



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:30 PM BST

PDB ID : 6Q27
Title : N-acetylmannosamine kinase with N-acetylmannosamine from *Staphylococcus aureus*
Authors : Coombes, D.; Horne, C.R.; Davies, J.S.; Dobson, R.C.J.
Deposited on : 2019-08-07
Resolution : 2.20 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 : 2.13.1
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) : 2.13.1

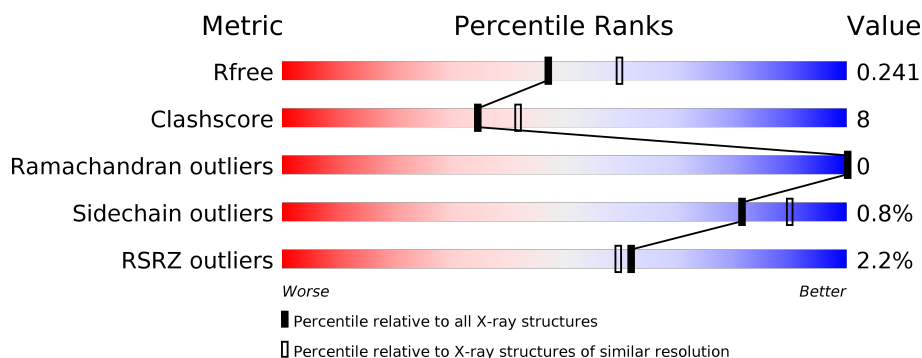
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	285	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>15%</div> </div> </div>
1	B	285	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
1	C	285	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
1	D	285	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>11%</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
2	BM3	A	301	-	-	X	-
2	BM3	B	301	-	-	X	-
2	BM3	D	301	-	-	X	-

2 Entry composition [i](#)

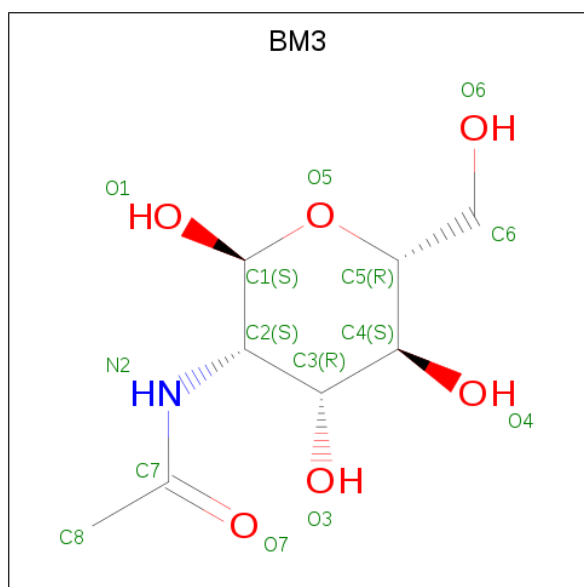
There are 3 unique types of molecules in this entry. The entry contains 9049 atoms, of which 60 are hydrogens and 0 are deuteriums.

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 Glucokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2207	1409	364	427	7			
1	B	285	Total	C	N	O	S	0	0	0
			2211	1411	365	428	7			
1	C	285	Total	C	N	O	S	0	0	0
			2211	1411	365	428	7			
1	D	285	Total	C	N	O	S	0	0	0
			2211	1411	365	428	7			

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-mannopyranose (three-letter code: BM3) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			30	8	15	1	6		
2	B	1	Total	C	H	N	O	0	0
			30	8	15	1	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			30	8	15	1	6		
2	D	1	Total	C	H	N	O	0	0
			30	8	15	1	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	25	Total	O	0	0
			25	25		
3	C	19	Total	O	0	0
			19	19		
3	D	14	Total	O	0	0
			14	14		

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.

Chain A:

85% 15%

Y2 Y3 Q21 L22 F25 I58 V61 S65 G68 V69 E72 Y79 A80 G81 V105 D108 A111 G115 E116 L117 I136 G137 K141 H146 K154 V158 L161 E172 A175 K181 K182 R183 M184 T193 H194 E200

E204 G205 D206 D207 I208 A209 I212 L213 D219 M230 Y231 D232 I242 L249 V266 A279 G283 Q286

Chain B:

Category	Value (%)
Green	84%
Yellow	16%

Chain C:

Category	Percentage
Green	86%
Yellow	14%

Chain D:

Category	Value (%)
Y2	89%
L22	11%
F25	11%
P33	11%
K36	11%
S37	11%
E38	11%
G50	11%
Y51	11%
Q54	11%
Y55	11%
Q56	11%
L57	11%
I58	11%
S65	11%
G68	11%
E72	11%
A80	11%
G81	11%
P85	11%
V105	11%
A111	11%
L117	11%
I136	11%
G137	11%
K141	11%
E172	11%
K181	11%
K182	11%
R183	11%
I184	11%
I185	11%
A186	11%
G187	11%
T190	11%
H194	11%
D206	11%
D207	11%
F208	11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.24Å 101.35Å 133.22Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	44.56 – 2.20 44.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.56-2.20) 100.0 (44.56-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.232 0.205 , 0.241	Depositor DCC
R_{free} test set	6342 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9049	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: BM3

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	0.48	0/2249	0.63	0/3049
1	B	0.46	0/2253	0.61	0/3054
1	C	0.43	0/2253	0.57	0/3054
1	D	0.44	0/2253	0.60	0/3054
All	All	0.45	0/9008	0.60	0/12211

