Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 08:51 PM EDT

PDB ID	:	6APV
Title	:	Trypanosoma brucei hypoxanthine guanine phosphoribosyltransferase in complex with [(2-{[2-(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)ethyl][(E)-2-phosphonoethenyl]amino}ethoxy)methyl]phosphonic acid
Authors	:	Teran, D.; Guddat, L.W.
Deposited on	:	2017-08-18
Resolution	:	1.99 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 (i) 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 (i)) were used in the production of this report:

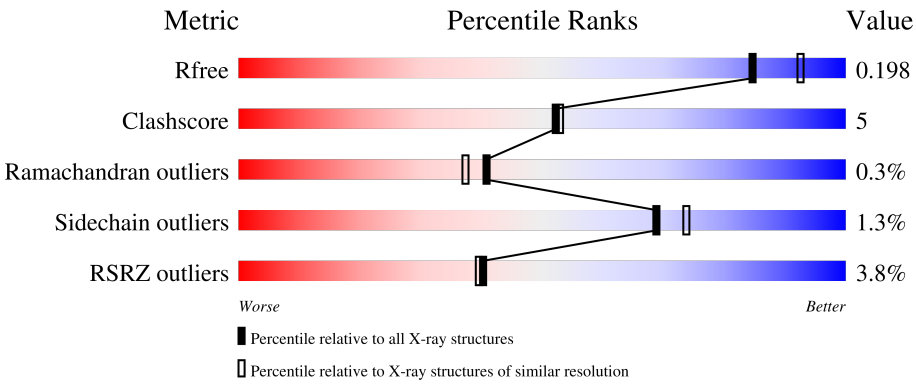
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	216	% 71% 10% 19%
1	B	216	5% 73% 11% 15%
1	C	216	4% 72% 8% 19%
1	D	216	3% 71% 10% 19%

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
4	PEG	C	304	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6518 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 Hypoxanthine-guanine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	1418	911	234	269	4	0	5	0
1	B	183	1511	968	252	287	4	0	10	0
1	C	174	1411	907	233	267	4	0	6	0
1	D	176	1440	927	240	269	4	0	7	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q07010
A	-4	HIS	-	expression tag	UNP Q07010
A	-3	HIS	-	expression tag	UNP Q07010
A	-2	HIS	-	expression tag	UNP Q07010
A	-1	HIS	-	expression tag	UNP Q07010
A	0	HIS	-	expression tag	UNP Q07010
B	-5	HIS	-	expression tag	UNP Q07010
B	-4	HIS	-	expression tag	UNP Q07010
B	-3	HIS	-	expression tag	UNP Q07010
B	-2	HIS	-	expression tag	UNP Q07010
B	-1	HIS	-	expression tag	UNP Q07010
B	0	HIS	-	expression tag	UNP Q07010
C	-5	HIS	-	expression tag	UNP Q07010
C	-4	HIS	-	expression tag	UNP Q07010
C	-3	HIS	-	expression tag	UNP Q07010
C	-2	HIS	-	expression tag	UNP Q07010
C	-1	HIS	-	expression tag	UNP Q07010
C	0	HIS	-	expression tag	UNP Q07010
D	-5	HIS	-	expression tag	UNP Q07010
D	-4	HIS	-	expression tag	UNP Q07010
D	-3	HIS	-	expression tag	UNP Q07010

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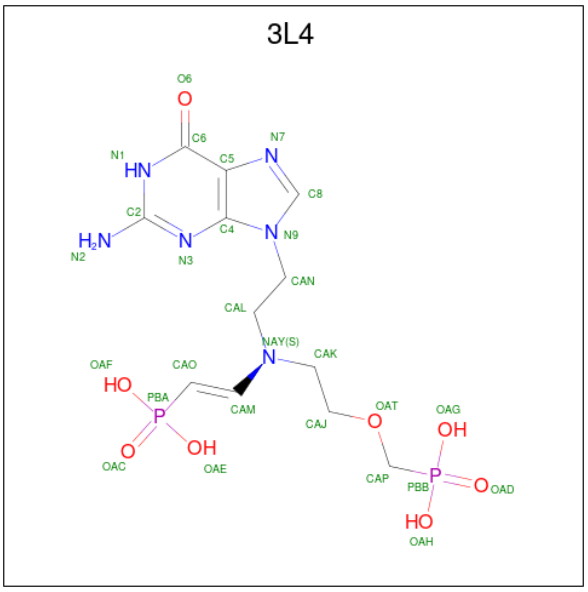
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	expression tag	UNP Q07010
D	-1	HIS	-	expression tag	UNP Q07010
D	0	HIS	-	expression tag	UNP Q07010

- Molecule 2 is [(2-{[2-(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)ethyl][(E)-2-phosphonoethenyl]amino}ethoxy)methyl]phosphonic acid (three-letter code: 3L4) (formula: $C_{12}H_{20}N_6O_8P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	12	6	8	2		
2	B	1	Total	C	N	O	P	0	0
			28	12	6	8	2		
2	C	1	Total	C	N	O	P	0	0
			28	12	6	8	2		
2	D	1	Total	C	N	O	P	0	0
			28	12	6	8	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	1
			3	3		

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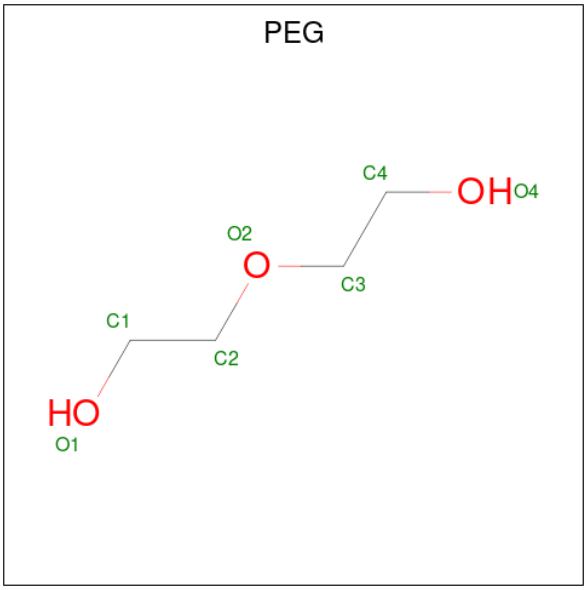
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	D	2	2	2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is water.

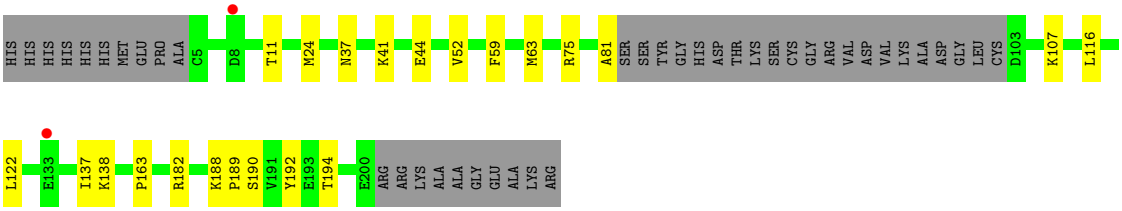
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	157	161	161	0	4
			Total	O		
5	B	155	162	162	0	7
			Total	O		
5	C	142	145	145	0	3
			Total	O		
5	D	120	121	121	0	1

