Authors : Li, G.-B.; Liu, S.
Deposited on : 2019-03-13
Resolution : 2.22 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

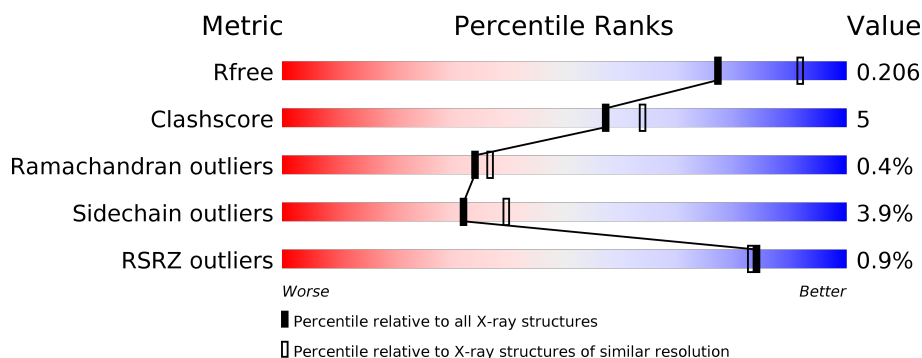
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 on 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	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	265	<div> <div>%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	C	265	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	D	265	<div> <div>%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	A	303	-	-	X	-
4	ACY	B	305	-	-	X	-
4	ACY	C	303	-	-	X	-
4	ACY	D	303	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8559 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.

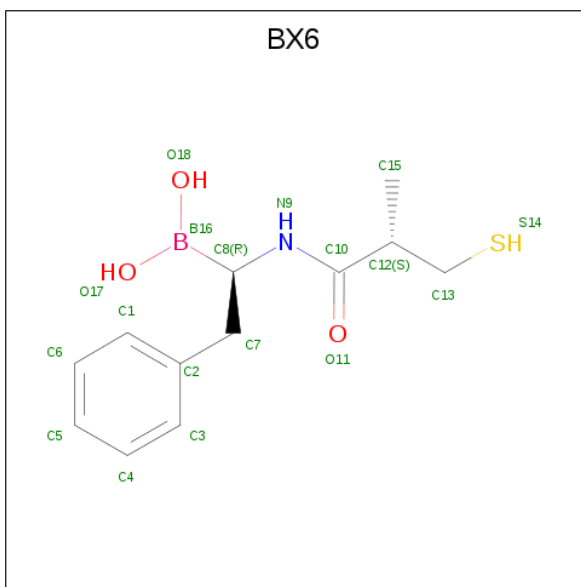
- Molecule 1 is a protein called Serine Beta-Lactamase KPC-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	1
			1974	1242	347	380	5			
1	B	264	Total	C	N	O	S	0	1	1
			1977	1244	347	381	5			
1	C	265	Total	C	N	O	S	0	0	1
			1974	1242	347	380	5			
1	D	260	Total	C	N	O	S	0	0	1
			1938	1220	341	372	5			

There are 4 discrepancies between the modelled and reference sequences:

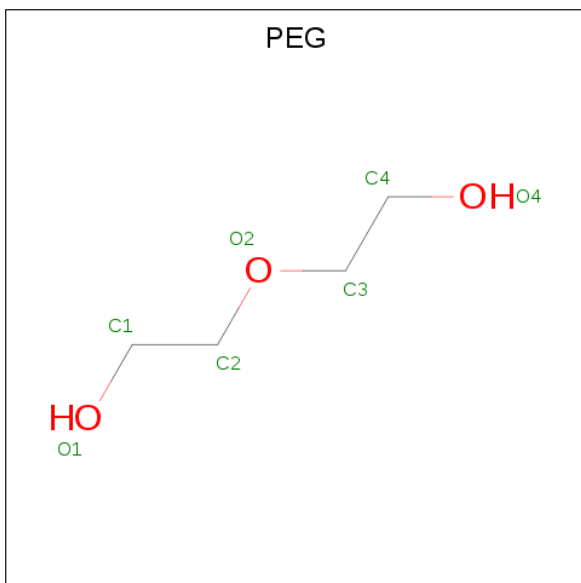
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	SER	-	expression tag	UNP Q93LQ9
B	25	SER	-	expression tag	UNP Q93LQ9
C	25	SER	-	expression tag	UNP Q93LQ9
D	25	SER	-	expression tag	UNP Q93LQ9

- Molecule 2 is [(1R)-1-[[[(2S)-2-methyl-3-sulfanyl-propanoyl]amino]-2-phenyl-ethyl]boronic acid (three-letter code: BX6) (formula: C₁₂H₁₈BNO₃S).



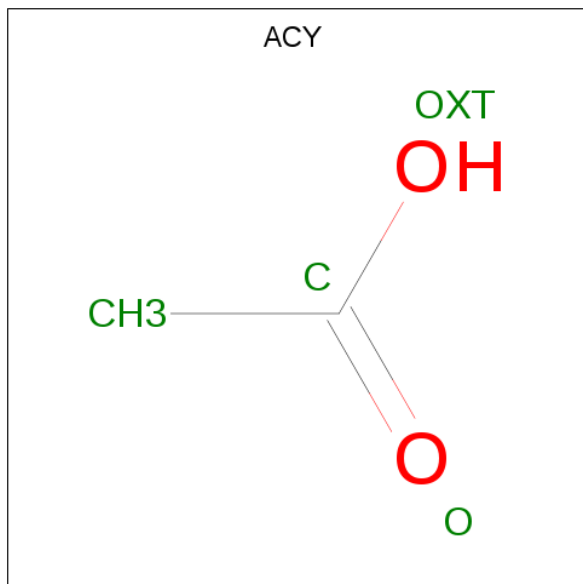
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 18	B 1	C 12	N 1	O 3	S 1	0	0
2	B	1	Total 18	B 1	C 12	N 1	O 3	S 1	0	0
2	C	1	Total 18	B 1	C 12	N 1	O 3	S 1	0	0
2	D	1	Total 18	B 1	C 12	N 1	O 3	S 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

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


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total	O	0	0
			166	166		
5	B	155	Total	O	0	2
			157	157		
5	C	94	Total	O	0	0
			94	94		
5	D	136	Total	O	0	1
			137	137		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Serine Beta-Lactamase KPC-2

Chain A: 




• Molecule 1: Serine Beta-Lactamase KPC-2

Chain B: 