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2207	0	2190	53	0
1	B	2211	0	2196	51	0
1	C	2211	0	2196	33	0
1	D	2211	0	2196	30	0
2	A	15	15	14	11	0
2	B	15	15	14	9	0
2	C	15	15	15	2	0
2	D	15	15	15	9	0
3	A	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	1	0
3	C	19	0	0	0	0
3	D	14	0	0	0	0
All	All	8989	60	8836	147	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 8.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ASP:OD2	2:C:301:BM3:O6	1.77	1.03
1:D:80:ALA:HA	2:D:301:BM3:H8C1	1.48	0.95
1:B:81:GLY:H	2:B:301:BM3:H8C1	1.31	0.94
1:D:68:GLY:HA2	2:D:301:BM3:H8C2	1.47	0.94
1:A:161:LEU:HD21	1:B:230:MET:HE3	1.49	0.92
1:A:230:MET:HG3	1:B:230:MET:HG3	1.54	0.90
1:A:68:GLY:HA2	2:A:301:BM3:H8C2	1.52	0.89
1:A:80:ALA:HA	2:A:301:BM3:H8C1	1.54	0.87
1:A:158:VAL:HG12	1:B:230:MET:HE1	1.57	0.85
1:A:158:VAL:HG12	1:B:230:MET:CE	2.06	0.84
1:B:81:GLY:N	2:B:301:BM3:H8C1	1.91	0.84
1:B:241:GLY:O	1:B:244:GLU:HG2	1.80	0.81
1:D:33:PRO:HB3	1:D:38:GLU:HG3	1.62	0.81
1:C:206:ASP:OD1	1:C:208:ILE:HG22	1.79	0.81
1:D:80:ALA:CA	2:D:301:BM3:H8C1	2.10	0.80
1:B:80:ALA:HA	2:B:301:BM3:H8C1	1.63	0.80
1:B:33:PRO:HB3	1:B:38:GLU:HG3	1.64	0.80
1:C:187:GLY:O	1:C:208:ILE:HD11	1.85	0.77
1:A:206:ASP:OD1	1:A:208:ILE:HG22	1.85	0.76
1:B:68:GLY:HA2	2:B:301:BM3:H8C2	1.68	0.76
1:A:80:ALA:CA	2:A:301:BM3:H8C1	2.15	0.75
1:D:68:GLY:CA	2:D:301:BM3:H8C2	2.16	0.75
1:B:81:GLY:H	2:B:301:BM3:C8	2.02	0.72
1:D:206:ASP:OD2	1:D:208:ILE:HG22	1.89	0.71
1:D:136:ILE:HD12	1:D:172:GLU:HA	1.73	0.71
1:B:206:ASP:OD1	1:B:208:ILE:HG22	1.91	0.70
1:D:208:ILE:O	1:D:208:ILE:HD12	1.92	0.70
1:A:136:ILE:HD12	1:A:172:GLU:HA	1.75	0.69
1:A:68:GLY:CA	2:A:301:BM3:H8C2	2.21	0.69
1:B:187:GLY:O	1:B:208:ILE:HD11	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:O	1:B:154:LYS:NZ	2.22	0.66
1:C:33:PRO:HA	1:C:38:GLU:OE2	1.96	0.65
1:B:80:ALA:CA	2:B:301:BM3:H8C1	2.29	0.63
1:D:184:MET:HA	1:D:212:ILE:HD13	1.81	0.63
1:D:68:GLY:HA2	2:D:301:BM3:C8	2.26	0.61
1:D:183:ARG:NH2	1:D:219:ASP:OD2	2.30	0.61
1:C:181:LYS:HE3	1:C:193:THR:O	2.01	0.60
1:A:25:PHE:CE2	1:C:194:HIS:HB2	2.37	0.60
1:A:25:PHE:HE2	1:C:194:HIS:HB2	1.67	0.59
1:C:33:PRO:HB3	1:C:38:GLU:HG3	1.84	0.59
1:B:33:PRO:HB3	1:B:38:GLU:CG	2.31	0.59
1:C:184:MET:HA	1:C:212:ILE:HD13	1.84	0.59
1:D:36:LYS:HE3	1:D:85:PRO:HG3	1.84	0.59
1:B:33:PRO:CB	1:B:38:GLU:HG3	2.31	0.58
1:A:230:MET:HE3	1:A:230:MET:HA	1.85	0.58
1:C:33:PRO:HA	1:C:38:GLU:CD	2.24	0.58
1:C:185:ILE:HD11	1:C:193:THR:HG22	1.85	0.57
1:A:230:MET:CE	1:B:231:TYR:HE2	2.18	0.57
1:A:232:ASP:OD1	1:B:154:LYS:HE3	2.04	0.56
1:A:81:GLY:N	2:A:301:BM3:H8C1	2.20	0.56
1:D:50:GLY:O	1:D:54:GLN:HG2	2.05	0.56
1:A:80:ALA:HA	2:A:301:BM3:C8	2.31	0.56
1:A:161:LEU:HD11	1:B:230:MET:HE1	1.87	0.56
1:B:200:GLU:O	1:B:204:GLU:HG2	2.06	0.55
1:A:154:LYS:NZ	1:B:266:VAL:O	2.36	0.55
1:A:3:TYR:HD2	1:A:61:VAL:HB	1.72	0.55
1:D:230:MET:CE	1:D:230:MET:HA	2.37	0.55
1:A:230:MET:HE1	1:B:231:TYR:HE2	1.72	0.54
1:A:181:LYS:HE3	1:A:193:THR:HG22	1.89	0.54
1:C:275:SER:OG	1:C:279:ALA:HB2	2.08	0.53
1:A:154:LYS:HE3	1:B:232:ASP:OD1	2.08	0.53
1:A:242:ILE:HG23	1:A:249:LEU:HD22	1.91	0.53
1:C:33:PRO:HB3	1:C:38:GLU:CG	2.39	0.53
1:D:33:PRO:CB	1:D:38:GLU:HG3	2.36	0.53
1:C:33:PRO:CB	1:C:38:GLU:HG3	2.39	0.52
1:D:81:GLY:N	2:D:301:BM3:H8C1	2.25	0.52
1:C:177:THR:O	1:C:181:LYS:HG3	2.09	0.52
1:D:80:ALA:HA	2:D:301:BM3:C8	2.31	0.52
1:D:117:LEU:CD1	1:D:141:LYS:HD3	2.40	0.51
1:D:58:ILE:HD12	1:D:58:ILE:N	2.25	0.51
1:B:275:SER:OG	1:B:279:ALA:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HD21	1:B:230:MET:CE	2.32	0.51
1:A:184:MET:HA	1:A:212:ILE:HD13	1.93	0.51
1:C:111:ALA:O	1:C:283:GLY:HA3	2.11	0.51
1:A:68:GLY:HA2	2:A:301:BM3:C8	2.33	0.50
