



Full wwPDB X-ray Structure Validation Report

Feb 22, 2024 – 03:04 AM EST

PDB ID : 4RAD
Title : Aza-acyclic nucleoside phosphonates containing a second phosphonate group as inhibitors of the human, Plasmodium falciparum and vivax 6-oxopurine phosphoribosyltransferases and their pro-drugs as antimalarial agents
Authors : Keough, D.T.; Hockova, D.; Janeba, Z.; Wang, T.-H.; Naesens, L.; Edstein, M.D.; Chavchich, M.; Guddat, L.W.
Deposited on : 2014-09-10
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

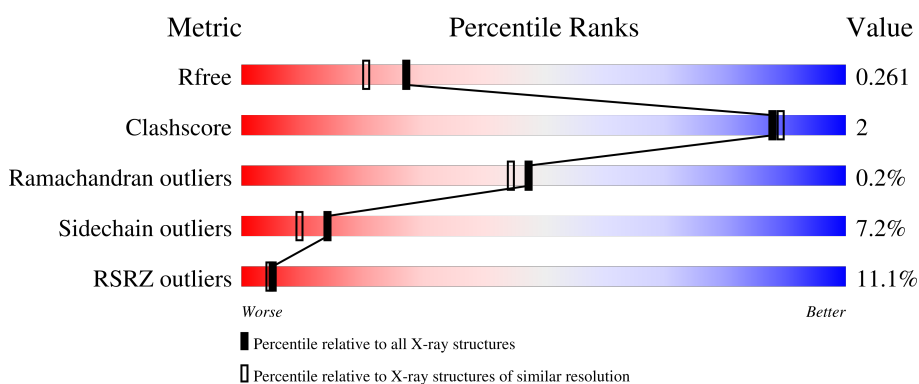
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



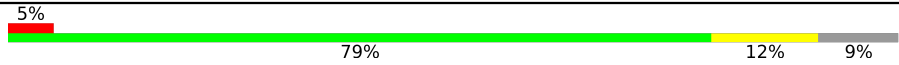


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	217	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">82% 8% • 9%</p>
1	B	217	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">86% 9% 5%</p>
1	C	217	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">82% 11% 7%</p>
1	D	217	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">84% 8% • 7%</p>
1	E	217	<div style="display: flex; align-items: center;"> <div style="width: 18%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">86% 8% 5%</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	217	
1	G	217	
1	H	217	

2 Entry composition

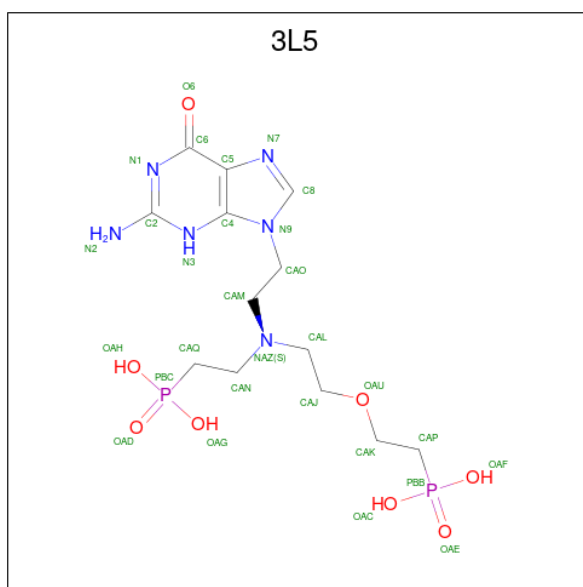
There are 4 unique types of molecules in this entry. The entry contains 26882 atoms, of which 13106 are hydrogens and 0 are deuteriums.

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	H	N	O	S				
1	A	197	3112	999	1558	259	289	7	0	0	0	
1	B	207	3277	1048	1644	274	304	7	0	0	0	
1	C	202	3210	1030	1611	268	294	7	0	0	0	
1	D	202	3189	1024	1597	265	296	7	0	0	0	
1	E	206	3238	1043	1616	269	303	7	0	0	0	
1	F	197	3141	1007	1581	262	284	7	0	0	0	
1	G	200	3171	1019	1589	264	292	7	0	0	0	
1	H	208	3313	1061	1663	276	306	7	0	0	0	

- Molecule 2 is (2-{[2-(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)ethyl][2-(2-phosphonoethoxy)ethyl]amino}ethyl)phosphonic acid (three-letter code: 3L5) (formula: C₁₃H₂₄N₆O₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	1
			96	26	38	12	16	4		
2	B	1	Total	C	H	N	O	P	0	0
			48	13	19	6	8	2		
2	C	1	Total	C	H	N	O	P	0	1
			96	26	38	12	16	4		
2	D	1	Total	C	H	N	O	P	0	1
			96	26	38	12	16	4		
2	E	1	Total	C	H	N	O	P	0	1
			96	26	38	12	16	4		
2	F	1	Total	C	H	N	O	P	0	0
			48	13	19	6	8	2		
2	G	1	Total	C	H	N	O	P	0	0
			48	13	19	6	8	2		
2	H	1	Total	C	H	N	O	P	0	1
			96	26	38	12	16	4		

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total 2	Mg 2	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0

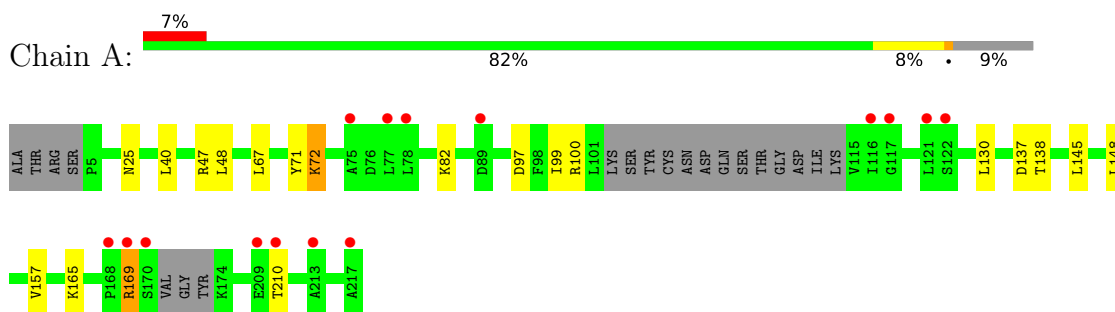
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total 78	O 78	0	0
4	B	88	Total 88	O 88	0	0
4	C	72	Total 72	O 72	0	0
4	D	94	Total 94	O 94	0	0
4	E	62	Total 62	O 62	0	0
4	F	98	Total 98	O 98	0	0
4	G	37	Total 37	O 37	0	0
4	H	69	Total 69	O 69	0	0

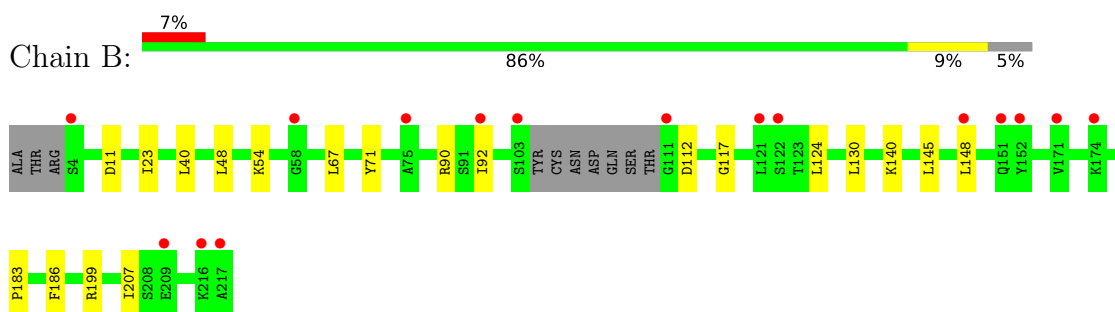
3 Residue-property plots [i](#)

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.

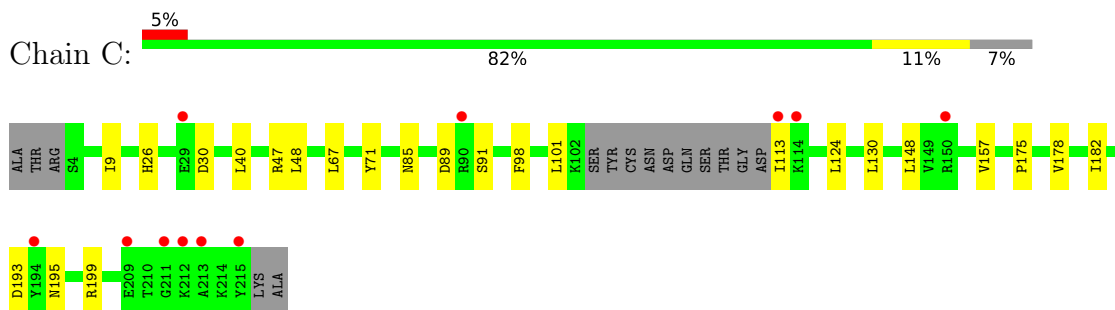
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



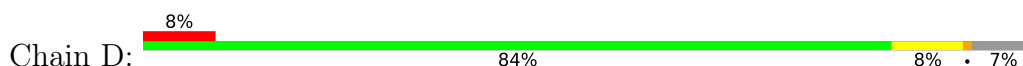
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

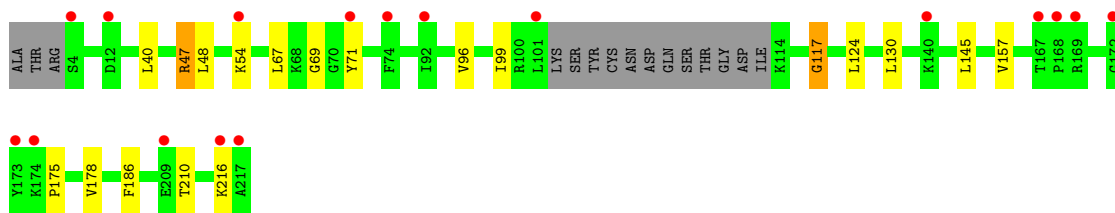


- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

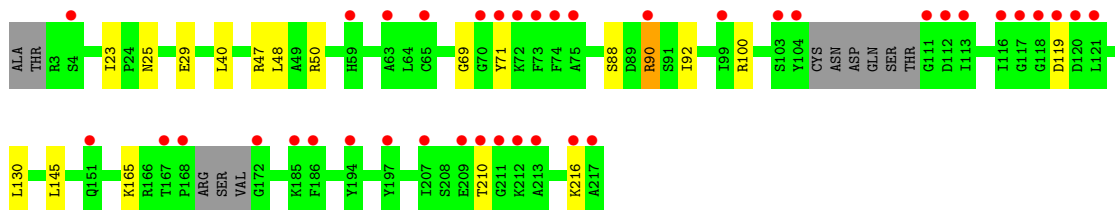
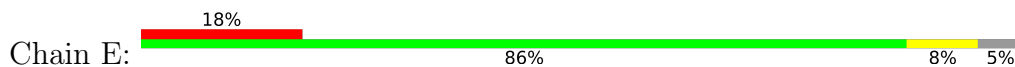


- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

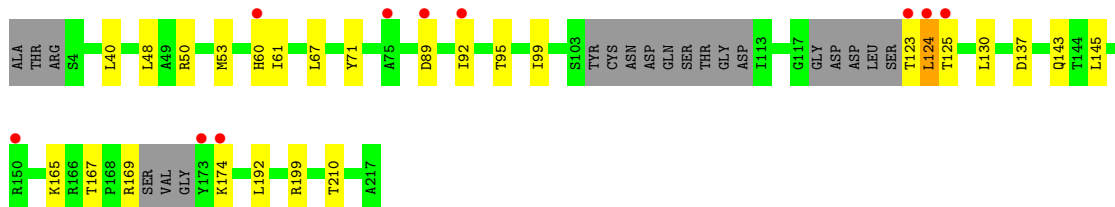
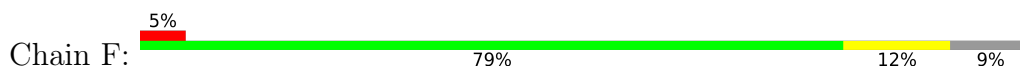




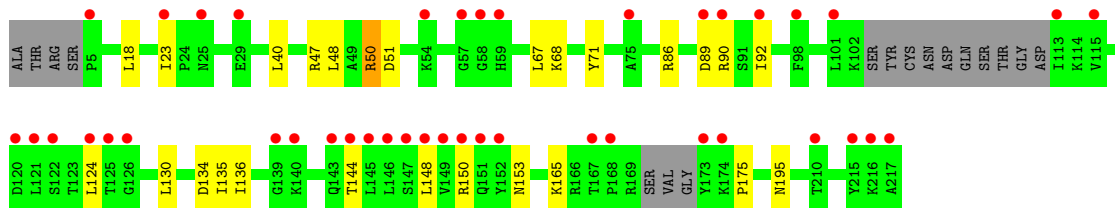
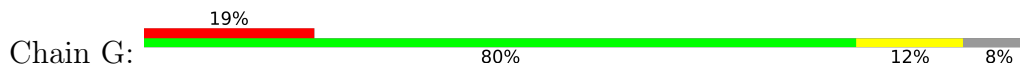
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



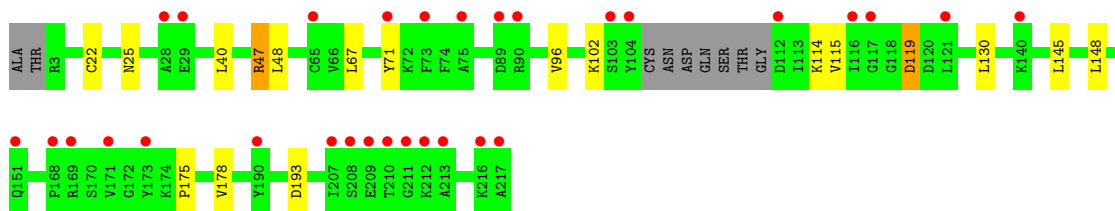
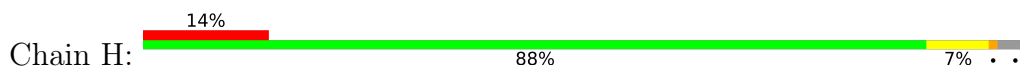
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.05Å 114.93Å 97.54Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	35.56 – 2.00 35.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.56-2.00) 98.7 (35.56-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.259 0.212 , 0.261	Depositor DCC
R_{free} test set	2000 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtrriage
Anisotropy	0.315	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26882	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: 3L5, 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	0.27	0/1583	0.52	0/2138
1	B	0.27	0/1664	0.49	0/2247
1	C	0.26	0/1630	0.50	0/2204
1	D	0.26	0/1623	0.49	0/2194
1	E	0.26	0/1653	0.47	0/2233
1	F	0.27	0/1588	0.52	0/2141
1	G	0.24	0/1612	0.46	0/2175
1	H	0.25	0/1682	0.49	0/2271
All	All	0.26	0/13035	0.49	0/17603

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	1554	1558	1558	9	0
1	B	1633	1644	1644	5	0
1	C	1599	1611	1611	9	0
1	D	1592	1597	1597	6	0
1	E	1622	1616	1616	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1560	1581	1581	8	0
1	G	1582	1589	1589	9	0
1	H	1650	1663	1663	7	0
2	A	58	38	44	0	0
2	B	29	19	22	0	0
2	C	58	38	44	2	0
2	D	58	38	44	1	0
2	E	58	38	44	1	0
2	F	29	19	22	0	0
2	G	29	19	22	0	0
2	H	58	38	44	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	78	0	0	3	0
4	B	88	0	0	1	0
4	C	72	0	0	3	0
4	D	94	0	0	3	0
4	E	62	0	0	2	0
4	F	98	0	0	0	0
4	G	37	0	0	2	0
4	H	69	0	0	1	0
All	All	13776	13106	13145	53	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 2.

