



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:58 PM UTC

PDB ID : 4RAD / pdb_00004rad
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:

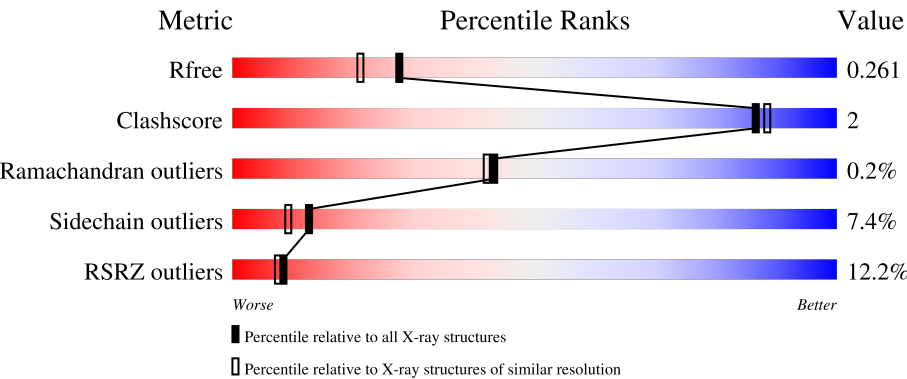
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	9% 82%9%9%
1	B	217	9% 85%10%5%
1	C	217	5% 82%12%7%
1	D	217	11% 84%7%7%
1	E	217	15% 85%10%5%

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Mol	Chain	Length	Quality of chain
1	F	217	9% 77% 12% • 9%
1	G	217	25% 80% 12% 8%
1	H	217	8% 88% 7% • •

2 Entry composition

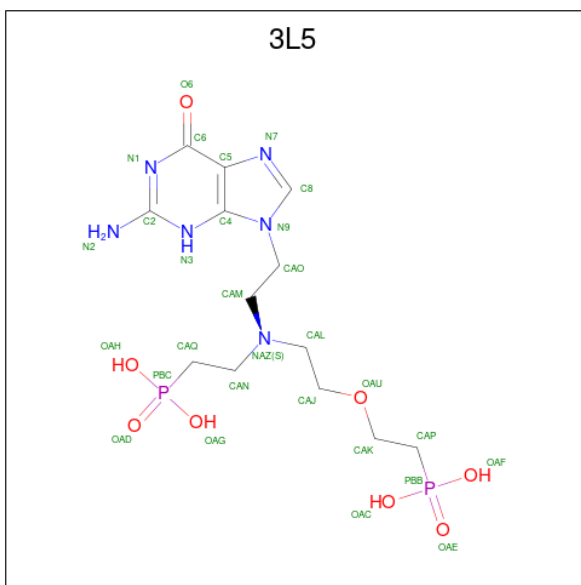
There are 4 unique types of molecules in this entry. The entry contains 26882 atoms, of which 13106 are hydrogens and 0 are deuteriums.

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

- 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 (CCD ID: 3L5) (formula: C₁₃H₂₄N₆O₈P₂).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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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

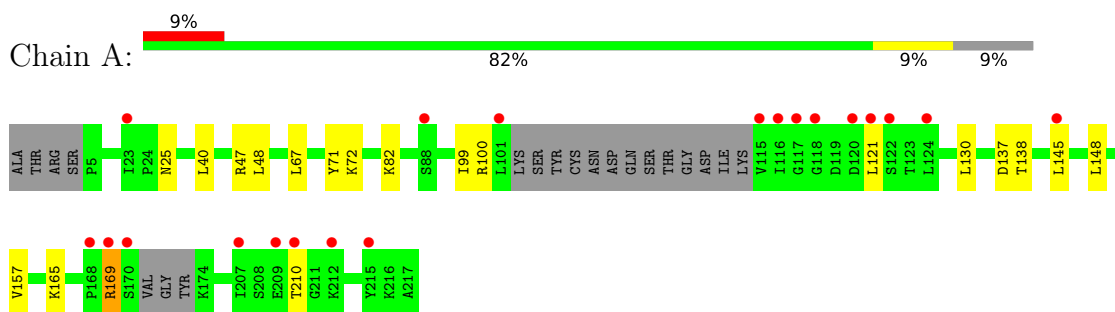
- Molecule 4 is water.

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

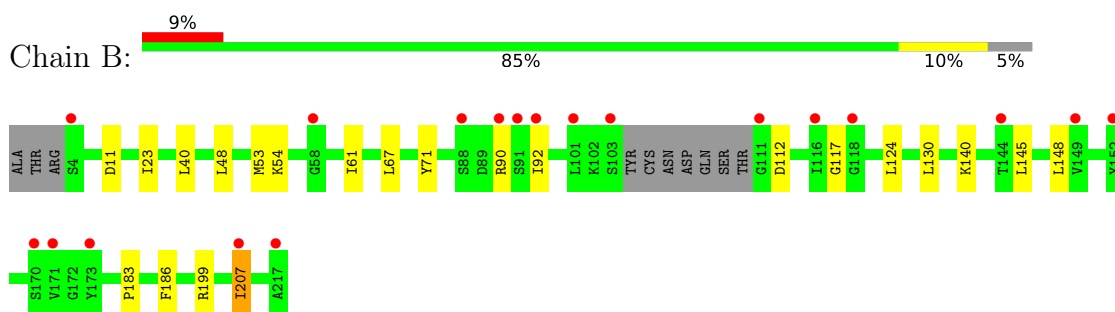
3 Residue-property plots

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.

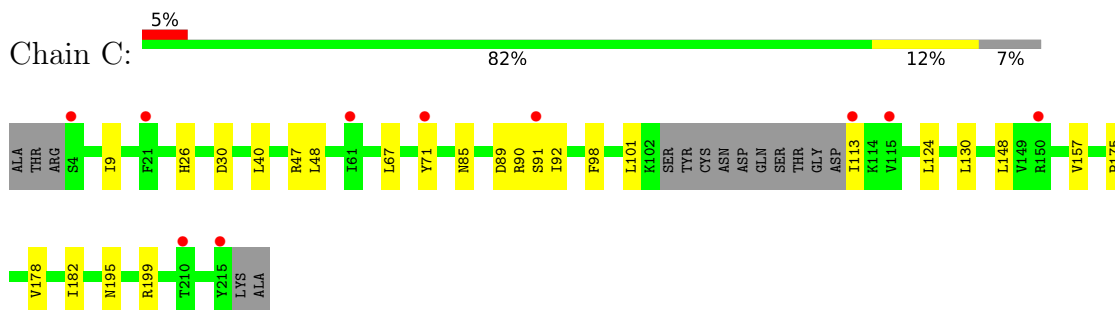
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



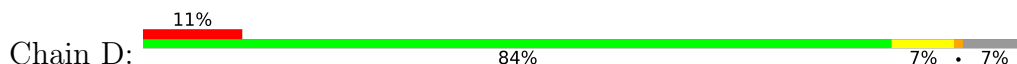
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

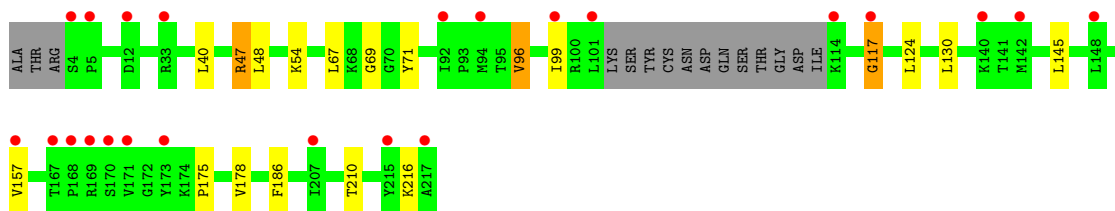


- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

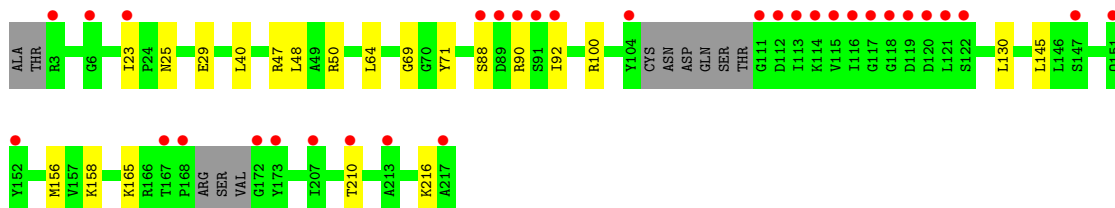
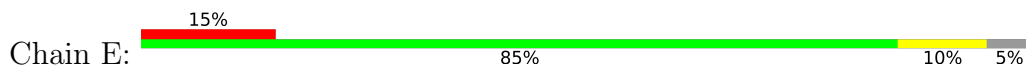


- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

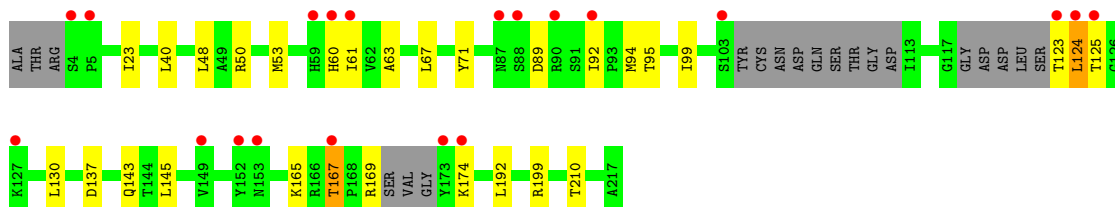
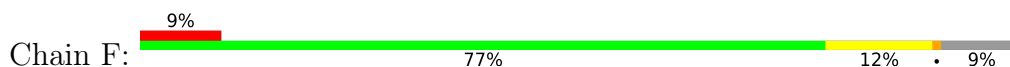




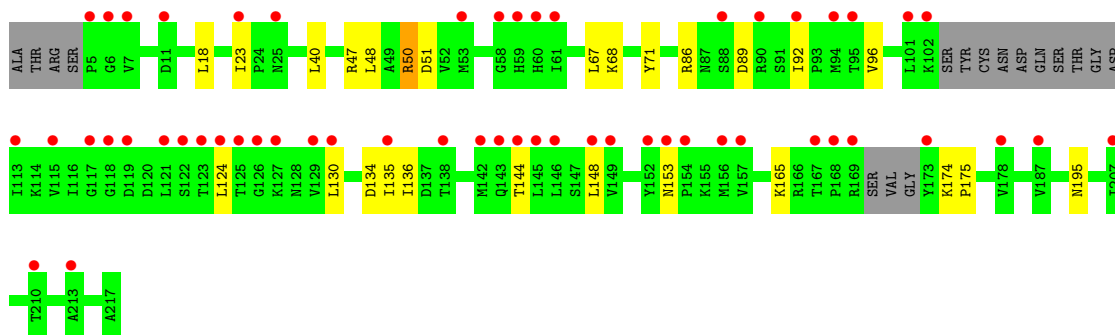
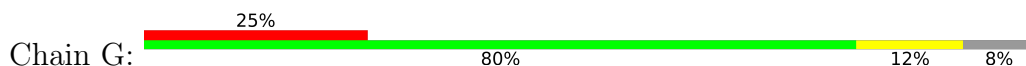
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



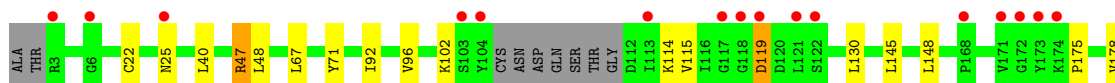
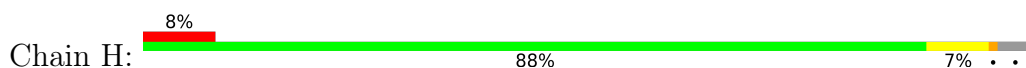
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- 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) 98.6 (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)	Xtriage
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	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.33	0/1583	0.67	0/2138
1	B	0.34	0/1664	0.64	0/2247
1	C	0.32	0/1630	0.64	0/2204
1	D	0.33	0/1623	0.64	0/2194
1	E	0.33	0/1653	0.64	0/2233
1	F	0.34	0/1588	0.68	0/2141
1	G	0.31	0/1612	0.63	0/2175
1	H	0.31	0/1682	0.65	0/2271
All	All	0.33	0/13035	0.65	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	6	0
1	C	1599	1611	1611	9	0
1	D	1592	1597	1597	6	0
1	E	1622	1616	1616	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1560	1581	1581	9	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	56	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 (56) 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:C:199:ARG:NH1	2:C:301[B]:3L5:OAE	2.34	0.61
1:G:68:LYS:NZ	4:G:429:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:NZ	4:A:428:HOH:O	2.32	0.59
1:B:112:ASP:N	1:B:112:ASP:OD1	2.34	0.59
1:A:72:LYS:NZ	4:A:447:HOH:O	2.30	0.58
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: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:B:53:MET:HE1	1:B:61:ILE:HD12	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:PRO:HG2	1:C:178:VAL:HG22	2.02	0.41
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:F:63:ALA:HB2	1:F:94:MET:HE2	2.03	0.41
1:B:199:ARG:HD2	1:D:96:VAL:HG22	2.02	0.41
1:E:156:MET:HE2	1:E:158:LYS:HE3	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