1:B:184:MET:HA	1:B:212:ILE:HD13	1.93	0.50
1:A:117:LEU:CD1	1:A:141:LYS:HD3	2.42	0.50
1:C:136:ILE:HD12	1:C:172:GLU:HA	1.93	0.50
1:A:200:GLU:O	1:A:204:GLU:HG3	2.12	0.49
1:B:136:ILE:HD12	1:B:172:GLU:HA	1.94	0.49
1:C:72:GLU:HG2	1:C:105:VAL:O	2.12	0.49
1:A:137:GLY:HA3	2:A:301:BM3:H5	1.94	0.49
1:A:81:GLY:H	2:A:301:BM3:H8C1	1.77	0.49
1:B:108:ASP:OD1	1:B:108:ASP:N	2.45	0.49
1:B:68:GLY:CA	2:B:301:BM3:H8C2	2.40	0.49
1:B:12:GLN:NE2	1:B:29:GLN:OE1	2.45	0.49
1:B:184:MET:HG2	1:B:198:LEU:HD22	1.95	0.48
1:C:22:LEU:HD21	1:C:118:LYS:HG2	1.95	0.48
1:D:230:MET:HE1	1:D:230:MET:HA	1.93	0.48
1:A:230:MET:CE	1:A:230:MET:HA	2.43	0.48
1:D:36:LYS:HE3	1:D:85:PRO:CG	2.43	0.48
1:B:72:GLU:HG2	1:B:105:VAL:O	2.13	0.48
1:C:128:PHE:CE1	1:C:227:ILE:HD13	2.48	0.48
1:B:33:PRO:HA	1:B:38:GLU:OE2	2.13	0.48
1:A:181:LYS:CE	1:A:193:THR:HG22	2.44	0.48
1:A:111:ALA:O	1:A:283:GLY:HA3	2.15	0.47
1:D:137:GLY:HA3	2:D:301:BM3:H5	1.96	0.47
1:A:108:ASP:OD1	1:A:108:ASP:N	2.46	0.47
1:B:233:PRO:O	1:B:268:ALA:HB2	2.14	0.47
1:A:136:ILE:HD11	1:A:175:ALA:HB3	1.95	0.47
1:B:137:GLY:HA3	2:B:301:BM3:H5	1.97	0.47
1:A:181:LYS:HE3	1:A:193:THR:CG2	2.45	0.46
1:D:81:GLY:H	2:D:301:BM3:H8C1	1.81	0.46
1:C:38:GLU:HG3	1:C:38:GLU:O	2.15	0.46
1:B:11:THR:HG22	1:B:12:GLN:HG3	1.98	0.46
1:C:16:ALA:HB1	1:C:24:MET:HG3	1.98	0.46
1:A:183:ARG:NH2	1:A:219:ASP:OD2	2.39	0.46
1:B:154:LYS:HE2	3:B:425:HOH:O	2.15	0.46
1:B:245:GLN:HB2	1:B:249:LEU:HB2	1.98	0.46
1:A:58:ILE:N	1:A:58:ILE:HD12	2.30	0.45
1:D:181:LYS:O	1:D:185:ILE:HG13	2.16	0.45
1:B:22:LEU:HD21	1:B:118:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:CG1	1:B:230:MET:HE1	2.37	0.45
1:C:81:GLY:N	2:C:301:BM3:H8C1	2.32	0.44
1:C:183:ARG:NH2	1:C:219:ASP:OD2	2.41	0.44
1:A:161:LEU:HD11	1:B:230:MET:CE	2.47	0.44
1:B:117:LEU:HD23	1:B:117:LEU:HA	1.77	0.44
1:B:184:MET:CG	1:B:198:LEU:HD22	2.48	0.43
1:C:34:ASP:N	1:C:38:GLU:OE2	2.49	0.43
1:A:208:ILE:HG23	1:A:209:ALA:N	2.33	0.43
1:A:230:MET:HE2	1:B:231:TYR:CE2	2.53	0.43
1:D:65:SER:HB2	1:D:111:ALA:CB	2.48	0.43
1:C:181:LYS:O	1:C:185:ILE:HD13	2.17	0.43
1:A:72:GLU:HG2	1:A:105:VAL:O	2.19	0.43
1:B:184:MET:SD	1:B:198:LEU:HD22	2.58	0.43
1:A:230:MET:CE	1:B:156:ASN:OD1	2.67	0.43
1:C:208:ILE:HD12	1:C:208:ILE:HA	1.86	0.43
1:B:202:ALA:O	1:B:210:LYS:HE3	2.19	0.42
1:B:25:PHE:CZ	1:D:194:HIS:HB2	2.53	0.42
1:A:194:HIS:HB2	1:C:25:PHE:CZ	2.54	0.42
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.90	0.42
1:D:51:TYR:HD1	1:D:54:GLN:HE21	1.67	0.42
1:A:137:GLY:CA	2:A:301:BM3:H5	2.49	0.42
1:C:181:LYS:CE	1:C:193:THR:O	2.66	0.42
1:D:187:GLY:O	1:D:208:ILE:HD11	2.19	0.42
1:C:69:VAL:HB	1:C:79:TYR:HB3	2.02	0.41
1:B:16:ALA:HB1	1:B:24:MET:HG3	2.02	0.41
1:A:115:GLY:HA3	1:A:279:ALA:O	2.21	0.41
1:A:69:VAL:HB	1:A:79:TYR:HB3	2.02	0.41
1:C:3:TYR:HB3	1:C:285:LEU:HD22	2.03	0.41
1:D:117:LEU:HD13	1:D:141:LYS:HD3	2.03	0.41
1:B:80:ALA:HA	2:B:301:BM3:C8	2.41	0.41
1:A:136:ILE:CD1	1:A:175:ALA:HB3	2.51	0.40
1:C:73:GLN:HG2	1:C:74:LYS:N	2.36	0.40
1:D:72:GLU:HG2	1:D:105:VAL:O	2.21	0.40
1:A:108:ASP:OD2	2:A:301:BM3:H6C1	2.21	0.40
1:C:64:ILE:O	1:C:105:VAL:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/285 (99%)	277 (98%)	6 (2%)	0	100	100
1	B	283/285 (99%)	278 (98%)	5 (2%)	0	100	100
1	C	283/285 (99%)	279 (99%)	4 (1%)	0	100	100
1	D	283/285 (99%)	277 (98%)	6 (2%)	0	100	100
All	All	1132/1140 (99%)	1111 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/236 (98%)	231 (100%)	1 (0%)	91	96
1	B	233/236 (99%)	232 (100%)	1 (0%)	91	96
1	C	233/236 (99%)	231 (99%)	2 (1%)	78	88
1	D	233/236 (99%)	230 (99%)	3 (1%)	69	81
All	All	931/944 (99%)	924 (99%)	7 (1%)	81	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	B	65	SER