All (53) 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:F:123:THR:O	1:F:125:THR:N	2.24	0.70
1:G:47:ARG:NH1	1:G:51:ASP:OD1	2.25	0.69
1:C:30:ASP:OD2	4:C:434:HOH:O	2.13	0.67
2:C:301[B]:3L5:H22	2:C:301[B]:3L5:H6	1.60	0.67
1:E:25:ASN:ND2	1:G:89:ASP:O	2.29	0.66
1:A:165:LYS:NZ	4:A:428:HOH:O	2.32	0.62
1:C:199:ARG:NH1	2:C:301[B]:3L5:OAE	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:LYS:NZ	4:G:429:HOH:O	2.34	0.60
1:B:112:ASP:N	1:B:112:ASP:OD1	2.34	0.59
1:D:117:GLY:O	4:D:444:HOH:O	2.16	0.58
1:H:47:ARG:NH2	4:H:443:HOH:O	2.37	0.58
1:C:26:HIS:O	4:C:434:HOH:O	2.17	0.57
1:A:138:THR:HA	1:A:169:ARG:CB	2.38	0.54
1:A:72:LYS:NZ	4:A:447:HOH:O	2.30	0.54
1:H:102:LYS:O	1:H:114:LYS:N	2.39	0.54
1:A:138:THR:HA	1:A:169:ARG:HB2	1.90	0.53
1:A:99:ILE:HD12	1:A:145:LEU:HD22	1.90	0.53
1:D:47:ARG:NH2	4:D:408:HOH:O	2.42	0.51
1:F:137:ASP:OD1	1:F:167:THR:HG21	2.11	0.50
1:G:134:ASP:OD1	1:G:135:ILE:N	2.45	0.50
1:F:165:LYS:O	1:F:169:ARG:NH2	2.39	0.49
1:D:175:PRO:HG2	1:D:178:VAL:HG22	1.94	0.48
1:D:186:PHE:O	4:D:461:HOH:O	2.20	0.48
1:E:69:GLY:H	2:E:301[A]:3L5:H4	1.79	0.48
1:E:50:ARG:NH2	4:E:403:HOH:O	2.43	0.47
1:B:186:PHE:HB3	1:B:207:ILE:HD11	1.96	0.47
1:F:53:MET:HA	1:F:92:ILE:HD11	1.97	0.47
1:A:82:LYS:NZ	4:A:453:HOH:O	2.48	0.46
1:A:137:ASP:OD2	1:A:169:ARG:NH2	2.49	0.46
1:F:50:ARG:NH1	1:G:86:ARG:O	2.49	0.46
1:G:165:LYS:NZ	4:G:411:HOH:O	2.49	0.46
1:F:60:HIS:NE2	1:F:95:THR:HG23	2.32	0.45
1:G:18:LEU:HB3	1:G:23:ILE:HD13	2.00	0.44
1:C:85:ASN:OD1	1:C:91:SER:OG	2.25	0.44
1:H:119:ASP:OD2	1:H:119:ASP:N	2.49	0.43
1:H:175:PRO:HG2	1:H:178:VAL:HG22	1.99	0.43
1:A:138:THR:HA	1:A:169:ARG:HG3	1.99	0.43
1:H:115:VAL:HG11	1:H:148:LEU:HD21	2.00	0.43
1:C:47:ARG:NH2	4:C:411:HOH:O	2.53	0.42
1:B:117:GLY:O	4:B:440:HOH:O	2.22	0.42
1:A:25:ASN:ND2	1:C:89:ASP:O	2.48	0.42
1:B:11:ASP:HA	1:B:183:PRO:HG3	2.01	0.42
1:C:9:ILE:HD12	1:C:182:ILE:HG22	2.02	0.42
1:F:199:ARG:HD2	1:H:96:VAL:HG22	2.01	0.41
1:F:123:THR:OG1	1:F:124:LEU:N	2.53	0.41
1:G:50:ARG:NH2	1:H:22:CYS:HA	2.35	0.41
1:E:88:SER:OG	1:E:90:ARG:NH1	2.54	0.41
1:C:175:PRO:HG2	1:C:178:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:ILE:HD12	1:G:175:PRO:HG3	2.01	0.41
1:D:69:GLY:H	2:D:301[B]:3L5:H3	1.86	0.41
1:B:199:ARG:HD2	1:D:96:VAL:HG22	2.02	0.41
1:E:165:LYS:NZ	4:E:422:HOH:O	2.54	0.40
1:C:67:LEU:HD21	1:C:98:PHE:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/217 (88%)	185 (97%)	6 (3%)	0	100	100
1	B	203/217 (94%)	197 (97%)	6 (3%)	0	100	100
1	C	198/217 (91%)	192 (97%)	6 (3%)	0	100	100
1	D	198/217 (91%)	191 (96%)	6 (3%)	1 (0%)	29	23
1	E	200/217 (92%)	193 (96%)	7 (4%)	0	100	100
1	F	189/217 (87%)	181 (96%)	7 (4%)	1 (0%)	29	23
1	G	194/217 (89%)	186 (96%)	7 (4%)	1 (0%)	29	23
1	H	204/217 (94%)	199 (98%)	5 (2%)	0	100	100
All	All	1577/1736 (91%)	1524 (97%)	50 (3%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	124	LEU
1	G	153	ASN
1	D	117	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/191 (89%)	157 (92%)	13 (8%)	13	8
1	B	179/191 (94%)	166 (93%)	13 (7%)	14	9
1	C	175/191 (92%)	164 (94%)	11 (6%)	18	13
1	D	174/191 (91%)	161 (92%)	13 (8%)	13	9
1	E	176/191 (92%)	162 (92%)	14 (8%)	12	7
1	F	170/191 (89%)	157 (92%)	13 (8%)	13	8
1	G	172/191 (90%)	159 (92%)	13 (8%)	13	8
1	H	181/191 (95%)	171 (94%)	10 (6%)	21	17
All	All	1397/1528 (91%)	1297 (93%)	100 (7%)	14	9

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	47	ARG
1	A	48	LEU
1	A	67	LEU
1	A	71	TYR
1	A	72	LYS
1	A	97	ASP
1	A	100	ARG
1	A	130	LEU
1	A	148	LEU
1	A	157	VAL
1	A	169	ARG
1	A	210	THR
1	B	23	ILE
1	B	40	LEU
1	B	48	LEU
1	B	54	LYS
1	B	67	LEU
1	B	71	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	90	ARG
1	B	92	ILE
1	B	124	LEU
1	B	130	LEU
1	B	140	LYS
1	B	145	LEU
1	B	148	LEU
1	C	40	LEU
1	C	48	LEU
1	C	71	TYR
1	C	101	LEU
1	C	113	ILE
1	C	124	LEU
1	C	130	LEU
1	C	148	LEU
1	C	157	VAL
1	C	193	ASP
1	C	195	ASN
1	D	40	LEU
1	D	47	ARG
1	D	48	LEU
1	D	54	LYS
1	D	67	LEU
1	D	71	TYR
1	D	99	ILE
1	D	124	LEU
1	D	130	LEU
1	D	145	LEU
1	D	157	VAL
1	D	210	THR
1	D	216	LYS
1	E	23	ILE
1	E	29	GLU
1	E	40	LEU
1	E	47	ARG
1	E	48	LEU
1	E	71	TYR
1	E	90	ARG
1	E	92	ILE
1	E	100	ARG
1	E	119	ASP
1	E	130	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	145	LEU
1	E	210	THR
1	E	216	LYS
1	F	40	LEU
1	F	48	LEU
1	F	61	ILE
1	F	67	LEU
1	F	71	TYR
1	F	89	ASP
1	F	99	ILE
1	F	130	LEU
1	F	143	GLN
1	F	145	LEU
1	F	174	LYS
1	F	192	LEU
1	F	210	THR
1	G	40	LEU
1	G	48	LEU
1	G	50	ARG
1	G	67	LEU
1	G	71	TYR
1	G	90	ARG
1	G	92	ILE
1	G	124	LEU
1	G	130	LEU
1	G	144	THR
1	G	148	LEU
1	G	150	ARG
1	G	195	ASN
1	H	25	ASN
1	H	40	LEU
1	H	47	ARG
1	H	48	LEU
1	H	67	LEU
1	H	71	TYR
1	H	119	ASP
1	H	130	LEU
1	H	145	LEU
1	H	193	ASP

Sometimes 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](#)

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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	3L5	A	301[A]	-	24,30,30	3.18	6 (25%)	31,43,43	1.00	1 (3%)
2	3L5	E	301[B]	-	24,30,30	3.13	6 (25%)	31,43,43	1.17	2 (6%)
2	3L5	B	301	-	24,30,30	3.03	6 (25%)	31,43,43	1.14	2 (6%)
2	3L5	E	301[A]	-	24,30,30	3.13	6 (25%)	31,43,43	1.22	2 (6%)
2	3L5	H	301[B]	-	24,30,30	3.18	5 (20%)	31,43,43	1.49	4 (12%)
2	3L5	C	301[B]	-	24,30,30	3.18	5 (20%)	31,43,43	1.05	1 (3%)
2	3L5	H	301[A]	-	24,30,30	3.21	5 (20%)	31,43,43	1.26	3 (9%)
2	3L5	C	301[A]	-	24,30,30	3.24	5 (20%)	31,43,43	1.33	3 (9%)
2	3L5	D	301[B]	3	24,30,30	3.14	6 (25%)	31,43,43	1.19	3 (9%)
2	3L5	G	301	-	24,30,30	3.19	6 (25%)	31,43,43	1.11	1 (3%)
2	3L5	D	301[A]	-	24,30,30	3.18	6 (25%)	31,43,43	1.04	1 (3%)
2	3L5	A	301[B]	-	24,30,30	3.23	6 (25%)	31,43,43	1.08	1 (3%)
2	3L5	F	301	3	24,30,30	3.08	6 (25%)	31,43,43	1.10	2 (6%)