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	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%)	24	21
1	E	200/217 (92%)	193 (96%)	7 (4%)	0	100	100
1	F	189/217 (87%)	181 (96%)	7 (4%)	1 (0%)	24	21
1	G	194/217 (89%)	186 (96%)	7 (4%)	1 (0%)	24	21
1	H	204/217 (94%)	199 (98%)	5 (2%)	0	100	100
All	All	1577/1736 (91%)	1524 (97%)	50 (3%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	124	LEU
1	G	153	ASN

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Mol	Chain	Res	Type
1	D	117	GLY

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	170/191 (89%)	158 (93%)	12 (7%)	13	10
1	B	179/191 (94%)	165 (92%)	14 (8%)	11	8
1	C	175/191 (92%)	163 (93%)	12 (7%)	14	11
1	D	174/191 (91%)	160 (92%)	14 (8%)	11	8
1	E	176/191 (92%)	163 (93%)	13 (7%)	13	9
1	F	170/191 (89%)	155 (91%)	15 (9%)	9	6
1	G	172/191 (90%)	159 (92%)	13 (8%)	12	9
1	H	181/191 (95%)	171 (94%)	10 (6%)	19	17
All	All	1397/1528 (91%)	1294 (93%)	103 (7%)	13	9

All (103) 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	100	ARG
1	A	121	LEU
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

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Mol	Chain	Res	Type
1	B	48	LEU
1	B	54	LYS
1	B	67	LEU
1	B	71	TYR
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	B	207	ILE
1	C	40	LEU
1	C	48	LEU
1	C	71	TYR
1	C	90	ARG
1	C	92	ILE
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	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	96	VAL
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

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Mol	Chain	Res	Type
1	E	48	LEU
1	E	64	LEU
1	E	71	TYR
1	E	92	ILE
1	E	100	ARG
1	E	130	LEU
1	E	145	LEU
1	E	210	THR
1	E	216	LYS
1	F	23	ILE
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	167	THR
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	92	ILE
1	G	96	VAL
1	G	124	LEU
1	G	130	LEU
1	G	144	THR
1	G	148	LEU
1	G	174	LYS
1	G	195	ASN
1	H	25	ASN
1	H	40	LEU
1	H	47	ARG
1	H	48	LEU
1	H	67	LEU

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Mol	Chain	Res	Type
1	H	71	TYR
1	H	92	ILE
1	H	119	ASP
1	H	130	LEU
1	H	145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	151	GLN
1	G	128	ASN
1	H	25	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 oligosaccharides 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	D	301[B]	3	29,30,30	2.79	6 (20%)	36,43,43	1.50	6 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3L5	H	301[A]	-	29,30,30	2.86	6 (20%)	36,43,43	1.54	6 (16%)
2	3L5	B	301	-	29,30,30	2.68	6 (20%)	36,43,43	1.56	5 (13%)
2	3L5	A	301[B]	-	29,30,30	2.87	6 (20%)	36,43,43	1.39	5 (13%)
2	3L5	H	301[B]	-	29,30,30	2.83	6 (20%)	36,43,43	1.69	7 (19%)
2	3L5	F	301	3	29,30,30	2.75	6 (20%)	36,43,43	1.41	5 (13%)
2	3L5	C	301[A]	-	29,30,30	2.90	6 (20%)	36,43,43	1.59	7 (19%)
2	3L5	G	301	-	29,30,30	2.83	6 (20%)	36,43,43	1.44	4 (11%)
2	3L5	C	301[B]	-	29,30,30	2.84	6 (20%)	36,43,43	1.37	4 (11%)
2	3L5	E	301[A]	-	29,30,30	2.78	6 (20%)	36,43,43	1.50	5 (13%)
2	3L5	D	301[A]	-	29,30,30	2.83	6 (20%)	36,43,43	1.35	4 (11%)
2	3L5	A	301[A]	-	29,30,30	2.83	6 (20%)	36,43,43	1.35	5 (13%)
2	3L5	E	301[B]	-	29,30,30	2.77	6 (20%)	36,43,43	1.48	4 (11%)

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	D	301[B]	3	-	7/20/20/20	0/2/2/2
2	3L5	H	301[A]	-	-	3/20/20/20	0/2/2/2
2	3L5	B	301	-	-	2/20/20/20	0/2/2/2
2	3L5	A	301[B]	-	-	2/20/20/20	0/2/2/2
2	3L5	H	301[B]	-	-	6/20/20/20	0/2/2/2
2	3L5	F	301	3	-	1/20/20/20	0/2/2/2
2	3L5	C	301[A]	-	-	7/20/20/20	0/2/2/2
2	3L5	G	301	-	-	7/20/20/20	0/2/2/2
2	3L5	C	301[B]	-	-	4/20/20/20	0/2/2/2
2	3L5	E	301[A]	-	-	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[A]	-	-	5/20/20/20	0/2/2/2
2	3L5	E	301[B]	-	-	9/20/20/20	0/2/2/2

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	3L5	O6-C6	10.85	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[B]	3L5	O6-C6	10.82	1.43	1.23
2	H	301[B]	3L5	O6-C6	10.81	1.43	1.23
2	H	301[A]	3L5	O6-C6	10.80	1.43	1.23
2	D	301[A]	3L5	O6-C6	10.75	1.43	1.23
2	A	301[A]	3L5	O6-C6	10.68	1.43	1.23
2	A	301[B]	3L5	O6-C6	10.66	1.43	1.23
2	E	301[A]	3L5	O6-C6	10.64	1.43	1.23
2	D	301[B]	3L5	O6-C6	10.63	1.43	1.23
2	E	301[B]	3L5	O6-C6	10.59	1.43	1.23
2	G	301	3L5	O6-C6	10.53	1.42	1.23
2	F	301	3L5	O6-C6	10.48	1.42	1.23
2	B	301	3L5	O6-C6	10.37	1.42	1.23
2	A	301[B]	3L5	PBC-CAQ	6.96	1.86	1.78
2	C	301[B]	3L5	PBC-CAQ	6.87	1.86	1.78
2	H	301[A]	3L5	PBC-CAQ	6.86	1.86	1.78
2	G	301	3L5	PBC-CAQ	6.86	1.86	1.78
2	A	301[A]	3L5	PBC-CAQ	6.69	1.86	1.78
2	H	301[B]	3L5	PBC-CAQ	6.68	1.86	1.78
2	C	301[A]	3L5	PBC-CAQ	6.63	1.85	1.78
2	D	301[A]	3L5	PBC-CAQ	6.61	1.85	1.78
2	D	301[B]	3L5	PBC-CAQ	6.58	1.85	1.78
2	E	301[A]	3L5	PBC-CAQ	6.58	1.85	1.78
2	E	301[B]	3L5	PBC-CAQ	6.56	1.85	1.78
2	F	301	3L5	PBC-CAQ	6.30	1.85	1.78
2	B	301	3L5	PBC-CAQ	5.77	1.85	1.78
2	C	301[A]	3L5	PBB-CAP	5.47	1.84	1.78
2	A	301[B]	3L5	PBB-CAP	5.29	1.84	1.78
2	G	301	3L5	PBB-CAP	5.02	1.84	1.78
2	A	301[A]	3L5	PBB-CAP	4.93	1.84	1.78
2	D	301[A]	3L5	PBB-CAP	4.93	1.84	1.78
2	H	301[A]	3L5	PBB-CAP	4.88	1.84	1.78
2	D	301[B]	3L5	PBB-CAP	4.61	1.83	1.78
2	H	301[B]	3L5	PBB-CAP	4.60	1.83	1.78
2	E	301[B]	3L5	PBB-CAP	4.58	1.83	1.78
2	B	301	3L5	PBB-CAP	4.54	1.83	1.78
2	E	301[A]	3L5	PBB-CAP	4.52	1.83	1.78
2	F	301	3L5	PBB-CAP	4.34	1.83	1.78
2	C	301[B]	3L5	PBB-CAP	4.28	1.83	1.78
2	D	301[A]	3L5	C2-N2	3.93	1.43	1.34
2	B	301	3L5	C2-N2	3.93	1.43	1.34
2	C	301[A]	3L5	C2-N2	3.93	1.43	1.34
2	G	301	3L5	C2-N2	3.92	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[B]	3L5	C2-N2	3.92	1.43	1.34
2	H	301[B]	3L5	C2-N2	3.92	1.43	1.34
2	E	301[B]	3L5	C2-N2	3.92	1.43	1.34
2	F	301	3L5	C2-N2	3.92	1.43	1.34
2	D	301[B]	3L5	C2-N2	3.88	1.43	1.34
2	H	301[A]	3L5	C2-N2	3.88	1.43	1.34
2	E	301[A]	3L5	C2-N2	3.85	1.43	1.34
2	A	301[A]	3L5	C2-N2	3.81	1.43	1.34
2	A	301[B]	3L5	C2-N2	3.76	1.43	1.34
2	C	301[B]	3L5	C5-C4	2.64	1.42	1.38
2	H	301[B]	3L5	C5-C4	2.64	1.42	1.38
2	A	301[B]	3L5	C5-C4	2.59	1.42	1.38
2	C	301[A]	3L5	C5-C4	2.56	1.42	1.38
2	H	301[A]	3L5	C5-C4	2.54	1.42	1.38
2	A	301[A]	3L5	C5-C4	2.52	1.42	1.38
2	F	301	3L5	C5-C4	2.51	1.42	1.38
2	D	301[A]	3L5	C5-C4	2.49	1.42	1.38
2	E	301[B]	3L5	C6-N1	-2.49	1.33	1.38
2	E	301[A]	3L5	C6-N1	-2.49	1.33	1.38
2	B	301	3L5	C6-N1	-2.47	1.33	1.38
2	G	301	3L5	C6-N1	-2.47	1.33	1.38
2	G	301	3L5	C5-C4	2.46	1.42	1.38
2	F	301	3L5	C6-N1	-2.44	1.33	1.38
2	A	301[B]	3L5	C6-N1	-2.43	1.33	1.38
2	H	301[B]	3L5	C6-N1	-2.41	1.33	1.38
2	A	301[A]	3L5	C6-N1	-2.41	1.33	1.38
2	D	301[B]	3L5	C5-C4	2.40	1.42	1.38
2	E	301[A]	3L5	C5-C4	2.39	1.42	1.38
2	H	301[A]	3L5	C6-N1	-2.39	1.33	1.38
2	C	301[B]	3L5	C6-N1	-2.38	1.34	1.38
2	D	301[B]	3L5	C6-N1	-2.37	1.34	1.38
2	C	301[A]	3L5	C6-N1	-2.35	1.34	1.38
2	E	301[B]	3L5	C5-C4	2.33	1.42	1.38
2	D	301[A]	3L5	C6-N1	-2.32	1.34	1.38
2	B	301	3L5	C5-C4	2.19	1.42	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	3L5	N9-C8-N7	-4.94	108.37	113.52
2	G	301	3L5	N9-C8-N7	-4.54	108.78	113.52
2	E	301[B]	3L5	N9-C8-N7	-4.52	108.80	113.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301[B]	3L5	N9-C8-N7	-4.45	108.89	113.52
2	E	301[A]	3L5	N9-C8-N7	-4.43	108.91	113.52
2	C	301[A]	3L5	N9-C8-N7	-4.40	108.94	113.52
2	A	301[A]	3L5	N9-C8-N7	-4.35	108.98	113.52
2	H	301[A]	3L5	N9-C8-N7	-4.34	108.99	113.52
2	F	301	3L5	N9-C8-N7	-4.31	109.03	113.52
2	D	301[A]	3L5	N9-C8-N7	-4.29	109.05	113.52
2	H	301[B]	3L5	N9-C8-N7	-4.28	109.06	113.52
2	A	301[B]	3L5	N9-C8-N7	-4.25	109.08	113.52
2	C	301[B]	3L5	N9-C8-N7	-4.13	109.21	113.52
2	F	301	3L5	CAM-CAO-N9	-3.85	104.85	111.66
2	E	301[A]	3L5	CAM-CAO-N9	-3.84	104.87	111.66
2	H	301[B]	3L5	CAM-NAZ-CAN	3.78	120.43	111.44
2	B	301	3L5	C8-N9-C4	3.66	109.91	106.81
2	E	301[B]	3L5	CAM-CAO-N9	-3.61	105.27	111.66
2	B	301	3L5	CAM-CAO-N9	-3.57	105.34	111.66
2	C	301[A]	3L5	OAU-CAK-CAP	3.41	119.00	109.19
2	C	301[A]	3L5	CAJ-OAU-CAK	3.08	126.75	113.26
2	E	301[B]	3L5	C8-N9-C4	3.04	109.38	106.81
2	G	301	3L5	C8-N9-C4	2.96	109.31	106.81
2	D	301[B]	3L5	CAM-CAO-N9	-2.88	106.57	111.66
2	D	301[B]	3L5	C8-N9-C4	2.85	109.22	106.81
2	H	301[A]	3L5	CAM-CAO-N9	-2.81	106.69	111.66
2	C	301[B]	3L5	C8-N7-C5	2.77	109.20	104.26
2	C	301[A]	3L5	C8-N9-C4	2.77	109.16	106.81
2	E	301[A]	3L5	C8-N9-C4	2.77	109.15	106.81
2	H	301[B]	3L5	C8-N7-C5	2.75	109.16	104.26
2	B	301	3L5	C8-N7-C5	2.73	109.13	104.26
2	E	301[A]	3L5	C8-N7-C5	2.73	109.12	104.26
2	H	301[A]	3L5	C8-N9-C4	2.72	109.11	106.81
2	H	301[A]	3L5	C8-N7-C5	2.72	109.11	104.26
2	A	301[A]	3L5	C8-N7-C5	2.71	109.08	104.26
2	G	301	3L5	C8-N7-C5	2.71	109.08	104.26
2	C	301[A]	3L5	C8-N7-C5	2.69	109.06	104.26
2	E	301[B]	3L5	C8-N7-C5	2.69	109.06	104.26
2	D	301[A]	3L5	C8-N7-C5	2.69	109.05	104.26
2	D	301[B]	3L5	C8-N7-C5	2.68	109.04	104.26
2	F	301	3L5	C8-N9-C4	2.67	109.07	106.81
2	A	301[B]	3L5	C8-N7-C5	2.66	108.99	104.26
2	F	301	3L5	C8-N7-C5	2.61	108.92	104.26
2	H	301[B]	3L5	C8-N9-C4	2.60	109.01	106.81
2	D	301[A]	3L5	C8-N9-C4	2.59	109.00	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[A]	3L5	C8-N9-C4	2.58	109.00	106.81
2	C	301[B]	3L5	C4-C5-N7	-2.57	105.92	109.26
2	A	301[B]	3L5	C8-N9-C4	2.52	108.95	106.81
2	H	301[A]	3L5	C4-C5-N7	-2.40	106.15	109.26
2	H	301[B]	3L5	C4-C5-N7	-2.40	106.15	109.26
2	H	301[B]	3L5	CAJ-OAU-CAK	2.39	123.72	113.26
2	C	301[A]	3L5	C4-C5-N7	-2.37	106.18	109.26
2	C	301[B]	3L5	C8-N9-C4	2.29	108.75	106.81
2	B	301	3L5	CAO-N9-C4	-2.26	123.72	127.08
2	A	301[A]	3L5	C4-C5-N7	-2.24	106.36	109.26
2	D	301[B]	3L5	C4-C5-N7	-2.22	106.39	109.26
2	D	301[A]	3L5	C4-C5-N7	-2.21	106.39	109.26
2	A	301[B]	3L5	C4-C5-N7	-2.20	106.40	109.26
2	H	301[A]	3L5	OAE-PBB-CAP	-2.19	107.33	111.45
2	F	301	3L5	C4-C5-N7	-2.18	106.44	109.26
2	D	301[B]	3L5	CAM-NAZ-CAL	2.14	116.53	111.44
2	E	301[A]	3L5	C4-C5-N7	-2.11	106.52	109.26
2	A	301[A]	3L5	CAM-CAO-N9	-2.11	107.93	111.66
2	A	301[B]	3L5	CAM-CAO-N9	-2.04	108.06	111.66
2	G	301	3L5	C4-C5-N7	-2.02	106.64	109.26
2	H	301[B]	3L5	OAG-PBC-CAQ	2.01	111.72	106.91
2	C	301[A]	3L5	CAO-N9-C4	-2.01	124.09	127.08

