



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:42 am BST

PDB ID : 2JG3
Title : MtaqI with BAZ
Authors : Pljevaljcic, G.; Scheidig, A.J.; Weinhold, E.
Deposited on : 2007-02-07
Resolution : 1.90 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

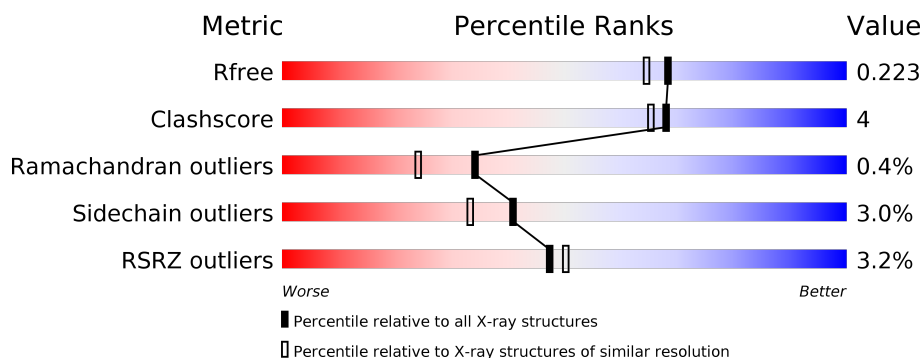
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	421	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>
1	D	421	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>
2	B	10	<div> <div>30%</div> <div>60%</div> <div>10%</div> </div>
2	E	10	<div> <div>40%</div> <div>50%</div> <div>10%</div> </div>
3	C	10	<div> <div>40%</div> <div>60%</div> </div>
3	F	10	<div> <div>20%</div> <div>70%</div> <div>10%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7895 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 MODIFICATION METHYLASE TAQI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	1
			3168	2074	544	544	6			
1	D	392	Total	C	N	O	S	0	0	1
			3174	2077	547	544	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ALA	GLY	conflict	UNP P14385
D	64	ALA	GLY	conflict	UNP P14385

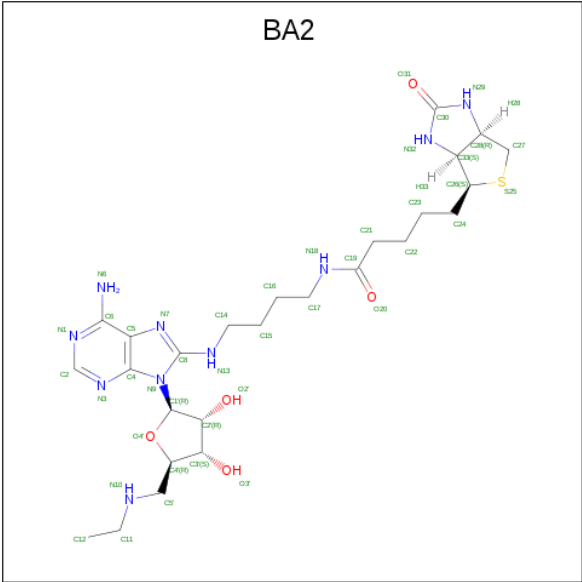
- Molecule 2 is a DNA chain called 5'-D(*GP*TP*TP*CP*GP*AP*TP*GP*TP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	0	0
			202	98	34	61	9			
2	E	10	Total	C	N	O	P	0	0	0
			202	98	34	61	9			

- Molecule 3 is a DNA chain called 5'-D(*GP*AP*CP*AP*TP*CP*GP*6MAP*AP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	P	0	0	0
			203	98	41	55	9			
3	F	10	Total	C	N	O	P	0	0	0
			203	98	41	55	9			

- Molecule 4 is 5'-DEOXY-5'-(ETHYLAMINO)-8-{[4-({5-[(3AS,4S,6AR)-2-OXOHEXAHYDRO-1H-THIENO[3,4-D]IMIDAZOL-4-YL]PENTANOYL}AMINO)BUTYL]AMINO}ADENOSINE (three-letter code: BA2) (formula: C₂₆H₄₂N₁₀O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	13	7	3		
4	D	1	Total	C	N	O	0	0
			26	16	7	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0