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	3L5	A	301[A]	-	-	6/20/20/20	0/2/2/2
2	3L5	E	301[B]	-	-	9/20/20/20	0/2/2/2
2	3L5	B	301	-	-	3/20/20/20	0/2/2/2
2	3L5	E	301[A]	-	-	8/20/20/20	0/2/2/2
2	3L5	H	301[B]	-	-	5/20/20/20	0/2/2/2
2	3L5	C	301[B]	-	-	4/20/20/20	0/2/2/2
2	3L5	H	301[A]	-	-	3/20/20/20	0/2/2/2
2	3L5	C	301[A]	-	-	7/20/20/20	0/2/2/2
2	3L5	D	301[B]	3	-	8/20/20/20	0/2/2/2
2	3L5	G	301	-	-	8/20/20/20	0/2/2/2
2	3L5	D	301[A]	-	-	8/20/20/20	0/2/2/2
2	3L5	A	301[B]	-	-	3/20/20/20	0/2/2/2
2	3L5	F	301	3	-	2/20/20/20	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	3L5	O6-C6	11.39	1.43	1.23
2	C	301[B]	3L5	O6-C6	11.35	1.43	1.23
2	H	301[B]	3L5	O6-C6	11.34	1.43	1.23
2	H	301[A]	3L5	O6-C6	11.34	1.43	1.23
2	D	301[A]	3L5	O6-C6	11.28	1.43	1.23
2	A	301[A]	3L5	O6-C6	11.20	1.43	1.23
2	A	301[B]	3L5	O6-C6	11.18	1.43	1.23
2	E	301[A]	3L5	O6-C6	11.17	1.43	1.23
2	D	301[B]	3L5	O6-C6	11.15	1.43	1.23
2	E	301[B]	3L5	O6-C6	11.11	1.43	1.23
2	G	301	3L5	O6-C6	11.05	1.42	1.23
2	F	301	3L5	O6-C6	11.00	1.42	1.23
2	B	301	3L5	O6-C6	10.88	1.42	1.23
2	A	301[B]	3L5	PBC-CAQ	7.31	1.86	1.78
2	C	301[B]	3L5	PBC-CAQ	7.22	1.86	1.78
2	H	301[A]	3L5	PBC-CAQ	7.21	1.86	1.78
2	G	301	3L5	PBC-CAQ	7.20	1.86	1.78
2	A	301[A]	3L5	PBC-CAQ	7.03	1.86	1.78
2	H	301[B]	3L5	PBC-CAQ	7.02	1.86	1.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	3L5	PBC-CAQ	6.97	1.85	1.78
2	D	301[A]	3L5	PBC-CAQ	6.95	1.85	1.78
2	D	301[B]	3L5	PBC-CAQ	6.91	1.85	1.78
2	E	301[A]	3L5	PBC-CAQ	6.91	1.85	1.78
2	E	301[B]	3L5	PBC-CAQ	6.89	1.85	1.78
2	F	301	3L5	PBC-CAQ	6.62	1.85	1.78
2	B	301	3L5	PBC-CAQ	6.07	1.85	1.78
2	C	301[A]	3L5	PBB-CAP	5.75	1.84	1.78
2	A	301[B]	3L5	PBB-CAP	5.56	1.84	1.78
2	G	301	3L5	PBB-CAP	5.28	1.84	1.78
2	A	301[A]	3L5	PBB-CAP	5.18	1.84	1.78
2	D	301[A]	3L5	PBB-CAP	5.18	1.84	1.78
2	H	301[A]	3L5	PBB-CAP	5.13	1.84	1.78
2	D	301[B]	3L5	PBB-CAP	4.85	1.83	1.78
2	H	301[B]	3L5	PBB-CAP	4.84	1.83	1.78
2	E	301[B]	3L5	PBB-CAP	4.81	1.83	1.78
2	B	301	3L5	PBB-CAP	4.77	1.83	1.78
2	E	301[A]	3L5	PBB-CAP	4.75	1.83	1.78
2	F	301	3L5	PBB-CAP	4.56	1.83	1.78
2	C	301[B]	3L5	PBB-CAP	4.50	1.83	1.78
2	D	301[A]	3L5	C2-N2	3.86	1.43	1.34
2	B	301	3L5	C2-N2	3.85	1.43	1.34
2	C	301[A]	3L5	C2-N2	3.85	1.43	1.34
2	G	301	3L5	C2-N2	3.85	1.43	1.34
2	C	301[B]	3L5	C2-N2	3.85	1.43	1.34
2	H	301[B]	3L5	C2-N2	3.85	1.43	1.34
2	E	301[B]	3L5	C2-N2	3.85	1.43	1.34
2	F	301	3L5	C2-N2	3.85	1.43	1.34
2	D	301[B]	3L5	C2-N2	3.81	1.43	1.34
2	H	301[A]	3L5	C2-N2	3.81	1.43	1.34
2	E	301[A]	3L5	C2-N2	3.78	1.43	1.34
2	A	301[A]	3L5	C2-N2	3.74	1.43	1.34
2	A	301[B]	3L5	C2-N2	3.69	1.43	1.34
2	E	301[B]	3L5	C6-N1	-2.50	1.33	1.39
2	E	301[A]	3L5	C6-N1	-2.50	1.33	1.39
2	B	301	3L5	C6-N1	-2.48	1.33	1.39
2	G	301	3L5	C6-N1	-2.48	1.33	1.39
2	F	301	3L5	C6-N1	-2.46	1.33	1.39
2	A	301[B]	3L5	C6-N1	-2.45	1.33	1.39
2	H	301[B]	3L5	C6-N1	-2.44	1.33	1.39
2	A	301[A]	3L5	C6-N1	-2.43	1.33	1.39
2	H	301[A]	3L5	C6-N1	-2.42	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[B]	3L5	C6-N1	-2.41	1.34	1.39
2	D	301[B]	3L5	C6-N1	-2.40	1.34	1.39
2	C	301[A]	3L5	C6-N1	-2.39	1.34	1.39
2	D	301[A]	3L5	C6-N1	-2.36	1.34	1.39
2	B	301	3L5	C5-C6	-2.31	1.42	1.47
2	E	301[B]	3L5	C5-C6	-2.23	1.43	1.47
2	D	301[B]	3L5	C5-C6	-2.14	1.43	1.47
2	A	301[B]	3L5	C5-C6	-2.14	1.43	1.47
2	A	301[A]	3L5	C5-C6	-2.08	1.43	1.47
2	G	301	3L5	C5-C6	-2.08	1.43	1.47
2	F	301	3L5	C5-C6	-2.07	1.43	1.47
2	D	301[A]	3L5	C5-C6	-2.07	1.43	1.47
2	E	301[A]	3L5	C5-C6	-2.06	1.43	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301[B]	3L5	CAM-NAZ-CAN	3.78	120.43	111.44
2	F	301	3L5	CAM-CAO-N9	-3.50	104.85	110.80
2	E	301[A]	3L5	CAM-CAO-N9	-3.49	104.87	110.80
2	C	301[A]	3L5	OAU-CAK-CAP	3.41	119.00	109.19
2	C	301[B]	3L5	C8-N7-C5	3.26	109.20	102.99
2	E	301[B]	3L5	CAM-CAO-N9	-3.25	105.27	110.80
2	H	301[B]	3L5	C8-N7-C5	3.24	109.16	102.99
2	B	301	3L5	C8-N7-C5	3.22	109.13	102.99
2	E	301[A]	3L5	C8-N7-C5	3.22	109.12	102.99
2	H	301[A]	3L5	C8-N7-C5	3.21	109.11	102.99
2	B	301	3L5	CAM-CAO-N9	-3.21	105.34	110.80
2	A	301[A]	3L5	C8-N7-C5	3.20	109.08	102.99
2	G	301	3L5	C8-N7-C5	3.20	109.08	102.99
2	C	301[A]	3L5	C8-N7-C5	3.19	109.06	102.99
2	E	301[B]	3L5	C8-N7-C5	3.18	109.06	102.99
2	D	301[A]	3L5	C8-N7-C5	3.18	109.05	102.99
2	D	301[B]	3L5	C8-N7-C5	3.17	109.04	102.99
2	A	301[B]	3L5	C8-N7-C5	3.15	108.99	102.99
2	F	301	3L5	C8-N7-C5	3.11	108.92	102.99
2	C	301[A]	3L5	CAJ-OAU-CAK	3.11	126.75	113.29
2	D	301[B]	3L5	CAM-CAO-N9	-2.49	106.57	110.80
2	H	301[A]	3L5	CAM-CAO-N9	-2.42	106.69	110.80
2	H	301[B]	3L5	CAJ-OAU-CAK	2.41	123.72	113.29
2	H	301[A]	3L5	OAE-PBB-CAP	-2.20	107.33	111.40
2	D	301[B]	3L5	CAM-NAZ-CAL	2.14	116.53	111.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301[B]	3L5	OAG-PBC-CAQ	2.03	111.72	106.95

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[A]	3L5	CAK-CAP-PBB-OAE
2	A	301[A]	3L5	CAK-CAP-PBB-OAF
2	A	301[A]	3L5	CAK-CAP-PBB-OAC
2	A	301[A]	3L5	OAU-CAK-CAP-PBB
2	A	301[B]	3L5	OAU-CAK-CAP-PBB
2	C	301[A]	3L5	CAK-CAP-PBB-OAE
2	C	301[A]	3L5	CAK-CAP-PBB-OAF
2	C	301[A]	3L5	CAK-CAP-PBB-OAC
2	C	301[A]	3L5	OAU-CAK-CAP-PBB
2	C	301[A]	3L5	CAP-CAK-OAU-CAJ
2	D	301[A]	3L5	CAK-CAP-PBB-OAE
2	D	301[A]	3L5	CAK-CAP-PBB-OAF
2	D	301[A]	3L5	CAK-CAP-PBB-OAC
2	D	301[B]	3L5	CAK-CAP-PBB-OAE
2	E	301[A]	3L5	OAU-CAK-CAP-PBB
2	E	301[A]	3L5	CAQ-CAN-NAZ-CAL
2	E	301[A]	3L5	CAQ-CAN-NAZ-CAM
2	E	301[A]	3L5	CAN-CAQ-PBC-OAD
2	E	301[B]	3L5	CAQ-CAN-NAZ-CAL
2	E	301[B]	3L5	CAQ-CAN-NAZ-CAM
2	E	301[B]	3L5	CAN-CAQ-PBC-OAG
2	E	301[B]	3L5	CAN-CAQ-PBC-OAH
2	E	301[B]	3L5	CAN-CAQ-PBC-OAD
2	G	301	3L5	CAK-CAP-PBB-OAE
2	G	301	3L5	CAK-CAP-PBB-OAF
2	G	301	3L5	CAK-CAP-PBB-OAC
2	H	301[A]	3L5	OAU-CAK-CAP-PBB
2	H	301[B]	3L5	CAP-CAK-OAU-CAJ
2	H	301[B]	3L5	CAQ-CAN-NAZ-CAL
2	H	301[B]	3L5	CAQ-CAN-NAZ-CAM
2	C	301[A]	3L5	CAO-CAM-NAZ-CAL
2	D	301[B]	3L5	OAU-CAJ-CAL-NAZ
2	B	301	3L5	OAU-CAJ-CAL-NAZ
2	C	301[B]	3L5	OAU-CAJ-CAL-NAZ
2	E	301[B]	3L5	NAZ-CAM-CAO-N9
2	D	301[A]	3L5	OAU-CAJ-CAL-NAZ

Continued on next page...

Continued from previous page...

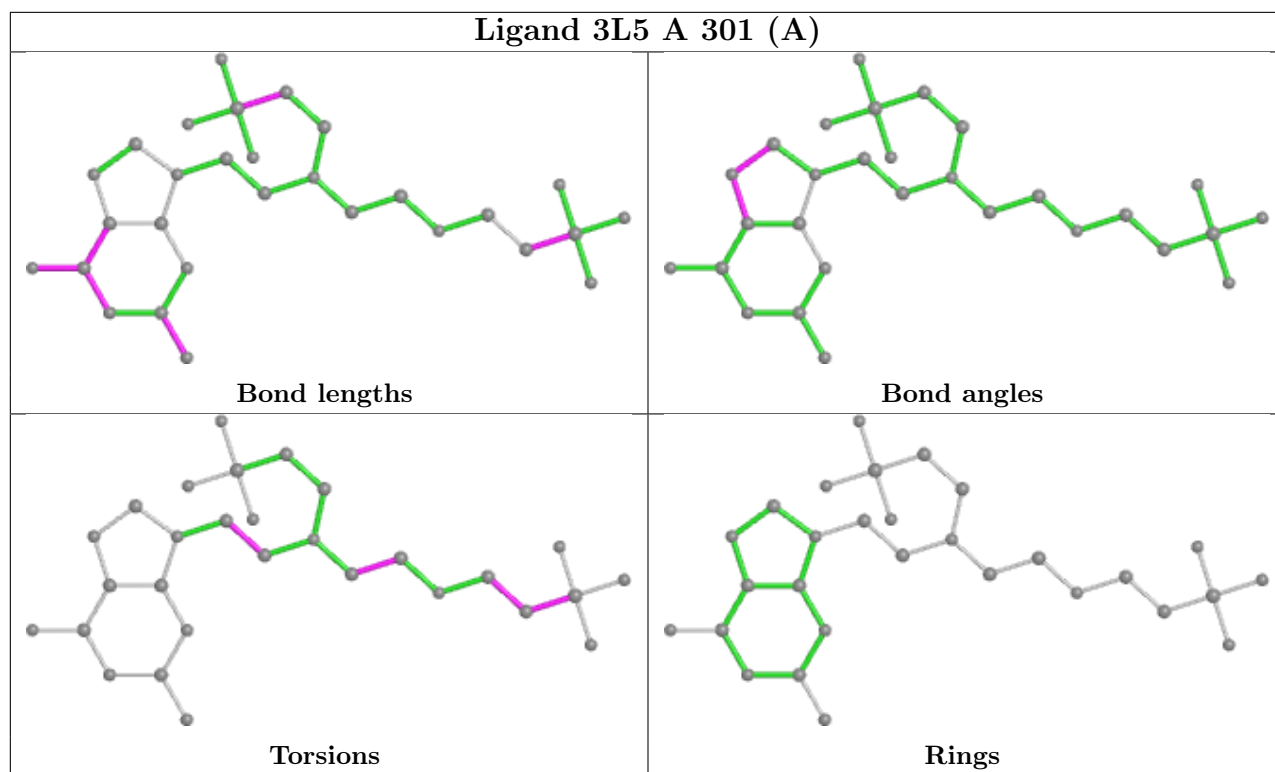
Mol	Chain	Res	Type	Atoms
2	D	301[B]	3L5	OAU-CAK-CAP-PBB
2	E	301[B]	3L5	OAU-CAK-CAP-PBB
2	E	301[A]	3L5	NAZ-CAM-CAO-N9
2	D	301[A]	3L5	CAL-CAJ-OAU-CAK
2	B	301	3L5	CAP-CAK-OAU-CAJ
2	D	301[A]	3L5	NAZ-CAM-CAO-N9
2	C	301[B]	3L5	CAP-CAK-OAU-CAJ
2	D	301[A]	3L5	CAO-CAM-NAZ-CAL
2	G	301	3L5	CAP-CAK-OAU-CAJ
2	C	301[A]	3L5	CAL-CAJ-OAU-CAK
2	H	301[B]	3L5	CAL-CAJ-OAU-CAK
2	C	301[B]	3L5	CAL-CAJ-OAU-CAK
2	D	301[B]	3L5	NAZ-CAM-CAO-N9
2	E	301[B]	3L5	OAU-CAJ-CAL-NAZ
2	A	301[B]	3L5	OAU-CAJ-CAL-NAZ
2	E	301[A]	3L5	CAN-CAQ-PBC-OAG
2	E	301[A]	3L5	CAN-CAQ-PBC-OAH
2	D	301[A]	3L5	CAP-CAK-OAU-CAJ
2	E	301[B]	3L5	CAP-CAK-OAU-CAJ
2	H	301[A]	3L5	CAP-CAK-OAU-CAJ
2	G	301	3L5	CAO-CAM-NAZ-CAN
2	B	301	3L5	NAZ-CAM-CAO-N9
2	D	301[B]	3L5	CAO-CAM-NAZ-CAL
2	D	301[B]	3L5	CAP-CAK-OAU-CAJ
2	E	301[A]	3L5	CAP-CAK-OAU-CAJ
2	F	301	3L5	NAZ-CAM-CAO-N9
2	F	301	3L5	CAL-CAJ-OAU-CAK
2	G	301	3L5	CAJ-CAL-NAZ-CAN
2	H	301[B]	3L5	CAJ-CAL-NAZ-CAM
2	A	301[A]	3L5	NAZ-CAM-CAO-N9
2	H	301[A]	3L5	CAL-CAJ-OAU-CAK
2	A	301[A]	3L5	OAU-CAJ-CAL-NAZ
2	C	301[B]	3L5	CAO-CAM-NAZ-CAN
2	D	301[B]	3L5	CAK-CAP-PBB-OAF
2	G	301	3L5	CAJ-CAL-NAZ-CAM
2	A	301[B]	3L5	NAZ-CAM-CAO-N9
2	G	301	3L5	NAZ-CAM-CAO-N9
2	D	301[B]	3L5	CAO-CAM-NAZ-CAN