• Molecule 1: Serine Beta-Lactamase KPC-2

Chain C: 



• Molecule 1: Serine Beta-Lactamase KPC-2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.51Å 165.51Å 94.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.78 – 2.22 47.78 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.78-2.22) 60.5 (47.78-1.78)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.167 , 0.201 0.175 , 0.206	Depositor DCC
R_{free} test set	1630 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.104 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8559	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, PEG, BX6

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	0.58	0/2014	0.76	4/2744 (0.1%)
1	B	0.60	0/2017	0.73	0/2748
1	C	0.57	0/2014	0.67	0/2744
1	D	0.59	0/1978	0.73	1/2694 (0.0%)
All	All	0.59	0/8023	0.72	5/10930 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	266	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	D	96	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	204	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	204	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	28	LEU	Peptide
1	C	252	PRO	Peptide

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	1974	0	1954	14	0
1	B	1977	0	1954	11	0
1	C	1974	0	1954	27	0
1	D	1938	0	1916	16	0
2	A	18	0	0	2	0
2	B	18	0	0	3	0
2	C	18	0	0	5	0
2	D	18	0	0	2	0
3	A	7	0	10	0	0
3	B	21	0	30	2	0
3	C	7	0	10	2	0
3	D	7	0	10	0	0
4	A	8	0	6	5	0
4	B	4	0	3	2	0
4	C	8	0	6	7	0
4	D	8	0	6	7	0
5	A	166	0	0	7	0
5	B	157	0	0	1	2
5	C	94	0	0	2	0
5	D	137	0	0	0	1
All	All	8559	0	7859	77	2

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 (77) 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:D:237:THR:N	4:D:303:ACY:H2	1.95	0.81
1:C:228:ASP:OD1	5:C:401:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:OE2	5:A:401:HOH:O	2.11	0.67
1:D:70:SER:HB2	4:D:303:ACY:H3	1.76	0.66
1:A:276:GLU:H	4:A:304:ACY:H2	1.61	0.66
1:C:26:THR:HG23	1:C:56:THR:H	1.62	0.65
5:A:482:HOH:O	1:C:26:THR:HG22	1.98	0.63
1:A:28:LEU:HD12	1:C:29:VAL:HG23	1.80	0.63
1:C:26:THR:HG21	1:C:55:ALA:HA	1.81	0.61
2:A:301:BX6:C7	4:A:303:ACY:H3	2.32	0.60
1:C:229:TRP:CE2	1:C:252:PRO:HB3	2.37	0.59
2:D:301:BX6:C1	4:D:303:ACY:H1	2.32	0.59
1:B:83:ARG:HG2	1:B:90:LEU:HD22	1.84	0.59
1:C:26:THR:CG2	1:C:56:THR:H	2.16	0.57
1:A:236:GLY:HA2	4:A:303:ACY:H2	1.85	0.57
1:D:237:THR:H	4:D:303:ACY:H2	1.72	0.55
1:D:50:ASP:OD2	1:D:256:ARG:NH1	2.34	0.54
1:B:26:THR:OG1	1:B:27:ASN:N	2.43	0.52
1:C:266:ARG:NH1	5:C:404:HOH:O	2.34	0.52
1:C:106:SER:O	1:C:110:GLU:HG3	2.10	0.52
1:D:30:ALA:N	1:D:32:PRO:HD2	2.25	0.51
1:B:26:THR:O	1:B:27:ASN:O	2.28	0.51
1:B:275:SER:OG	1:B:278:VAL:HG23	2.10	0.51
1:A:25:SER:HB3	1:A:184:ARG:NH2	2.26	0.51
2:C:301:BX6:C3	4:C:303:ACY:H2	2.41	0.51
2:A:301:BX6:O18	4:A:303:ACY:CH3	2.59	0.50
1:D:31:GLU:N	1:D:32:PRO:CD	2.74	0.50
1:D:276:GLU:H	4:D:304:ACY:H2	1.77	0.49
1:C:166:GLU:HB3	1:C:167:LEU:HD12	1.94	0.49
1:D:70:SER:CB	4:D:303:ACY:H3	2.42	0.49
1:C:229:TRP:CD2	1:C:252:PRO:HB3	2.49	0.48
1:D:225:VAL:HG13	1:D:229:TRP:HB2	1.95	0.48
1:A:204:ARG:HD3	5:A:475:HOH:O	2.13	0.48
1:A:70:SER:HB2	4:A:303:ACY:H2	1.96	0.48
1:C:63:GLU:OE1	1:C:184:ARG:NH1	2.47	0.47
1:A:212:LYS:NZ	5:A:406:HOH:O	2.47	0.47
1:B:104:PRO:HB2	1:B:105:TRP:CE3	2.50	0.47
1:A:266:ARG:HB2	1:A:266:ARG:CZ	2.45	0.47
1:C:225:VAL:HG13	1:C:226:PRO:HD2	1.97	0.46
1:A:31:GLU:HG3	5:A:524:HOH:O	2.15	0.46
2:C:301:BX6:O18	4:C:303:ACY:CH3	2.64	0.46
1:C:100:ASN:ND2	3:C:302:PEG:O1	2.46	0.46
1:C:70:SER:HB3	1:C:73:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:SER:HB2	4:C:303:ACY:H1	1.96	0.45
1:A:100:ASN:HB2	5:A:411:HOH:O	2.16	0.45
1:C:229:TRP:CZ2	1:C:252:PRO:HB3	2.52	0.45
1:D:166:GLU:HB3	1:D:167:LEU:HD12	1.99	0.45
1:C:70:SER:OG	2:C:301:BX6:O18	2.30	0.45
1:B:73:LYS:HB2	1:B:234:LYS:HE3	2.00	0.44
1:C:37:GLU:HG3	1:C:42:GLY:O	2.18	0.43
1:C:230:ALA:HB3	1:C:251:TRP:HB2	2.01	0.43
1:B:229:TRP:HE3	1:B:250:VAL:CG1	2.31	0.43
2:B:301:BX6:C2	4:B:305:ACY:H2	2.49	0.43
2:D:301:BX6:C7	4:D:303:ACY:H1	2.49	0.43
1:B:28:LEU:HA	1:B:28:LEU:HD12	1.73	0.43
1:B:29:VAL:O	1:B:32:PRO:HD2	2.18	0.42
2:B:301:BX6:O18	4:B:305:ACY:H3	2.19	0.42
1:C:237:THR:N	4:C:303:ACY:H3	2.35	0.42
1:D:70:SER:HB3	1:D:73:LYS:HD2	1.99	0.42
2:C:301:BX6:C7	4:C:303:ACY:H2	2.49	0.42
1:A:168:GLU:OE2	5:A:402:HOH:O	2.22	0.42
1:A:252:PRO:HB2	1:A:256:ARG:HD3	2.00	0.42
1:C:229:TRP:CE2	1:C:252:PRO:CB	3.00	0.42
1:B:88:ALA:HB2	3:B:304:PEG:H41	2.00	0.42
1:D:69:CYS:SG	1:D:243:THR:HG22	2.60	0.42
1:D:73:LYS:HB2	1:D:234:LYS:HE3	2.01	0.42
1:D:46:VAL:HG11	1:D:286:ALA:HB2	2.00	0.42
3:B:302:PEG:H21	5:B:430:HOH:O	2.19	0.41
1:A:229:TRP:HZ2	1:D:168:GLU:HG2	1.85	0.41
1:B:168[B]:GLU:OE1	1:C:288:GLU:OE2	2.39	0.41
1:C:25:SER:HB2	1:C:59:SER:HB3	2.01	0.41
1:C:100:ASN:OD1	3:C:302:PEG:C4	2.69	0.41
1:C:252:PRO:O	1:C:256:ARG:HB3	2.21	0.41
2:B:301:BX6:C3	2:B:301:BX6:N9	2.84	0.41
2:C:301:BX6:O18	4:C:303:ACY:H3	2.20	0.41
1:C:70:SER:CB	4:C:303:ACY:H1	2.52	0.40
1:D:225:VAL:CG1	1:D:229:TRP:HB2	2.52	0.40