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Mol	Chain	Res	Type
1	C	26	ASP
1	C	65	SER
1	D	65	SER
1	D	190	THR
1	D	208	ILE

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	BM3	A	301	-	15,15,15	1.99	4 (26%)	21,21,21	3.78	6 (28%)
2	BM3	B	301	-	15,15,15	1.87	4 (26%)	21,21,21	3.45	9 (42%)
2	BM3	C	301	-	15,15,15	2.20	5 (33%)	21,21,21	2.78	9 (42%)
2	BM3	D	301	-	15,15,15	1.94	4 (26%)	21,21,21	3.50	7 (33%)

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	BM3	A	301	-	-	0/6/26/26	0/1/1/1
2	BM3	B	301	-	-	0/6/26/26	0/1/1/1
2	BM3	C	301	-	-	1/6/26/26	0/1/1/1
2	BM3	D	301	-	-	0/6/26/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	BM3	C2-N2	4.01	1.52	1.45
2	C	301	BM3	C7-N2	3.95	1.47	1.34
2	D	301	BM3	C2-N2	3.91	1.52	1.45
2	A	301	BM3	C2-N2	3.87	1.52	1.45
2	C	301	BM3	C3-C2	-3.52	1.46	1.53
2	A	301	BM3	C7-N2	3.49	1.46	1.34
2	B	301	BM3	C2-N2	3.49	1.51	1.45
2	C	301	BM3	O5-C1	3.45	1.51	1.42
2	A	301	BM3	C3-C2	-3.36	1.46	1.53
2	D	301	BM3	C7-N2	3.27	1.45	1.34
2	B	301	BM3	C7-N2	3.23	1.45	1.34
2	D	301	BM3	C3-C2	-3.01	1.47	1.53
2	B	301	BM3	C3-C2	-2.81	1.47	1.53
2	C	301	BM3	C1-C2	2.70	1.56	1.52
2	A	301	BM3	O5-C1	2.69	1.49	1.42
2	D	301	BM3	O5-C1	2.66	1.49	1.42
2	B	301	BM3	O5-C1	2.55	1.49	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	BM3	C1-C2-N2	-12.11	96.70	110.73
2	D	301	BM3	C1-C2-N2	-11.75	97.11	110.73
2	B	301	BM3	C1-C2-N2	-11.35	97.58	110.73
2	A	301	BM3	O5-C1-C2	9.98	119.55	109.52
2	C	301	BM3	C1-C2-N2	-7.30	102.27	110.73
2	D	301	BM3	O5-C1-C2	6.92	116.47	109.52
2	C	301	BM3	O5-C1-C2	5.57	115.12	109.52
2	B	301	BM3	O5-C1-C2	5.22	114.76	109.52
2	B	301	BM3	C1-C2-C3	5.22	117.66	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	BM3	C1-C2-C3	5.06	117.44	110.54
2	C	301	BM3	O4-C4-C3	-4.92	98.97	110.35
2	B	301	BM3	O4-C4-C3	-4.78	99.30	110.35
2	A	301	BM3	O4-C4-C3	-4.23	100.58	110.35
2	D	301	BM3	O4-C4-C3	-3.78	101.60	110.35
2	C	301	BM3	O3-C3-C2	-3.46	102.67	109.66
2	A	301	BM3	C1-C2-C3	3.22	114.93	110.54
2	C	301	BM3	C3-C2-N2	3.08	116.44	110.62
2	B	301	BM3	O5-C5-C4	2.94	115.03	109.69
2	C	301	BM3	C3-C4-C5	2.86	115.35	110.24
2	C	301	BM3	C4-C3-C2	2.68	114.27	110.34
2	D	301	BM3	O5-C5-C4	2.68	114.57	109.69
2	B	301	BM3	O3-C3-C4	2.60	116.36	110.35
2	B	301	BM3	C2-N2-C7	2.41	129.04	123.18
2	B	301	BM3	C3-C2-N2	-2.38	106.12	110.62
2	D	301	BM3	C6-C5-C4	-2.35	107.50	113.00
2	A	301	BM3	C2-N2-C7	2.35	128.88	123.18
2	B	301	BM3	C3-C4-C5	2.28	114.30	110.24
2	C	301	BM3	O3-C3-C4	2.15	115.32	110.35
2	D	301	BM3	C3-C2-N2	-2.08	106.69	110.62
2	C	301	BM3	C6-C5-C4	-2.07	108.15	113.00
2	A	301	BM3	C3-C4-C5	2.01	113.82	110.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	BM3	O5-C5-C6-O6