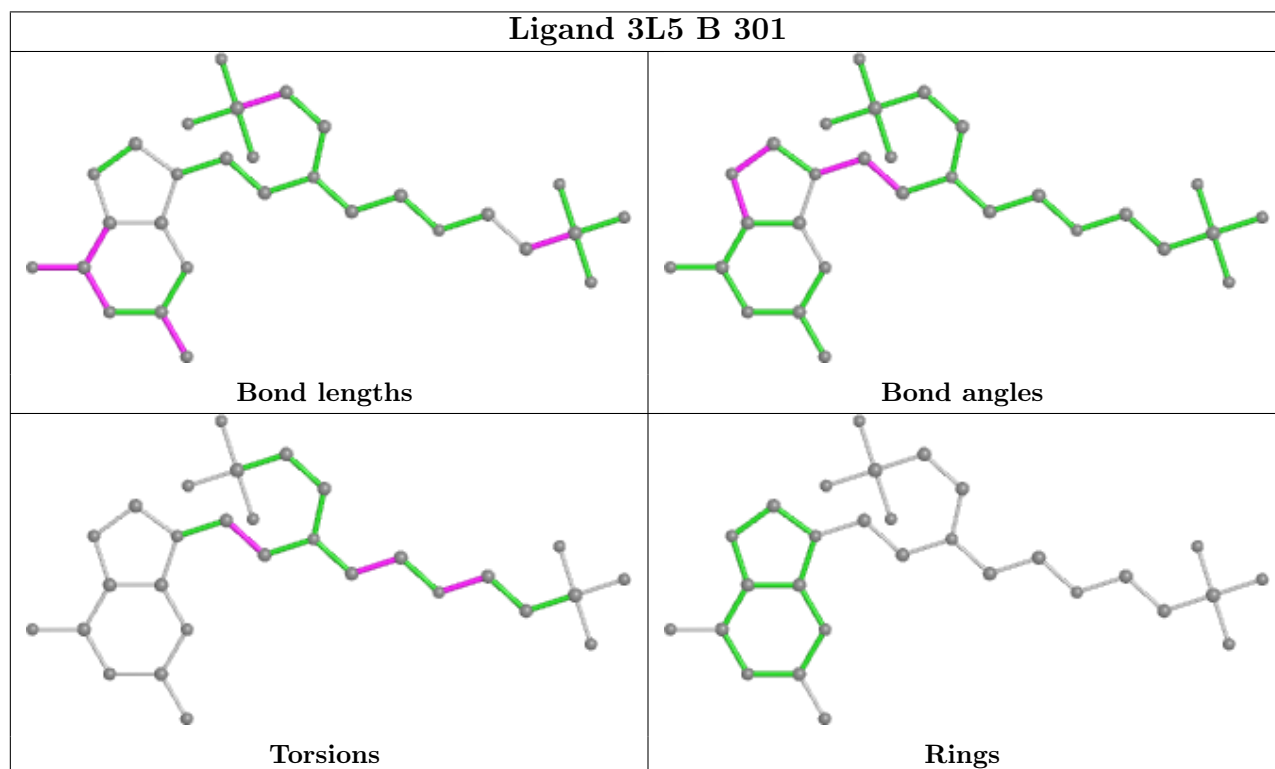
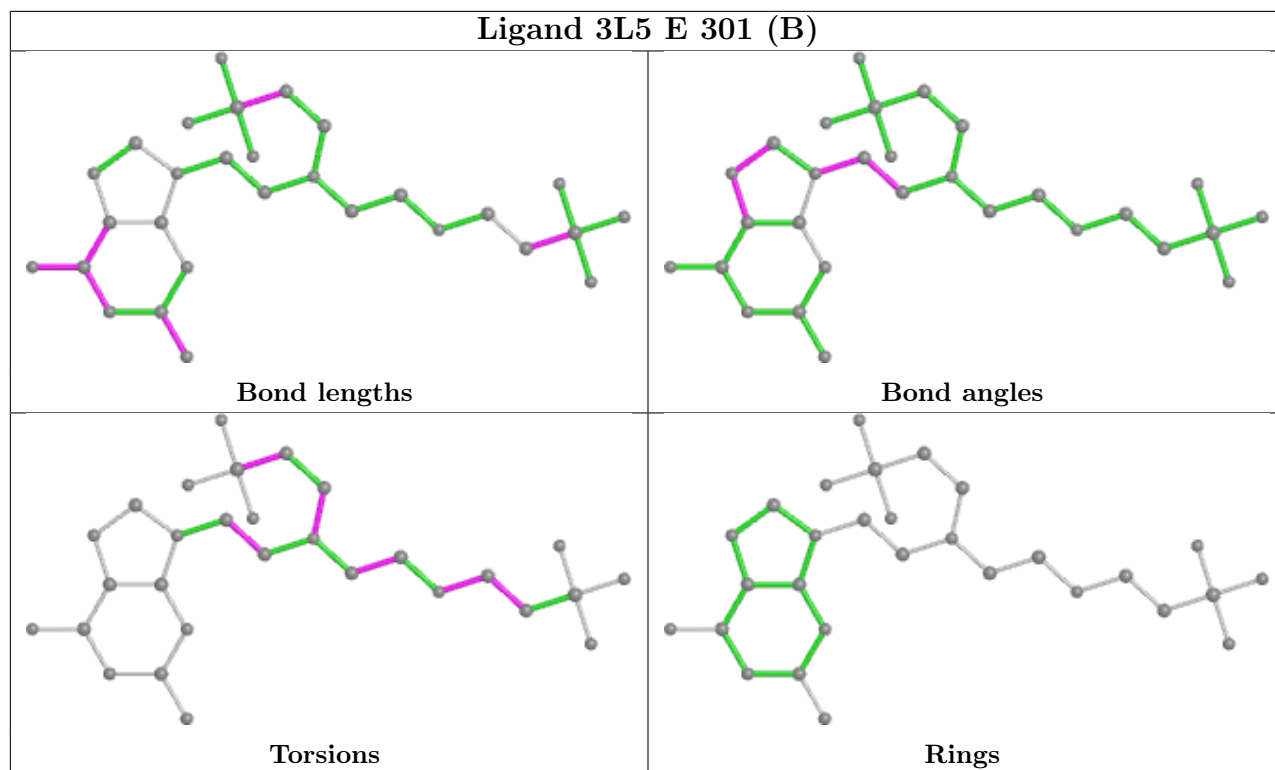
There are no ring outliers.

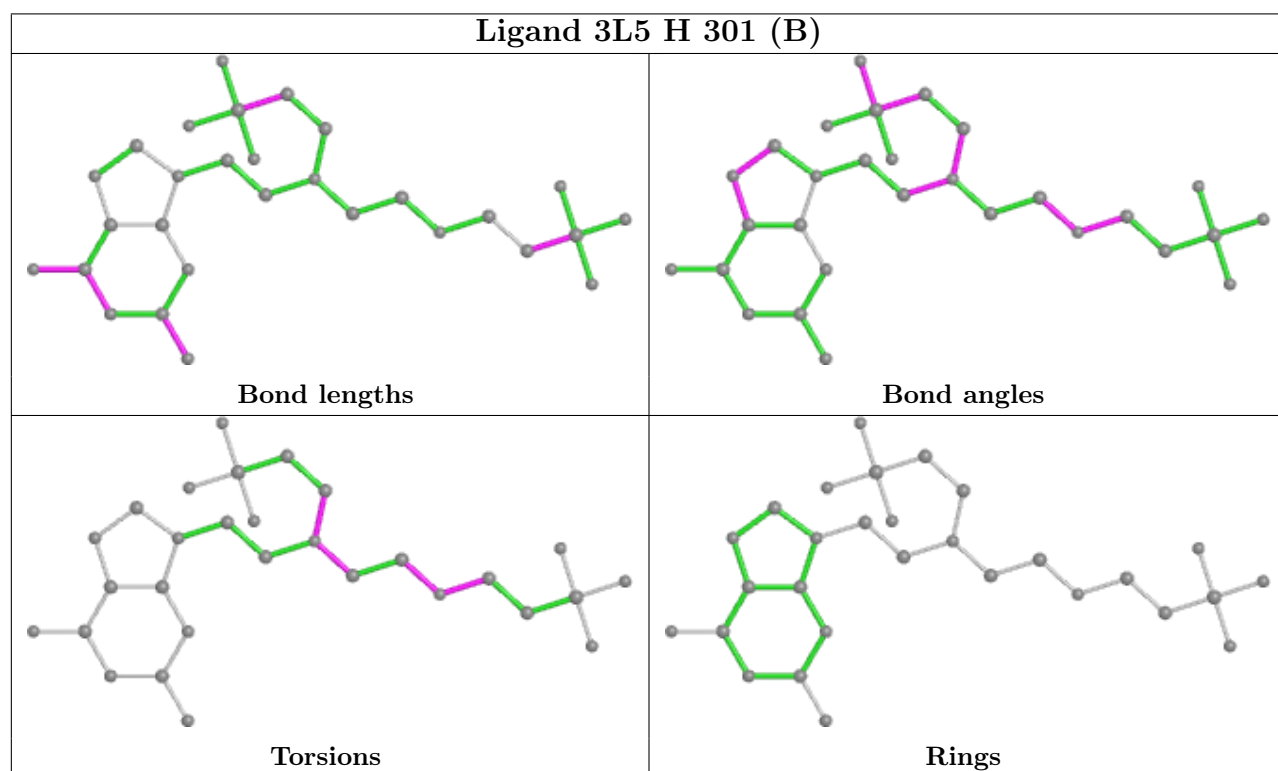
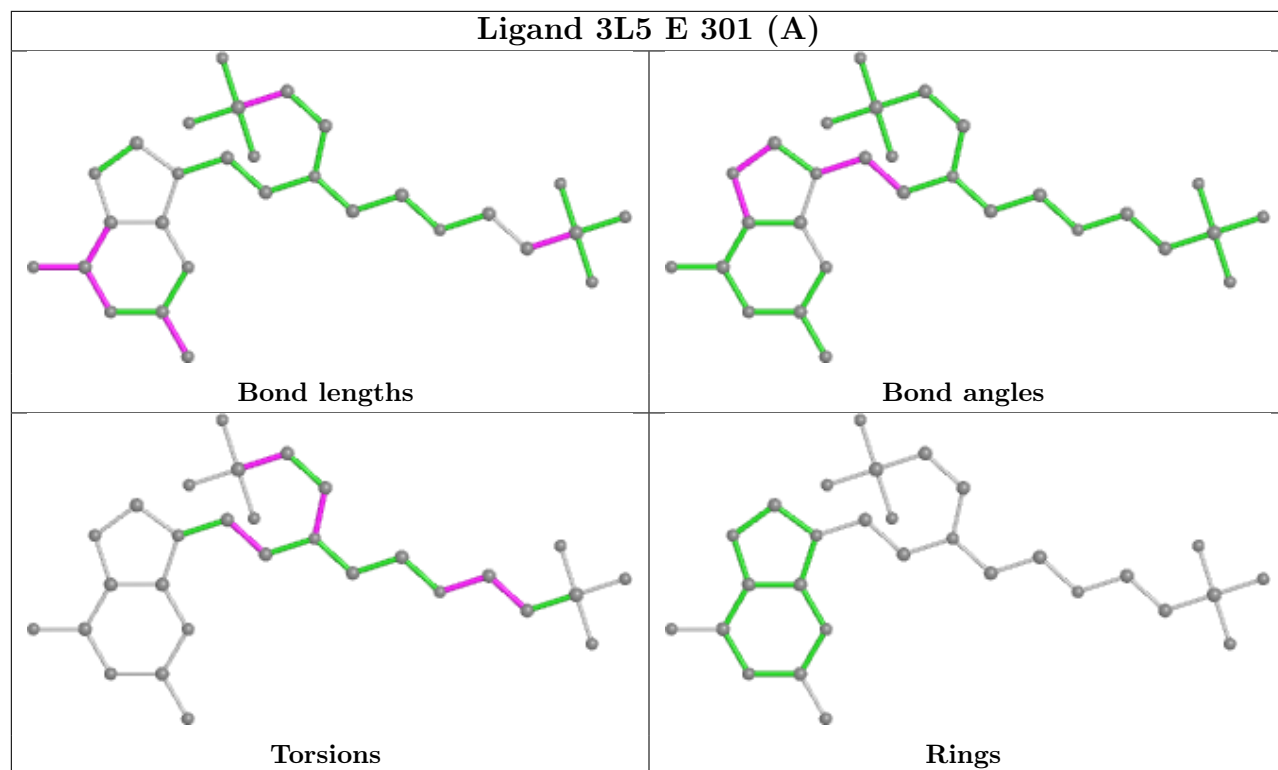
3 monomers are involved in 4 short contacts:

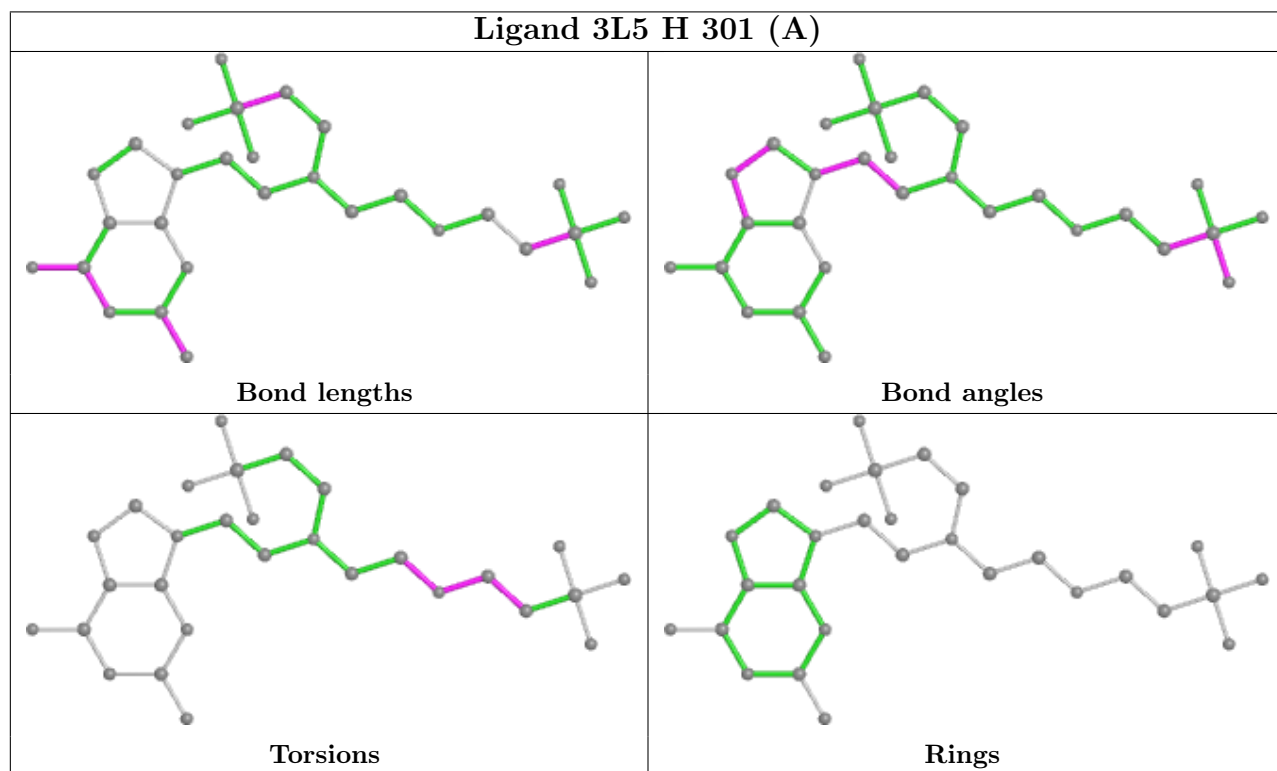
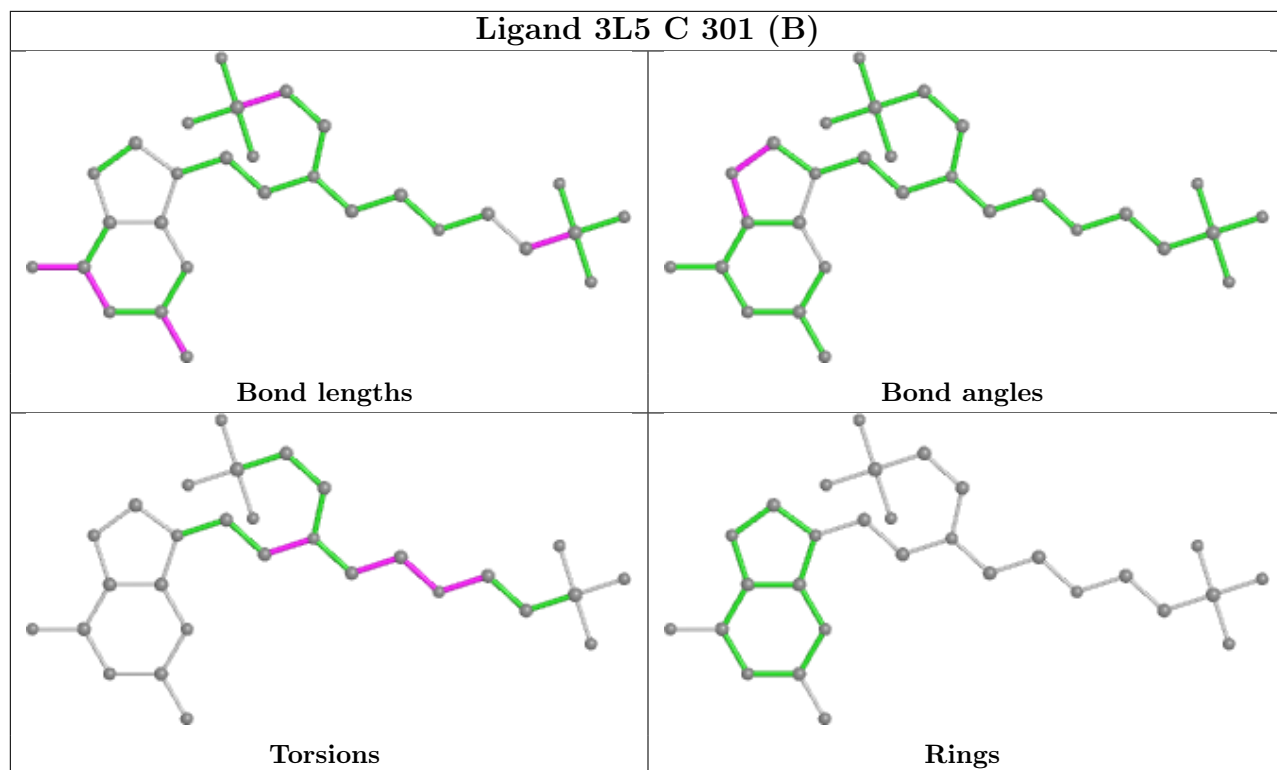
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301[A]	3L5	1	0
2	C	301[B]	3L5	2	0
2	D	301[B]	3L5	1	0