3 Residue-property plots (i)

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

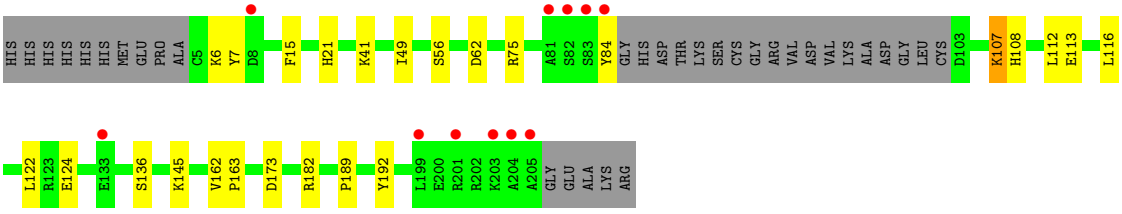
• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

Chain A:



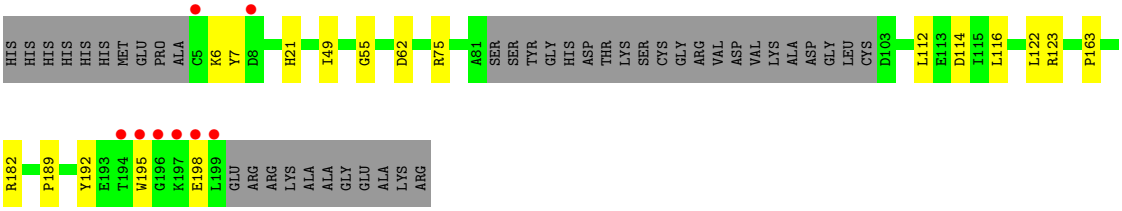
• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

Chain B:



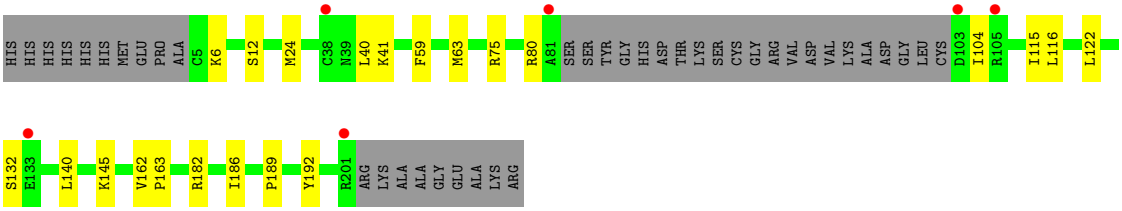
• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

Chain C:



• Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

Chain D:


HIS
HIS
HIS
HIS
HIS
MET
GLU
PRO
ALA
C5
K6
S12
M24
C38
N39
L40
K41
F59
M63
R75
R80
A81
SER
SER
TYR
GLY
HIS
ASP
THR
LYS
SER
CYS
GLY
ARG
VAL
ASP
VAL
LYS
ALA
ASP
GLY
LEU
CYS
D103
I104
R105
I115
L116
L122
S132
E133
L140
K145
V162
P163
R182
I186
P189
Y192
R201
ARG
LYS
ALA
ALA
GLY
GLU
ALA
LYS
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	89.48Å 94.56Å 109.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.28 – 1.99 47.28 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.28-1.99) 99.5 (47.28-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.164 , 0.198 0.164 , 0.198	Depositor DCC
R_{free} test set	2005 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6518	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6007e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 3L4, PEG, MG

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	0.47	0/1446	0.63	0/1961
1	B	0.47	0/1546	0.62	0/2096
1	C	0.48	0/1442	0.62	0/1956
1	D	0.43	0/1472	0.59	0/1995
All	All	0.46	0/5906	0.61	0/8008

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	1418	0	1437	19	1
1	B	1511	0	1536	17	1
1	C	1411	0	1434	11	0
1	D	1440	0	1472	17	0
2	A	28	0	17	0	0
2	B	28	0	17	1	0
2	C	28	0	17	0	0
2	D	28	0	17	1	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	7	0	10	1	0
4	B	7	0	10	1	0
4	C	7	0	10	3	1
4	D	7	0	10	1	1
5	A	161	0	0	1	0
5	B	162	0	0	4	1
5	C	145	0	0	1	1
5	D	121	0	0	1	0
All	All	6518	0	5987	65	3

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 (65) 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:84:TYR:HD1	1:B:124:GLU:HG2	1.43	0.82
1:A:24:MET:HG2	1:A:63:MET:HE1	1.63	0.78
1:B:75:ARG:NH1	5:B:455[B]:HOH:O	2.16	0.73
1:A:190:SER:O	1:A:194:THR:HG23	1.90	0.72
1:D:24:MET:HG2	1:D:63:MET:HE1	1.78	0.66
2:D:301:3L4:H4	5:D:490:HOH:O	1.98	0.64
1:D:116:LEU:HD13	1:D:122[A]:LEU:HD12	1.84	0.59
1:D:24:MET:HG2	1:D:63:MET:CE	2.35	0.57
1:A:137:ILE:O	1:A:138:LYS:HD3	2.06	0.56
1:A:59:PHE:HE1	1:A:63:MET:CE	2.19	0.55
1:D:115:ILE:HD11	1:D:145:LYS:HD2	1.89	0.55
1:A:182:ARG:HH12	4:A:304:PEG:H21	1.72	0.54
1:A:59:PHE:CE1	1:A:63:MET:CE	2.91	0.53
1:B:108:HIS:HD2	1:B:136:SER:OG	1.91	0.53
1:B:107:LYS:HE2	5:B:474:HOH:O	2.09	0.52
1:A:24:MET:HG2	1:A:63:MET:CE	2.35	0.52
1:C:195:TRP:O	1:C:198:GLU:HB3	2.10	0.51
1:D:59:PHE:CE2	1:D:63:MET:HE2	2.45	0.51
1:B:75:ARG:HG3	5:B:401:HOH:O	2.13	0.49
1:D:59:PHE:HE2	1:D:63:MET:HE2	1.78	0.49
1:C:189:PRO:HA	1:C:192:TYR:CZ	2.49	0.48
1:B:182:ARG:HH22	4:B:304:PEG:H12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:HG2	1:B:162[A]:VAL:HG23	1.96	0.47
1:A:116:LEU:HD13	1:A:122[A]:LEU:HD12	1.96	0.47
1:B:15:PHE:HE2	1:B:162[A]:VAL:HG12	1.79	0.47
1:A:59:PHE:CE1	1:A:63:MET:HE3	2.50	0.47
1:A:24:MET:CE	1:A:63:MET:HE2	2.45	0.47
1:D:40:LEU:O	1:D:41:LYS:HD3	2.14	0.47
1:B:21:HIS:HD2	5:B:540[B]:HOH:O	1.98	0.47
1:A:11:THR:HG23	1:A:188:LYS:HA	1.97	0.46
1:A:59:PHE:CE1	1:A:63:MET:HE2	2.50	0.46
1:D:189:PRO:HA	1:D:192:TYR:CE2	2.50	0.46
1:A:24:MET:CG	1:A:63:MET:HE1	2.42	0.45
1:B:116:LEU:HD13	1:B:122[A]:LEU:HD12	1.97	0.45
1:C:21:HIS:HD2	5:C:531:HOH:O	2.00	0.45
1:A:37:ASN:HB2	5:A:468:HOH:O	2.16	0.44
1:B:173:ASP:O	2:B:301:3L4:N2	2.51	0.44
1:D:162:VAL:HG12	1:D:163[B]:PRO:O	2.18	0.44
1:C:116:LEU:HD13	1:C:122:LEU:HD12	2.00	0.44
1:B:21:HIS:HE1	1:B:62:ASP:OD1	2.01	0.43
1:C:182:ARG:HH12	4:C:304:PEG:H21	1.84	0.43
1:C:6:LYS:HE2	1:C:7:TYR:CZ	2.53	0.43
1:C:55:GLY:HA3	1:C:114:ASP:OD2	2.19	0.43
1:B:162[B]:VAL:HG12	1:B:163:PRO:O	2.19	0.43
1:B:189:PRO:HA	1:B:192:TYR:CZ	2.54	0.43
1:A:52:VAL:HG12	1:A:81:ALA:HB2	2.00	0.42
1:A:41:LYS:HB3	1:A:41:LYS:HE3	1.73	0.42
1:A:59:PHE:HE1	1:A:63:MET:HE2	1.84	0.42
1:C:49:ILE:HG23	1:C:112:LEU:HD13	2.01	0.42
1:B:6:LYS:HE3	1:B:7:TYR:CE2	2.54	0.42
1:B:49:ILE:HG23	1:B:112:LEU:HD13	2.01	0.42
1:D:122[B]:LEU:HD12	1:D:122[B]:LEU:HA	1.90	0.42
1:C:182:ARG:NH1	4:C:304:PEG:H21	2.35	0.42
1:B:56[A]:SER:OG	1:B:113[A]:GLU:OE1	2.38	0.41
1:A:189:PRO:HA	1:A:192:TYR:CZ	2.55	0.41
1:D:189:PRO:HA	1:D:192:TYR:CZ	2.56	0.41
1:D:59:PHE:CE2	1:D:63:MET:CE	3.03	0.41
1:C:21:HIS:HE1	1:C:62:ASP:OD1	2.03	0.41
1:D:12[A]:SER:OG	1:D:186:ILE:HD12	2.19	0.41
1:C:182:ARG:HH12	4:C:304:PEG:C2	2.34	0.41
1:D:63:MET:HG2	1:D:140:LEU:HD21	2.03	0.41
1:A:24:MET:HE2	1:A:63:MET:HE2	2.02	0.40
1:D:104:ILE:HD11	1:D:132:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:MET:CE	1:D:63:MET:HE2	2.52	0.40
1:D:182:ARG:HH12	4:D:304:PEG:H21	1.85	0.40