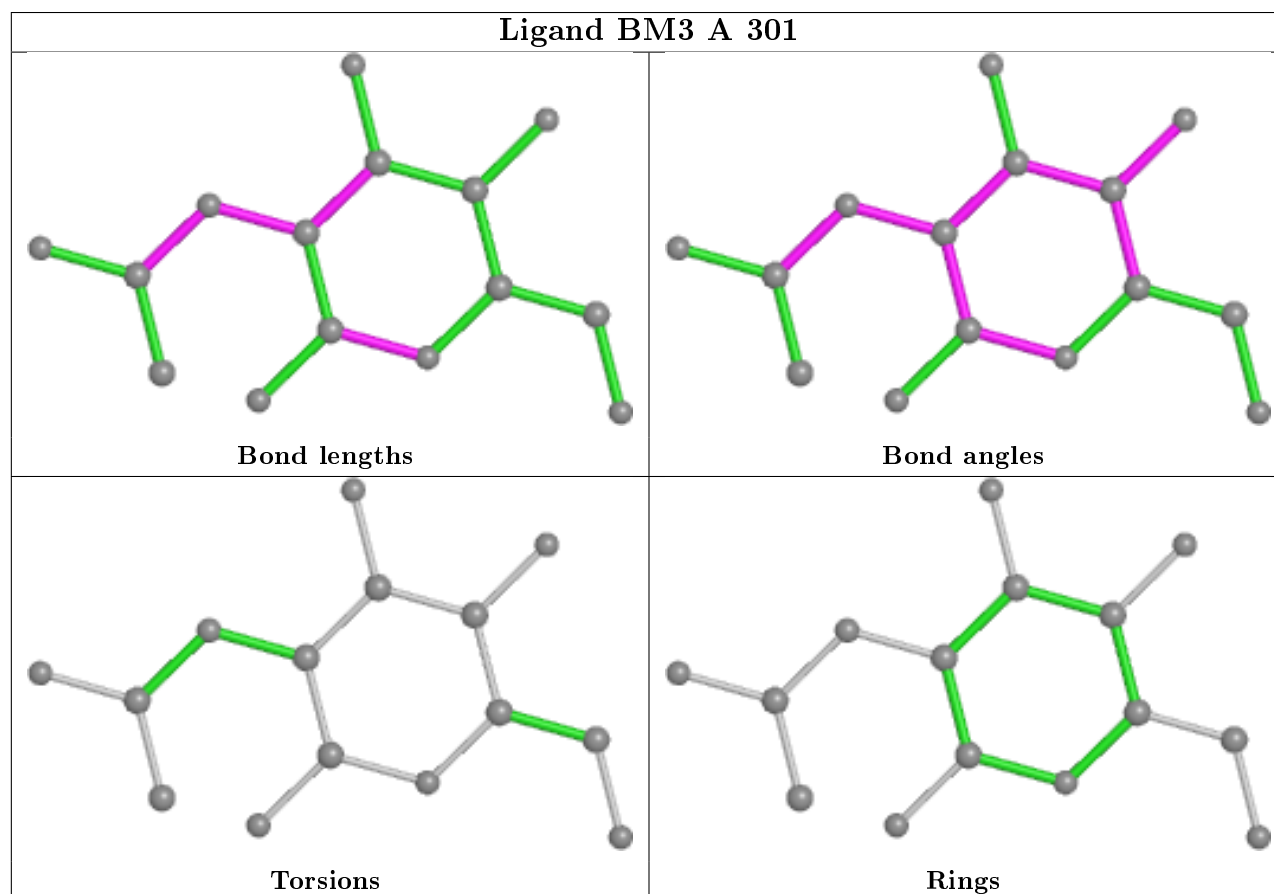
There are no ring outliers.

4 monomers are involved in 31 short contacts:

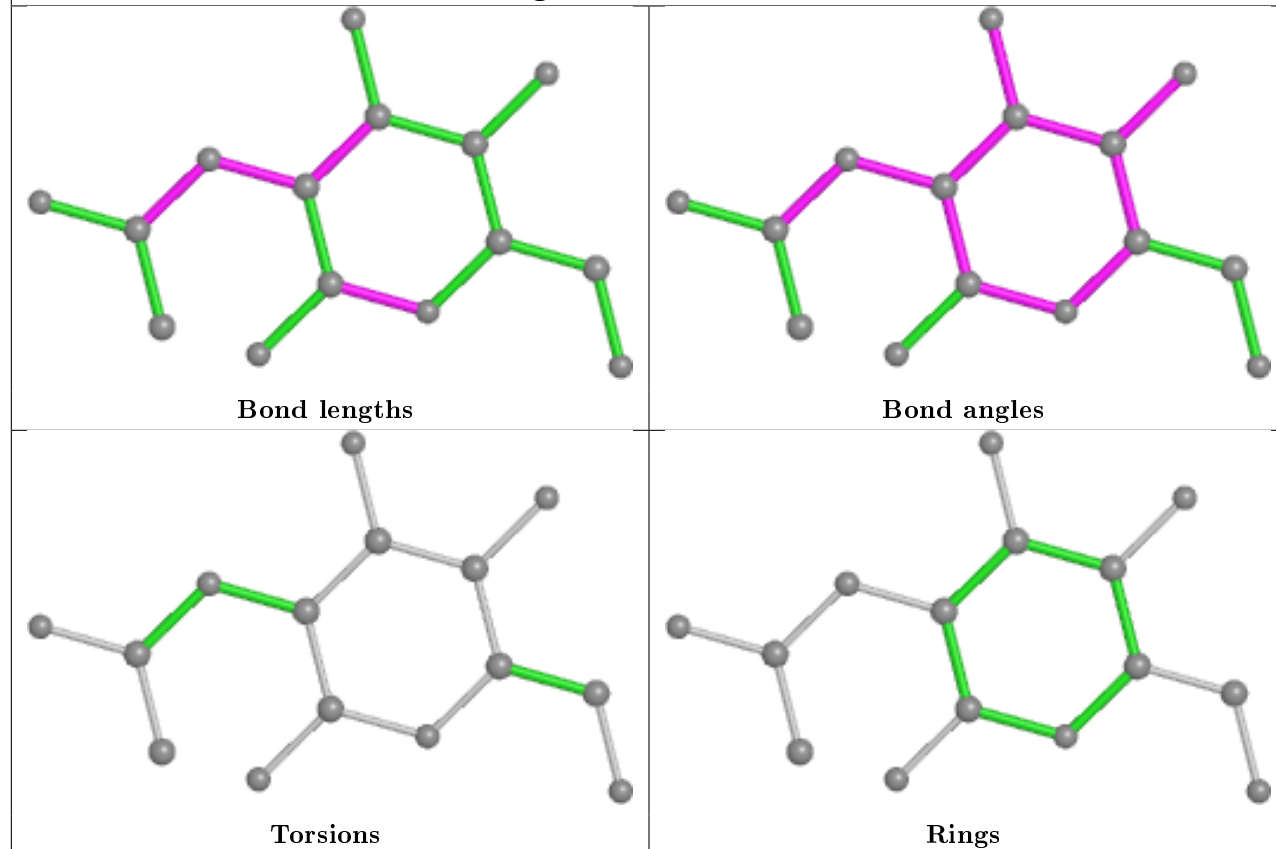
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	BM3	11	0
2	B	301	BM3	9	0
2	C	301	BM3	2	0
2	D	301	BM3	9	0