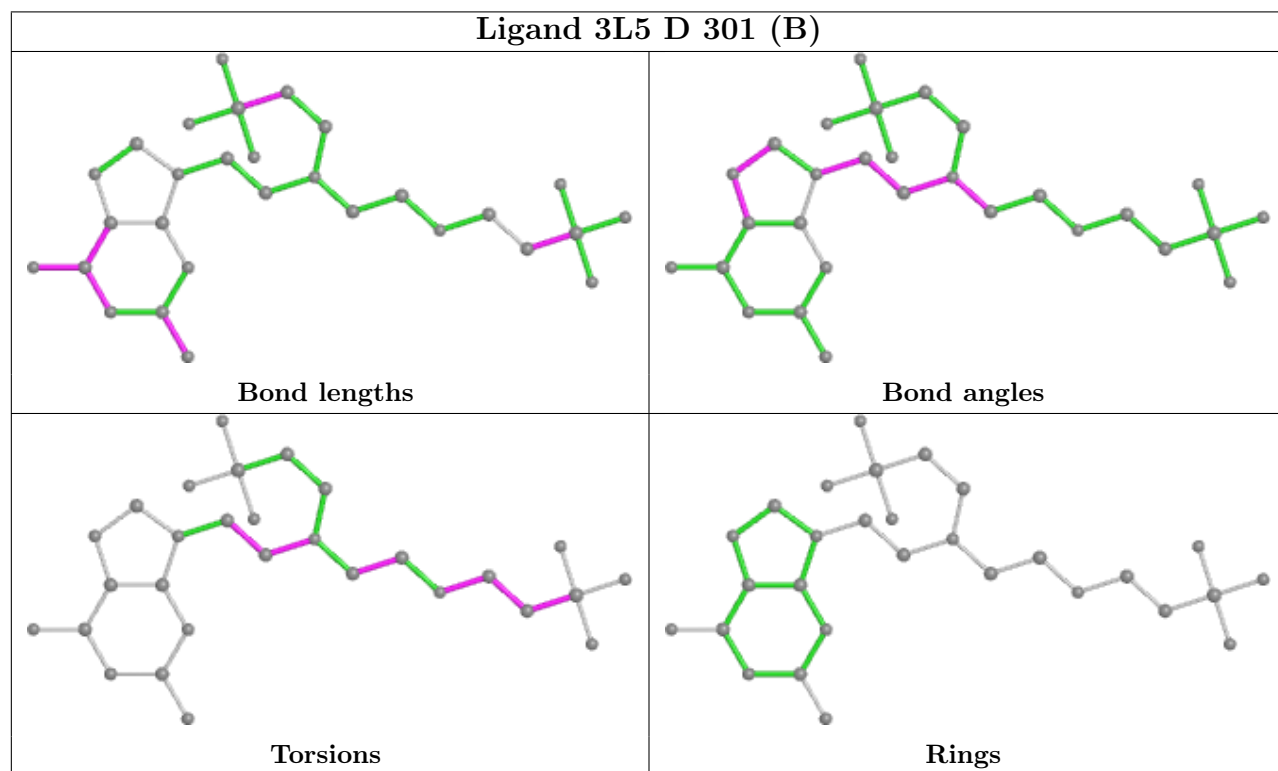
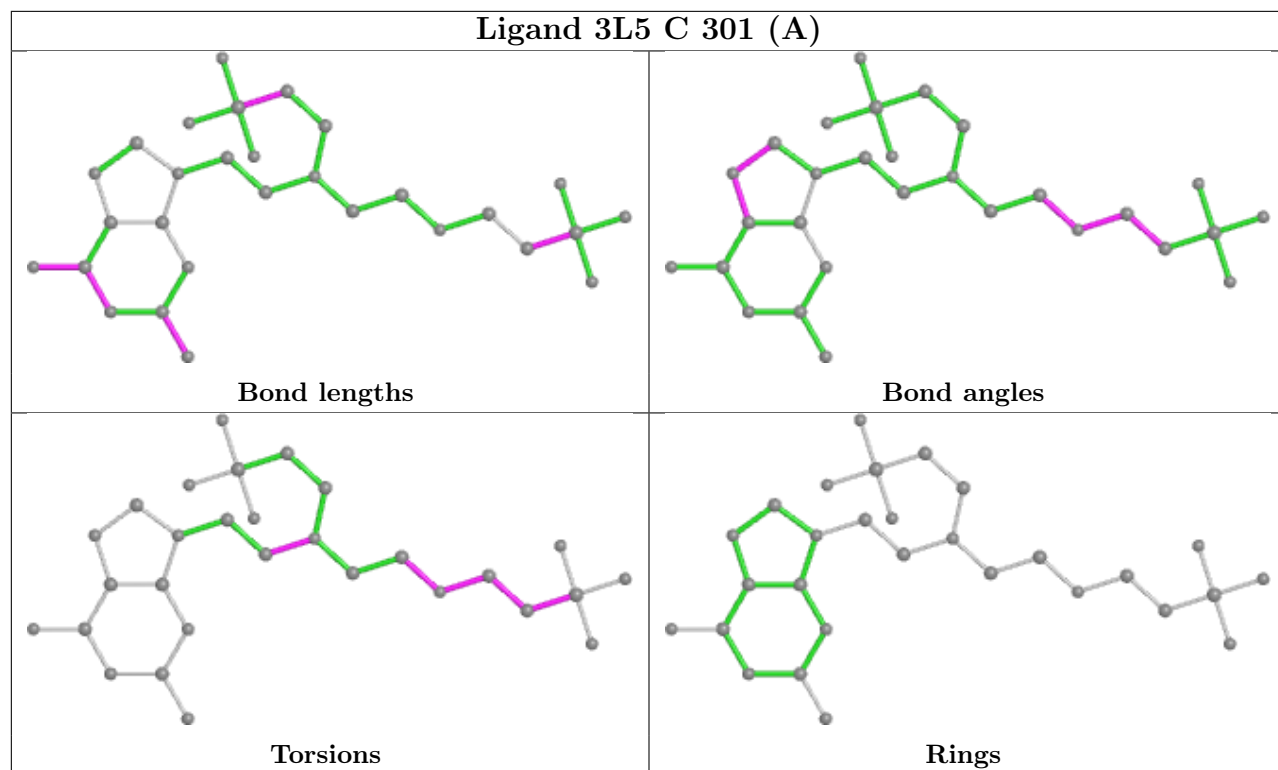
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

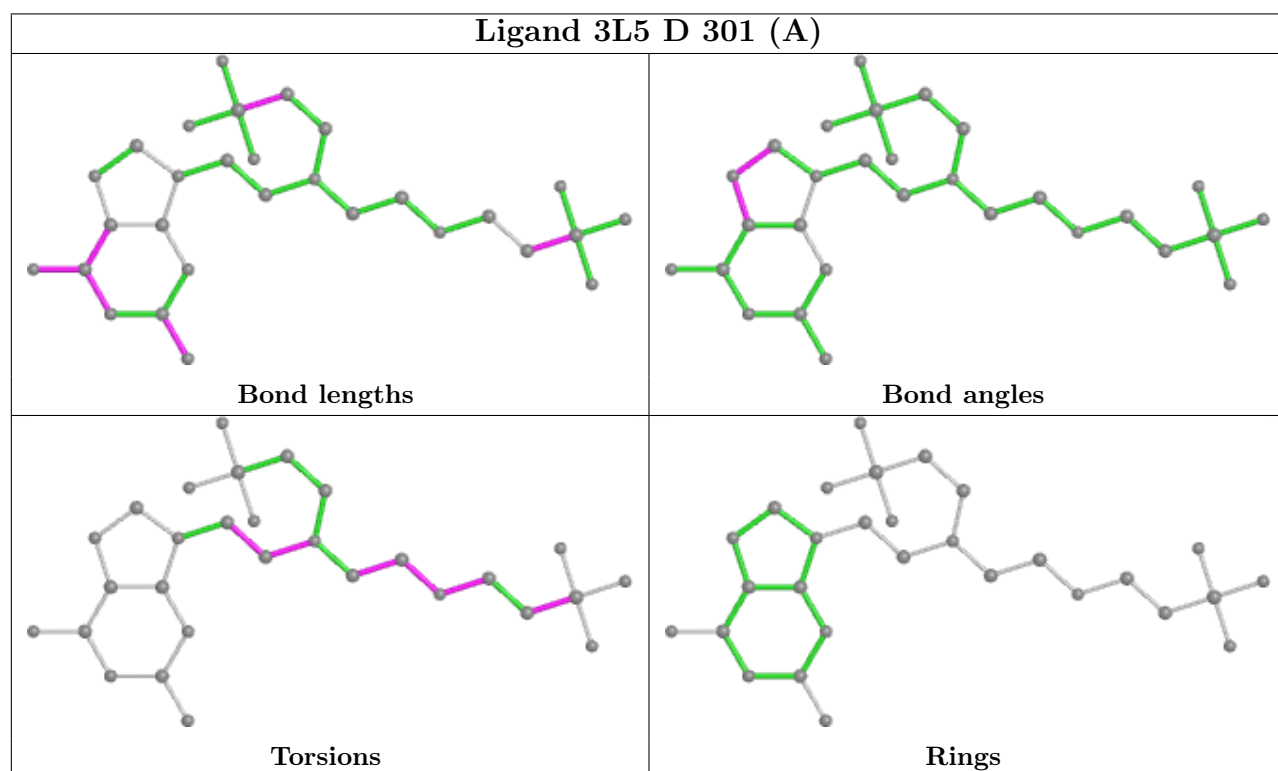
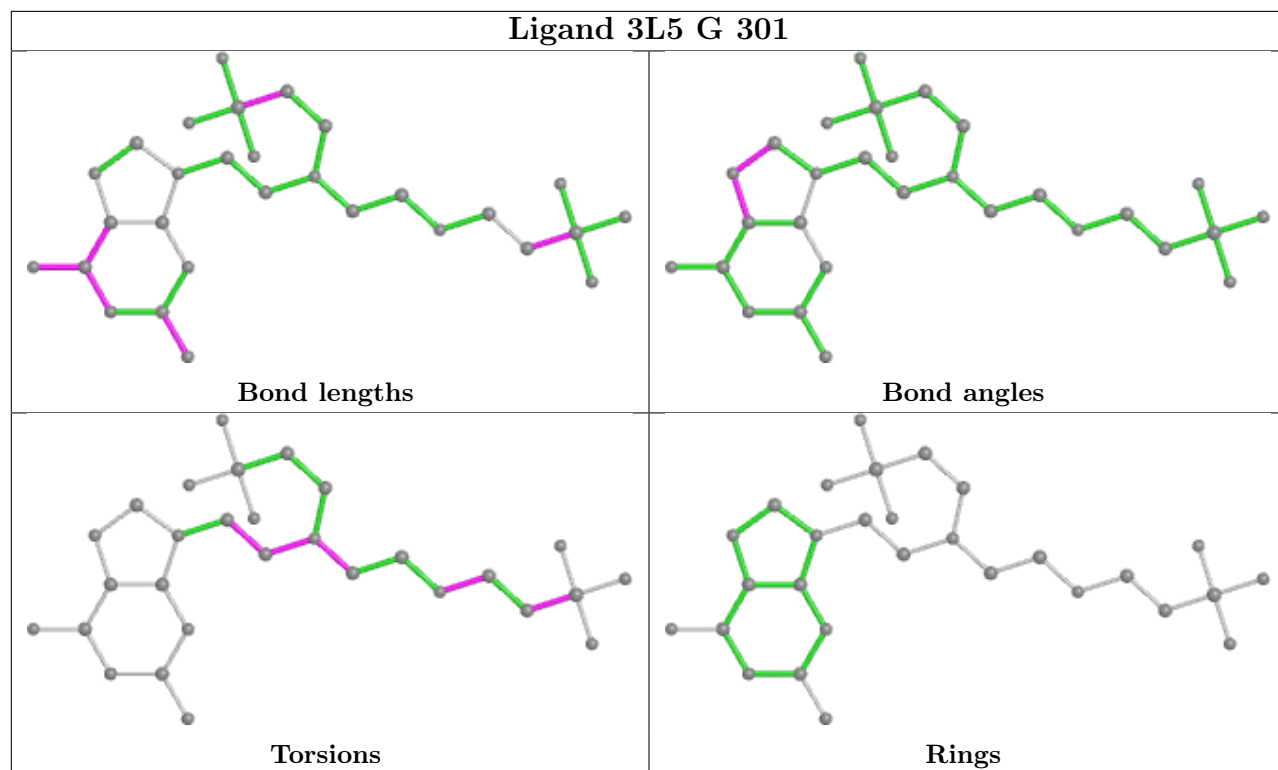