All (3) 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)
4:C:304:PEG:O1	4:D:304:PEG:O1[3_483]	1.88	0.32
5:B:522:HOH:O	5:C:502:HOH:O[3_573]	2.10	0.10
1:A:44[A]:GLU:OE2	1:B:41:LYS:NZ[4_574]	2.17	0.03

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	176/216 (82%)	170 (97%)	5 (3%)	1 (1%)	25 19
1	B	189/216 (88%)	184 (97%)	5 (3%)	0	100 100
1	C	176/216 (82%)	171 (97%)	4 (2%)	1 (1%)	25 19
1	D	179/216 (83%)	172 (96%)	7 (4%)	0	100 100
All	All	720/864 (83%)	697 (97%)	21 (3%)	2 (0%)	41 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PRO
1	C	163	PRO

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	159/186 (86%)	157 (99%)	2 (1%)	69	74
1	B	170/186 (91%)	169 (99%)	1 (1%)	86	90
1	C	159/186 (86%)	157 (99%)	2 (1%)	69	74
1	D	162/186 (87%)	159 (98%)	3 (2%)	57	61
All	All	650/744 (87%)	642 (99%)	8 (1%)	69	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	107	LYS
1	B	107	LYS
1	C	75	ARG
1	C	123	ARG
1	D	6	LYS
1	D	75	ARG
1	D	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	HIS
1	B	108	HIS
1	C	21	HIS
1	D	39	ASN

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)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	3L4	B	301	3	26,29,29	3.48	12 (46%)	26,42,42	2.19	6 (23%)
4	PEG	D	304	-	6,6,6	0.50	0	5,5,5	0.86	0
4	PEG	A	304	-	6,6,6	0.44	0	5,5,5	0.43	0
4	PEG	C	304	-	6,6,6	0.47	0	5,5,5	0.45	0
2	3L4	D	301	3	26,29,29	3.44	12 (46%)	26,42,42	2.19	7 (26%)
2	3L4	A	301	3	26,29,29	3.18	12 (46%)	26,42,42	3.25	5 (19%)
4	PEG	B	304	-	6,6,6	0.49	0	5,5,5	0.29	0
2	3L4	C	301	3	26,29,29	3.21	12 (46%)	26,42,42	3.05	5 (19%)