There are no chirality outliers.

All (69) 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

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

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

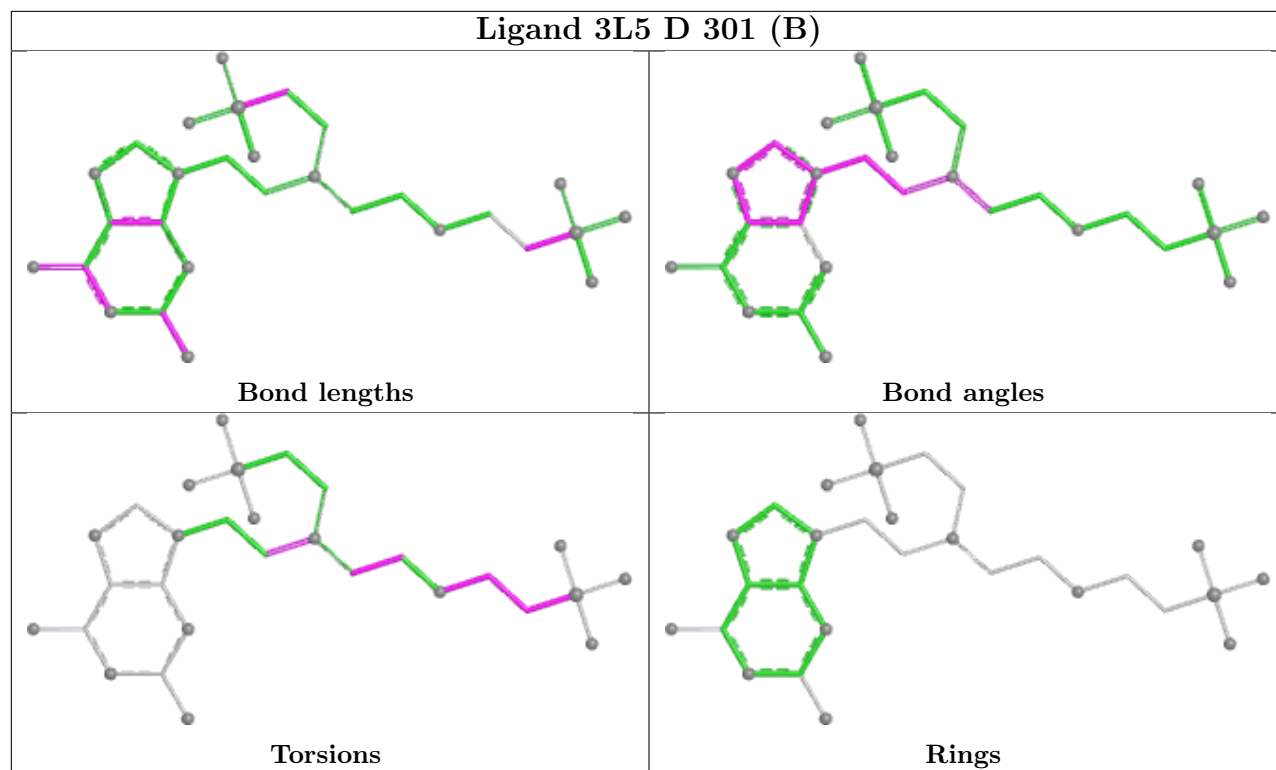
There are no ring outliers.

3 monomers are involved in 4 short contacts:

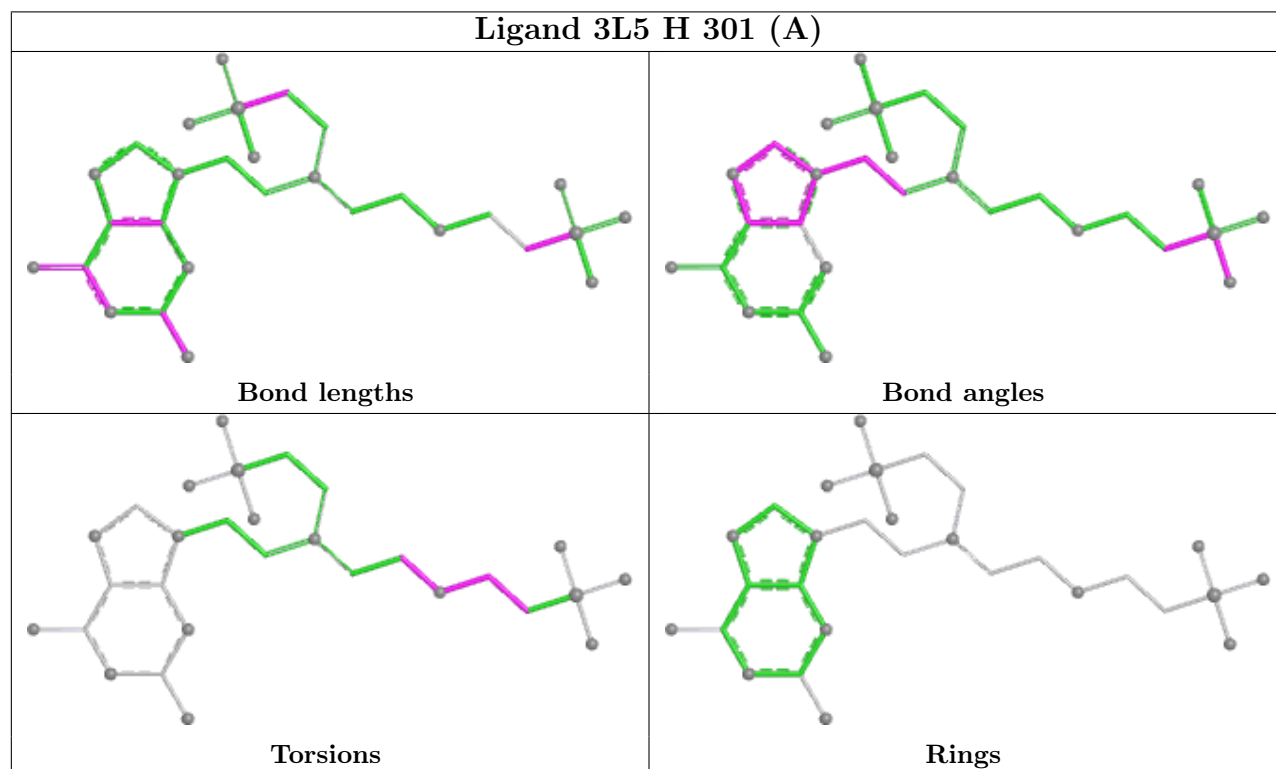
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301[B]	3L5	1	0
2	C	301[B]	3L5	2	0
2	E	301[A]	3L5	1	0

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.

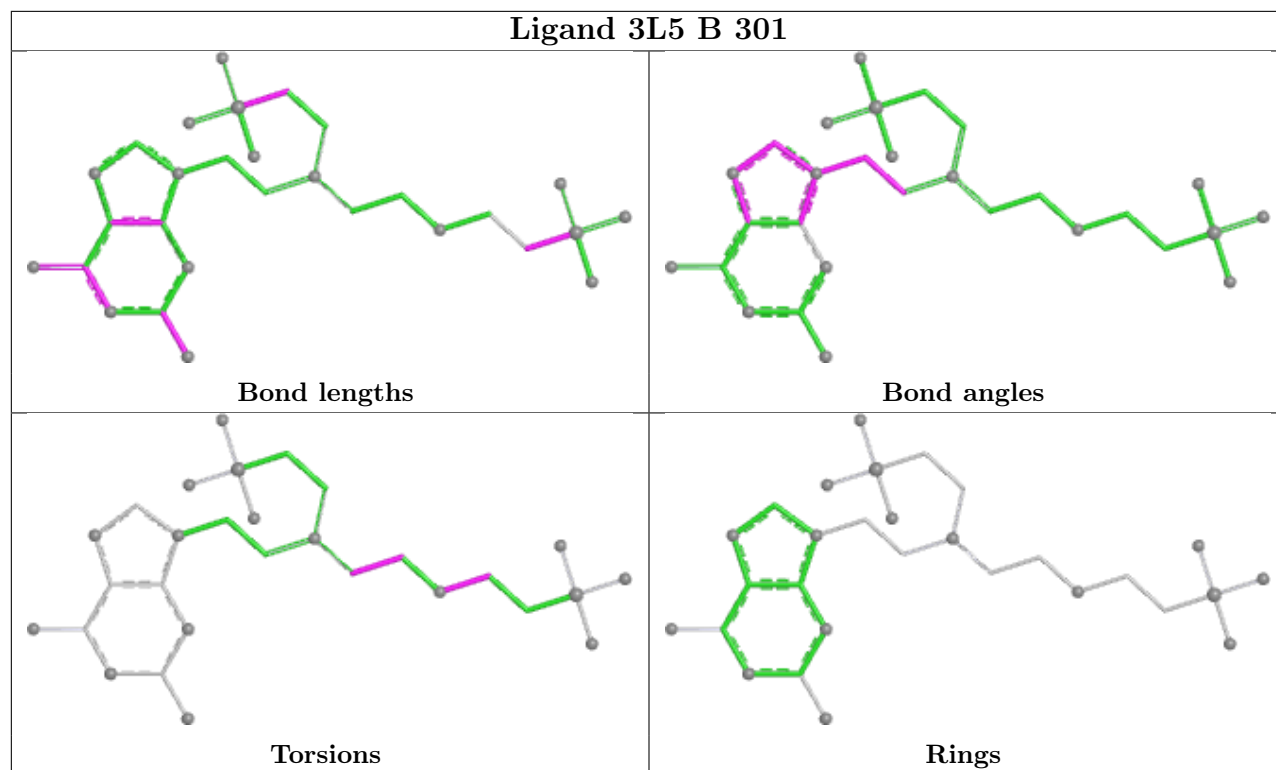
Ligand 3L5 D 301 (B)