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

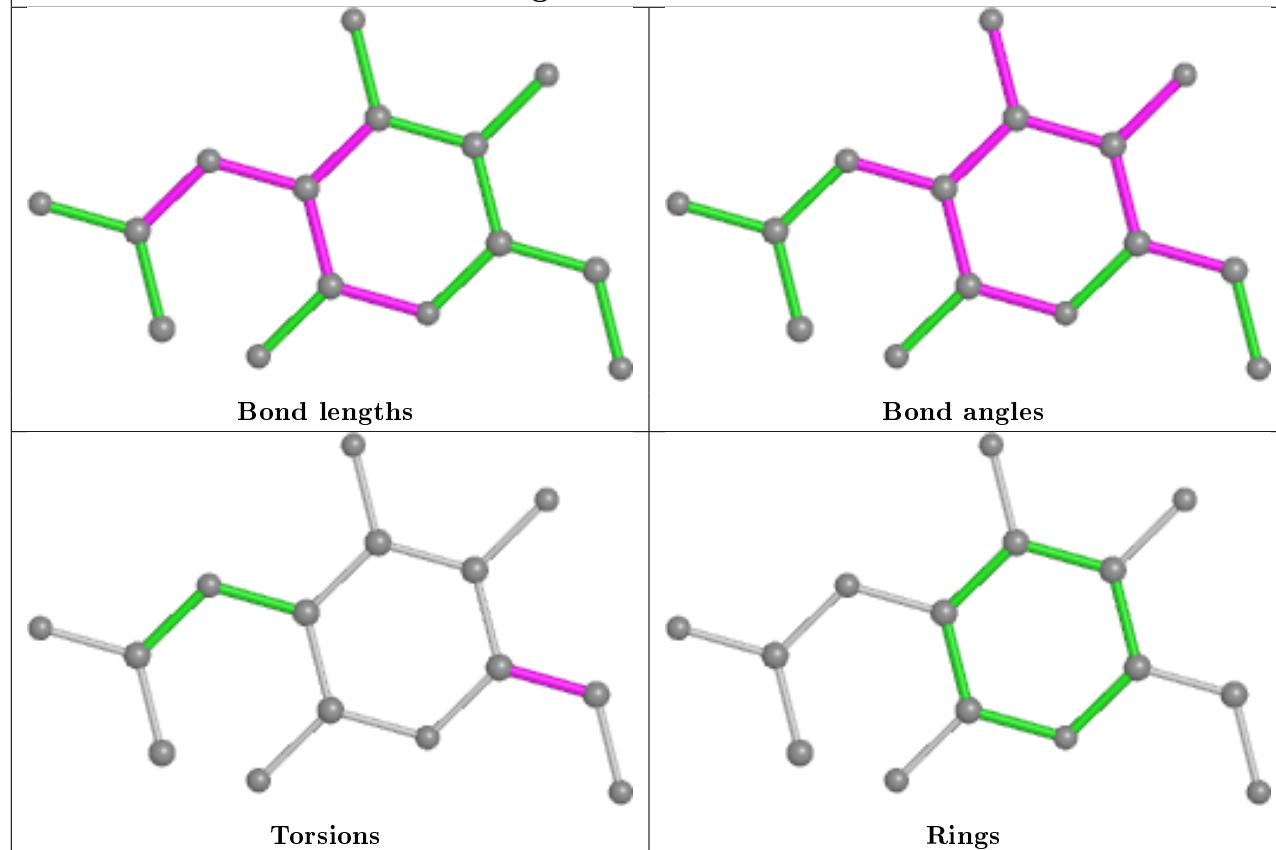
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