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	3L4	B	301	3	-	8/16/19/19	0/2/2/2
4	PEG	D	304	-	-	0/4/4/4	-
4	PEG	A	304	-	-	1/4/4/4	-
4	PEG	C	304	-	-	2/4/4/4	-
2	3L4	D	301	3	-	12/16/19/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3L4	A	301	3	-	12/16/19/19	0/2/2/2
4	PEG	B	304	-	-	3/4/4/4	-
2	3L4	C	301	3	-	14/16/19/19	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	3L4	CAO-CAM	10.30	1.53	1.32
2	D	301	3L4	CAO-CAM	10.25	1.53	1.32
2	C	301	3L4	CAO-CAM	10.16	1.53	1.32
2	A	301	3L4	CAO-CAM	9.80	1.52	1.32
2	B	301	3L4	PBA-CAO	7.74	1.87	1.76
2	D	301	3L4	PBA-CAO	7.50	1.87	1.76
2	C	301	3L4	PBA-CAO	6.32	1.85	1.76
2	A	301	3L4	PBA-CAO	5.66	1.84	1.76
2	A	301	3L4	C2-N3	5.38	1.46	1.33
2	D	301	3L4	C2-N3	5.02	1.45	1.33
2	B	301	3L4	C2-N3	4.91	1.45	1.33
2	C	301	3L4	C2-N3	4.88	1.45	1.33
2	D	301	3L4	C2-N2	4.78	1.45	1.34
2	B	301	3L4	CAM-NAY	4.48	1.47	1.33
2	B	301	3L4	C2-N2	4.44	1.44	1.34
2	D	301	3L4	C4-N3	4.37	1.48	1.37
2	D	301	3L4	CAM-NAY	4.31	1.47	1.33
2	B	301	3L4	C4-N3	4.29	1.47	1.37
2	A	301	3L4	CAM-NAY	4.00	1.46	1.33
2	A	301	3L4	C2-N2	3.99	1.43	1.34
2	A	301	3L4	C4-N3	3.95	1.47	1.37
2	C	301	3L4	C4-N3	3.92	1.46	1.37
2	C	301	3L4	C2-N2	3.77	1.43	1.34
2	C	301	3L4	CAM-NAY	3.73	1.45	1.33
2	B	301	3L4	C6-N1	3.47	1.43	1.37
2	A	301	3L4	C6-N1	3.32	1.42	1.37
2	D	301	3L4	C6-N1	3.22	1.42	1.37
2	B	301	3L4	PBB-CAP	3.00	1.87	1.80
2	B	301	3L4	C2-N1	2.92	1.44	1.37
2	C	301	3L4	C2-N1	2.89	1.44	1.37
2	A	301	3L4	C5-C6	2.83	1.53	1.47
2	D	301	3L4	OAT-CAP	-2.81	1.38	1.42
2	A	301	3L4	PBB-CAP	2.78	1.87	1.80
2	D	301	3L4	C2-N1	2.74	1.44	1.37
2	C	301	3L4	PBB-CAP	2.71	1.87	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	3L4	PBA-OAC	2.67	1.53	1.48
2	B	301	3L4	PBA-OAC	2.61	1.52	1.48
2	D	301	3L4	C5-C6	2.60	1.52	1.47
2	D	301	3L4	PBB-CAP	2.60	1.86	1.80
2	C	301	3L4	C6-N1	2.60	1.41	1.37
2	C	301	3L4	C5-C6	2.58	1.52	1.47
2	B	301	3L4	PBA-OAF	-2.57	1.50	1.54
2	B	301	3L4	C5-C6	2.51	1.52	1.47
2	C	301	3L4	PBA-OAE	-2.27	1.50	1.54
2	A	301	3L4	PBA-OAC	2.16	1.52	1.48
2	A	301	3L4	C2-N1	2.16	1.43	1.37
2	A	301	3L4	O6-C6	-2.06	1.19	1.23
2	D	301	3L4	O6-C6	-2.05	1.19	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	3L4	CAO-CAM-NAY	-15.03	102.82	126.89
2	C	301	3L4	CAO-CAM-NAY	-13.73	104.89	126.89
2	B	301	3L4	CAO-CAM-NAY	-7.93	114.19	126.89
2	D	301	3L4	CAO-CAM-NAY	-6.82	115.96	126.89
2	D	301	3L4	CAJ-CAK-NAY	-5.32	104.34	113.74
2	B	301	3L4	CAL-NAY-CAM	-3.03	110.65	121.14
2	C	301	3L4	C8-N7-C5	2.99	108.68	102.99
2	A	301	3L4	C5-C6-N1	2.97	119.19	113.95
2	D	301	3L4	C5-C6-N1	2.96	119.19	113.95
2	C	301	3L4	C2-N1-C6	-2.95	119.67	125.10
2	A	301	3L4	C2-N1-C6	-2.89	119.78	125.10
2	A	301	3L4	C8-N7-C5	2.83	108.39	102.99
2	B	301	3L4	C5-C6-N1	2.78	118.86	113.95
2	B	301	3L4	CAK-NAY-CAM	-2.70	111.81	121.14
2	B	301	3L4	C8-N7-C5	2.56	107.87	102.99
2	C	301	3L4	C5-C6-N1	2.52	118.41	113.95
2	C	301	3L4	CAK-NAY-CAM	-2.46	112.64	121.14
2	D	301	3L4	C2-N1-C6	-2.43	120.62	125.10
2	B	301	3L4	C2-N1-C6	-2.42	120.65	125.10
2	D	301	3L4	CAP-OAT-CAJ	2.30	118.52	112.90
2	A	301	3L4	CAK-NAY-CAM	-2.26	113.33	121.14
2	D	301	3L4	C8-N7-C5	2.13	107.05	102.99
2	D	301	3L4	CAL-NAY-CAK	-2.11	109.52	117.07

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	3L4	OAT-CAP-PBB-OAD
2	A	301	3L4	CAJ-CAK-NAY-CAM
2	A	301	3L4	CAO-CAM-NAY-CAK
2	A	301	3L4	CAO-CAM-NAY-CAL
2	A	301	3L4	CAN-CAL-NAY-CAM
2	A	301	3L4	CAM-CAO-PBA-OAC
2	A	301	3L4	NAY-CAL-CAN-N9
2	B	301	3L4	PBB-CAP-OAT-CAJ
2	B	301	3L4	CAJ-CAK-NAY-CAM
2	B	301	3L4	CAO-CAM-NAY-CAK
2	B	301	3L4	CAO-CAM-NAY-CAL
2	B	301	3L4	CAN-CAL-NAY-CAK
2	B	301	3L4	CAM-CAO-PBA-OAC
2	C	301	3L4	OAT-CAP-PBB-OAH
2	C	301	3L4	OAT-CAP-PBB-OAD
2	C	301	3L4	CAJ-CAK-NAY-CAM
2	C	301	3L4	CAO-CAM-NAY-CAK
2	C	301	3L4	CAO-CAM-NAY-CAL
2	C	301	3L4	CAN-CAL-NAY-CAM
2	C	301	3L4	CAM-CAO-PBA-OAC
2	C	301	3L4	NAY-CAL-CAN-N9
2	D	301	3L4	OAT-CAP-PBB-OAG
2	D	301	3L4	OAT-CAP-PBB-OAH
2	D	301	3L4	OAT-CAP-PBB-OAD
2	D	301	3L4	PBB-CAP-OAT-CAJ
2	D	301	3L4	CAJ-CAK-NAY-CAM
2	D	301	3L4	CAO-CAM-NAY-CAK
2	D	301	3L4	CAN-CAL-NAY-CAK
2	D	301	3L4	CAM-CAO-PBA-OAC
2	C	301	3L4	OAT-CAJ-CAK-NAY
2	D	301	3L4	OAT-CAJ-CAK-NAY
2	A	301	3L4	OAT-CAJ-CAK-NAY
4	B	304	PEG	O1-C1-C2-O2
4	A	304	PEG	O1-C1-C2-O2
2	C	301	3L4	CAN-CAL-NAY-CAK
2	D	301	3L4	NAY-CAL-CAN-N9
2	D	301	3L4	CAO-CAM-NAY-CAL
4	C	304	PEG	O1-C1-C2-O2
2	B	301	3L4	CAK-CAJ-OAT-CAP
2	B	301	3L4	NAY-CAL-CAN-N9
2	A	301	3L4	CAJ-CAK-NAY-CAL
2	C	301	3L4	CAJ-CAK-NAY-CAL

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Mol	Chain	Res	Type	Atoms
2	C	301	3L4	CAL-CAN-N9-C4
4	B	304	PEG	C1-C2-O2-C3
4	C	304	PEG	C1-C2-O2-C3
2	C	301	3L4	CAK-CAJ-OAT-CAP
4	B	304	PEG	O2-C3-C4-O4
2	A	301	3L4	CAK-CAJ-OAT-CAP
2	A	301	3L4	OAT-CAP-PBB-OAG
2	D	301	3L4	CAK-CAJ-OAT-CAP
2	A	301	3L4	PBB-CAP-OAT-CAJ
2	C	301	3L4	PBB-CAP-OAT-CAJ