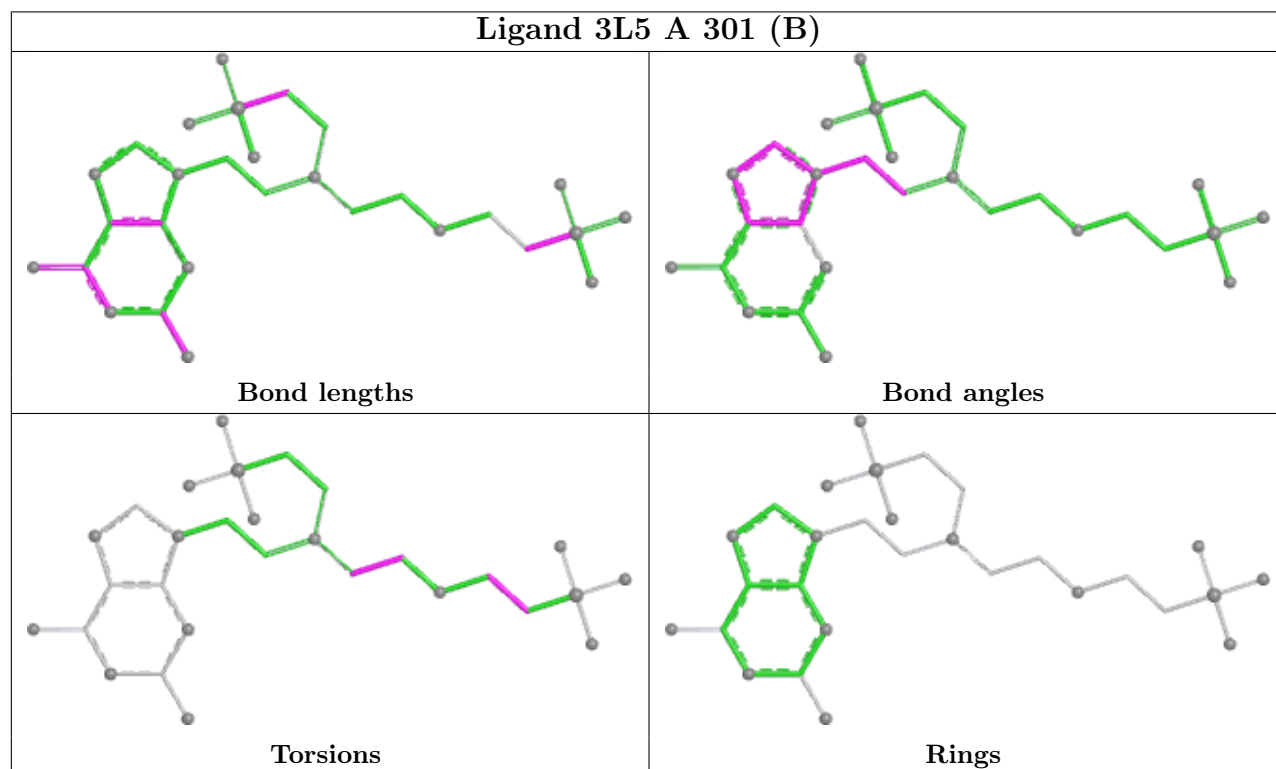
Ligand 3L5 H 301 (A)



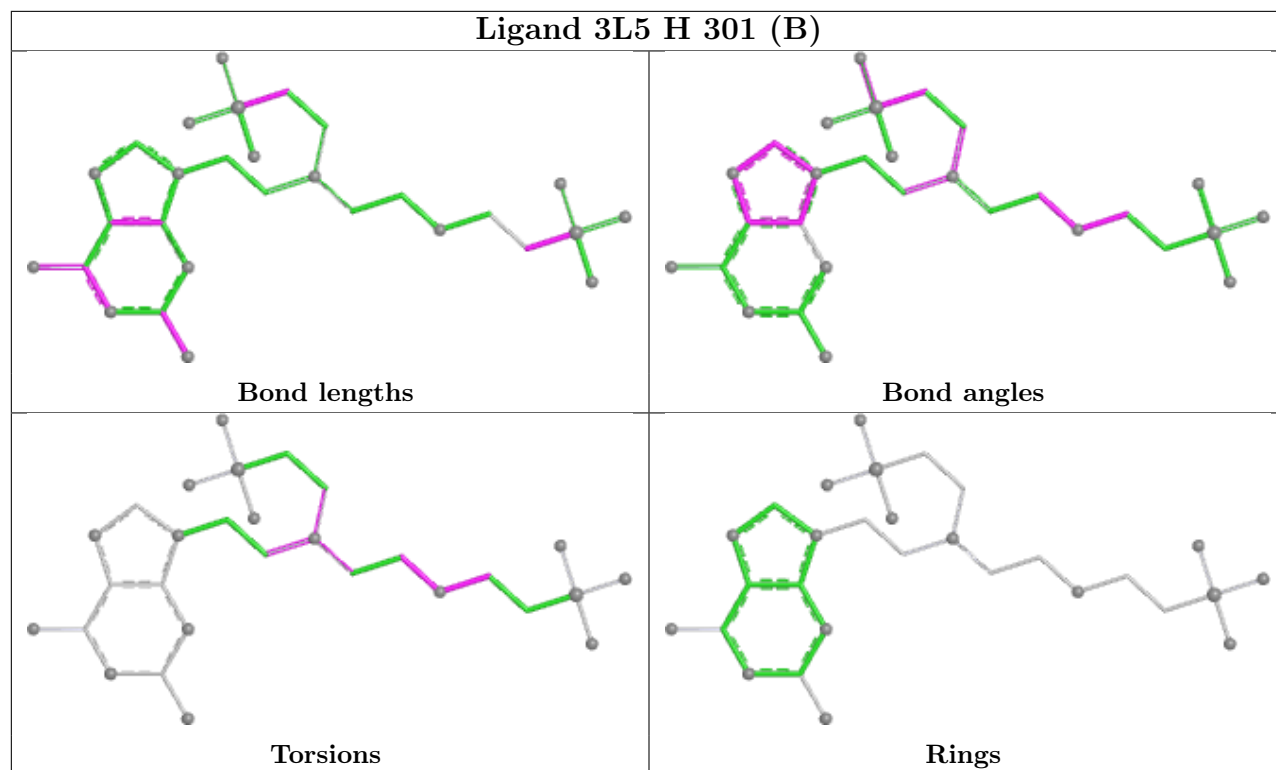
Ligand 3L5 B 301



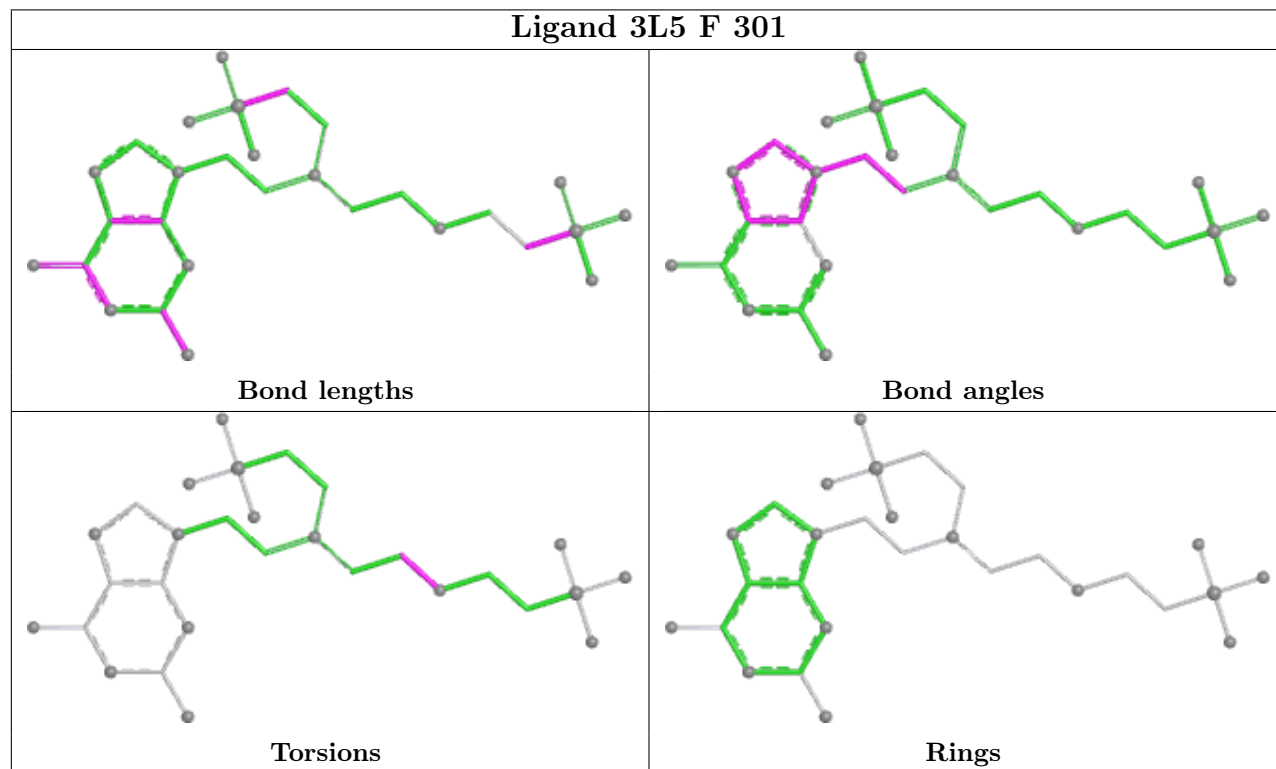
Ligand 3L5 A 301 (B)



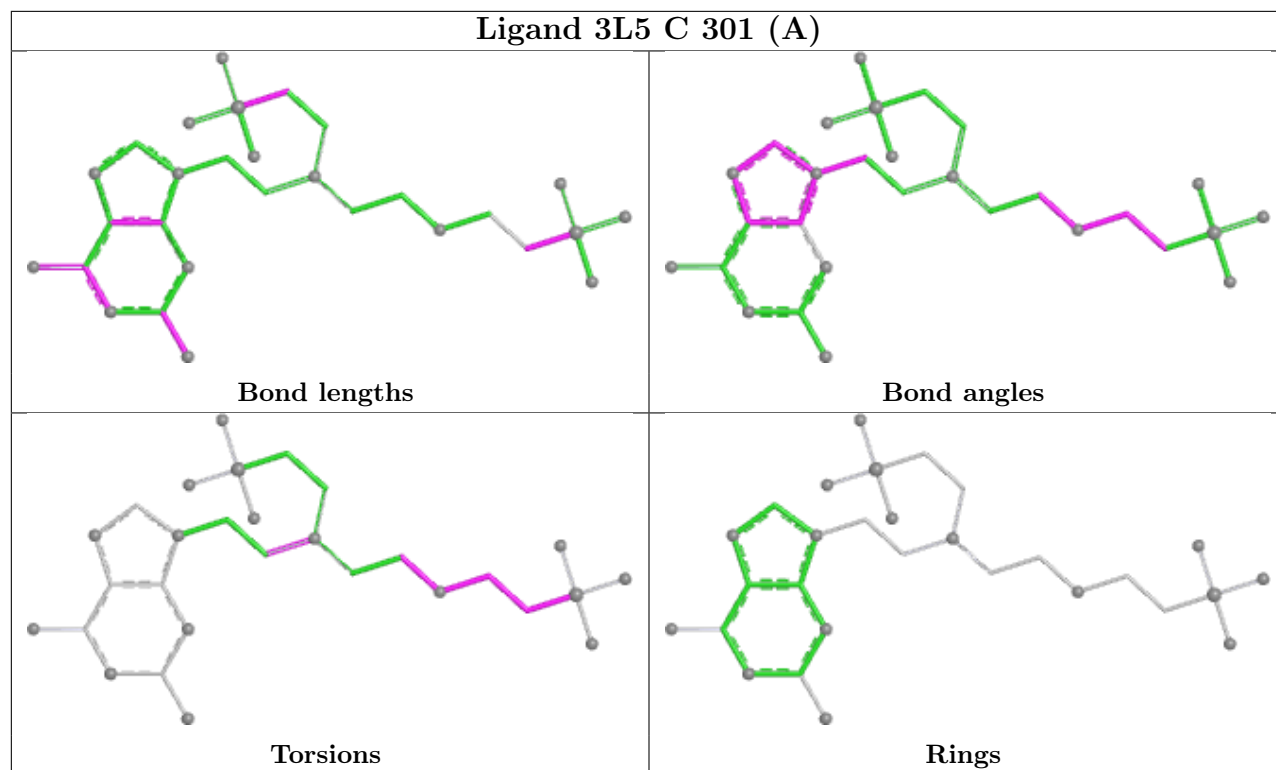
Ligand 3L5 H 301 (B)