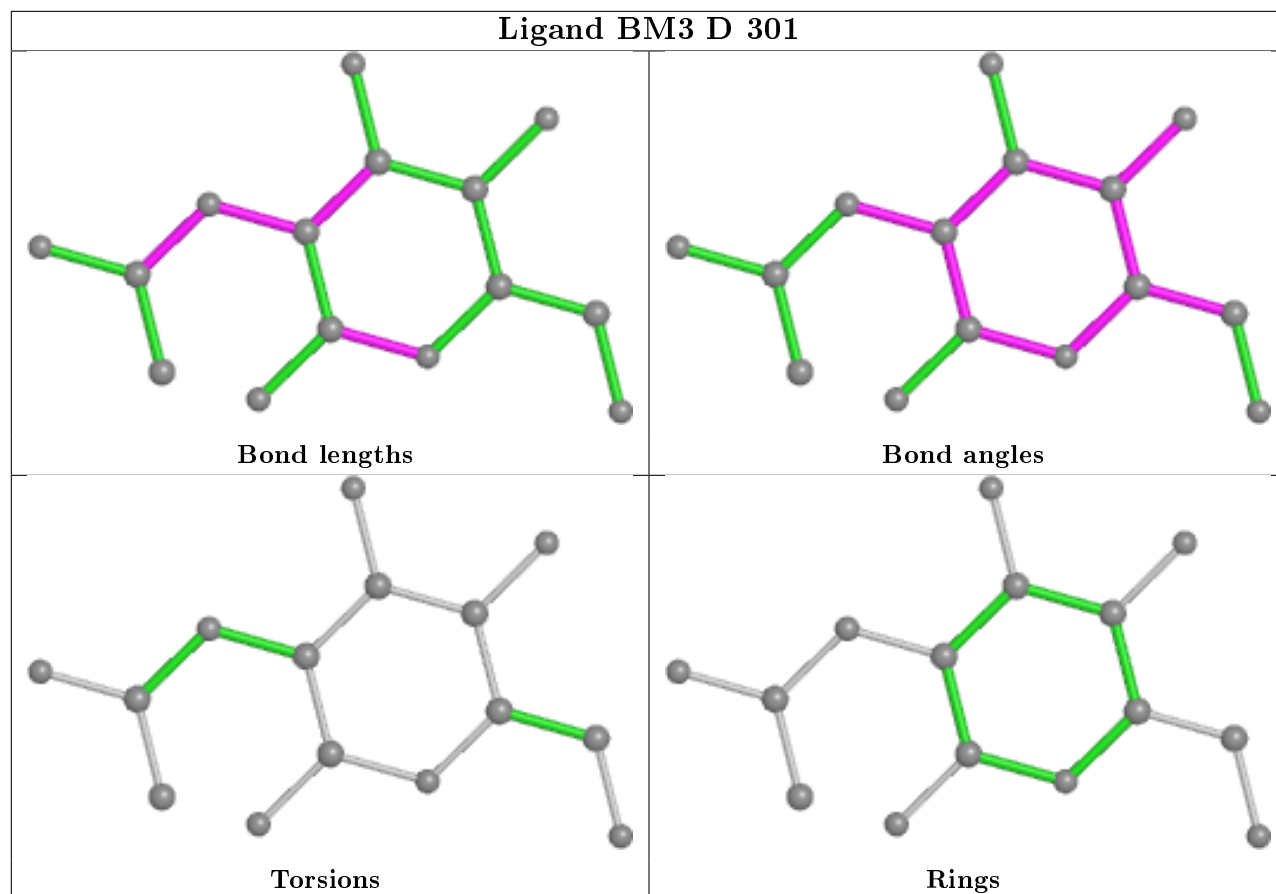


Ligand BM3 B 301



Ligand BM3 C 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	285/285 (100%)	-0.15	4 (1%) 75 73	30, 43, 75, 98	0
1	B	285/285 (100%)	-0.17	4 (1%) 75 73	30, 46, 87, 111	0
1	C	285/285 (100%)	-0.01	13 (4%) 32 31	30, 51, 92, 126	0
1	D	285/285 (100%)	-0.15	4 (1%) 75 73	33, 47, 79, 109	0
All	All	1140/1140 (100%)	-0.12	25 (2%) 62 59	30, 46, 85, 126	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	208	ILE	3.7
1	C	191	ARG	3.1
1	C	190	THR	3.1
1	C	198	LEU	3.0
1	A	22	LEU	3.0
1	C	186	ALA	2.9
1	D	25	PHE	2.8
1	B	188	GLY	2.8
1	C	188	GLY	2.5
1	C	193	THR	2.5
1	D	2	TYR	2.4
1	C	199	PHE	2.4
1	A	21	GLN	2.4
1	A	146	HIS	2.4
1	B	193	THR	2.4
1	C	189	PHE	2.3
1	C	212	ILE	2.3
1	B	25	PHE	2.2
1	D	22	LEU	2.2
1	C	181	LYS	2.1
1	C	185	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	56	GLN	2.1
1	C	207	ASP	2.0
1	A	2	TYR	2.0
1	B	190	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

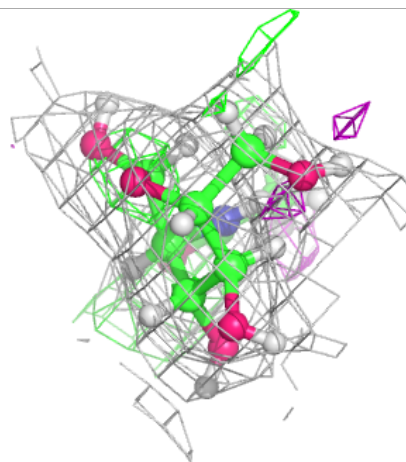
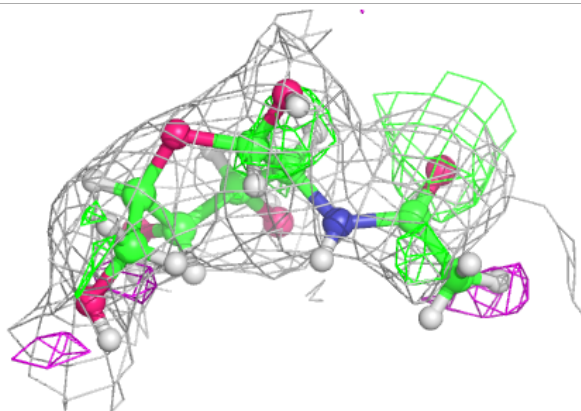
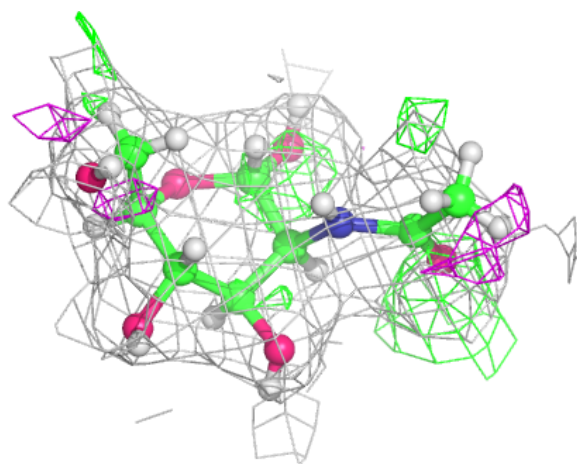
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BM3	C	301	15/15	0.83	0.20	59,77,95,95	0
2	BM3	B	301	15/15	0.90	0.20	57,74,92,92	0
2	BM3	D	301	15/15	0.91	0.28	68,83,105,105	0
2	BM3	A	301	15/15	0.92	0.19	57,73,95,95	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.