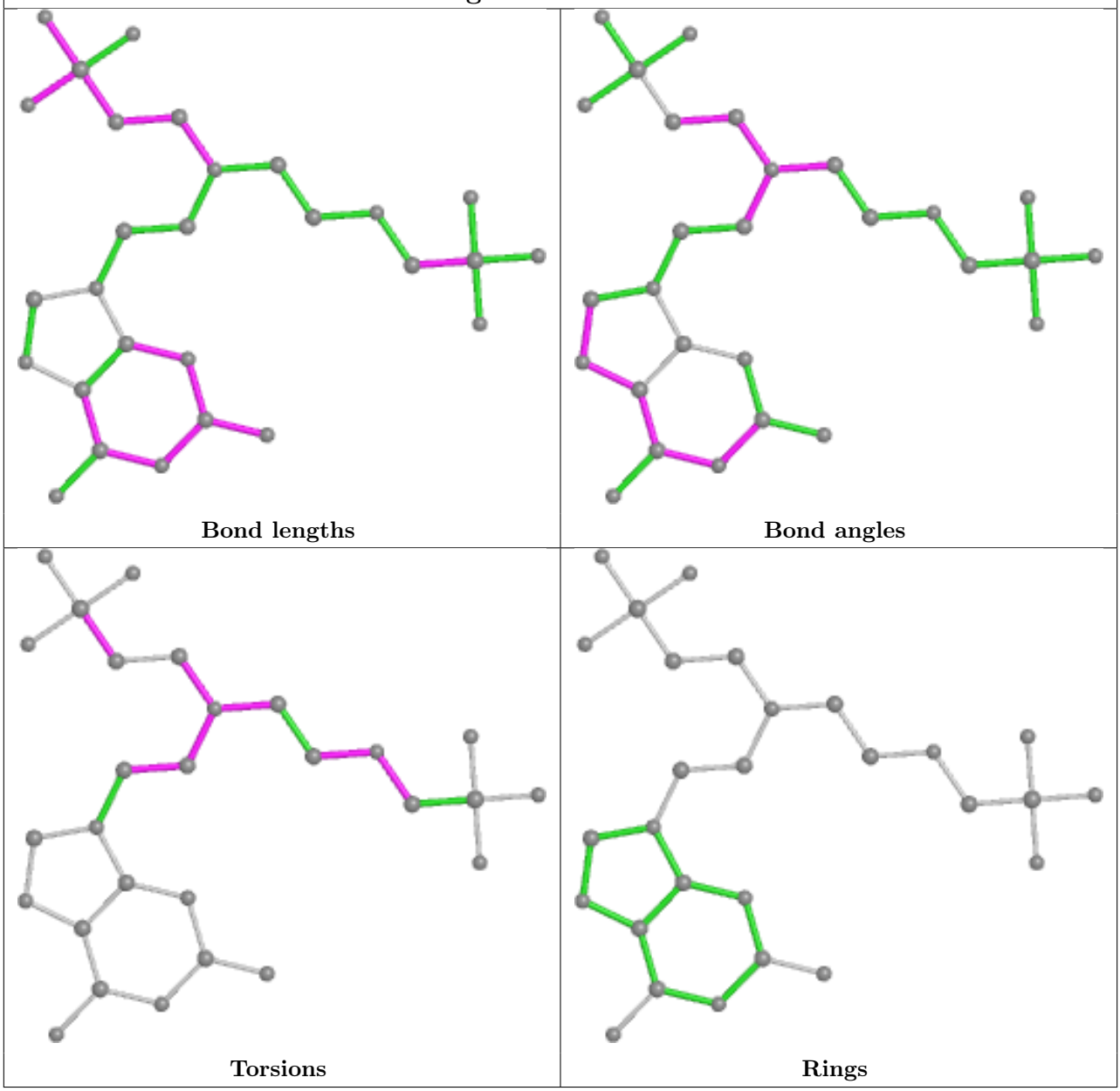
There are no ring outliers.

6 monomers are involved in 9 short contacts:

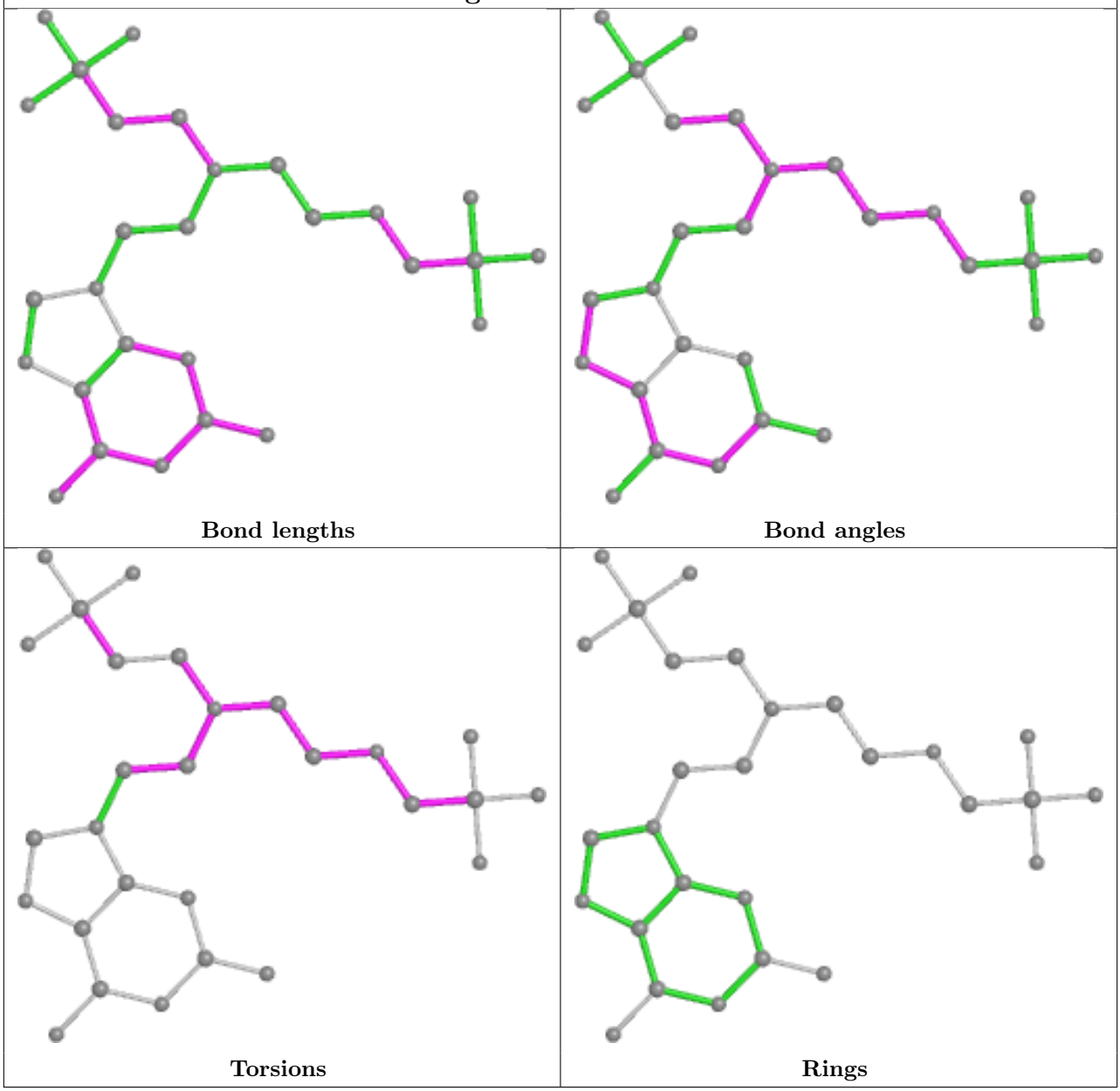
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	3L4	1	0
4	D	304	PEG	1	1
4	A	304	PEG	1	0
4	C	304	PEG	3	1
2	D	301	3L4	1	0
4	B	304	PEG	1	0

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 then 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.