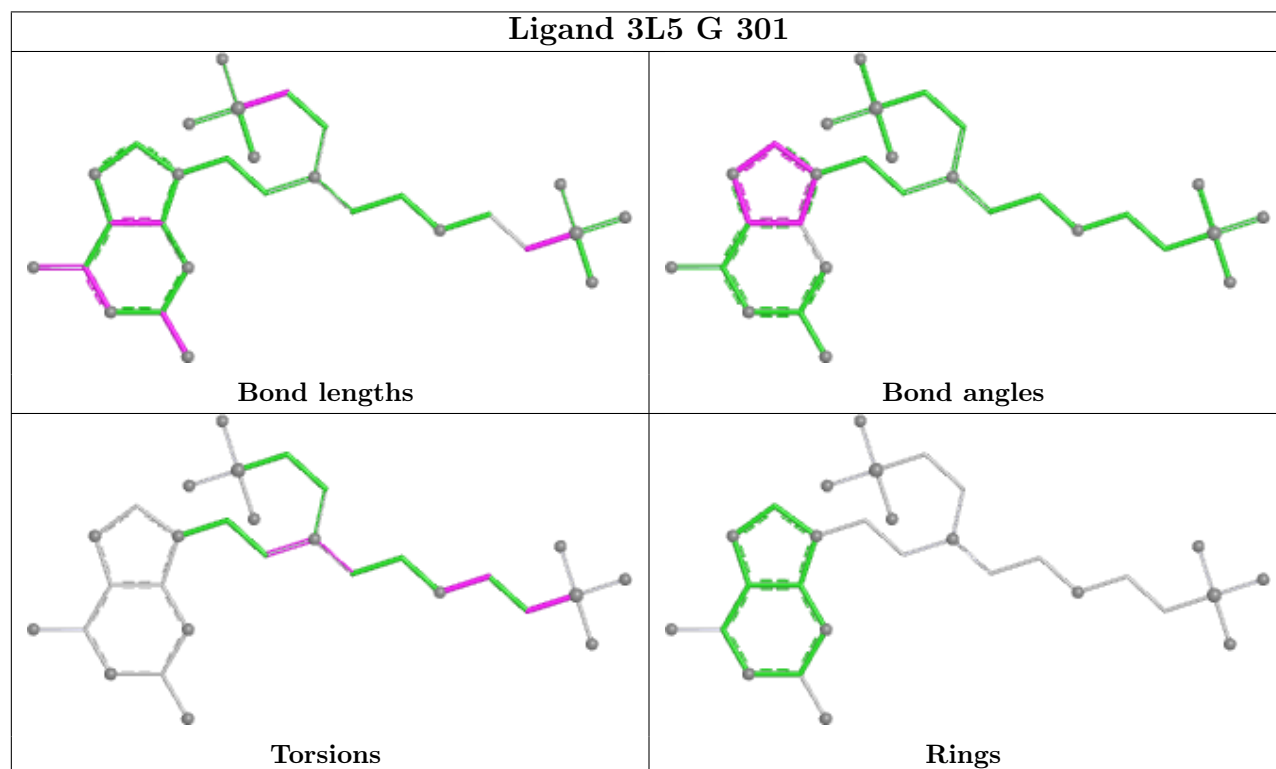
Ligand 3L5 F 301



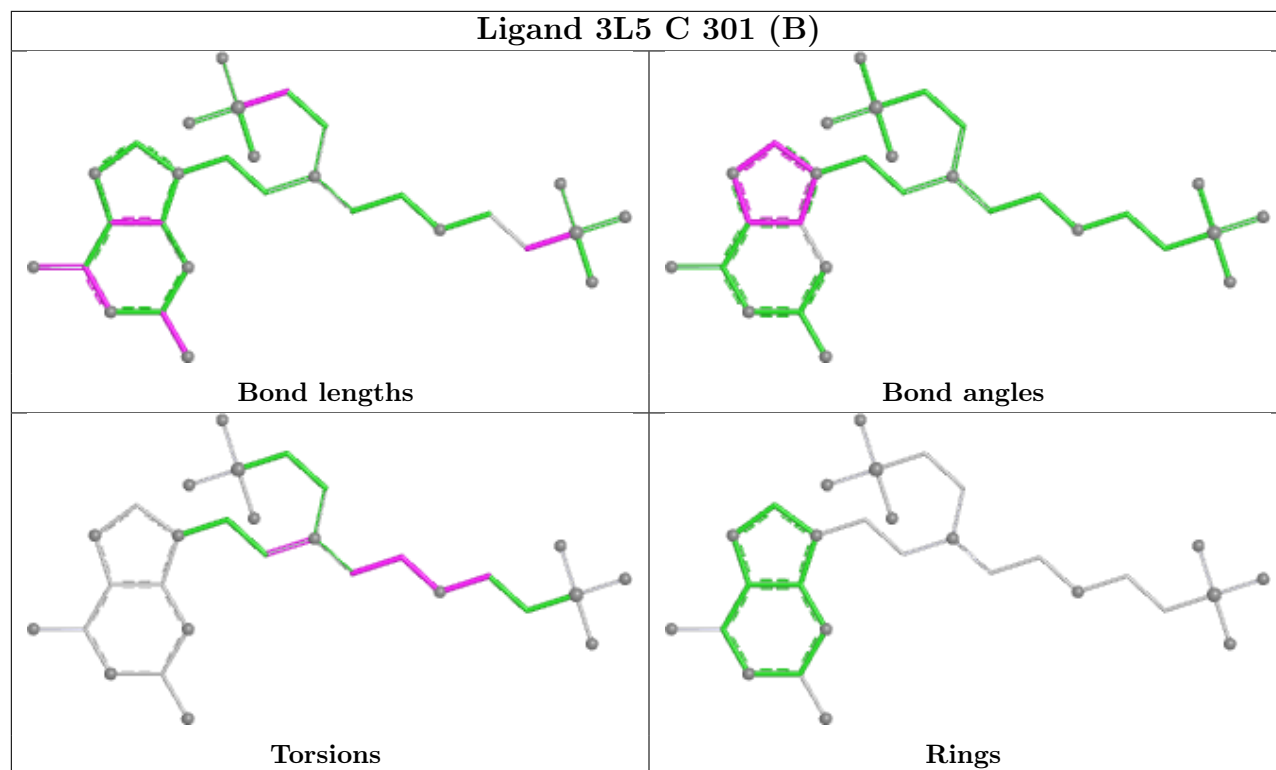
Ligand 3L5 C 301 (A)



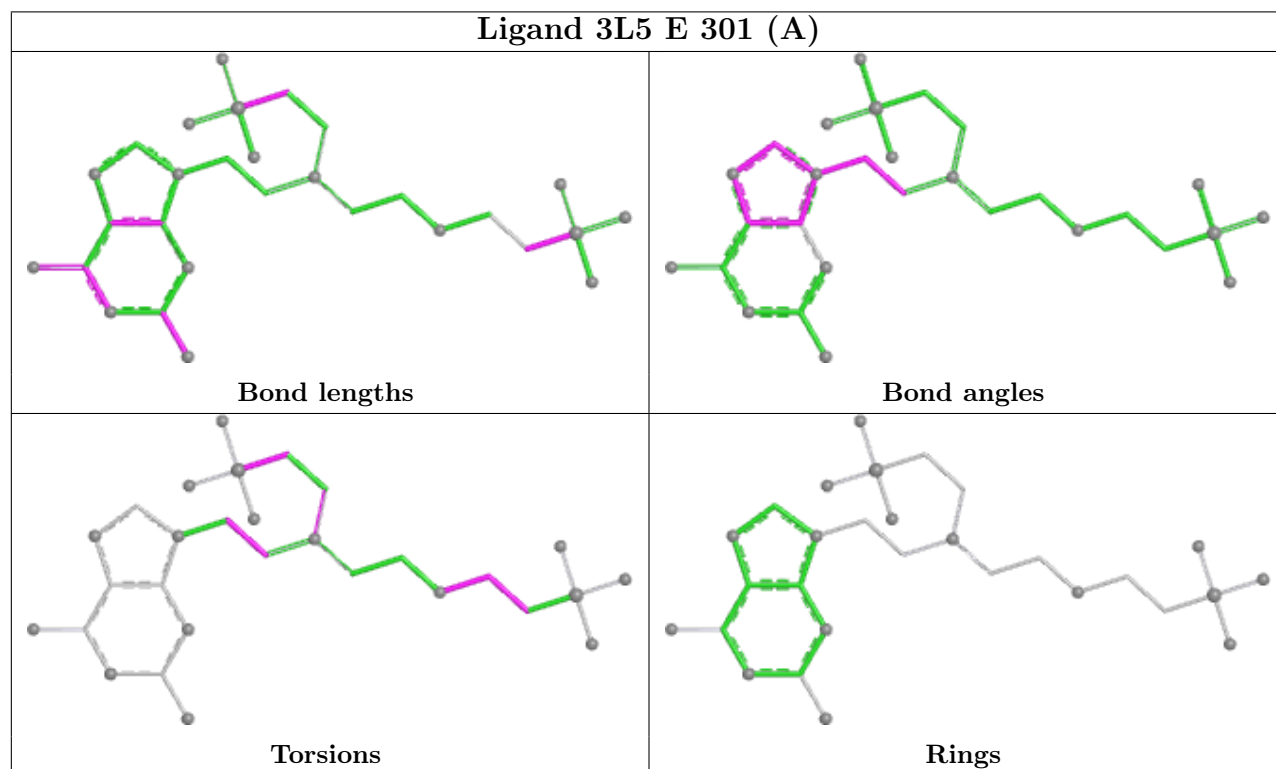
Ligand 3L5 G 301



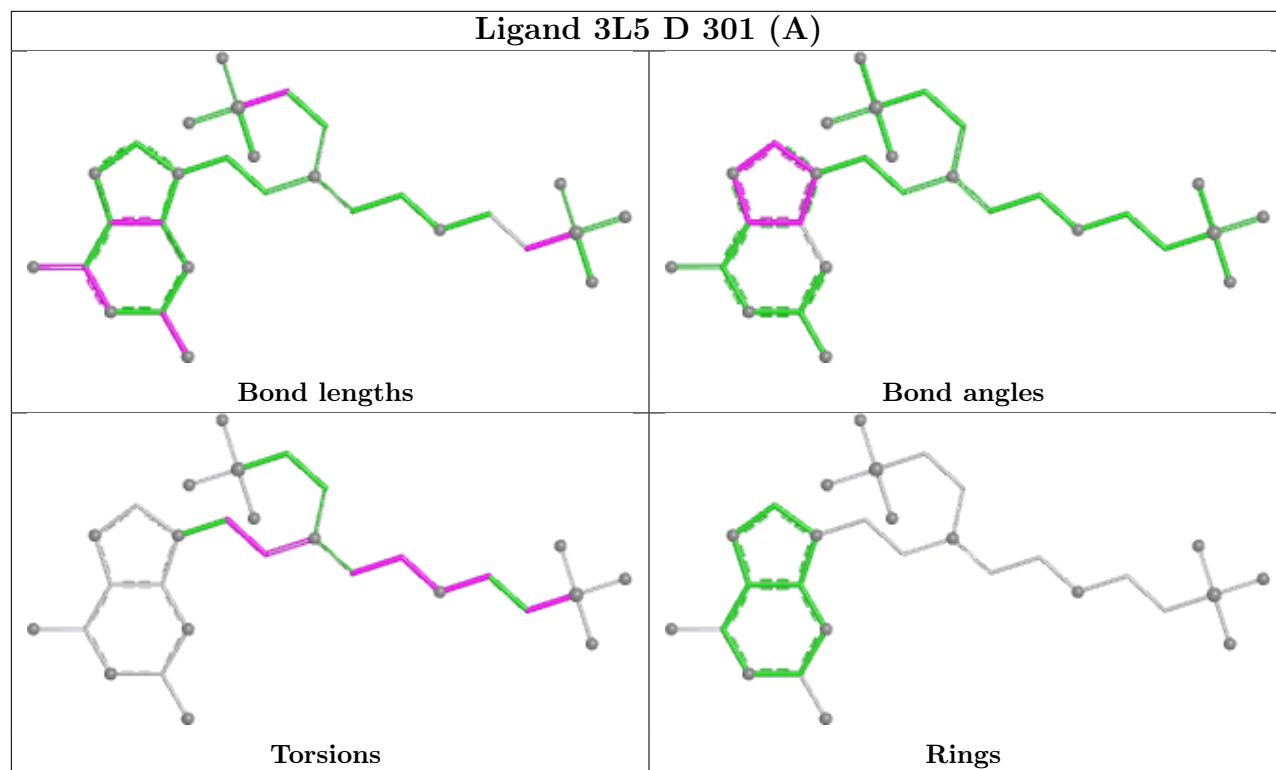
Ligand 3L5 C 301 (B)