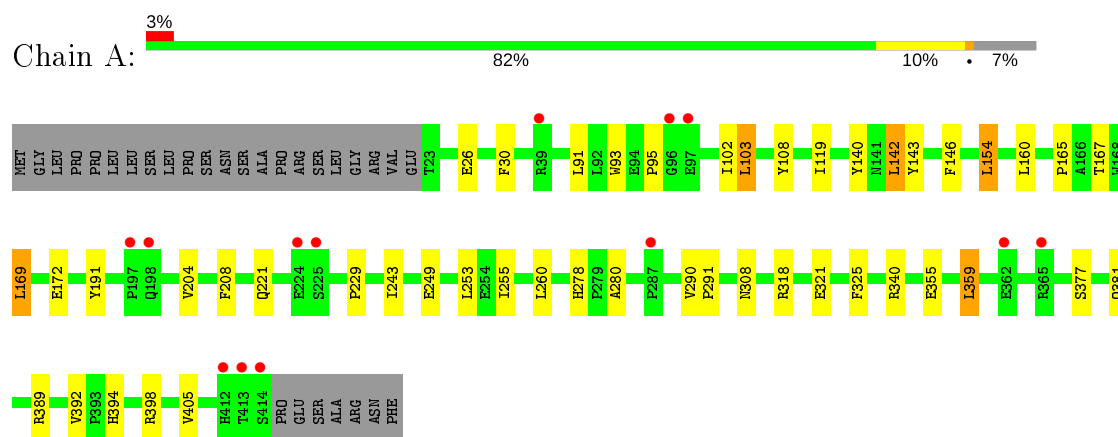
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	287	Total 287	O 287	0	0
7	B	48	Total 48	O 48	0	0
7	C	28	Total 28	O 28	0	0
7	D	259	Total 259	O 259	0	0
7	E	30	Total 30	O 30	0	0
7	F	28	Total 28	O 28	0	0

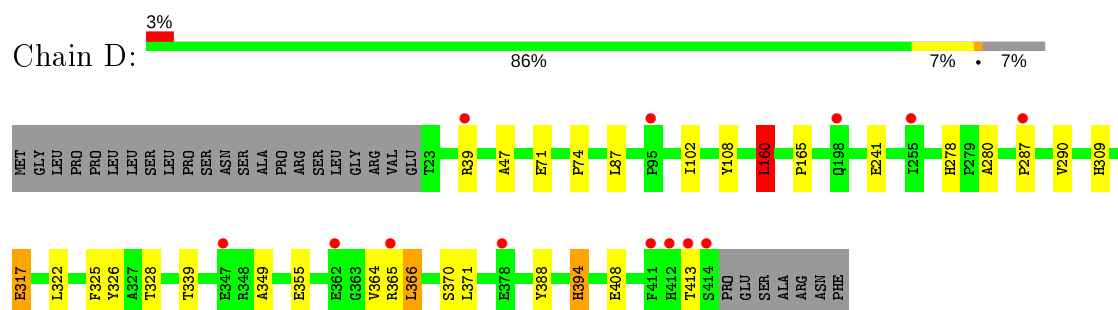
3 Residue-property plots [i](#)

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: MODIFICATION METHYLASE TAQI



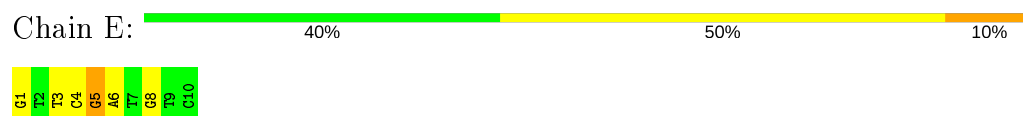
• Molecule 1: MODIFICATION METHYLASE TAQI



• Molecule 2: 5'-D(*GP*TP*TP*CP*GP*AP*TP*GP*TP*CP)-3'



• Molecule 2: 5'-D(*GP*TP*TP*CP*GP*AP*TP*GP*TP*CP)-3'



- Molecule 3: 5'-D(*GP*AP*CP*AP*TP*CP*GP*6MAP*AP*CP)-3'

Chain C:  40% 60%



- Molecule 3: 5'-D(*GP*AP*CP*AP*TP*CP*GP*6MAP*AP*CP)-3'

Chain F:  20% 70% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.40 Å 69.19 Å 114.39 Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	19.73 – 1.90 19.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.73-1.90) 99.5 (19.73-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 1.90 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.226 0.185 , 0.223	Depositor DCC
R_{free} test set	3639 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7895	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: GOL, K, BA2, 6MA