All (2) 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)
5:B:401:HOH:O	5:D:525:HOH:O[1_556]	2.01	0.19
5:B:532:HOH:O	5:B:533:HOH:O[3_655]	2.19	0.01

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	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	B	263/265 (99%)	259 (98%)	3 (1%)	1 (0%)	34	37
1	C	263/265 (99%)	253 (96%)	7 (3%)	3 (1%)	14	11
1	D	258/265 (97%)	251 (97%)	7 (3%)	0	100	100
All	All	1047/1060 (99%)	1022 (98%)	21 (2%)	4 (0%)	34	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	27	ASN
1	C	100	ASN
1	C	252	PRO
1	C	29	VAL

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	200/200 (100%)	188 (94%)	12 (6%)	19	21
1	B	200/200 (100%)	194 (97%)	6 (3%)	41	51
1	C	200/200 (100%)	194 (97%)	6 (3%)	41	51
1	D	195/200 (98%)	188 (96%)	7 (4%)	35	43
All	All	795/800 (99%)	764 (96%)	31 (4%)	32	40

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	35	LYS
1	A	59	SER
1	A	63	GLU
1	A	86	GLN
1	A	87	GLN
1	A	91	LEU
1	A	130	SER
1	A	141	GLU
1	A	142	LEU
1	A	228	ASP
1	A	233	ASP
1	B	26	THR
1	B	28	LEU
1	B	86	GLN
1	B	111	LYS
1	B	130	SER
1	B	271	ASP
1	C	86	GLN
1	C	142	LEU
1	C	191	GLN
1	C	254	THR
1	C	266	ARG
1	C	288	GLU
1	D	38	GLN
1	D	99	LYS
1	D	130	SER
1	D	142	LEU
1	D	225	VAL
1	D	233	ASP
1	D	256	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	100	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

17 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
2	BX6	D	301	-	15,18,18	1.61	3 (20%)	18,23,23	1.52	4 (22%)
3	PEG	B	303	-	6,6,6	0.60	0	5,5,5	1.07	0
2	BX6	B	301	-	15,18,18	1.88	4 (26%)	18,23,23	1.88	5 (27%)
4	ACY	C	303	-	1,3,3	5.71	1 (100%)	0,3,3	0.00	-
4	ACY	A	304	-	1,3,3	1.98	0	0,3,3	0.00	-
3	PEG	A	302	-	6,6,6	0.74	0	5,5,5	1.11	0
3	PEG	B	302	-	6,6,6	0.71	0	5,5,5	1.24	1 (20%)
3	PEG	C	302	-	6,6,6	0.62	0	5,5,5	0.56	0
4	ACY	D	303	-	1,3,3	2.76	1 (100%)	0,3,3	0.00	-
4	ACY	A	303	-	1,3,3	6.04	1 (100%)	0,3,3	0.00	-
4	ACY	D	304	-	1,3,3	2.45	1 (100%)	0,3,3	0.00	-
3	PEG	B	304	-	6,6,6	0.48	0	5,5,5	0.80	0
2	BX6	C	301	-	15,18,18	1.92	3 (20%)	18,23,23	1.71	4 (22%)
2	BX6	A	301	-	15,18,18	1.98	3 (20%)	18,23,23	1.90	5 (27%)
3	PEG	D	302	-	6,6,6	0.47	0	5,5,5	0.80	0
4	ACY	C	304	-	1,3,3	1.10	0	0,3,3	0.00	-
4	ACY	B	305	-	1,3,3	2.72	1 (100%)	0,3,3	0.00	-