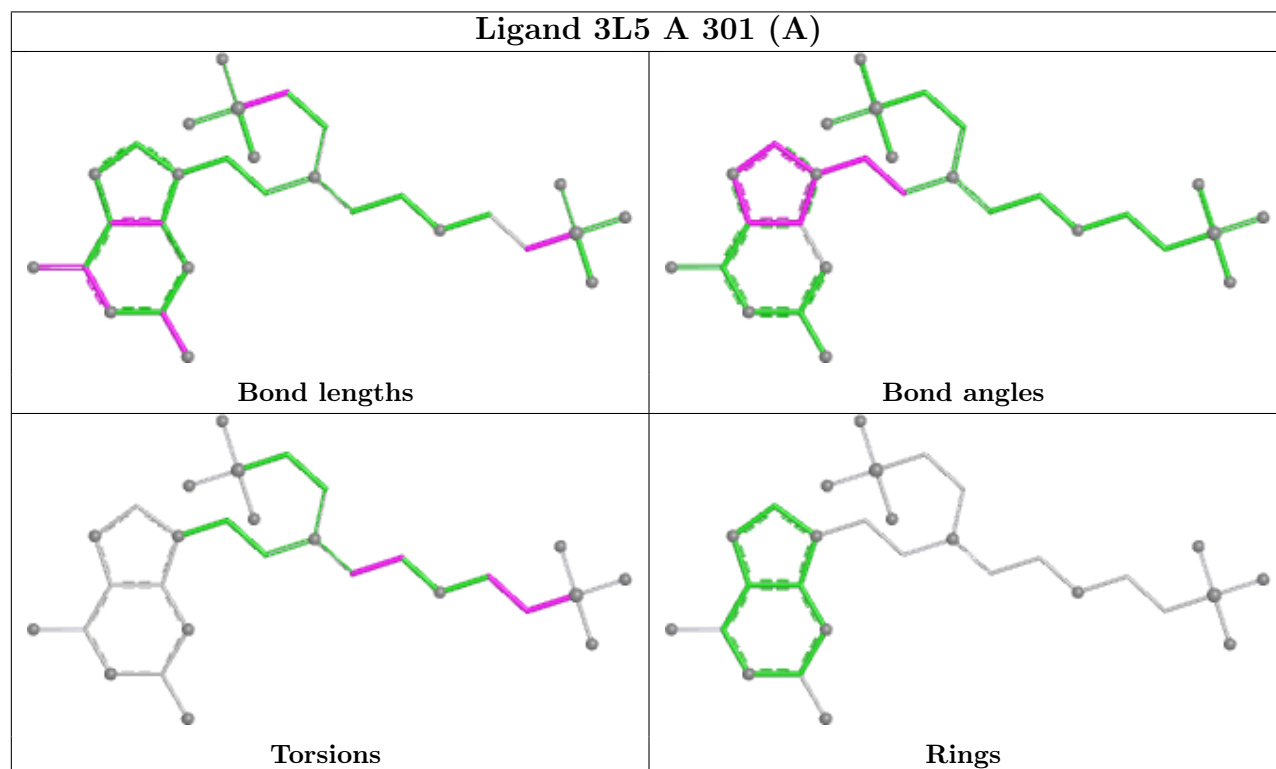
Ligand 3L5 E 301 (A)

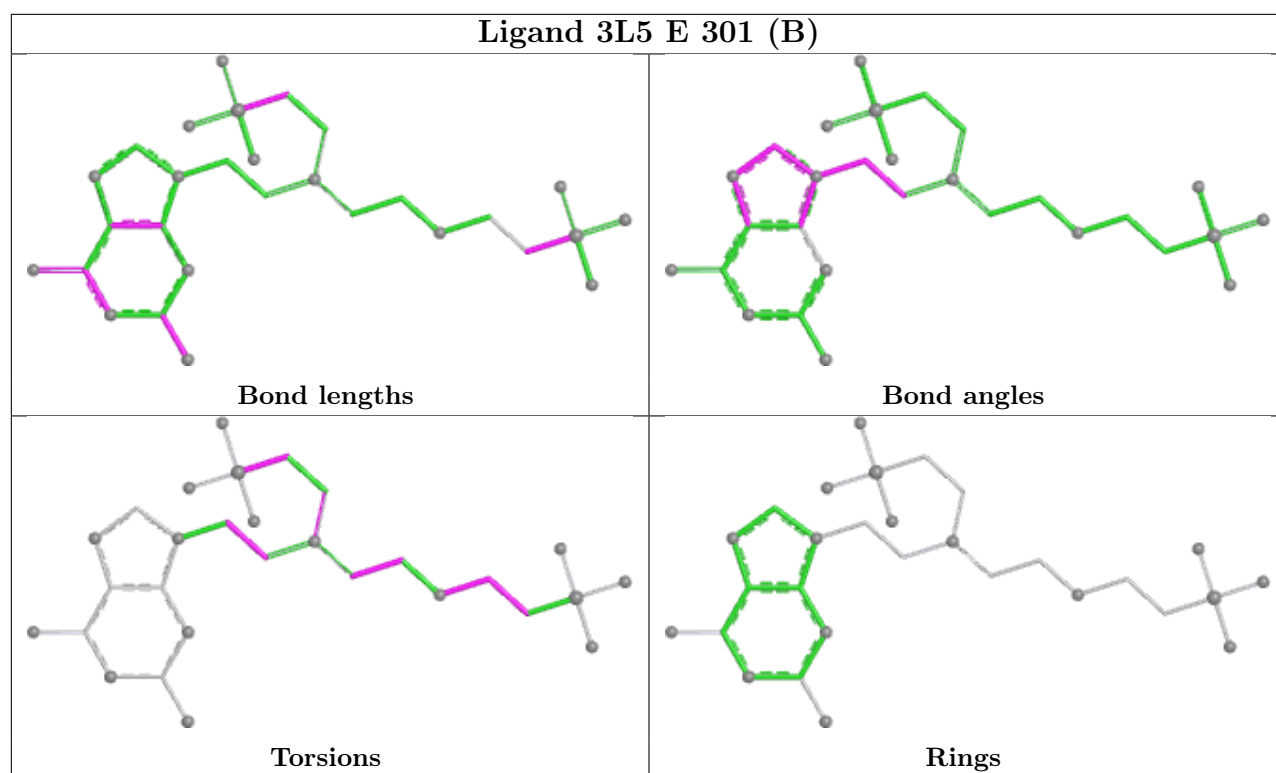


Ligand 3L5 D 301 (A)



Ligand 3L5 A 301 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	197/217 (90%)	0.48	20 (10%) 12 11	28, 43, 93, 114	0
1	B	207/217 (95%)	0.52	19 (9%) 14 13	28, 43, 89, 105	0
1	C	202/217 (93%)	0.42	10 (4%) 34 33	29, 47, 81, 101	0
1	D	202/217 (93%)	0.51	23 (11%) 10 9	27, 48, 74, 113	0
1	E	206/217 (94%)	0.88	32 (15%) 5 4	32, 53, 99, 152	0
1	F	197/217 (90%)	0.36	20 (10%) 12 11	27, 41, 90, 112	0
1	G	200/217 (92%)	1.40	55 (27%) 1 1	39, 72, 120, 134	0
1	H	208/217 (95%)	0.68	18 (8%) 16 15	31, 52, 94, 107	0
All	All	1619/1736 (93%)	0.66	197 (12%) 8 7	27, 49, 97, 152	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	121	LEU	8.7
1	A	121	LEU	6.2
1	G	102	LYS	6.0
1	E	111	GLY	5.6
1	A	169	ARG	4.8
1	B	111	GLY	4.7
1	A	170	SER	4.6
1	E	118	GLY	4.6
1	A	116	ILE	4.6
1	G	6	GLY	4.5
1	E	116	ILE	4.5
1	E	122	SER	4.4
1	A	168	PRO	4.3
1	H	122	SER	4.3
1	G	125	THR	4.3
1	G	126	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	118	GLY	4.1
1	G	152	TYR	4.1
1	H	173	TYR	4.1
1	E	117	GLY	4.1
1	G	149	VAL	4.1
1	B	58	GLY	4.0
1	H	171	VAL	4.0
1	A	117	GLY	4.0
1	G	118	GLY	4.0
1	A	122	SER	3.9
1	F	60	HIS	3.9
1	C	4	SER	3.8
1	E	88	SER	3.8
1	E	172	GLY	3.8
1	B	101	LEU	3.8
1	H	121	LEU	3.7
1	E	92	ILE	3.7
1	G	146	LEU	3.7
1	B	149	VAL	3.7
1	G	5	PRO	3.6
1	G	169	ARG	3.6
1	G	113	ILE	3.6
1	D	101	LEU	3.6
1	D	171	VAL	3.5
1	E	168	PRO	3.5
1	F	123	THR	3.5
1	D	5	PRO	3.5
1	H	118	GLY	3.5
1	G	156	MET	3.5
1	H	104	TYR	3.4
1	B	92	ILE	3.4
1	E	23	ILE	3.4
1	E	113	ILE	3.4
1	G	122	SER	3.4
1	C	215	TYR	3.3
1	F	173	TYR	3.3
1	G	124	LEU	3.3
1	E	114	LYS	3.3
1	A	88	SER	3.2
1	G	123	THR	3.2
1	D	92	ILE	3.2
1	G	7	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	115	VAL	3.2
1	B	217	ALA	3.2
1	F	125	THR	3.2
1	F	87	ASN	3.2
1	E	3	ARG	3.1
1	G	129	VAL	3.1
1	B	91	SER	3.1
1	E	104	TYR	3.0
1	F	174	LYS	3.0
1	G	94	MET	3.0
1	E	217	ALA	3.0
1	G	154	PRO	3.0
1	F	152	TYR	3.0
1	B	103	SER	2.9
1	D	157	VAL	2.9
1	A	23	ILE	2.9
1	E	207	ILE	2.9
1	A	210	THR	2.9
1	G	173	TYR	2.9
1	G	121	LEU	2.9
1	G	167	THR	2.9
1	G	59	HIS	2.8
1	G	101	LEU	2.8
1	G	168	PRO	2.8
1	D	117	GLY	2.8
1	E	210	THR	2.8
1	D	4	SER	2.8
1	E	91	SER	2.7
1	E	119	ASP	2.7
1	F	124	LEU	2.7
1	A	115	VAL	2.7
1	A	145	LEU	2.7
1	G	142	MET	2.7
1	E	213	ALA	2.7
1	G	145	LEU	2.7
1	F	103	SER	2.7
1	G	23	ILE	2.7
1	G	143	GLN	2.6
1	H	168	PRO	2.6
1	D	170	SER	2.6
1	G	25	ASN	2.6
1	G	144	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	148	LEU	2.6
1	F	88	SER	2.6
1	G	92	ILE	2.6
1	G	60	HIS	2.6
1	G	127	LYS	2.6
1	B	144	THR	2.6
1	E	115	VAL	2.5
1	G	58	GLY	2.5
1	H	6	GLY	2.5
1	C	210	THR	2.5
1	F	167	THR	2.5
1	G	130	LEU	2.5
1	F	92	ILE	2.5
1	G	61	ILE	2.5
1	D	114	LYS	2.5
1	A	101	LEU	2.5
1	F	59	HIS	2.5
1	F	127	LYS	2.5
1	H	117	GLY	2.5
1	F	149	VAL	2.5
1	G	157	VAL	2.5
1	B	152	TYR	2.5
1	D	167	THR	2.5
1	H	103	SER	2.5
1	D	168	PRO	2.5
1	E	120	ASP	2.4
1	G	11	ASP	2.4
1	G	119	ASP	2.4
1	H	25	ASN	2.4
1	E	151	GLN	2.4
1	G	207	ILE	2.4
1	B	173	TYR	2.4
1	E	152	TYR	2.4
1	G	53	MET	2.4
1	B	90	ARG	2.4
1	D	140	LYS	2.4
1	D	169	ARG	2.4
1	G	210	THR	2.4
1	D	217	ALA	2.4
1	H	113	ILE	2.4
1	C	71	TYR	2.3
1	D	173	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	172	GLY	2.3
1	A	120	ASP	2.3
1	C	113	ILE	2.3
1	H	119	ASP	2.3
1	B	4	SER	2.3
1	F	61	ILE	2.3
1	D	148	LEU	2.3
1	F	90	ARG	2.3
1	H	174	LYS	2.3
1	B	88	SER	2.3
1	A	207	ILE	2.3
1	G	138	THR	2.3
1	G	153	ASN	2.3
1	C	91	SER	2.2
1	C	61	ILE	2.2
1	D	99	ILE	2.2
1	G	178	VAL	2.2
1	E	6	GLY	2.2
1	A	215	TYR	2.2
1	E	173	TYR	2.2
1	H	3	ARG	2.2
1	B	207	ILE	2.2
1	E	167	THR	2.2
1	C	115	VAL	2.2
1	D	12	ASP	2.2
1	D	142	MET	2.2
1	G	88	SER	2.2
1	A	212	LYS	2.2
1	D	94	MET	2.2
1	E	112	ASP	2.2
1	G	135	ILE	2.2
1	H	207	ILE	2.2
1	C	150	ARG	2.2
1	D	33	ARG	2.2
1	F	4	SER	2.2
1	B	118	GLY	2.1
1	B	170	SER	2.1
1	A	209	GLU	2.1
1	E	89	ASP	2.1
1	B	116	ILE	2.1
1	D	207	ILE	2.1
1	B	171	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	213	ALA	2.1
1	E	147	SER	2.1
1	F	153	ASN	2.1
1	G	95	THR	2.1
1	C	21	PHE	2.1
1	G	90	ARG	2.1
1	G	117	GLY	2.1
1	H	217	ALA	2.1
1	E	90	ARG	2.0
1	D	215	TYR	2.0
1	G	187	VAL	2.0
1	A	124	LEU	2.0
1	F	5	PRO	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 oligosaccharides 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	G	302	1/1	0.59	0.21	118,118,118,118	0
2	3L5	A	301[B]	29/29	0.74	0.23	34,66,90,102	48
2	3L5	A	301[A]	29/29	0.74	0.23	35,73,93,127	48
3	MG	H	302	1/1	0.76	0.14	80,80,80,80	0
2	3L5	E	301[A]	29/29	0.77	0.25	47,68,87,112	48
2	3L5	E	301[B]	29/29	0.77	0.25	48,70,112,113	48
3	MG	A	302	1/1	0.78	0.21	69,69,69,69	0
3	MG	B	303	1/1	0.78	0.15	78,78,78,78	0
2	3L5	G	301	29/29	0.80	0.15	56,83,169,169	0
2	3L5	C	301[B]	29/29	0.83	0.21	31,45,172,173	48