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	0.60	0/3272	0.69	2/4448 (0.0%)
1	D	0.61	1/3278 (0.0%)	0.72	2/4455 (0.0%)
2	B	1.10	0/225	2.04	10/346 (2.9%)
2	E	1.08	0/225	1.91	8/346 (2.3%)
3	C	1.01	0/202	1.77	5/307 (1.6%)
3	F	1.08	0/202	1.93	8/307 (2.6%)
All	All	0.68	1/7404 (0.0%)	0.95	35/10209 (0.3%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	370	SER	C-N	-7.24	1.17	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	PRO	CB-CA-C	-11.89	82.27	112.00
2	E	8	DG	O4'-C1'-N9	-11.62	99.86	108.00
2	B	5	DG	O4'-C1'-N9	9.88	114.91	108.00
3	F	20	DC	O4'-C1'-N1	9.88	114.91	108.00
1	D	160	LEU	CA-CB-CG	8.76	135.45	115.30
2	B	2	DT	P-O3'-C3'	8.57	129.98	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	DG	O4'-C1'-N9	-8.48	102.06	108.00
3	F	19	DA	O4'-C1'-N9	8.29	113.80	108.00
3	F	12	DA	O4'-C1'-N9	-8.07	102.35	108.00
3	C	12	DA	O4'-C1'-N9	-7.44	102.79	108.00
2	E	3	DT	O4'-C1'-N1	-7.33	102.87	108.00
2	B	2	DT	C6-C5-C7	-7.09	118.65	122.90
2	E	4	DC	O4'-C1'-N1	-7.04	103.07	108.00
3	C	20	DC	O4'-C1'-N1	6.88	112.81	108.00
2	B	9	DT	P-O3'-C3'	6.67	127.71	119.70
2	B	2	DT	N3-C4-O4	6.38	123.73	119.90
3	F	15	DT	N3-C4-O4	6.36	123.71	119.90
2	B	9	DT	C1'-O4'-C4'	-6.22	103.88	110.10
3	C	13	DC	C1'-O4'-C4'	-6.11	103.99	110.10
1	A	169	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	103	LEU	CA-CB-CG	5.87	128.81	115.30
3	F	11	DG	P-O3'-C3'	5.87	126.74	119.70
3	F	15	DT	C5-C4-O4	-5.64	120.95	124.90
2	E	1	DG	P-O3'-C3'	5.63	126.45	119.70
2	B	4	DC	P-O3'-C3'	5.62	126.44	119.70
3	C	15	DT	C5-C4-O4	-5.61	120.97	124.90
3	C	15	DT	N3-C4-O4	5.53	123.22	119.90
2	E	5	DG	C5-C6-O6	-5.53	125.28	128.60
2	B	3	DT	O4'-C1'-N1	-5.45	104.19	108.00
2	E	3	DT	C4'-C3'-C2'	5.42	107.98	103.10
2	B	2	DT	C4-C5-C7	5.36	122.22	119.00
3	F	16	DC	C6-N1-C2	-5.19	118.23	120.30
2	E	5	DG	C5-C6-N1	5.12	114.06	111.50
3	F	13	DC	C1'-O4'-C4'	-5.11	104.99	110.10
2	E	3	DT	N1-C1'-C2'	5.05	122.20	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	394	HIS	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	3168	0	3158	25	0
1	D	3174	0	3168	15	0
2	B	202	0	116	10	0
2	E	202	0	116	5	0
3	C	203	0	114	1	0
3	F	203	0	114	1	0
4	A	23	0	18	8	0
4	D	26	0	24	6	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	287	0	0	3	0
7	B	48	0	0	0	0
7	C	28	0	0	0	0
7	D	259	0	0	2	0
7	E	30	0	0	0	0
7	F	28	0	0	0	0
All	All	7895	0	6844	54	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 4.