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
2	BX6	D	301	-	-	2/13/18/18	0/1/1/1
3	PEG	B	303	-	-	1/4/4/4	-
2	BX6	B	301	-	-	7/13/18/18	0/1/1/1
3	PEG	A	302	-	-	1/4/4/4	-
3	PEG	B	302	-	-	2/4/4/4	-
3	PEG	C	302	-	-	2/4/4/4	-
3	PEG	B	304	-	-	3/4/4/4	-
2	BX6	C	301	-	-	5/13/18/18	0/1/1/1
2	BX6	A	301	-	-	3/13/18/18	0/1/1/1
3	PEG	D	302	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	ACY	CH3-C	-6.04	1.41	1.48
4	C	303	ACY	CH3-C	-5.71	1.41	1.48
2	C	301	BX6	C10-N9	5.53	1.46	1.34
2	A	301	BX6	C10-N9	5.17	1.45	1.34
2	B	301	BX6	C10-N9	4.78	1.44	1.34
2	D	301	BX6	C10-N9	4.57	1.44	1.34
2	A	301	BX6	C7-C8	3.44	1.59	1.53
2	A	301	BX6	C7-C2	3.14	1.58	1.51
2	B	301	BX6	C7-C8	3.07	1.58	1.53
4	D	303	ACY	CH3-C	-2.76	1.45	1.48
4	B	305	ACY	CH3-C	-2.72	1.45	1.48
2	B	301	BX6	C7-C2	2.53	1.57	1.51
4	D	304	ACY	CH3-C	2.45	1.51	1.48
2	C	301	BX6	C13-C12	2.42	1.56	1.53
2	C	301	BX6	C7-C2	2.42	1.57	1.51
2	D	301	BX6	C7-C8	2.35	1.57	1.53
2	B	301	BX6	O11-C10	-2.04	1.19	1.23
2	D	301	BX6	O11-C10	-2.01	1.19	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	BX6	C2-C7-C8	5.03	124.44	113.35
2	A	301	BX6	C7-C2-C1	3.67	128.19	120.91
2	D	301	BX6	B16-C8-C7	3.39	121.11	112.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	BX6	O11-C10-N9	-3.26	116.90	122.93
2	A	301	BX6	B16-C8-C7	3.17	120.57	112.65
2	B	301	BX6	O11-C10-N9	-3.04	117.31	122.93
2	B	301	BX6	C12-C10-N9	3.02	119.66	116.42
2	C	301	BX6	C7-C2-C3	2.90	126.66	120.91
2	C	301	BX6	C12-C10-N9	2.82	119.44	116.42
2	A	301	BX6	C6-C1-C2	2.80	124.92	120.63
2	A	301	BX6	C3-C2-C1	-2.78	113.79	118.17
3	B	302	PEG	O2-C2-C1	2.59	121.43	110.07
2	A	301	BX6	O11-C10-N9	-2.40	118.49	122.93
2	B	301	BX6	B16-C8-C7	2.37	118.57	112.65
2	D	301	BX6	C6-C1-C2	2.27	124.12	120.63
2	D	301	BX6	O11-C10-N9	-2.26	118.74	122.93
2	B	301	BX6	C15-C12-C10	-2.22	105.85	109.42
2	D	301	BX6	O11-C10-C12	2.05	125.25	121.33
2	C	301	BX6	B16-C8-C7	2.01	117.67	112.65

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	BX6	C2-C7-C8-N9
2	D	301	BX6	C2-C7-C8-B16
2	B	301	BX6	C1-C2-C7-C8
2	B	301	BX6	C3-C2-C7-C8
2	B	301	BX6	C2-C7-C8-B16
2	B	301	BX6	C10-C12-C13-S14
2	B	301	BX6	C15-C12-C13-S14
2	C	301	BX6	C2-C7-C8-N9
2	C	301	BX6	C2-C7-C8-B16
2	A	301	BX6	C2-C7-C8-N9
2	A	301	BX6	C2-C7-C8-B16
3	B	302	PEG	O1-C1-C2-O2
3	B	304	PEG	O2-C3-C4-O4
3	C	302	PEG	O2-C3-C4-O4
3	D	302	PEG	O1-C1-C2-O2
3	B	304	PEG	O1-C1-C2-O2
3	B	303	PEG	C1-C2-O2-C3
3	D	302	PEG	C4-C3-O2-C2
3	B	304	PEG	C1-C2-O2-C3
2	C	301	BX6	N9-C10-C12-C13
3	C	302	PEG	C4-C3-O2-C2

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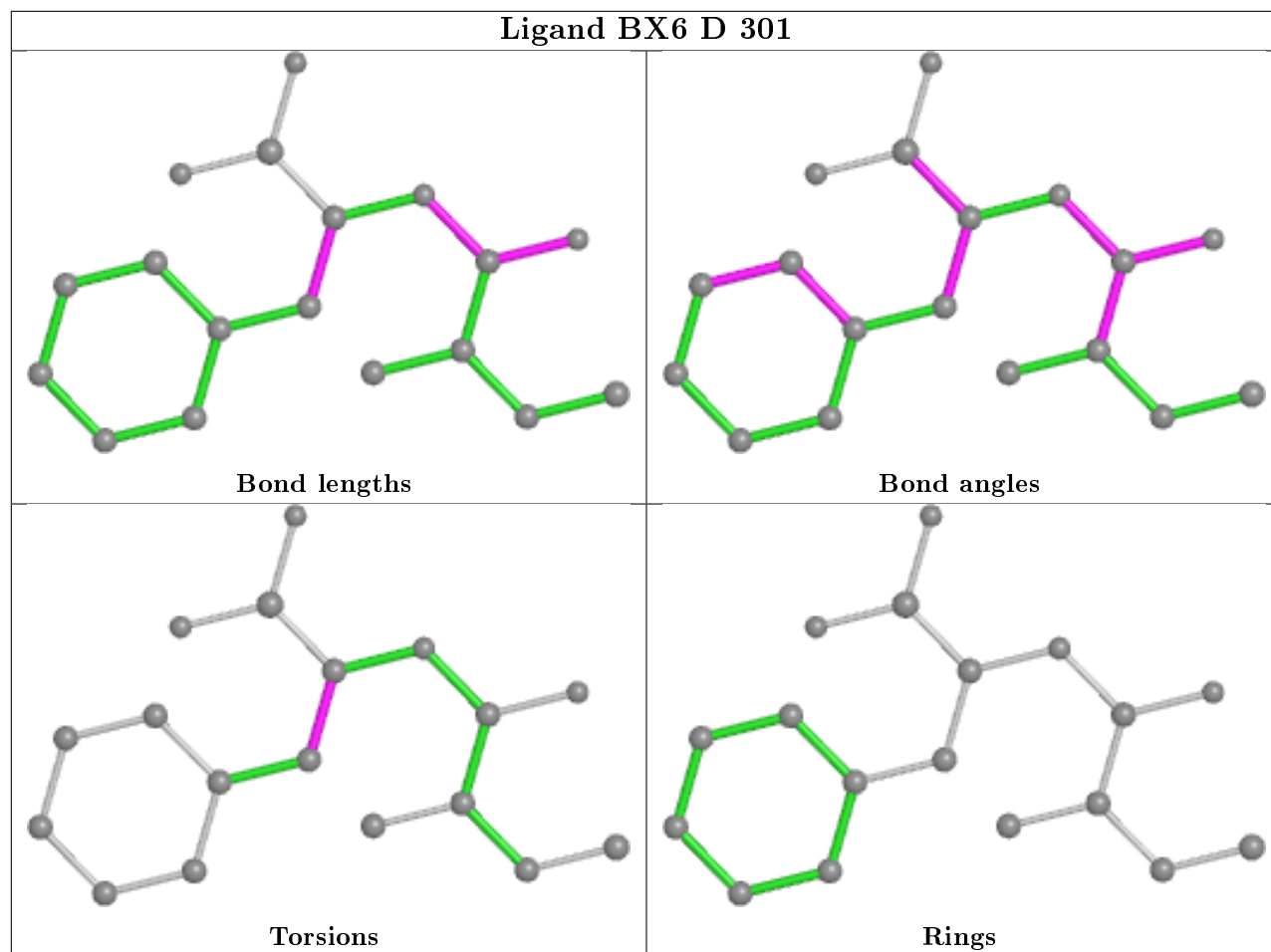
Mol	Chain	Res	Type	Atoms
2	B	301	BX6	C2-C7-C8-N9
3	A	302	PEG	O1-C1-C2-O2
2	B	301	BX6	C7-C8-N9-C10
2	A	301	BX6	C7-C8-N9-C10
3	B	302	PEG	O2-C3-C4-O4
2	C	301	BX6	C7-C8-N9-C10
2	C	301	BX6	O11-C10-C12-C13