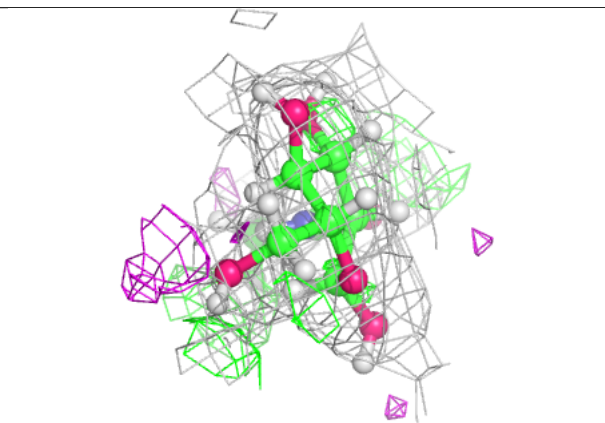
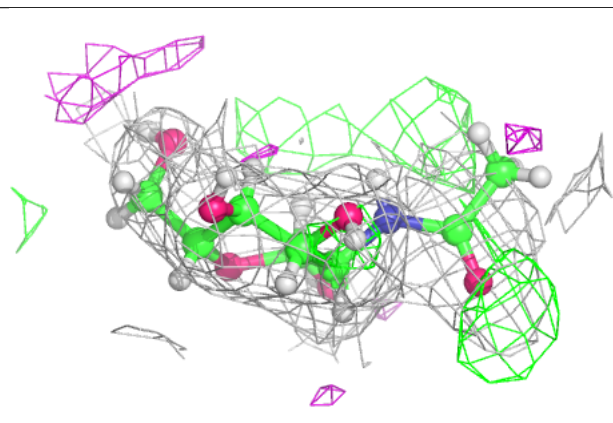
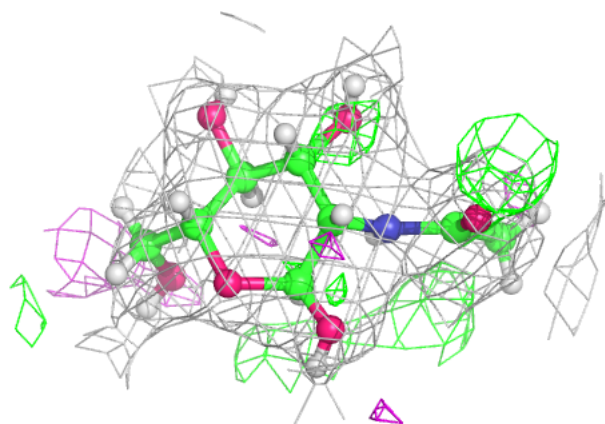
Electron density around BM3 C 301:

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



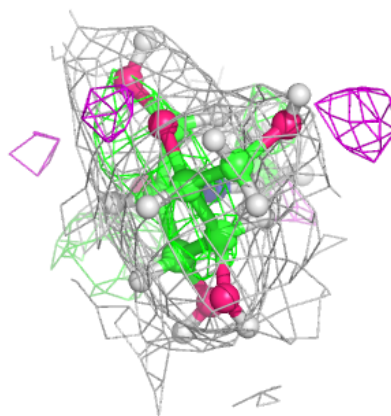
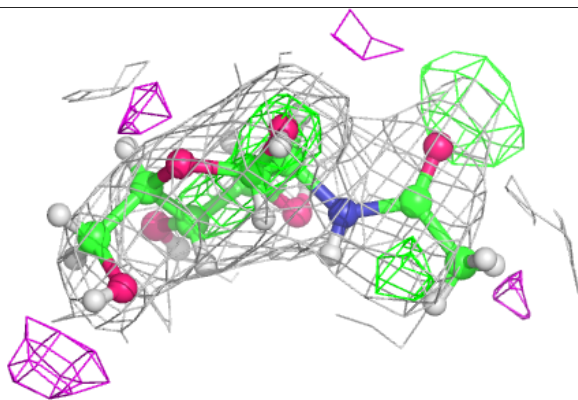
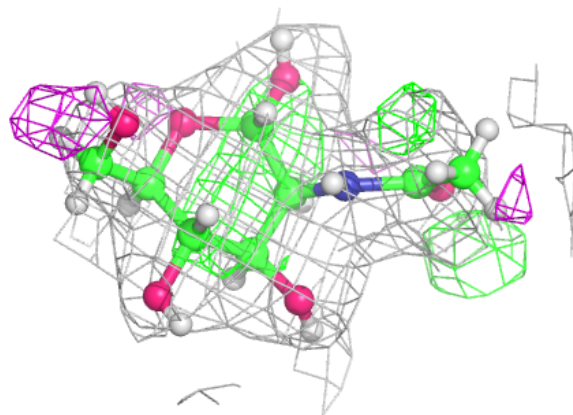
Electron density around BM3 B 301:

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



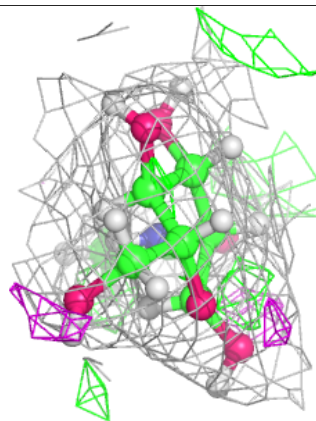
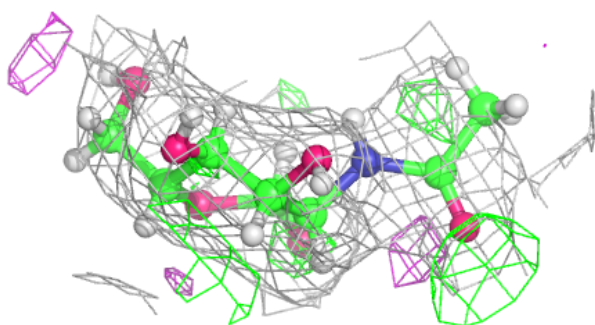
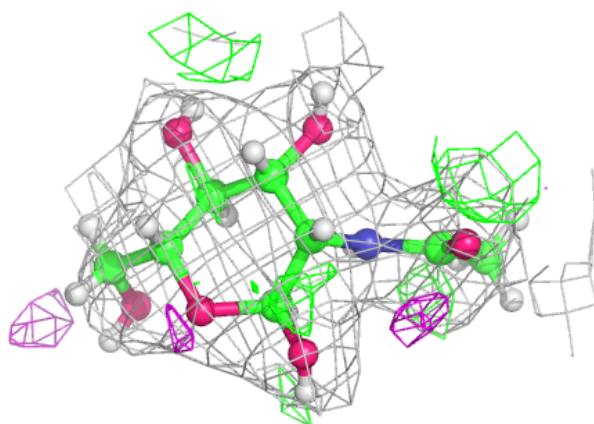
Electron density around BM3 D 301:

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



Electron density around BM3 A 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.