All (54) 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:A:1415:BA2:C12	2:B:6:DA:H61	1.33	1.40
4:A:1415:BA2:H123	2:B:6:DA:N6	1.62	1.14
4:A:1415:BA2:H123	2:B:6:DA:H61	0.95	1.10
4:D:1416:BA2:H111	2:E:6:DA:H61	1.15	1.08
4:D:1416:BA2:H111	2:E:6:DA:N6	1.70	1.04
4:A:1415:BA2:C12	2:B:6:DA:N6	2.18	0.97
4:A:1415:BA2:H121	2:B:6:DA:H61	1.46	0.81
1:A:394:HIS:HE1	2:B:5:DG:N7	1.89	0.69
4:A:1415:BA2:C11	2:B:6:DA:H61	2.05	0.68
7:A:2153:HOH:O	1:D:317:GLU:HG2	1.96	0.66
1:A:160:LEU:HG	1:A:208:PHE:HB3	1.80	0.63
1:D:394:HIS:HE1	2:E:5:DG:N7	1.96	0.62
4:A:1415:BA2:C11	2:B:6:DA:N6	2.63	0.59
1:D:365:ARG:NH1	7:D:2226:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1416:BA2:C11	2:E:6:DA:H61	2.04	0.59
1:D:339:THR:HG21	1:D:388:TYR:HB2	1.85	0.59
1:A:119:ILE:HG13	1:A:142:LEU:HD22	1.85	0.57
3:F:18:6MA:H2'	3:F:19:DA:O5'	2.03	0.57
1:A:169:LEU:HB3	1:A:243:ILE:HB	1.86	0.57
1:A:255:ILE:HD11	7:A:2073:HOH:O	2.03	0.57
3:C:18:6MA:H2'	3:C:19:DA:O5'	2.05	0.57
1:A:30:PHE:HE1	1:A:229:PRO:HG3	1.73	0.54
1:D:309:HIS:HE1	7:D:2194:HOH:O	1.91	0.52
1:A:278:HIS:CD2	1:A:280:ALA:H	2.28	0.51
4:A:1415:BA2:H111	2:B:6:DA:N6	2.27	0.50
1:A:249:GLU:HG2	7:A:2177:HOH:O	2.10	0.50
1:A:318:ARG:HD2	1:A:321:GLU:OE2	2.11	0.50
1:A:191:TYR:HA	1:A:204:VAL:HG12	1.95	0.48
1:A:260:LEU:HD13	1:A:405:VAL:HG21	1.95	0.48
1:A:26:GLU:CD	1:A:26:GLU:H	2.17	0.47
1:A:394:HIS:CE1	2:B:5:DG:N7	2.77	0.47
1:D:74:PRO:HA	1:D:87:LEU:HD21	1.96	0.47
1:D:47:ALA:HB1	4:D:1416:BA2:O4'	2.15	0.46
1:A:325:PHE:HB2	1:A:359:LEU:HD11	1.98	0.45
4:D:1416:BA2:C11	2:E:6:DA:N6	2.60	0.45
1:A:93:TRP:CZ2	1:A:95:PRO:HB3	2.52	0.45
1:A:167:THR:HG22	1:A:392:VAL:HG12	1.98	0.44
1:A:278:HIS:HD2	1:A:280:ALA:H	1.64	0.44
1:D:326:TYR:O	1:D:349:ALA:HB1	2.17	0.44
1:D:102:ILE:O	1:D:160:LEU:HA	2.16	0.44
1:A:377:SER:O	1:A:381:GLN:HG2	2.18	0.44
1:D:278:HIS:HD2	1:D:280:ALA:H	1.65	0.43
1:D:364:VAL:HG12	1:D:366:LEU:HD13	2.00	0.42
1:D:278:HIS:CD2	1:D:280:ALA:H	2.37	0.42
1:A:102:ILE:O	1:A:160:LEU:HA	2.20	0.42
1:A:291:PRO:HB3	1:A:308:ASN:HD22	1.84	0.42
1:A:108:TYR:CE1	1:A:165:PRO:HD3	2.55	0.41
1:D:71:GLU:OE2	4:D:1416:BA2:O2'	2.33	0.41
1:A:91:LEU:HD21	1:A:146:PHE:CD1	2.55	0.41
1:A:102:ILE:HD12	1:A:154:LEU:HD13	2.02	0.41
1:A:172:GLU:OE2	1:A:398:ARG:NE	2.51	0.41
1:D:325:PHE:O	1:D:328:THR:HG22	2.21	0.41
1:D:108:TYR:CE1	1:D:165:PRO:HD3	2.55	0.40
1:A:30:PHE:CE1	1:A:229:PRO:HG3	2.54	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	390/421 (93%)	378 (97%)	10 (3%)	2 (0%)	29	18
1	D	390/421 (93%)	377 (97%)	12 (3%)	1 (0%)	41	31
All	All	780/842 (93%)	755 (97%)	22 (3%)	3 (0%)	34	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	355	GLU
1	A	389	ARG
1	A	355	GLU

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	329/356 (92%)	319 (97%)	10 (3%)	41	33
1	D	330/356 (93%)	320 (97%)	10 (3%)	41	33
All	All	659/712 (93%)	639 (97%)	20 (3%)	41	33

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	A	140	TYR
1	A	142	LEU

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Mol	Chain	Res	Type
1	A	143	TYR
1	A	154	LEU
1	A	221	GLN
1	A	253	LEU
1	A	290	VAL
1	A	340	ARG
1	A	359	LEU
1	D	39	ARG
1	D	160	LEU
1	D	241	GLU
1	D	290	VAL
1	D	317	GLU
1	D	322	LEU
1	D	366	LEU
1	D	371	LEU
1	D	408	GLU
1	D	413	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	278	HIS
1	A	394	HIS
1	D	278	HIS
1	D	309	HIS
1	D	394	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	6MA	C	18	3,2	18,24,25	1.03	1 (5%)	15,34,37	2.56	7 (46%)
3	6MA	F	18	3,2	18,24,25	0.88	0	15,34,37	2.71	8 (53%)