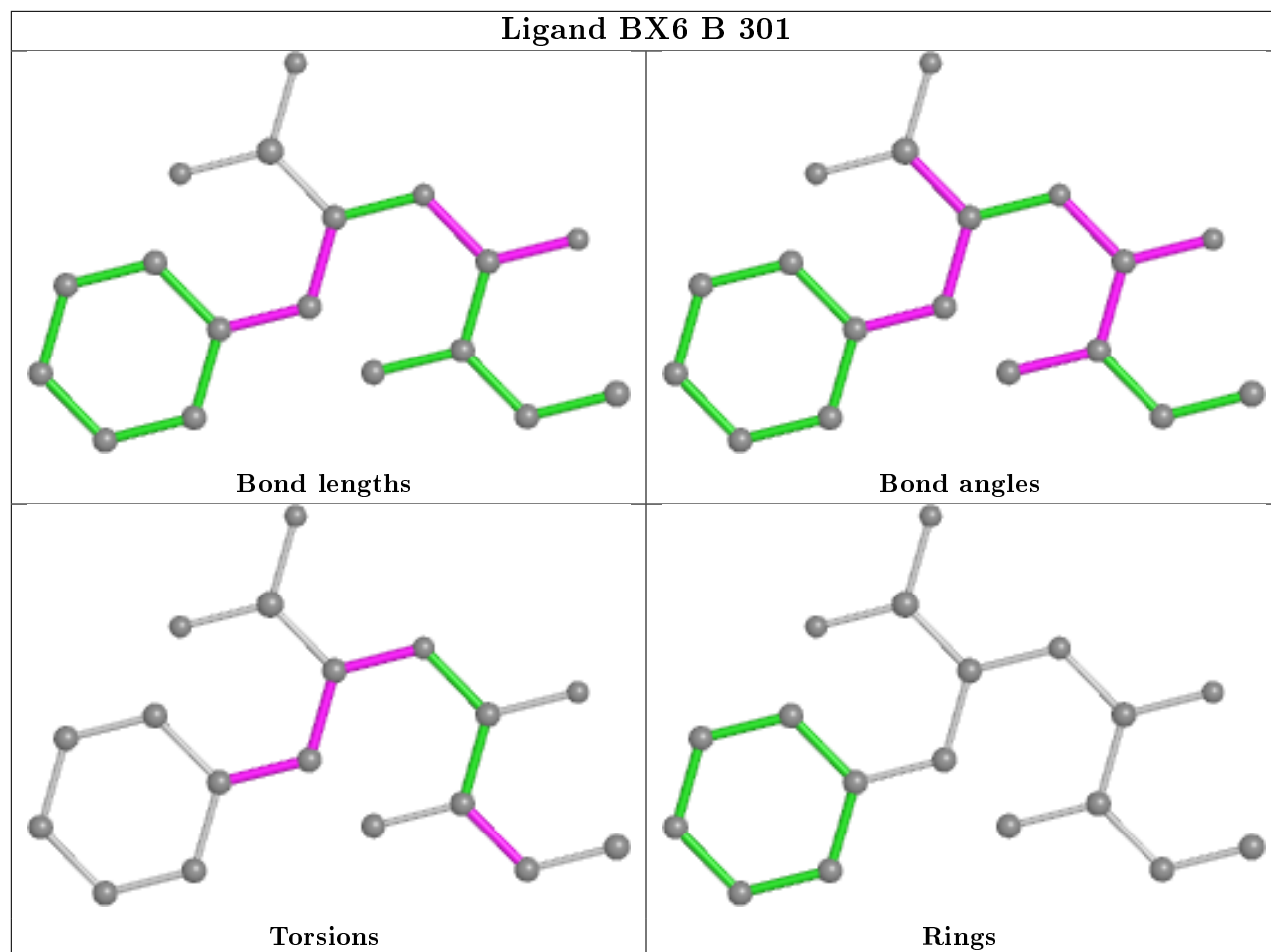
There are no ring outliers.