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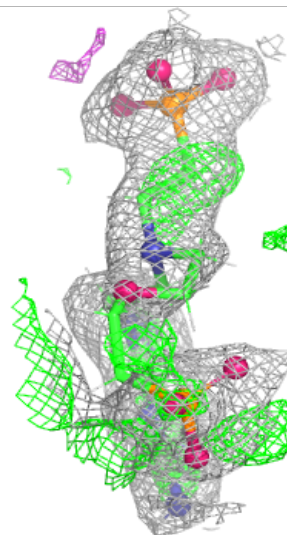
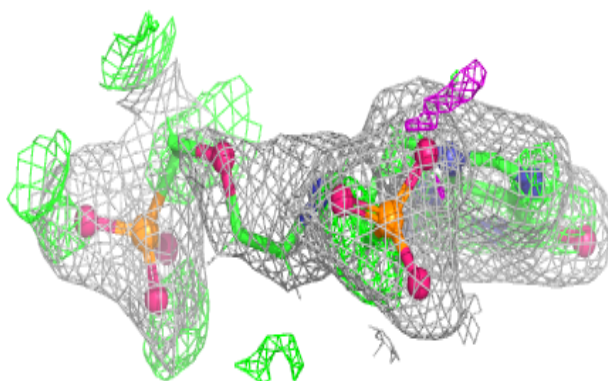
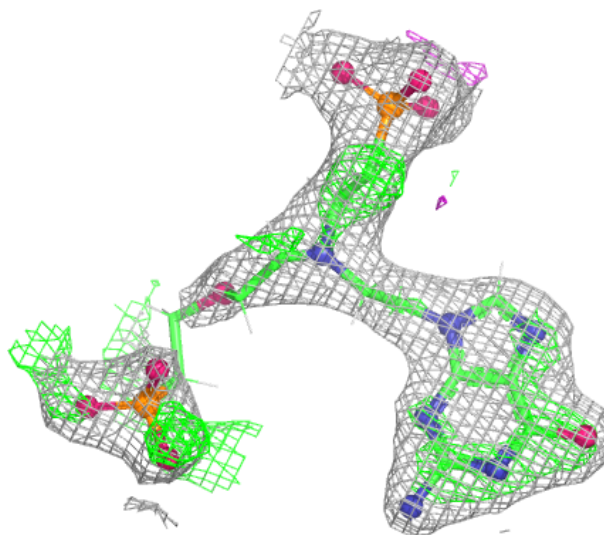
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3L5	C	301[A]	29/29	0.83	0.21	31,45,168,170	48
2	3L5	D	301[B]	29/29	0.86	0.14	36,44,85,86	48
2	3L5	D	301[A]	29/29	0.86	0.14	36,44,83,83	48
2	3L5	H	301[A]	29/29	0.88	0.12	35,42,53,54	48
2	3L5	H	301[B]	29/29	0.88	0.12	36,44,64,64	48
3	MG	F	302	1/1	0.91	0.10	48,48,48,48	0
3	MG	F	303	1/1	0.92	0.07	51,51,51,51	0
2	3L5	B	301	29/29	0.93	0.11	35,48,107,107	0
3	MG	D	302	1/1	0.93	0.08	55,55,55,55	0
3	MG	B	302	1/1	0.94	0.13	53,53,53,53	0
2	3L5	F	301	29/29	0.95	0.08	27,36,51,51	0
3	MG	C	302	1/1	0.97	0.05	53,53,53,53	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.

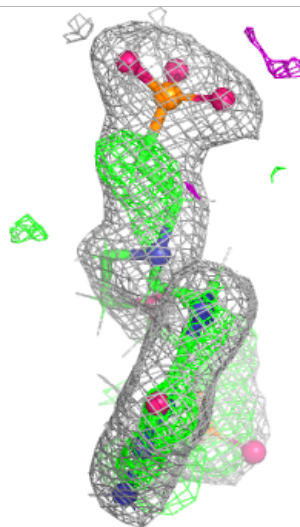
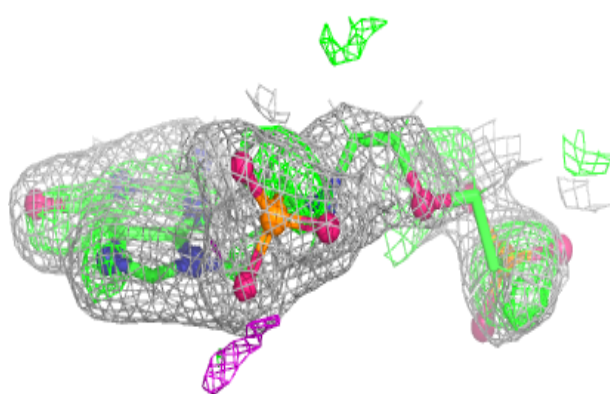
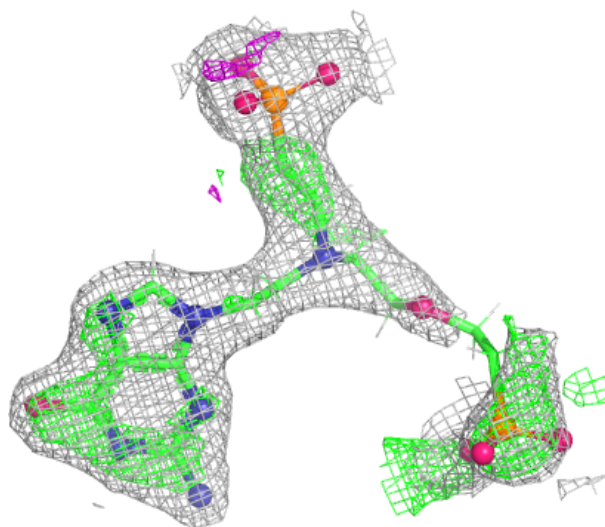
Electron density around 3L5 A 301 (B):

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



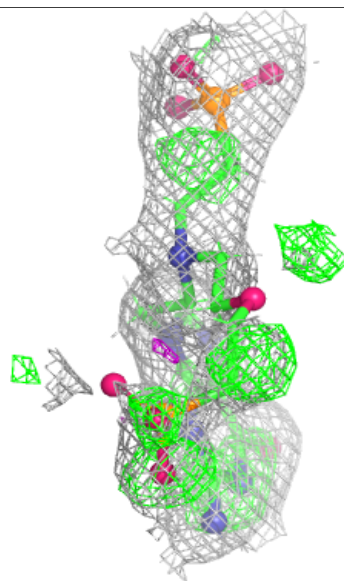
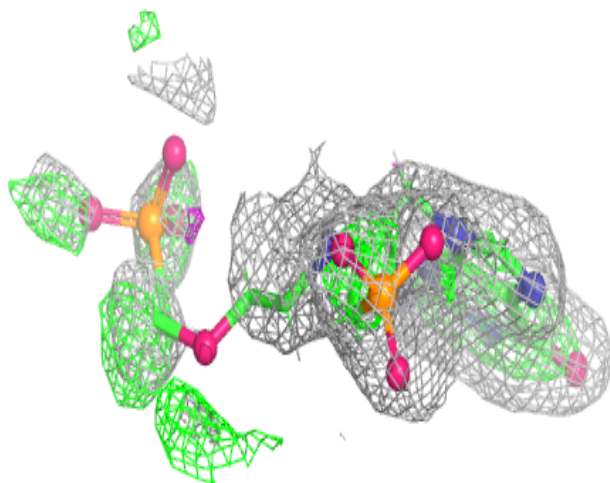
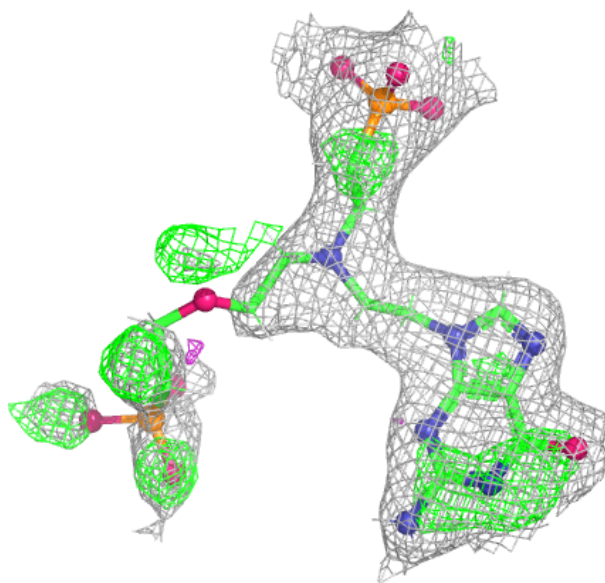
Electron density around 3L5 A 301 (A):

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



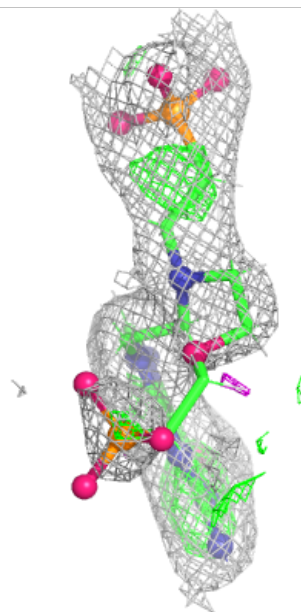
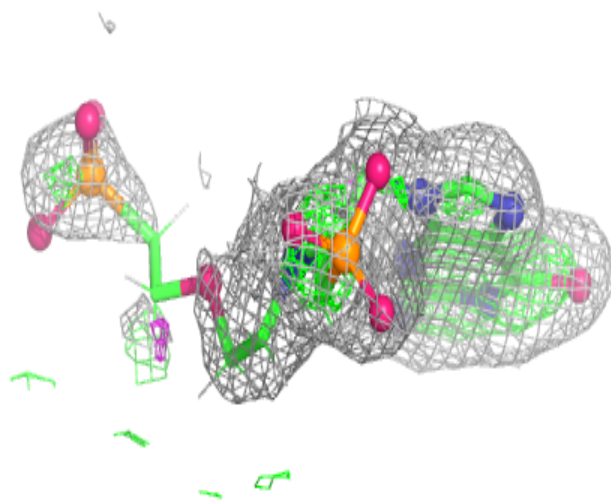
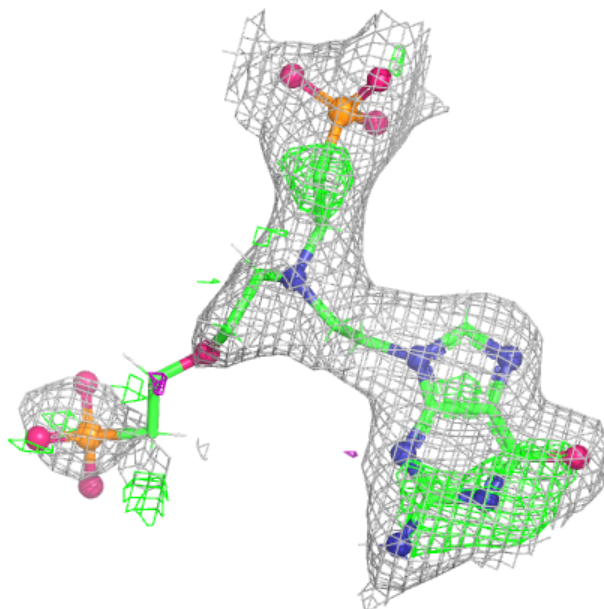
Electron density around 3L5 E 301 (A):

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



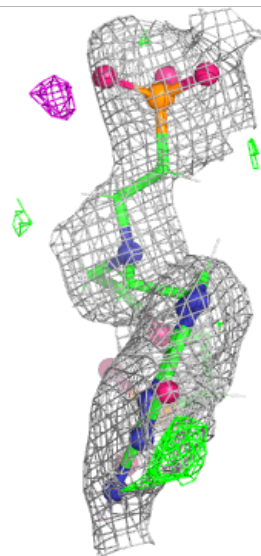
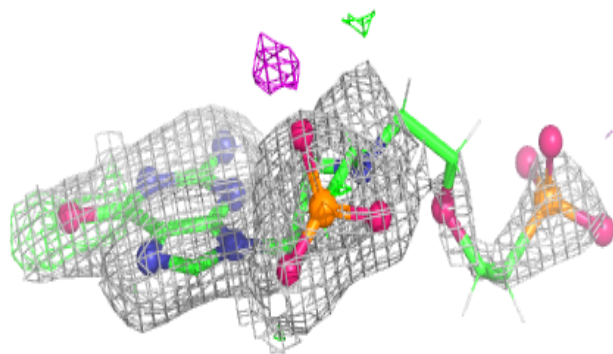
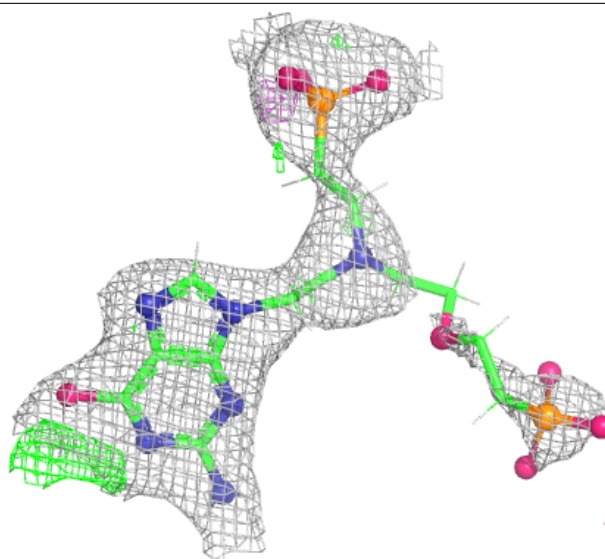
Electron density around 3L5 E 301 (B):