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
3	6MA	C	18	3,2	-	1/5/23/24	0/3/3/3
3	6MA	F	18	3,2	-	1/5/23/24	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	18	6MA	O4'-C4'	-2.33	1.39	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	18	6MA	C1-N6-C6	5.36	127.49	122.87
3	C	18	6MA	C2-N1-C6	5.20	121.05	116.59
3	F	18	6MA	C2-N1-C6	4.36	120.33	116.59
3	C	18	6MA	O5'-C5'-C4'	-4.20	94.71	108.99
3	F	18	6MA	O5'-C5'-C4'	-4.05	95.21	108.99
3	F	18	6MA	O4'-C4'-C3'	3.62	114.12	105.67
3	C	18	6MA	O4'-C4'-C3'	3.47	113.78	105.67
3	C	18	6MA	O3'-C3'-C2'	-3.11	99.77	110.90
3	C	18	6MA	O4'-C1'-C2'	2.77	111.49	106.25
3	F	18	6MA	O4'-C1'-C2'	2.77	111.47	106.25
3	C	18	6MA	C1-N6-C6	2.41	124.95	122.87
3	F	18	6MA	O3'-C3'-C2'	-2.41	102.29	110.90
3	C	18	6MA	C5'-C4'-C3'	2.33	128.41	114.74
3	F	18	6MA	O4'-C4'-C5'	2.30	116.95	109.37
3	F	18	6MA	C4'-O4'-C1'	-2.10	104.37	109.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	18	6MA	O4'-C4'-C5'-O5'
3	F	18	6MA	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	18	6MA	1	0
3	F	18	6MA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
5	GOL	B	1012	-	5,5,5	0.36	0	5,5,5	0.73	0
5	GOL	A	1416	-	5,5,5	0.50	0	5,5,5	0.60	0
4	BA2	A	1415	6	20,25,46	3.02	7 (35%)	18,36,64	3.45	10 (55%)
4	BA2	D	1416	6	24,28,46	3.46	8 (33%)	20,39,64	2.96	9 (45%)

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
5	GOL	B	1012	-	-	0/4/4/4	-
5	GOL	A	1416	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BA2	A	1415	6	-	2/4/26/61	0/3/3/5
4	BA2	D	1416	6	-	3/7/29/61	0/3/3/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1416	BA2	C2-N3	8.85	1.46	1.32
4	A	1415	BA2	C2-N3	8.37	1.45	1.32
4	D	1416	BA2	C8-N13	7.68	1.44	1.33
4	D	1416	BA2	C4-N3	7.47	1.46	1.35
4	D	1416	BA2	C2-N1	7.26	1.47	1.33
4	A	1415	BA2	C2-N1	6.49	1.46	1.33
4	A	1415	BA2	C4-N3	6.04	1.44	1.35
4	D	1416	BA2	C5-C4	3.66	1.50	1.40
4	A	1415	BA2	C5-C4	3.16	1.49	1.40
4	D	1416	BA2	C6-C5	2.75	1.53	1.43
4	A	1415	BA2	C6-N6	2.68	1.43	1.34
4	D	1416	BA2	C6-N6	2.62	1.43	1.34
4	A	1415	BA2	C6-C5	2.55	1.52	1.43
4	D	1416	BA2	C6-N1	2.38	1.47	1.37
4	A	1415	BA2	C6-N1	2.12	1.46	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1416	BA2	N3-C2-N1	-7.87	116.38	128.68
4	A	1415	BA2	N3-C2-N1	-7.67	116.69	128.68
4	A	1415	BA2	C14-N13-C8	-6.86	114.73	123.47
4	D	1416	BA2	C2-N1-C6	6.54	129.94	118.75
4	A	1415	BA2	C1'-N9-C4	-5.40	117.26	126.71
4	A	1415	BA2	C2-N1-C6	4.87	127.08	118.75
4	D	1416	BA2	C5-C6-N1	-4.22	110.78	120.35
4	A	1415	BA2	C5-C6-N1	-3.53	112.35	120.35
4	A	1415	BA2	C5-C6-N6	-3.50	115.04	120.35
4	D	1416	BA2	C1'-N9-C4	-2.98	121.50	126.71
4	D	1416	BA2	C4-C5-N7	-2.94	106.49	109.47
4	A	1415	BA2	O4'-C1'-C2'	2.91	111.17	106.93
4	D	1416	BA2	O2'-C2'-C1'	2.48	120.00	110.85
4	A	1415	BA2	O3'-C3'-C4'	-2.23	104.59	111.05
4	A	1415	BA2	O4'-C4'-C3'	2.19	109.45	105.11
4	D	1416	BA2	C3'-C2'-C1'	2.18	104.26	100.98
4	D	1416	BA2	O4'-C4'-C3'	2.17	109.41	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1415	BA2	C2'-C3'-C4'	2.15	106.81	102.64
4	D	1416	BA2	O3'-C3'-C2'	-2.06	105.14	111.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1416	GOL	O1-C1-C2-O2
5	A	1416	GOL	O1-C1-C2-C3
5	A	1416	GOL	C1-C2-C3-O3
5	A	1416	GOL	O2-C2-C3-O3
4	A	1415	BA2	O4'-C4'-C5'-N10
4	D	1416	BA2	N13-C14-C15-C16
4	D	1416	BA2	C4'-C5'-N10-C11
4	A	1415	BA2	C3'-C4'-C5'-N10
4	D	1416	BA2	C12-C11-N10-C5'