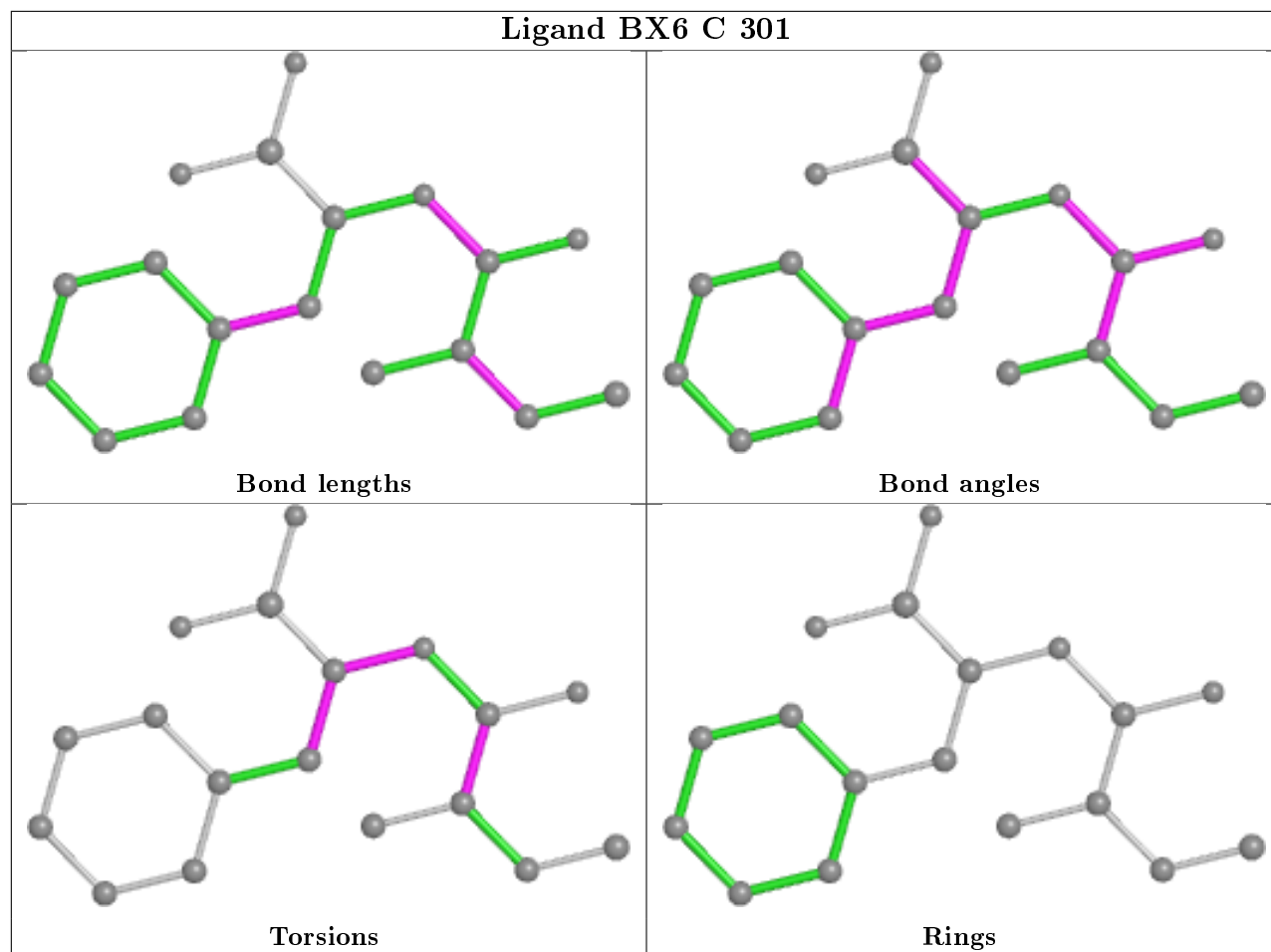
13 monomers are involved in 27 short contacts:

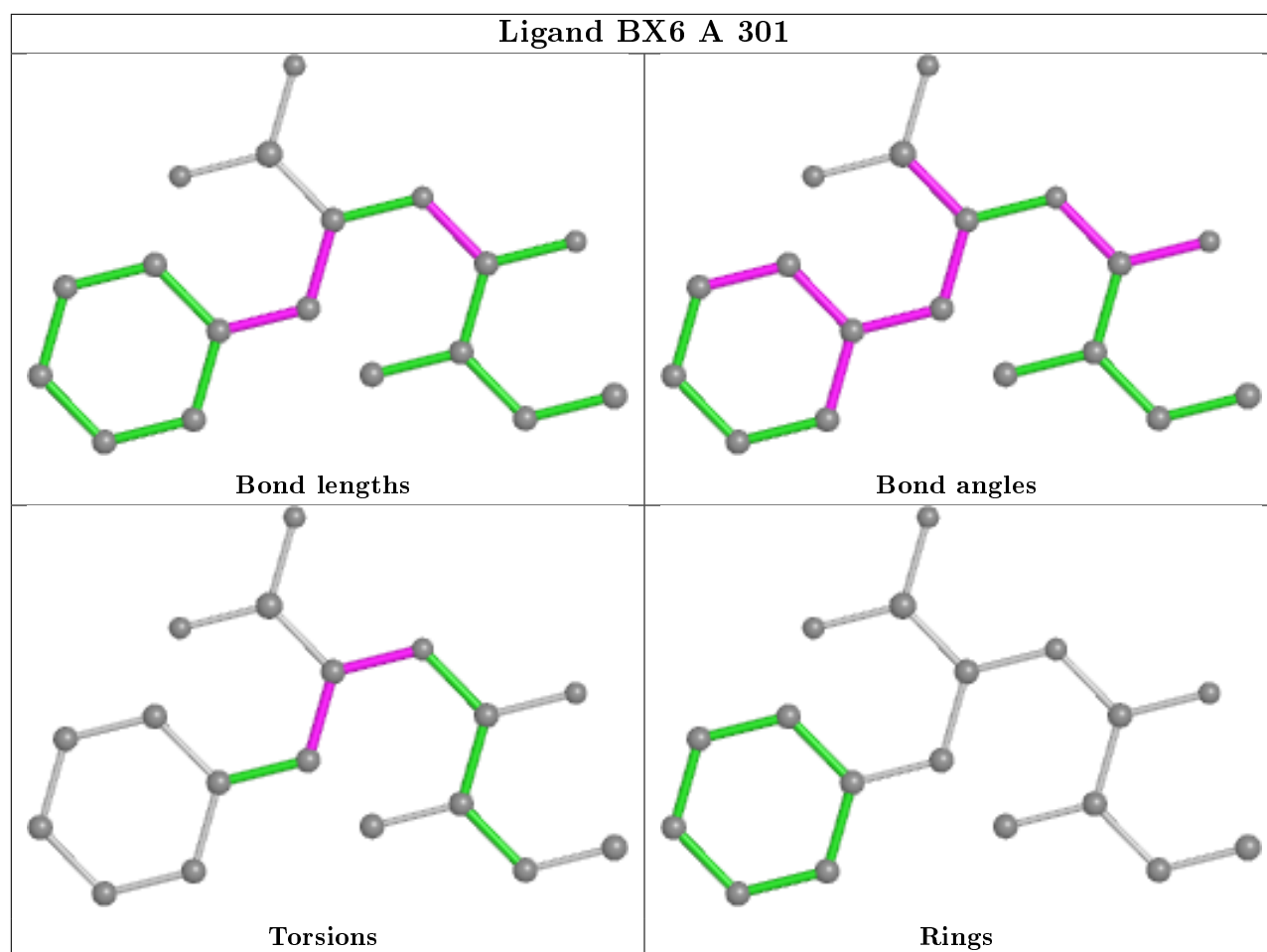
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	BX6	2	0
2	B	301	BX6	3	0
4	C	303	ACY	7	0
4	A	304	ACY	1	0
3	B	302	PEG	1	0
3	C	302	PEG	2	0
4	D	303	ACY	6	0
4	A	303	ACY	4	0
4	D	304	ACY	1	0
3	B	304	PEG	1	0
2	C	301	BX6	5	0
2	A	301	BX6	2	0
4	B	305	ACY	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/265 (100%)	-1.09	0 100 100	12, 19, 35, 49	0
1	B	264/265 (99%)	-1.03	2 (0%) 86 85	11, 17, 38, 80	0
1	C	265/265 (100%)	-0.84	4 (1%) 73 72	18, 29, 51, 70	0
1	D	260/265 (98%)	-0.97	3 (1%) 79 77	12, 20, 46, 71	0
All	All	1054/1060 (99%)	-0.98	9 (0%) 84 83	11, 21, 45, 80	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	ASN	7.5
1	B	26	THR	6.1
1	D	30	ALA	3.6
1	C	255	GLY	3.3
1	D	38	GLN	2.7
1	C	228	ASP	2.4
1	D	105	TRP	2.3
1	C	229	TRP	2.2
1	C	227	ALA	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