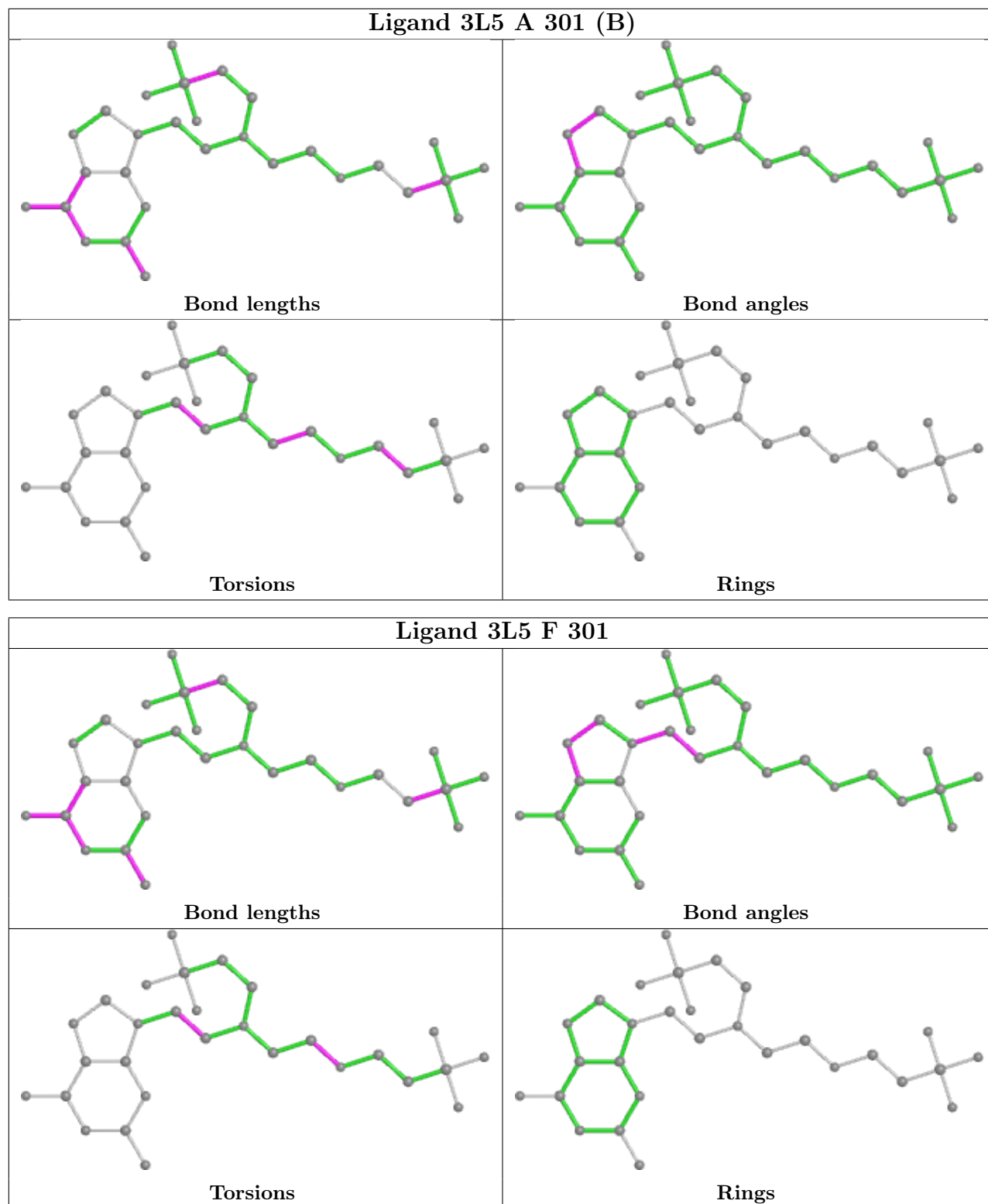












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	197/217 (90%)	0.55	15 (7%) 13 13	25, 39, 85, 107	0
1	B	207/217 (95%)	0.52	16 (7%) 13 12	26, 40, 83, 99	0
1	C	202/217 (93%)	0.29	11 (5%) 25 24	27, 43, 71, 91	0
1	D	202/217 (93%)	0.60	17 (8%) 11 10	25, 43, 67, 99	0
1	E	206/217 (94%)	1.04	39 (18%) 1 1	29, 48, 90, 134	0
1	F	197/217 (90%)	0.29	10 (5%) 28 27	24, 38, 82, 101	0
1	G	200/217 (92%)	1.18	42 (21%) 1 0	36, 66, 109, 123	0
1	H	208/217 (95%)	0.86	30 (14%) 2 2	28, 46, 86, 97	0
All	All	1619/1736 (93%)	0.67	180 (11%) 5 4	24, 44, 88, 134	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	173	TYR	11.1
1	E	121	LEU	8.6
1	C	113	ILE	6.7
1	G	144	THR	6.6
1	E	117	GLY	6.6
1	E	217	ALA	6.5
1	A	169	ARG	6.1
1	D	217	ALA	6.0
1	B	111	GLY	5.5
1	H	104	TYR	5.5
1	B	217	ALA	5.4
1	G	148	LEU	5.3
1	E	90	ARG	5.0
1	E	168	PRO	5.0
1	H	171	VAL	4.9
1	D	92	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	112	ASP	4.5
1	E	216	LYS	4.5
1	G	145	LEU	4.5
1	E	116	ILE	4.4
1	A	168	PRO	4.4
1	E	118	GLY	4.4
1	H	217	ALA	4.1
1	C	213	ALA	4.1
1	H	210	THR	4.0
1	E	59	HIS	4.0
1	E	210	THR	3.9
1	H	209	GLU	3.9
1	D	4	SER	3.9
1	A	210	THR	3.9
1	D	173	TYR	3.8
1	G	152	TYR	3.8
1	E	104	TYR	3.8
1	B	121	LEU	3.8
1	G	167	THR	3.8
1	E	211	GLY	3.8
1	E	71	TYR	3.7
1	C	211	GLY	3.7
1	H	169	ARG	3.7
1	B	152	TYR	3.6
1	G	125	THR	3.6
1	H	103	SER	3.6
1	G	143	GLN	3.6
1	E	209	GLU	3.4
1	G	58	GLY	3.4
1	G	217	ALA	3.4
1	E	167	THR	3.4
1	E	103	SER	3.3
1	E	113	ILE	3.3
1	A	121	LEU	3.3
1	A	209	GLU	3.3
1	G	140	LYS	3.3
1	G	120	ASP	3.3
1	G	5	PRO	3.3
1	G	89	ASP	3.3
1	F	60	HIS	3.3
1	C	90	ARG	3.3
1	C	114	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	211	GLY	3.2
1	A	117	GLY	3.2
1	E	197	TYR	3.1
1	G	121	LEU	3.1
1	D	140	LYS	3.1
1	A	170	SER	3.1
1	G	90	ARG	3.1
1	G	113	ILE	3.1
1	D	169	ARG	3.0
1	E	73	PHE	3.0
1	F	92	ILE	3.0
1	H	207	ILE	3.0
1	H	89	ASP	3.0
1	H	29	GLU	2.9
1	G	92	ILE	2.9
1	F	173	TYR	2.9
1	G	75	ALA	2.9
1	F	125	THR	2.9
1	B	209	GLU	2.9
1	G	150	ARG	2.9
1	F	124	LEU	2.9
1	E	120	ASP	2.9
1	D	172	GLY	2.9
1	B	103	SER	2.9
1	G	29	GLU	2.9
1	C	150	ARG	2.8
1	H	208	SER	2.8
1	D	168	PRO	2.8
1	H	173	TYR	2.8
1	G	124	LEU	2.8
1	G	149	VAL	2.8
1	E	119	ASP	2.7
1	G	115	VAL	2.7
1	C	209	GLU	2.7
1	E	72	LYS	2.7
1	G	98	PHE	2.7
1	B	174	LYS	2.7
1	H	216	LYS	2.7
1	F	89	ASP	2.7
1	B	151	GLN	2.7
1	E	207	ILE	2.7
1	G	122	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	147	SER	2.7
1	E	74	PHE	2.7
1	D	12	ASP	2.7
1	H	112	ASP	2.6
1	G	210	THR	2.6
1	H	117	GLY	2.6
1	H	168	PRO	2.6
1	G	25	ASN	2.6
1	C	194	TYR	2.6
1	H	73	PHE	2.6
1	A	89	ASP	2.5
1	B	148	LEU	2.6
1	G	23	ILE	2.5
1	D	216	LYS	2.5
1	E	213	ALA	2.5
1	D	54	LYS	2.5
1	H	212	LYS	2.5
1	D	71	TYR	2.4
1	E	185	LYS	2.4
1	D	74	PHE	2.4
1	D	167	THR	2.4
1	E	172	GLY	2.4
1	H	65	CYS	2.4
1	E	75	ALA	2.4
1	F	174	LYS	2.4
1	G	139	GLY	2.4
1	G	168	PRO	2.3
1	B	58	GLY	2.3
1	B	216	LYS	2.3
1	G	101	LEU	2.3
1	H	151	GLN	2.3
1	E	65	CYS	2.3
1	B	4	SER	2.3
1	D	209	GLU	2.3
1	E	212	LYS	2.3
1	B	92	ILE	2.3
1	G	215	TYR	2.3
1	D	101	LEU	2.3
1	C	215	TYR	2.3
1	E	186	PHE	2.3
1	H	28	ALA	2.3
1	G	59	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	99	ILE	2.3
1	C	212	LYS	2.2
1	G	174	LYS	2.2
1	E	4	SER	2.2
1	A	75	ALA	2.2
1	A	213	ALA	2.2
1	B	171	VAL	2.2
1	E	111	GLY	2.2
1	E	63	ALA	2.2
1	F	75	ALA	2.2
1	G	57	GLY	2.2
1	H	190	TYR	2.2
1	H	90	ARG	2.2
1	C	29	GLU	2.2
1	E	70	GLY	2.2
1	H	75	ALA	2.2
1	D	174	LYS	2.2
1	G	54	LYS	2.2
1	A	116	ILE	2.1
1	A	77	LEU	2.1
1	E	151	GLN	2.1
1	A	217	ALA	2.1
1	E	194	TYR	2.1
1	H	71	TYR	2.1
1	H	140	LYS	2.1
1	G	216	LYS	2.1
1	F	123	THR	2.1
1	H	121	LEU	2.0
1	B	75	ALA	2.0
1	A	122	SER	2.0
1	A	78	LEU	2.0
1	G	146	LEU	2.0
1	H	116	ILE	2.0
1	H	213	ALA	2.0
1	F	150	ARG	2.0
1	B	122	SER	2.0
1	G	126	GLY	2.0
1	G	151	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

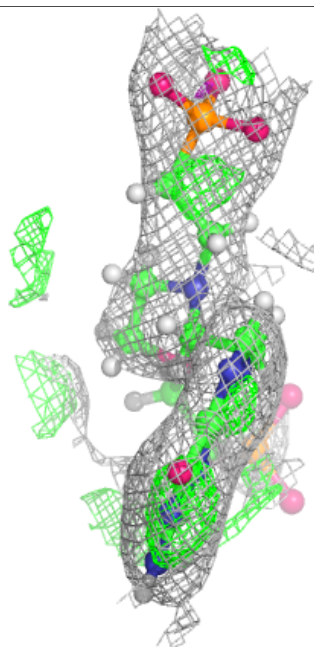
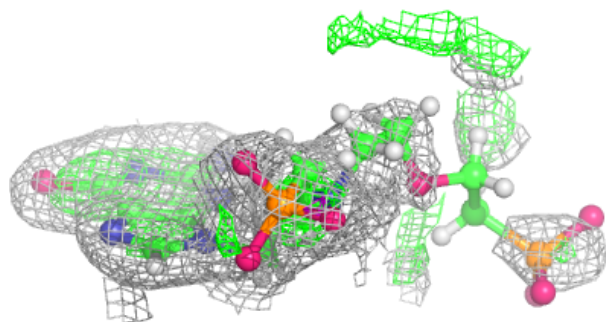
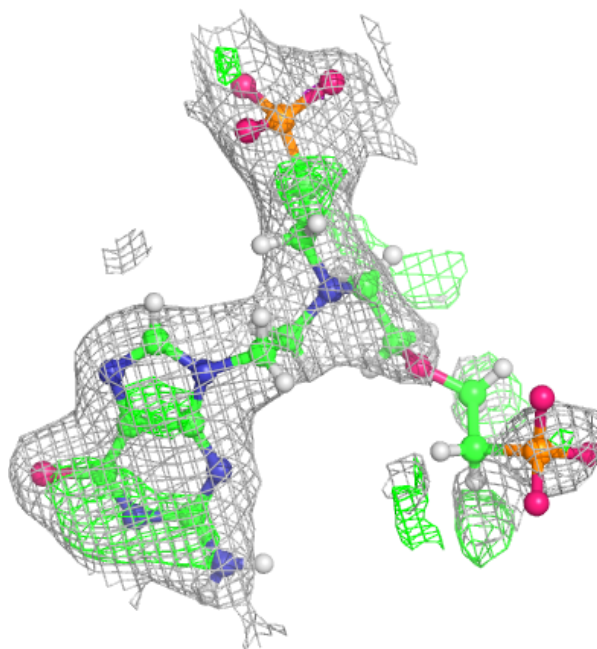
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	303	1/1	0.71	0.15	78,78,78,78	0
2	3L5	E	301[B]	29/29	0.82	0.26	48,70,112,113	48
2	3L5	E	301[A]	29/29	0.82	0.26	47,68,87,112	48
3	MG	D	302	1/1	0.82	0.10	55,55,55,55	0
2	3L5	G	301	29/29	0.85	0.22	56,83,169,169	0
2	3L5	C	301[A]	29/29	0.85	0.24	31,45,168,170	48
2	3L5	C	301[B]	29/29	0.85	0.24	31,45,172,173	48
2	3L5	A	301[B]	29/29	0.87	0.21	34,66,90,102	48
2	3L5	D	301[A]	29/29	0.87	0.19	36,44,83,83	48
3	MG	A	302	1/1	0.87	0.23	69,69,69,69	0
2	3L5	D	301[B]	29/29	0.87	0.19	36,44,85,86	48
2	3L5	A	301[A]	29/29	0.87	0.21	35,73,93,127	48
3	MG	H	302	1/1	0.88	0.14	80,80,80,80	0
2	3L5	H	301[A]	29/29	0.89	0.16	35,42,53,54	48
2	3L5	H	301[B]	29/29	0.89	0.16	36,44,64,64	48
3	MG	B	302	1/1	0.92	0.10	53,53,53,53	0
2	3L5	B	301	29/29	0.93	0.14	35,48,107,107	0
3	MG	C	302	1/1	0.94	0.12	53,53,53,53	0
3	MG	F	302	1/1	0.95	0.17	48,48,48,48	0
3	MG	F	303	1/1	0.97	0.06	51,51,51,51	0
3	MG	G	302	1/1	0.97	0.10	118,118,118,118	0
2	3L5	F	301	29/29	0.97	0.12	27,36,51,51	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.