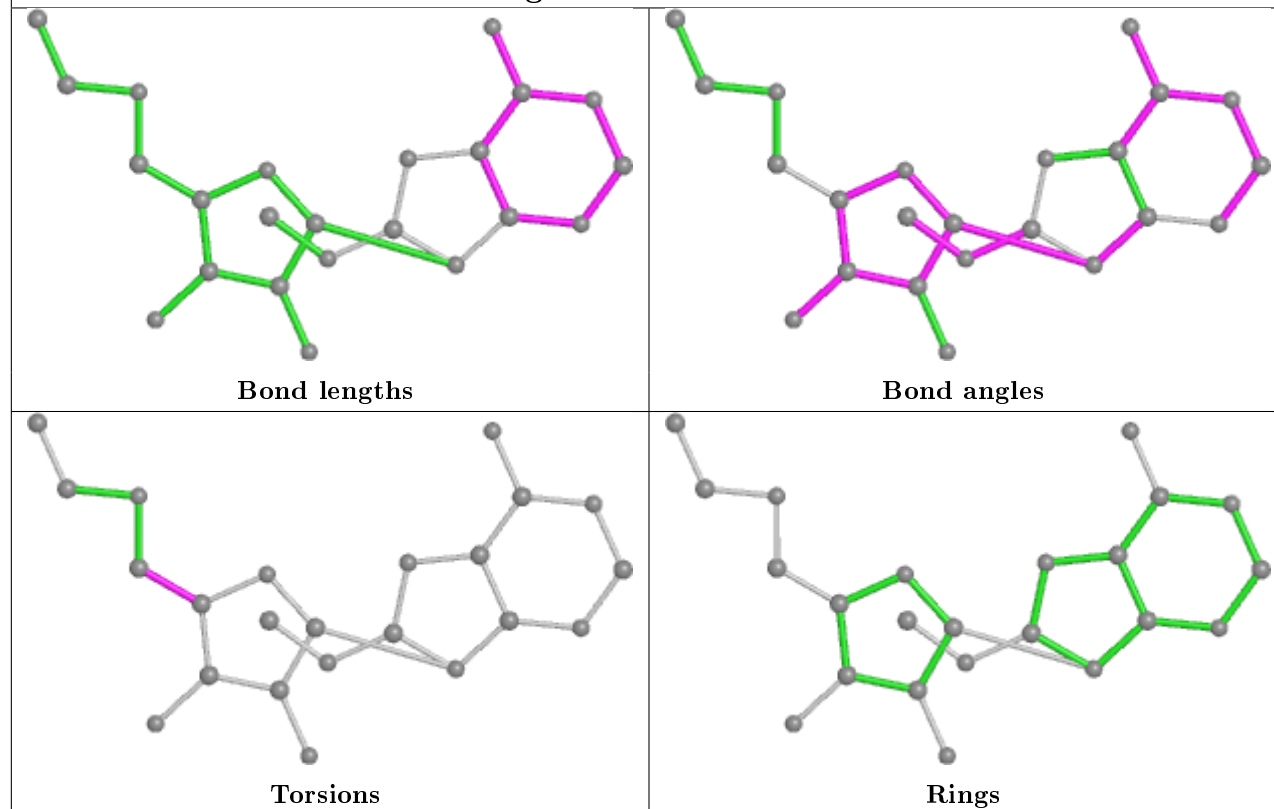
There are no ring outliers.

2 monomers are involved in 14 short contacts:

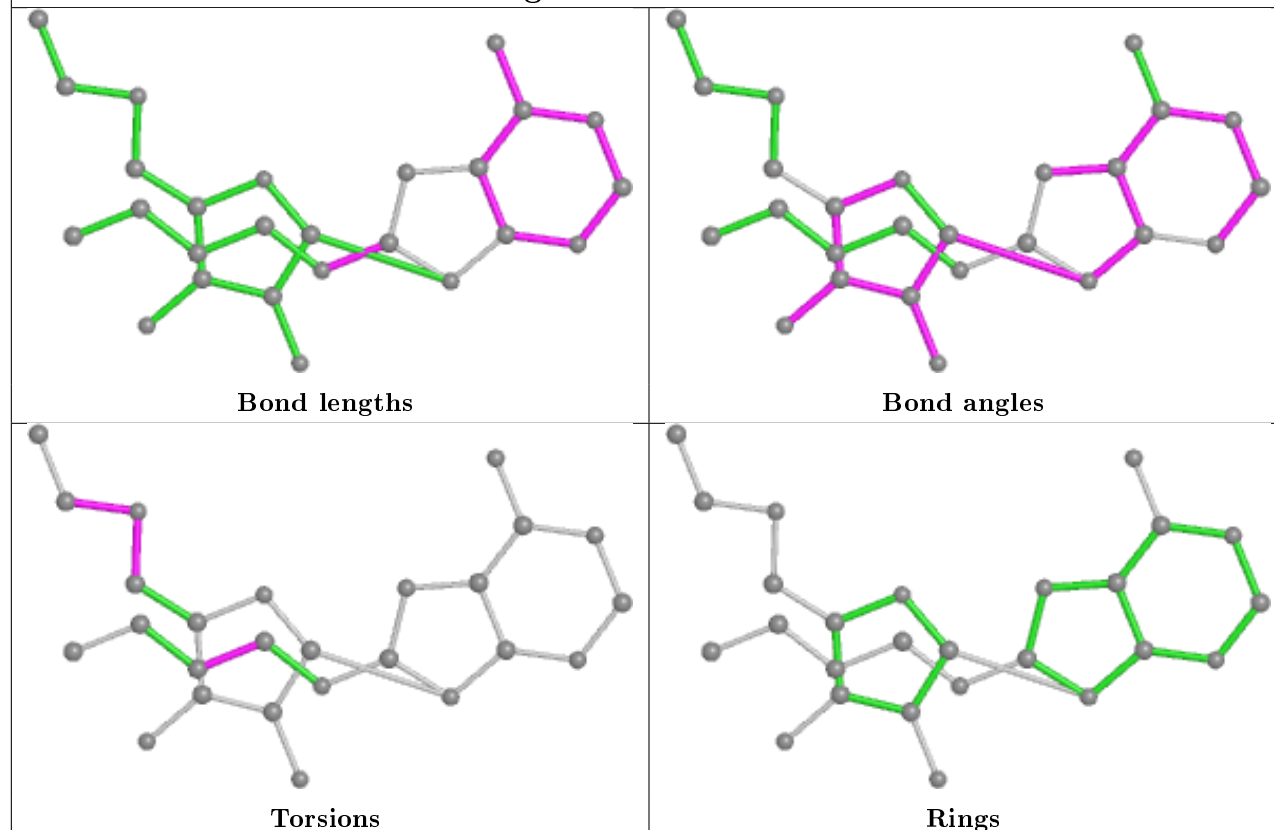
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1415	BA2	8	0
4	D	1416	BA2	6	0

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 BA2 A 1415



Ligand BA2 D 1416



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	370:SER	C	371:LEU	N	1.17

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	392/421 (93%)	0.12	13 (3%) 46 49	4, 10, 22, 36	0
1	D	392/421 (93%)	0.22	13 (3%) 46 49	5, 11, 21, 36	0
2	B	10/10 (100%)	-0.41	0 100 100	4, 6, 10, 11	0
2	E	10/10 (100%)	-0.38	0 100 100	5, 8, 10, 11	0
3	C	9/10 (90%)	-0.50	0 100 100	5, 6, 7, 13	0
3	F	9/10 (90%)	-0.39	0 100 100	7, 9, 14, 19	0
All	All	822/882 (93%)	0.14	26 (3%) 47 50	4, 10, 21, 36	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	413	THR	4.8
1	D	414	SER	4.7
1	D	287	PRO	4.2
1	A	414	SER	4.0
1	A	287	PRO	3.4
1	A	413	THR	3.2
1	A	198	GLN	3.1
1	D	255	ILE	3.0
1	A	97	GLU	2.9
1	A	96	GLY	2.8
1	A	225	SER	2.8
1	A	224	GLU	2.7
1	D	365	ARG	2.7
1	D	362	GLU	2.7
1	A	365	ARG	2.5
1	A	412	HIS	2.5
1	D	412	HIS	2.4
1	D	39	ARG	2.4
1	A	362	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	95	PRO	2.4
1	D	411	PHE	2.3
1	A	39	ARG	2.3
1	D	198	GLN	2.2
1	D	378	GLU	2.1
1	A	197	PRO	2.0
1	D	347	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	6MA	C	18	22/23	0.96	0.10	2,3,6,7	0
3	6MA	F	18	22/23	0.97	0.09	3,8,10,13	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