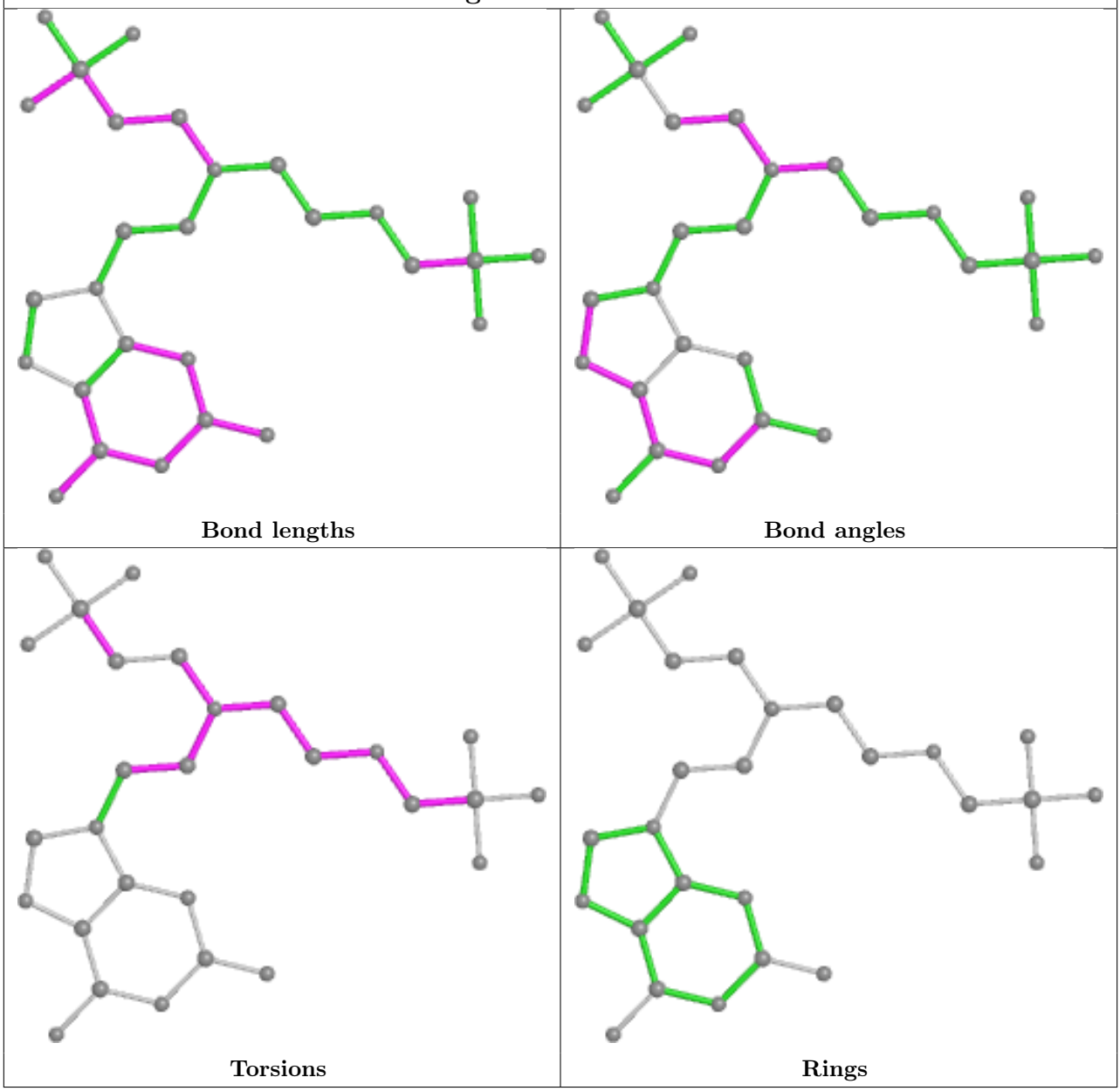
Ligand 3L4 B 301



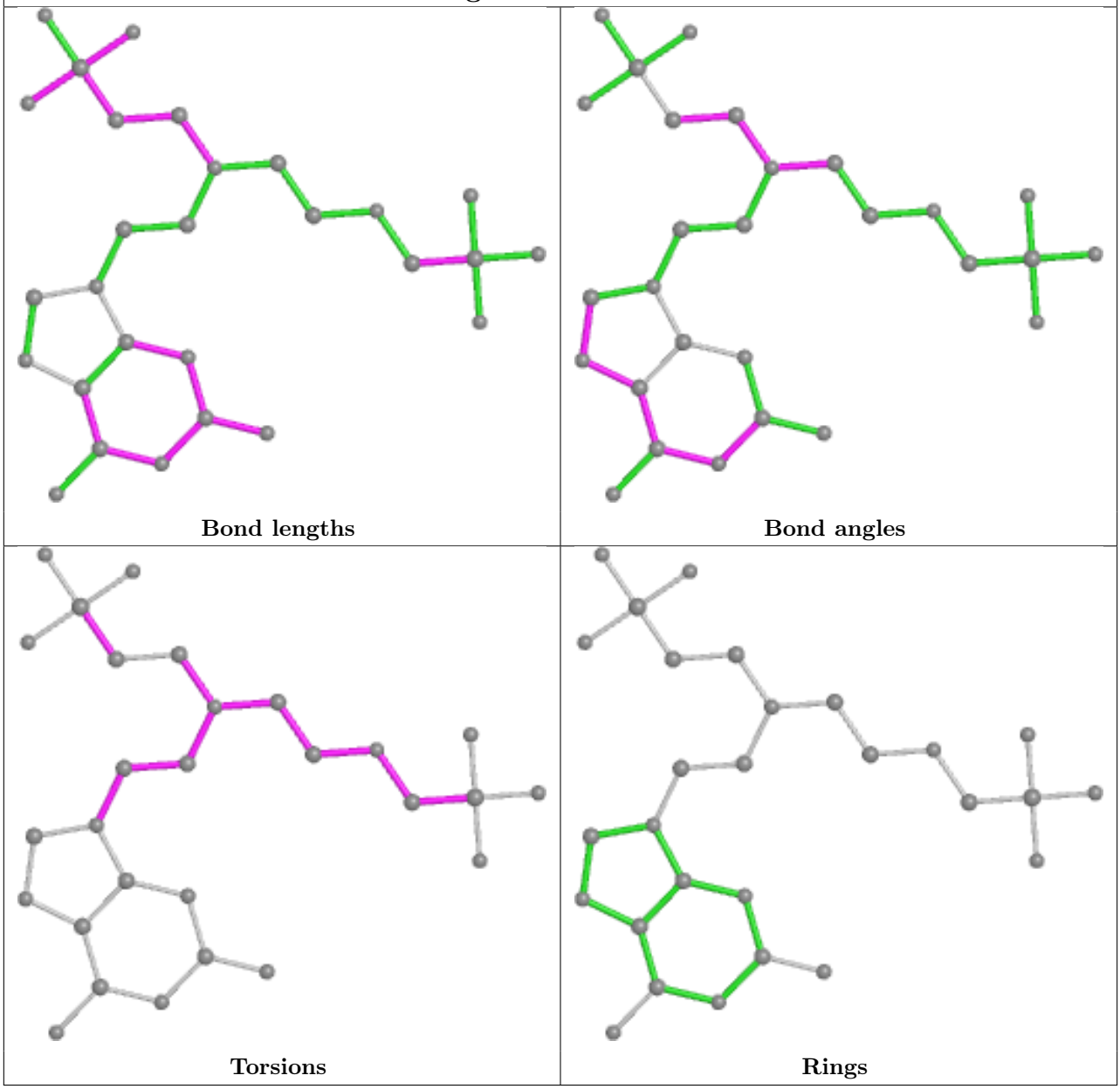
Ligand 3L4 D 301



Ligand 3L4 A 301



Ligand 3L4 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 (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	175/216 (81%)	-0.12	2 (1%)	80	79	9, 18, 47, 74	0
1	B	183/216 (84%)	0.07	11 (6%)	21	20	8, 18, 53, 78	0
1	C	174/216 (80%)	-0.05	8 (4%)	32	31	10, 20, 51, 74	0
1	D	176/216 (81%)	0.09	6 (3%)	45	44	10, 23, 52, 78	0
All	All	708/864 (81%)	0.00	27 (3%)	40	39	8, 20, 51, 78	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	ALA	6.3
1	B	205	ALA	4.1
1	B	203	LYS	3.9
1	C	197	LYS	3.5
1	D	81	ALA	3.2
1	A	8	ASP	3.2
1	B	8	ASP	3.1
1	B	84	TYR	3.1
1	B	82	SER	3.0
1	C	199	LEU	3.0
1	D	38	CYS	2.9
1	C	8	ASP	2.8
1	D	133	GLU	2.8
1	B	81	ALA	2.7
1	D	103	ASP	2.6
1	D	105	ARG	2.6
1	D	201	ARG	2.6
1	C	196	GLY	2.6
1	C	195	TRP	2.4
1	A	133	GLU	2.3
1	C	5	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	201	ARG	2.2
1	B	199	LEU	2.2
1	C	198	GLU	2.1
1	C	194	THR	2.1