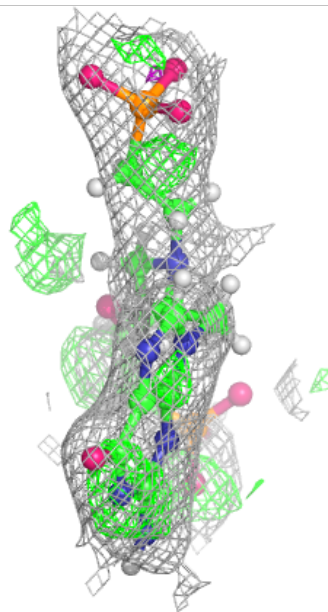
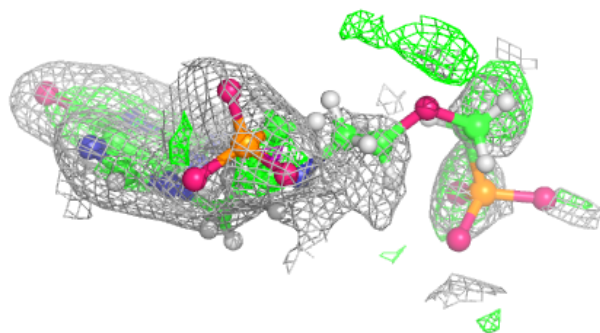
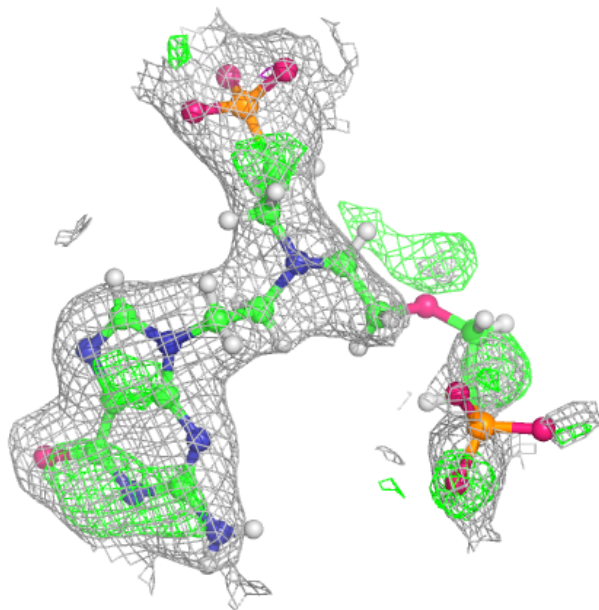
Electron density around 3L5 E 301 (B):

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



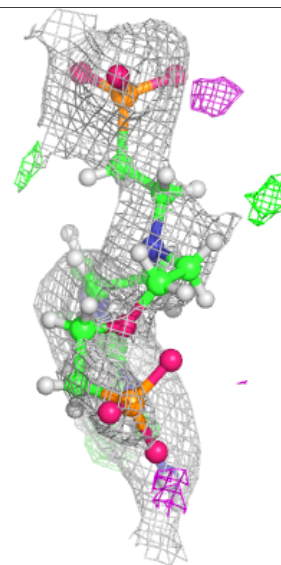
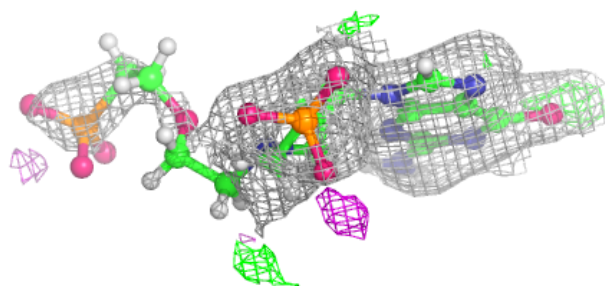
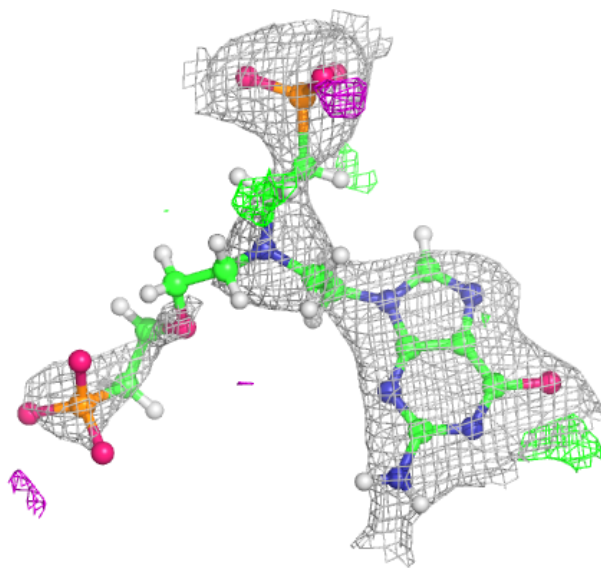
Electron density around 3L5 E 301 (A):

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



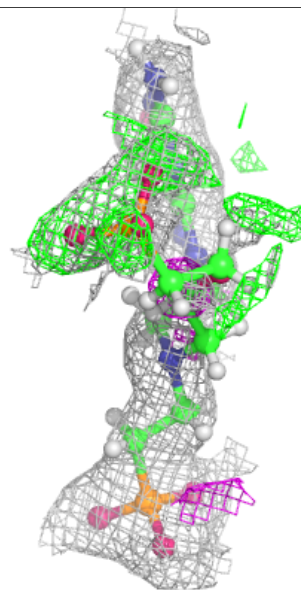
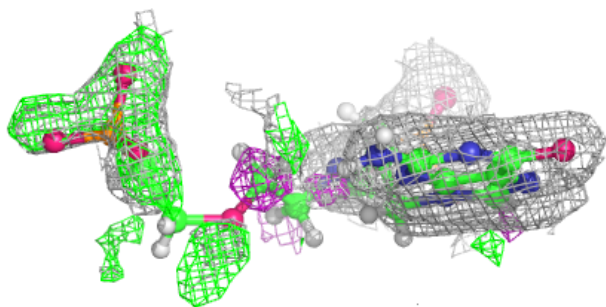
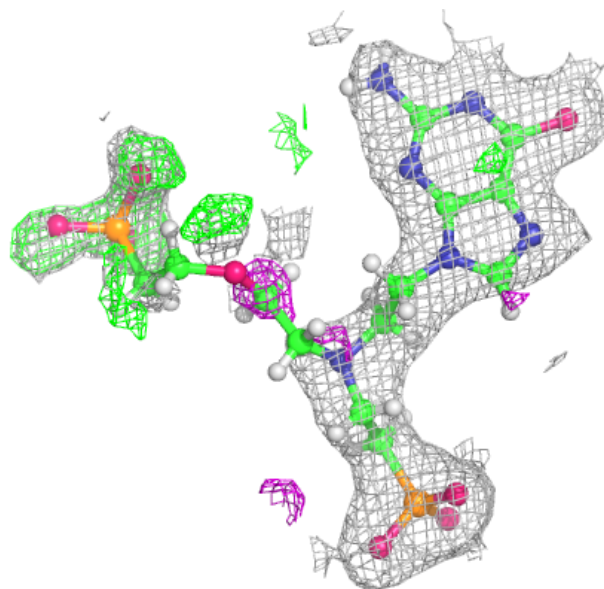
Electron density around 3L5 G 301:

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



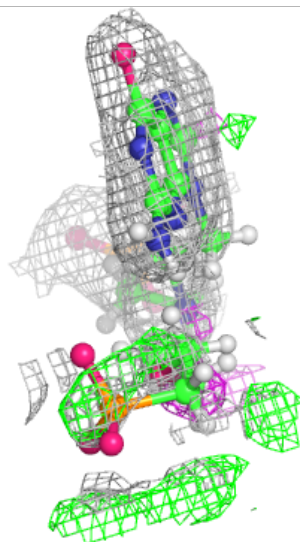
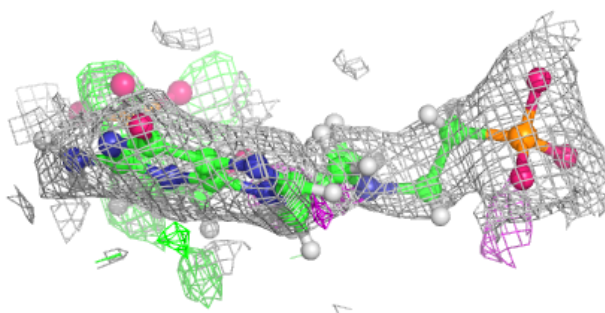
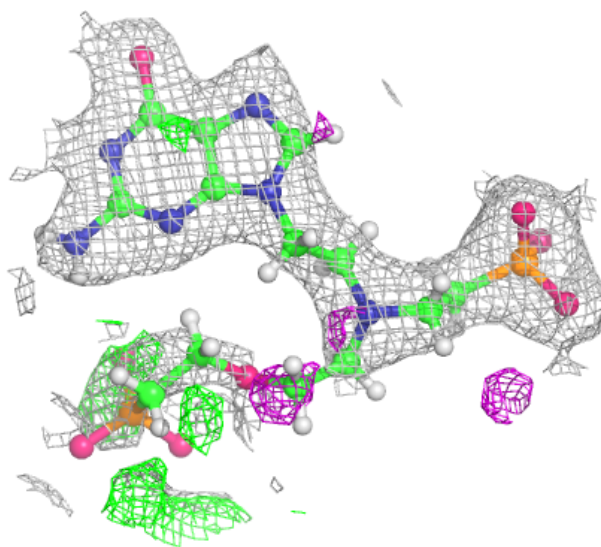
Electron density around 3L5 C 301 (A):

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



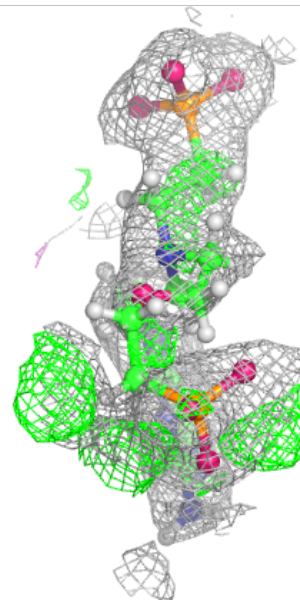
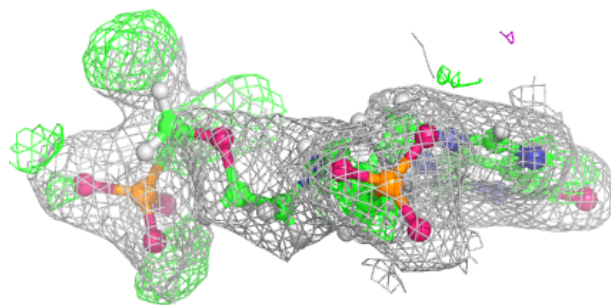
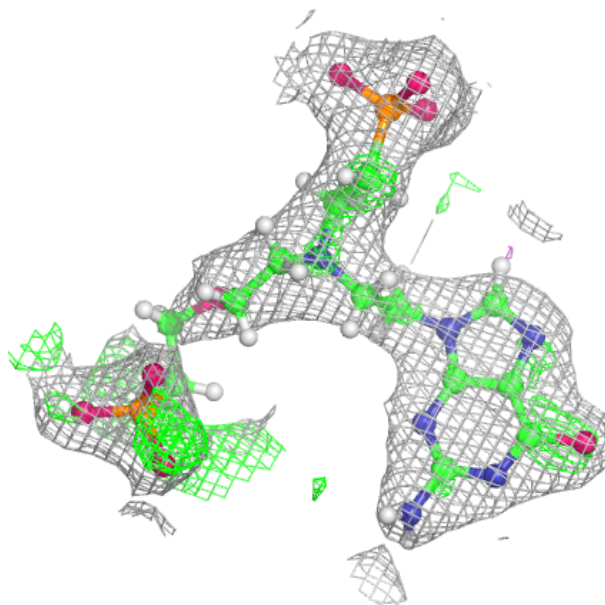
Electron density around 3L5 C 301 (B):

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



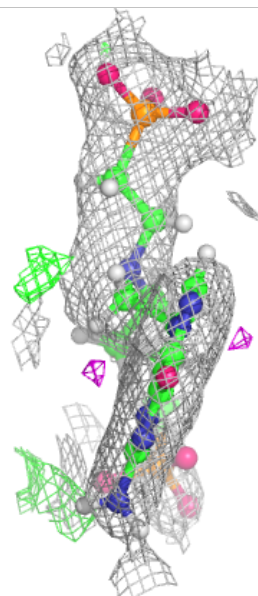
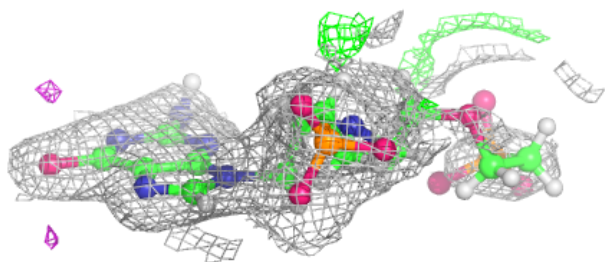
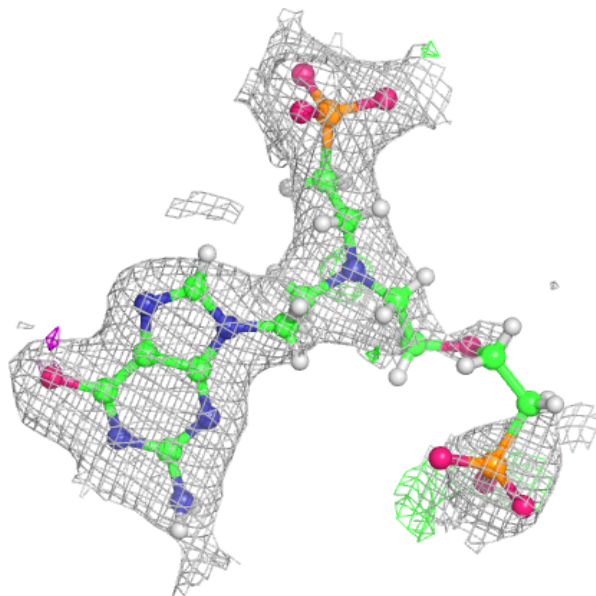
Electron density around 3L5 A 301 (B):