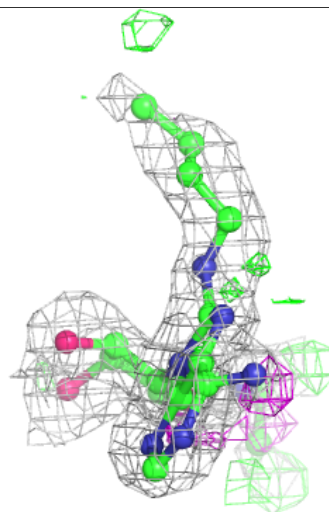
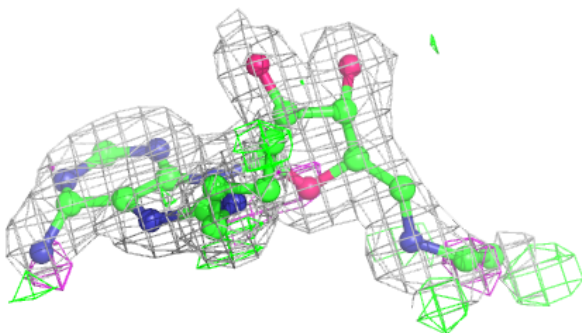
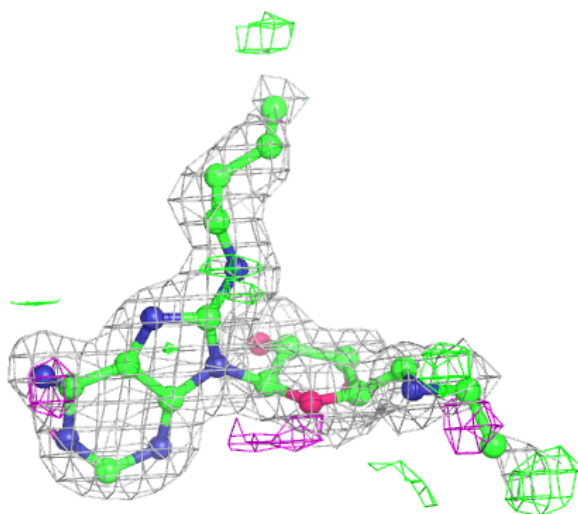
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	1416	6/6	0.84	0.24	28,31,32,33	0
4	BA2	D	1416	26/42	0.92	0.15	5,10,22,24	0
4	BA2	A	1415	23/42	0.93	0.12	4,8,15,19	0
5	GOL	B	1012	6/6	0.93	0.13	22,22,23,24	0
6	K	B	1011	1/1	0.97	0.13	23,23,23,23	0
6	K	D	1415	1/1	0.99	0.20	22,22,22,22	0

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.

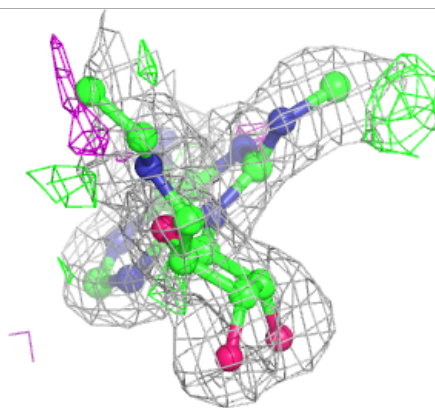
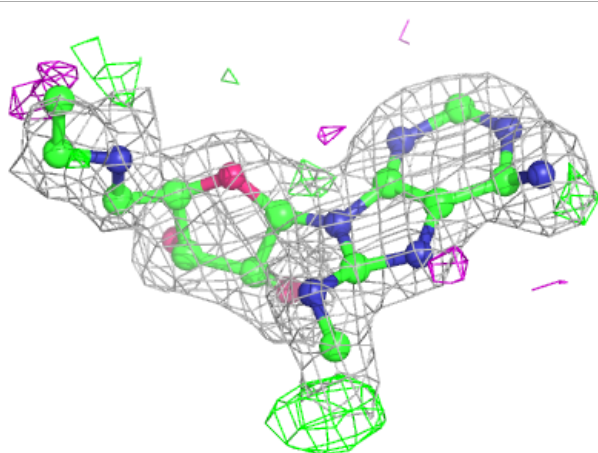
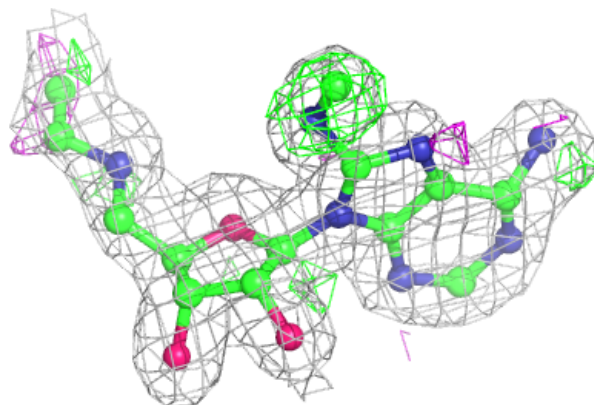
Electron density around BA2 D 1416:

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



Electron density around BA2 A 1415:

$2mF_o-DF_c$ (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.