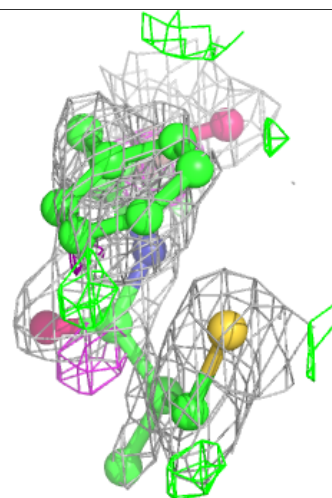
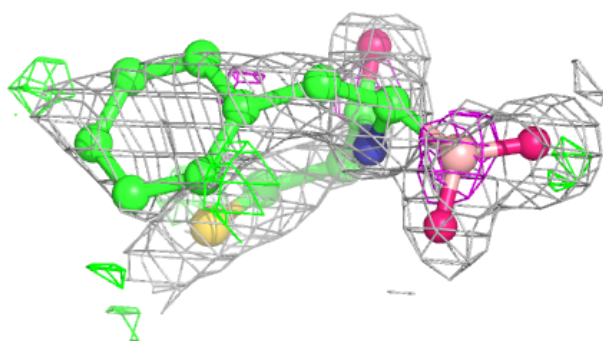
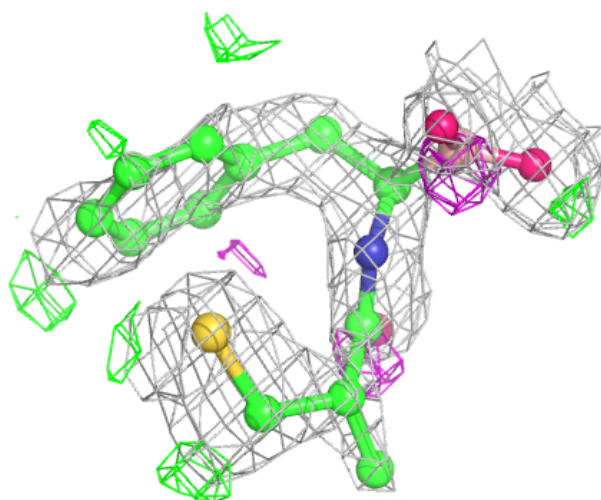
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BX6	C	301	18/18	0.77	0.28	32,50,58,73	0
3	PEG	A	302	7/7	0.78	0.15	30,34,39,40	0
3	PEG	D	302	7/7	0.83	0.14	27,42,47,51	0
2	BX6	A	301	18/18	0.84	0.29	25,42,57,65	0
2	BX6	B	301	18/18	0.85	0.20	26,43,59,64	0
2	BX6	D	301	18/18	0.86	0.22	21,42,58,62	0
3	PEG	C	302	7/7	0.87	0.11	33,36,39,40	0
3	PEG	B	304	7/7	0.90	0.10	29,34,40,42	0
3	PEG	B	302	7/7	0.94	0.10	14,17,25,29	0
3	PEG	B	303	7/7	0.95	0.10	18,23,30,30	0
4	ACY	A	304	4/4	0.95	0.15	19,21,32,38	0
4	ACY	D	304	4/4	0.95	0.08	32,34,38,47	0
4	ACY	D	303	4/4	0.97	0.17	7,20,32,44	0
4	ACY	A	303	4/4	0.97	0.17	3,24,25,29	0
4	ACY	C	303	4/4	0.97	0.16	10,27,29,39	0
4	ACY	C	304	4/4	0.97	0.13	21,28,30,32	0
4	ACY	B	305	4/4	0.97	0.14	7,26,33,36	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.

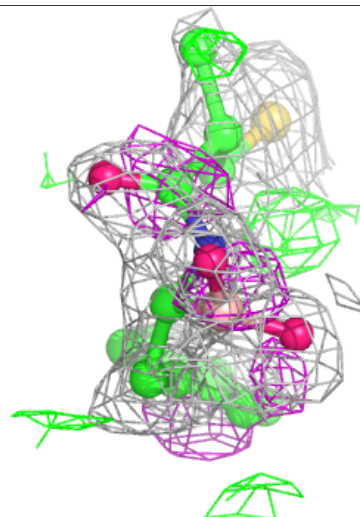
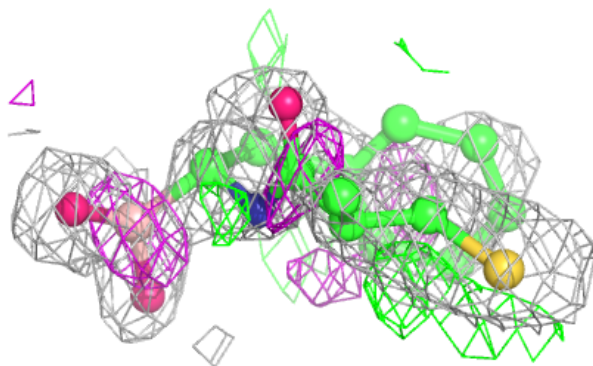
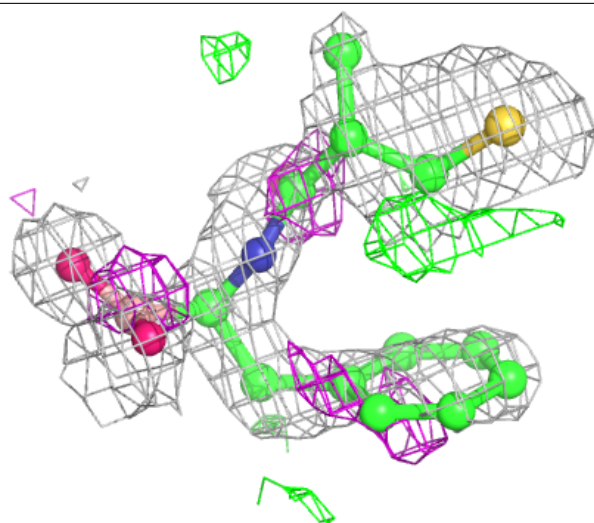
Electron density around BX6 C 301:

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



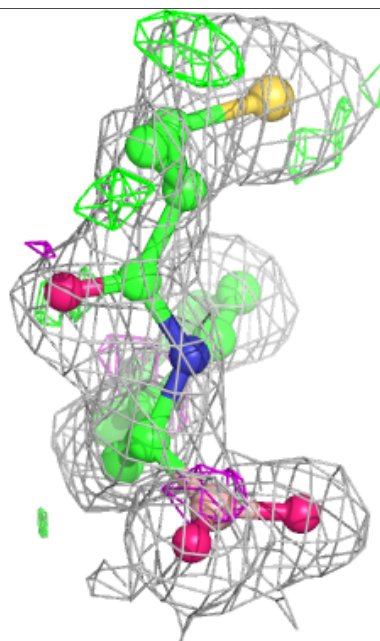
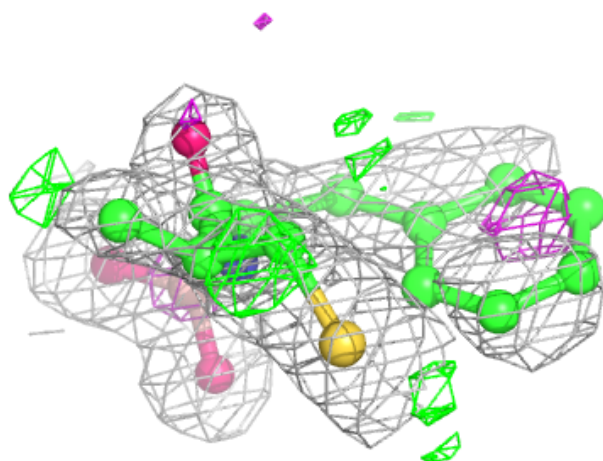
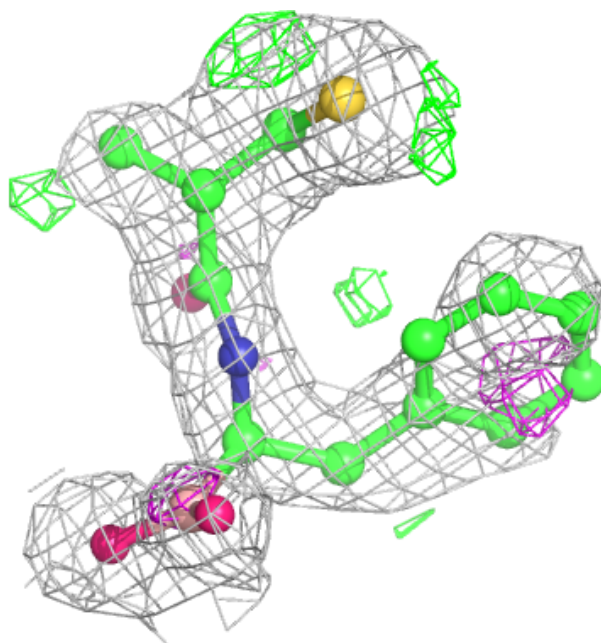
Electron density around BX6 A 301:

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



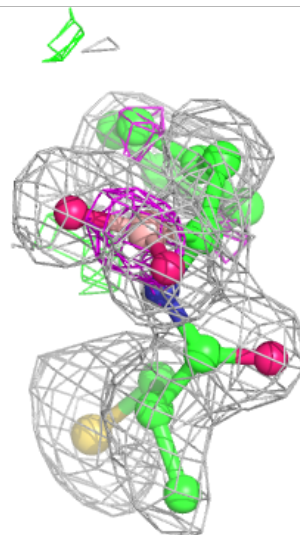
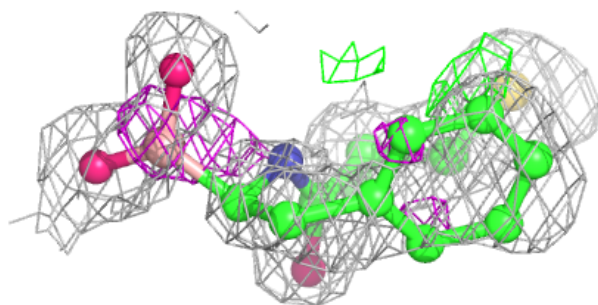
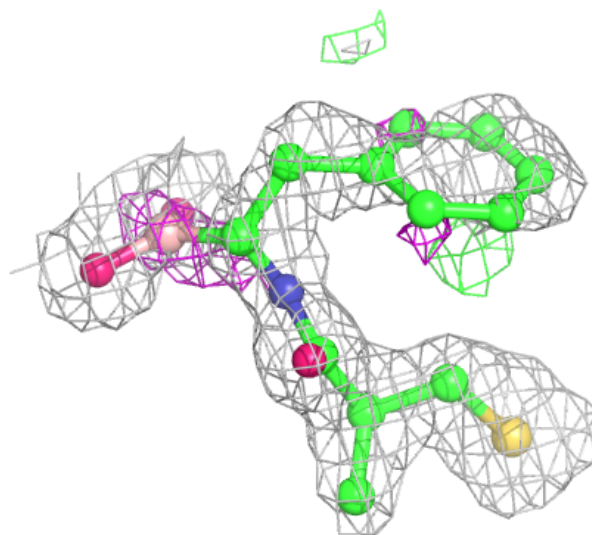
Electron density around BX6 B 301:

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



Electron density around BX6 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.