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



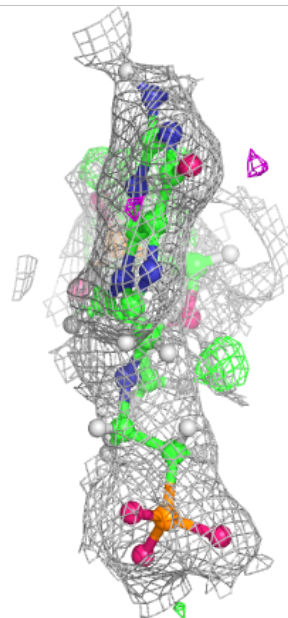
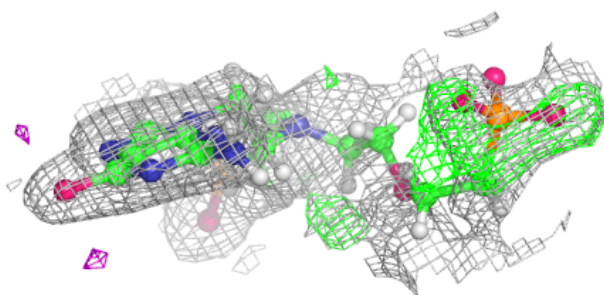
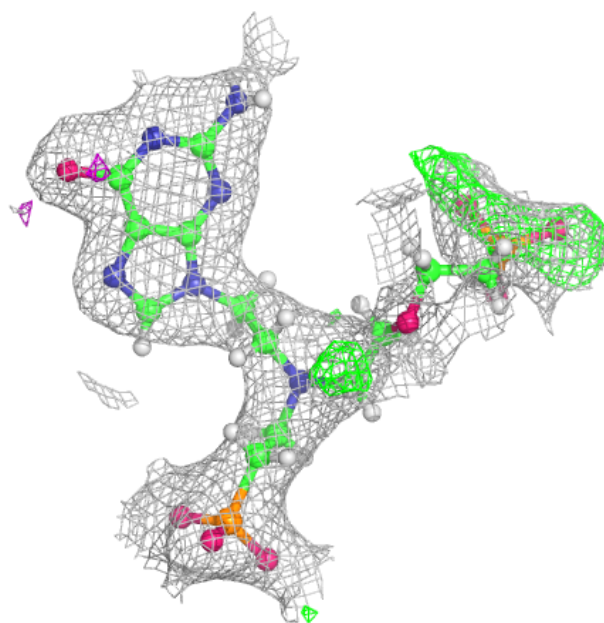
Electron density around 3L5 D 301 (A):

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



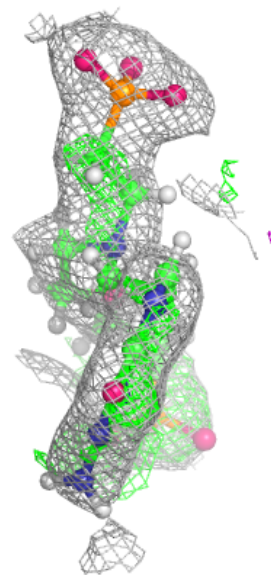
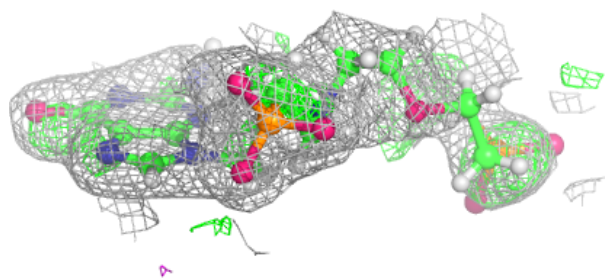
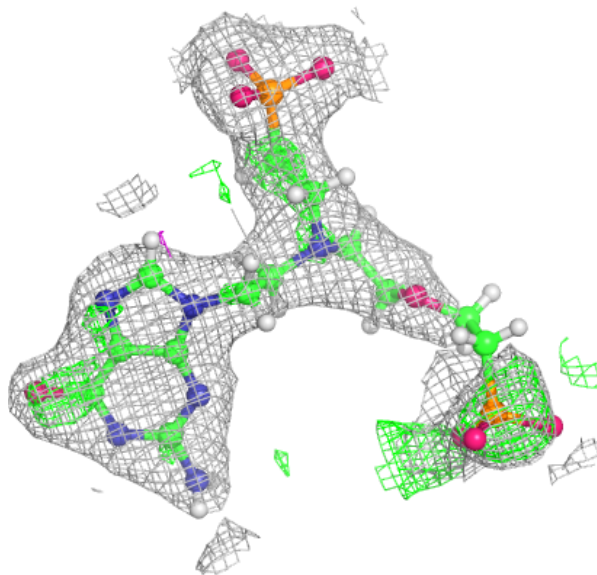
Electron density around 3L5 D 301 (B):

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



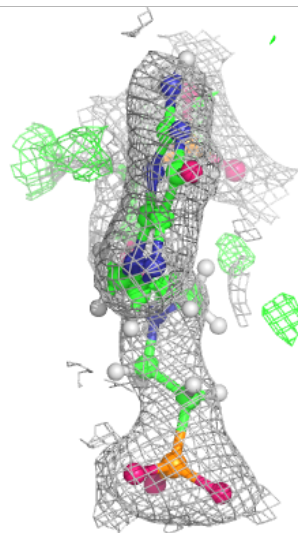
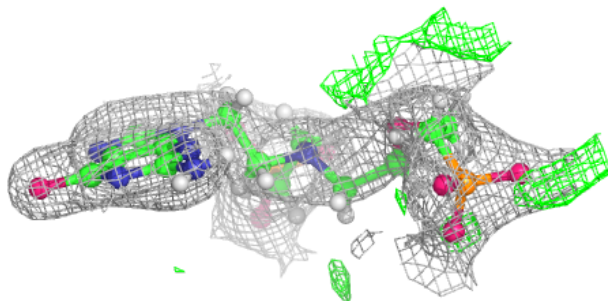
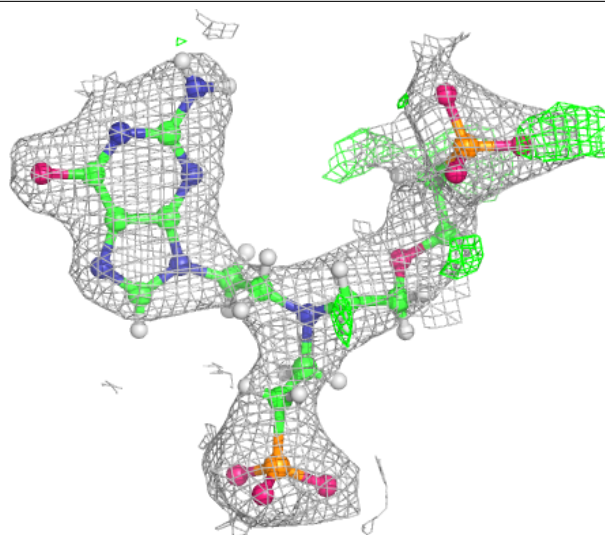
Electron density around 3L5 A 301 (A):

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



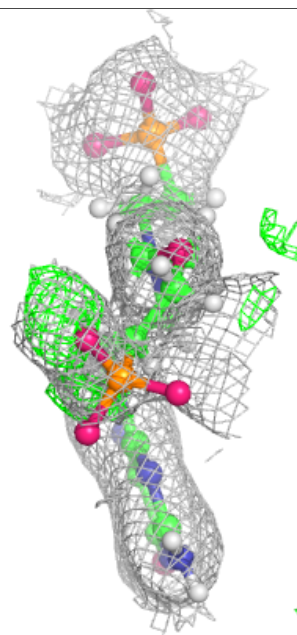
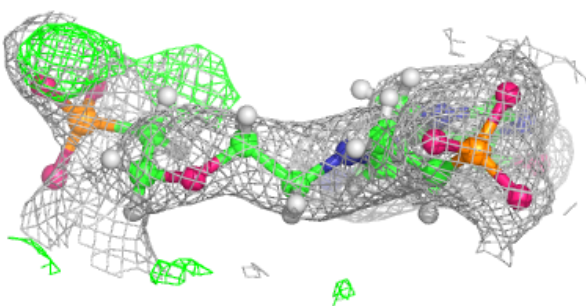
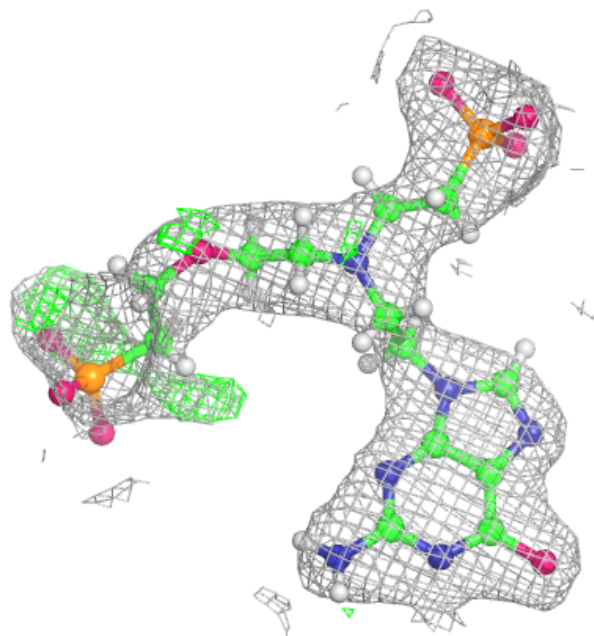
Electron density around 3L5 H 301 (A):

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



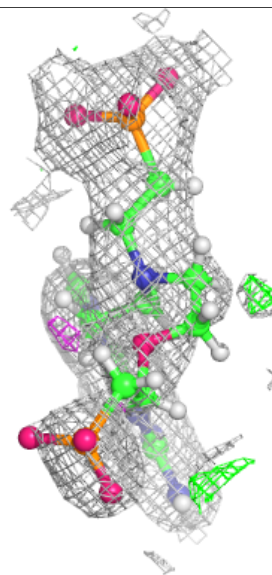
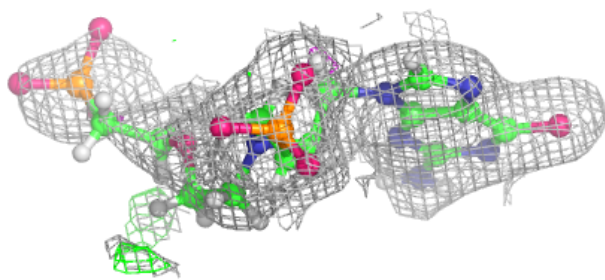
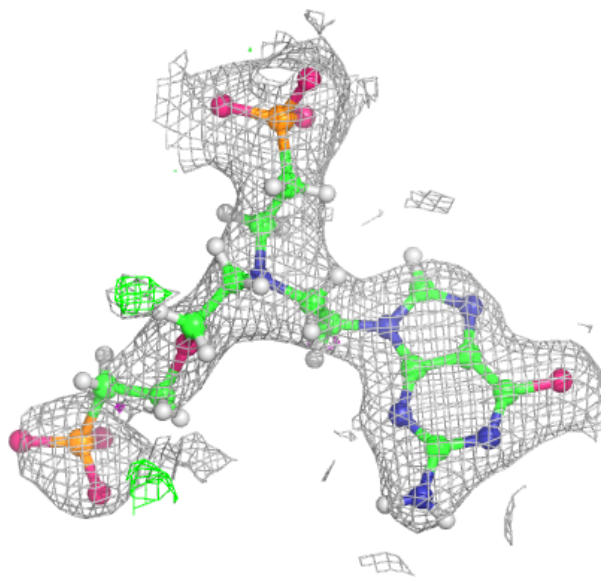
Electron density around 3L5 H 301 (B):

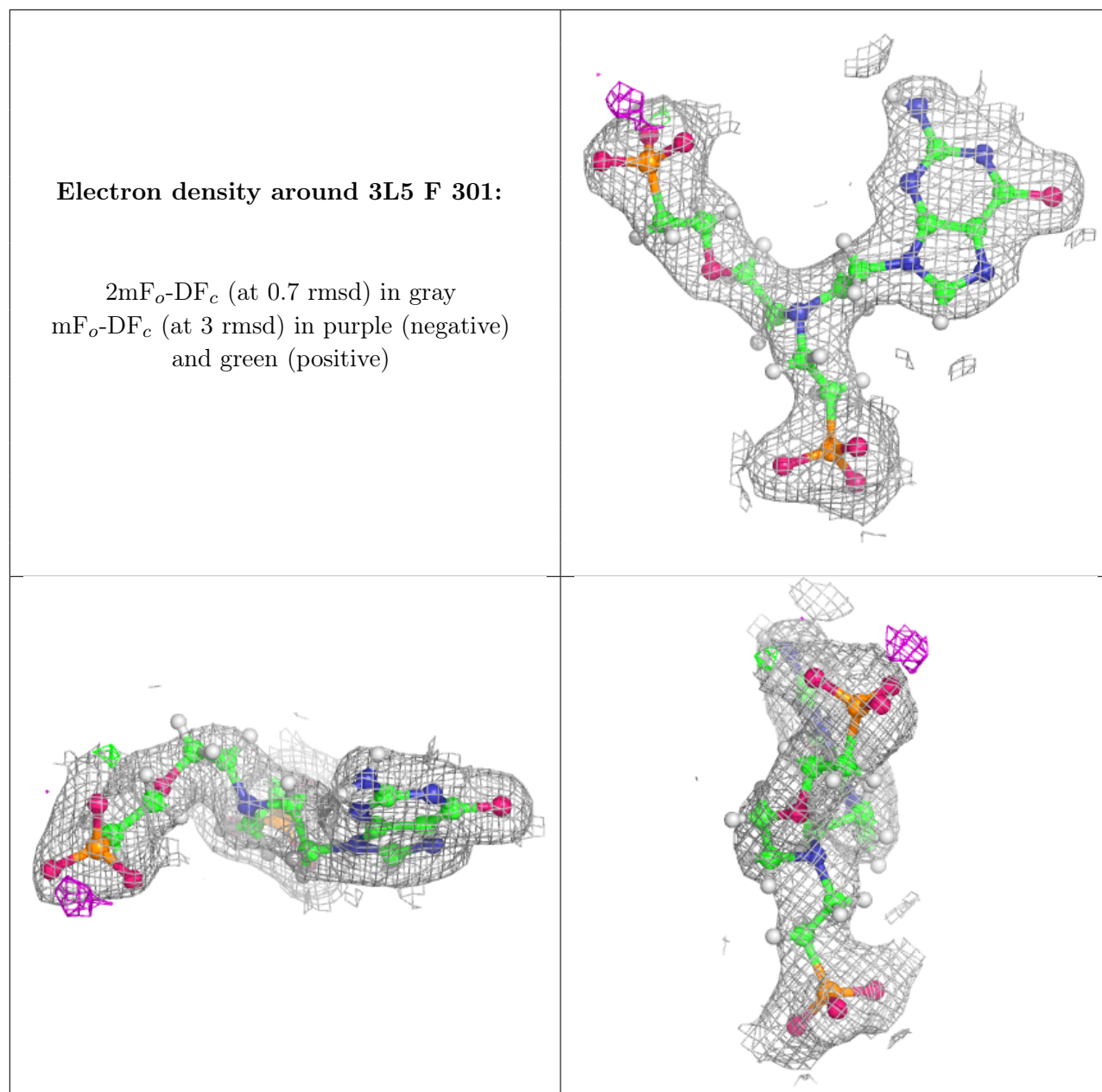
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3L5 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.