1	B	133	GLU	2.0
1	B	83	SER	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)

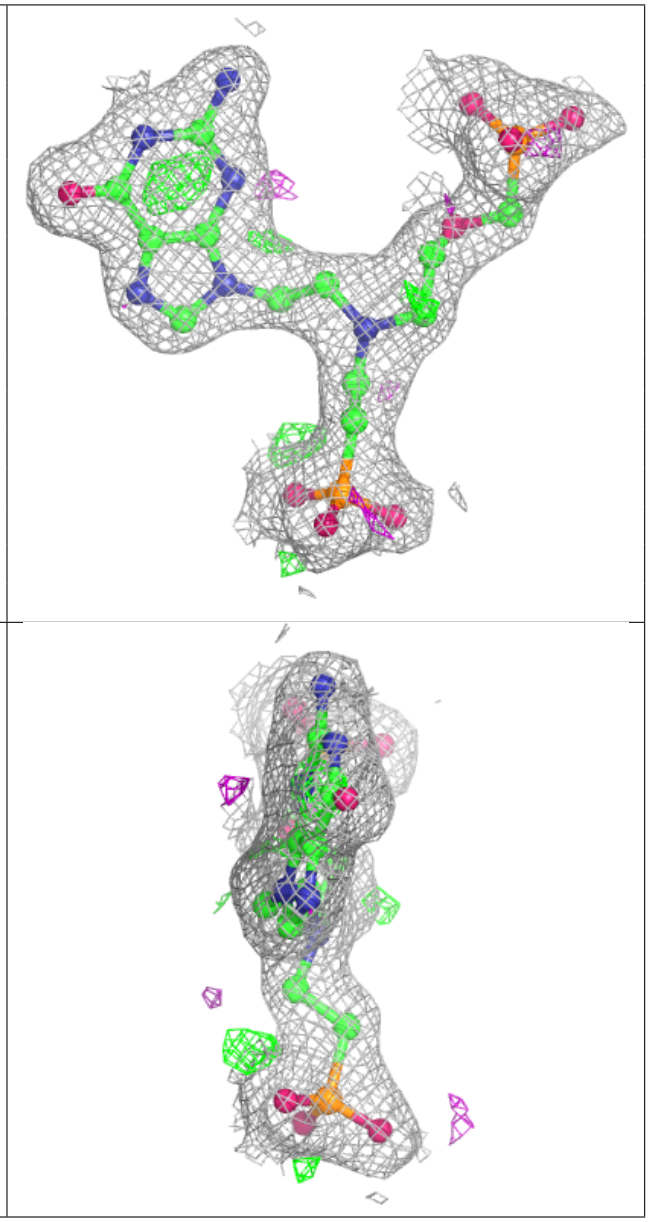
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	303[A]	1/1	0.82	0.19	39,39,39,39	1
3	MG	C	303[B]	1/1	0.82	0.19	15,15,15,15	1
4	PEG	A	304	7/7	0.90	0.16	28,29,40,41	0
4	PEG	B	304	7/7	0.90	0.14	22,26,31,33	0
4	PEG	C	304	7/7	0.90	0.16	27,32,39,39	0
3	MG	C	302	1/1	0.91	0.06	42,42,42,42	0
4	PEG	D	304	7/7	0.92	0.14	29,31,35,38	0
3	MG	B	302	1/1	0.93	0.06	21,21,21,21	0
3	MG	A	302	1/1	0.95	0.09	25,25,25,25	0
2	3L4	C	301	28/28	0.96	0.11	14,22,38,40	0
3	MG	A	303	1/1	0.96	0.26	54,54,54,54	0
2	3L4	A	301	28/28	0.97	0.10	12,19,35,38	0
2	3L4	D	301	28/28	0.97	0.10	13,17,31,38	0
2	3L4	B	301	28/28	0.98	0.09	10,17,29,32	0
3	MG	D	303	1/1	0.98	0.09	36,36,36,36	0
3	MG	B	303	1/1	0.98	0.14	50,50,50,50	0
3	MG	D	302	1/1	0.99	0.03	18,18,18,18	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.

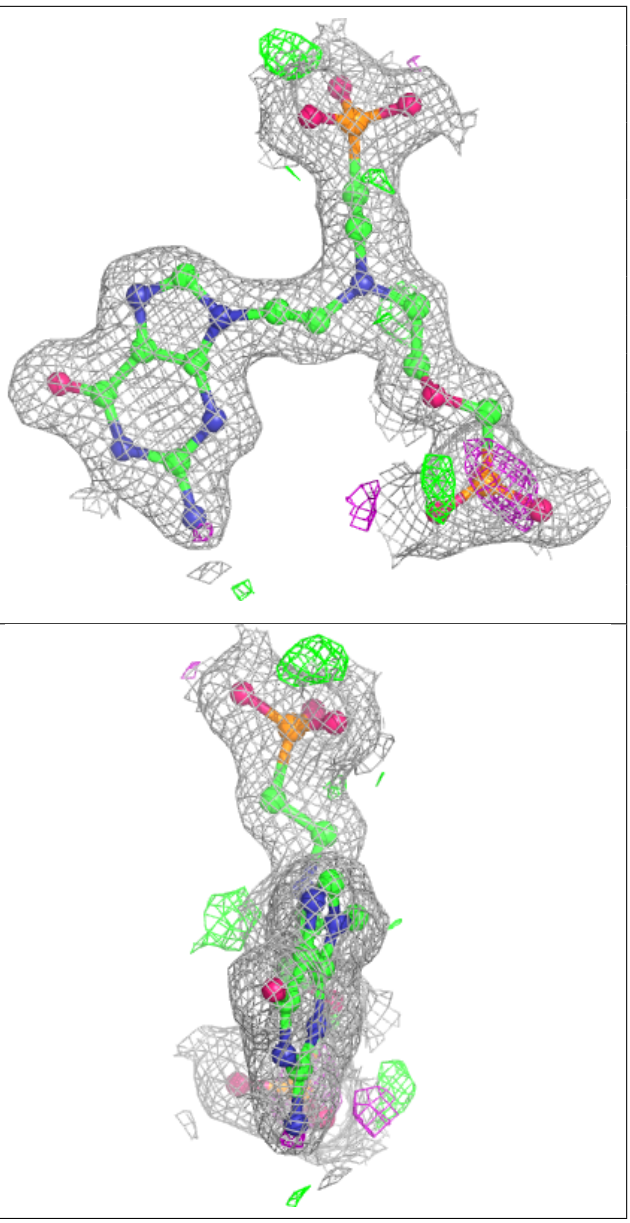
Electron density around 3L4 C 301:

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



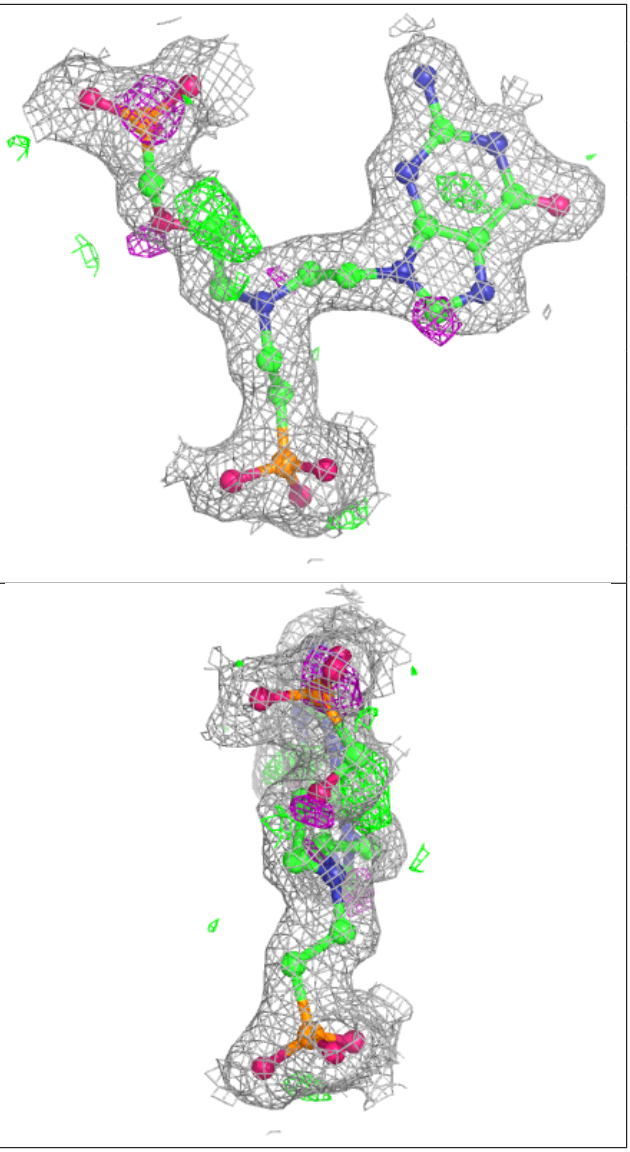
Electron density around 3L4 A 301:

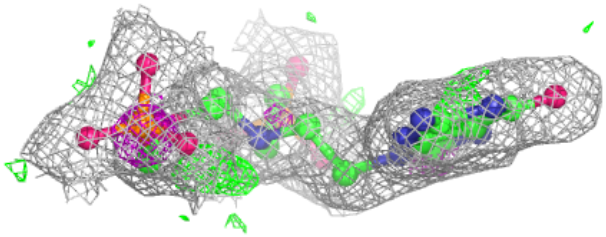
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3L4 D 301:

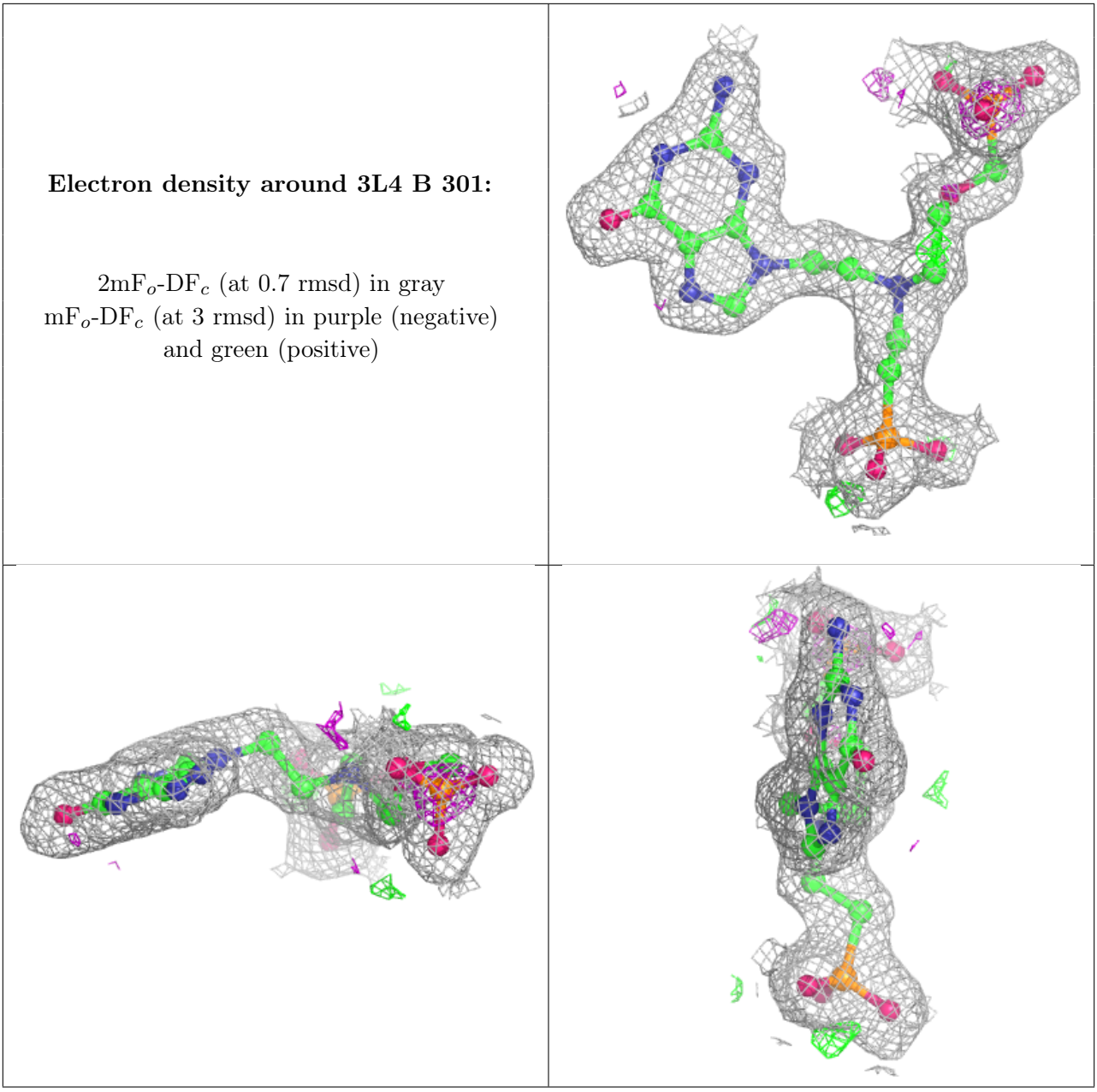
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around 3L4 B 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.