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



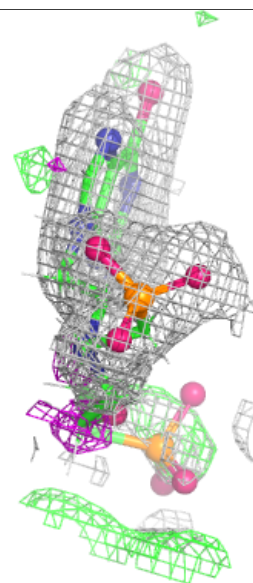
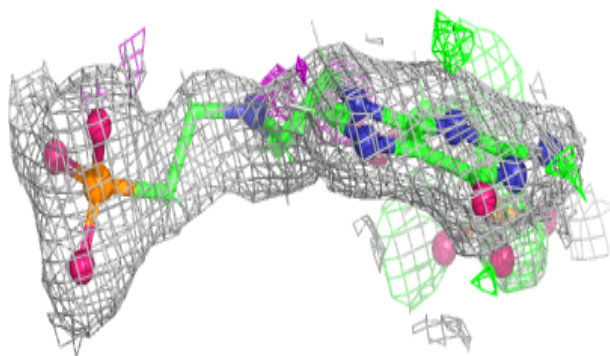
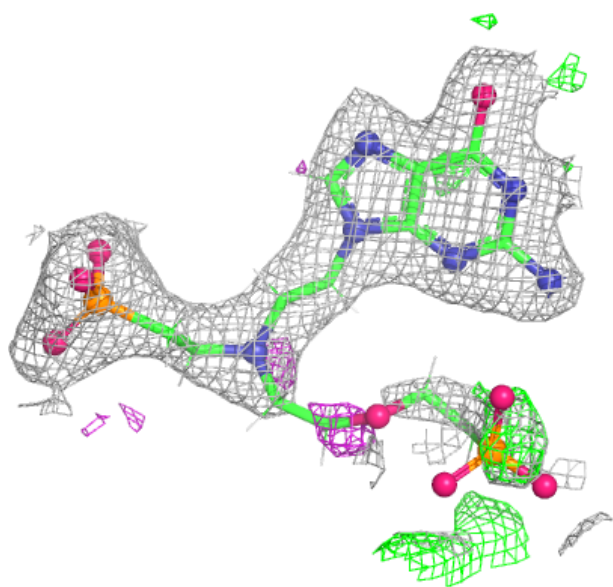
Electron density around 3L5 G 301:

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



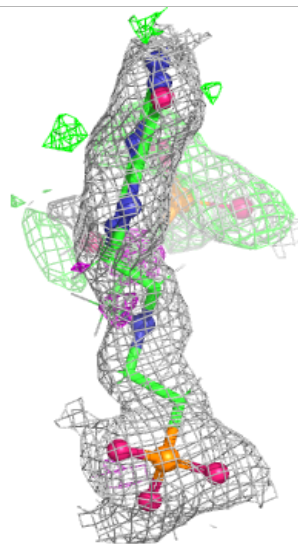
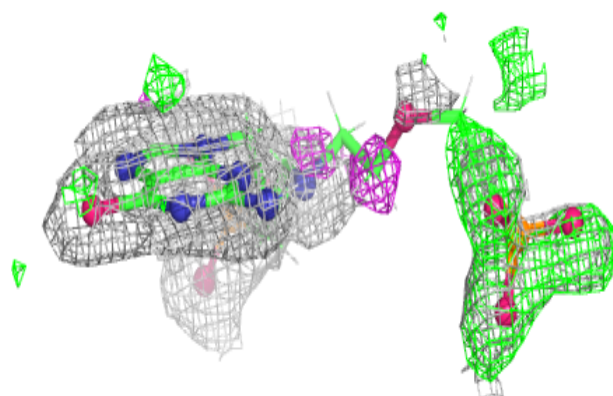
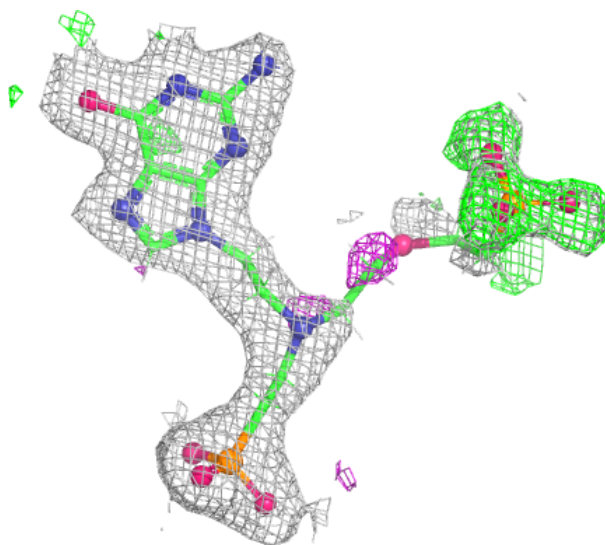
Electron density around 3L5 C 301 (B):

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



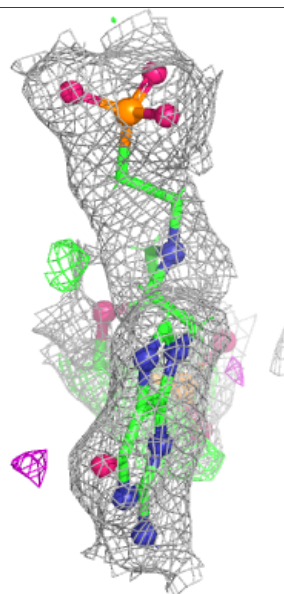
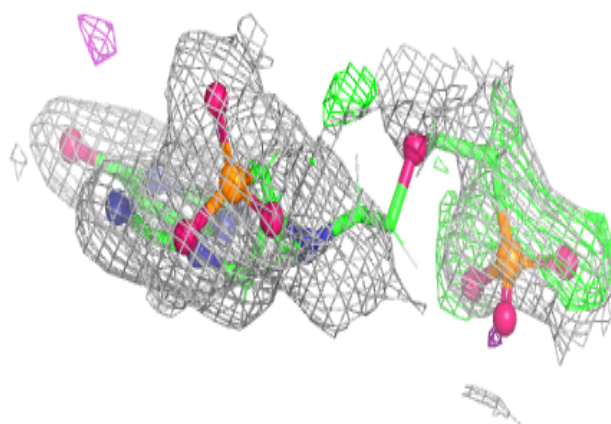
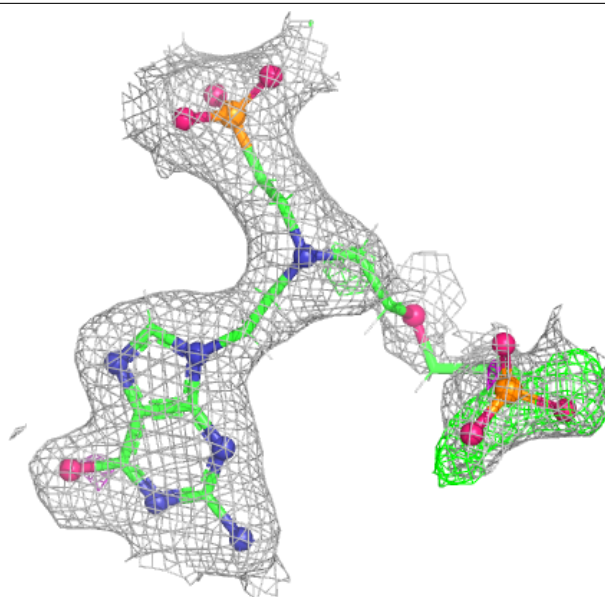
Electron density around 3L5 C 301 (A):

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



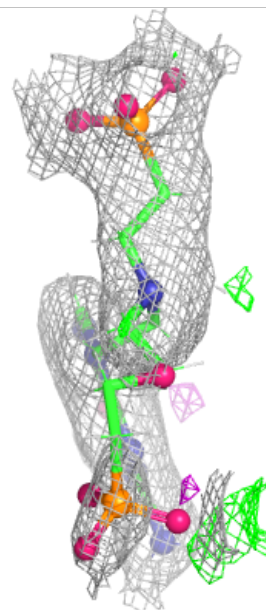
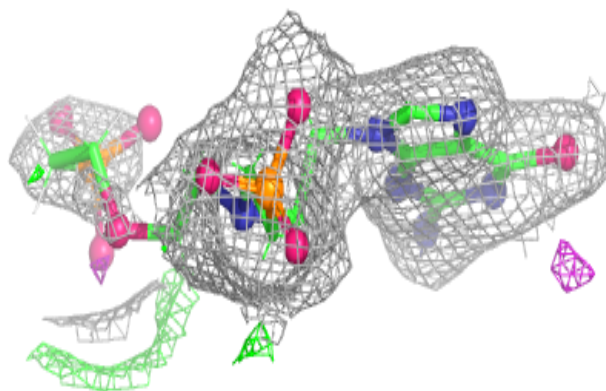
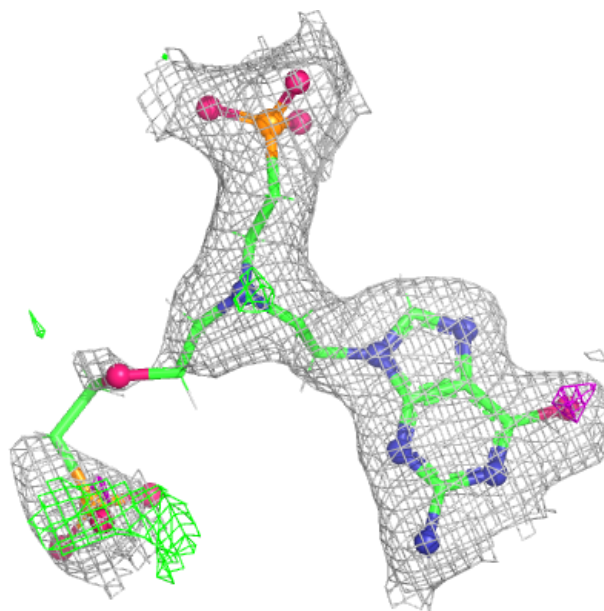
Electron density around 3L5 D 301 (B):

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



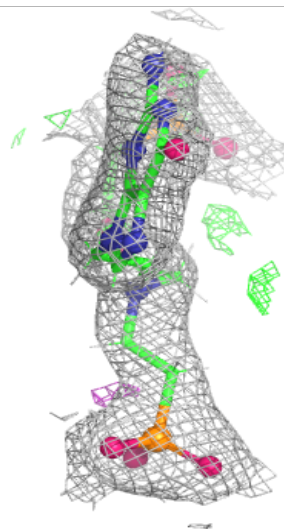
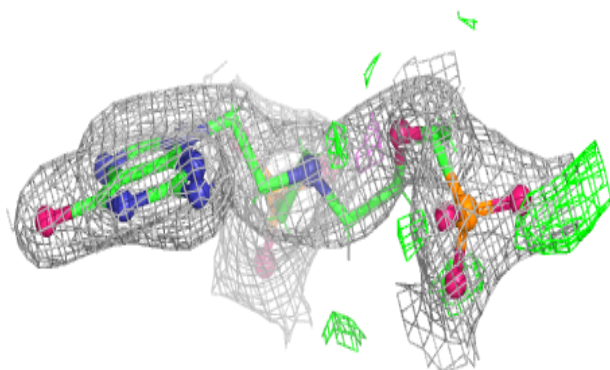
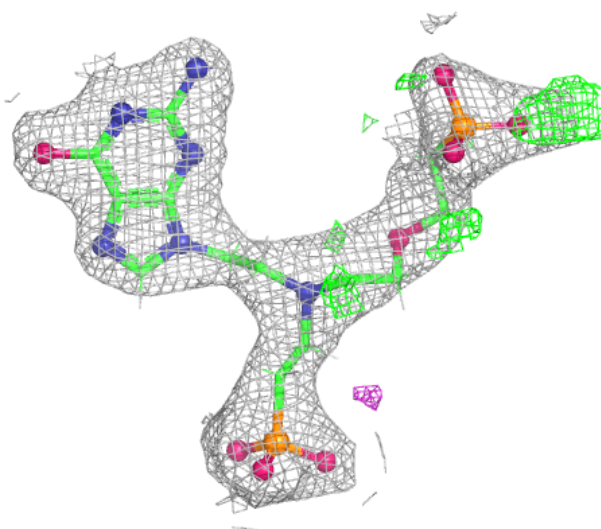
Electron density around 3L5 D 301 (A):

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



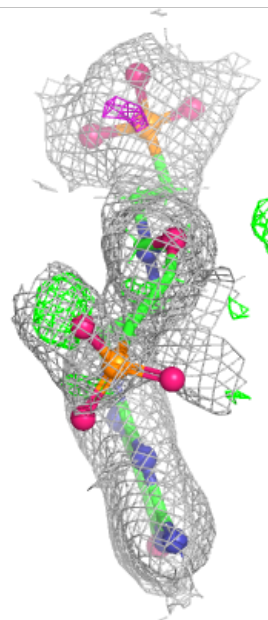
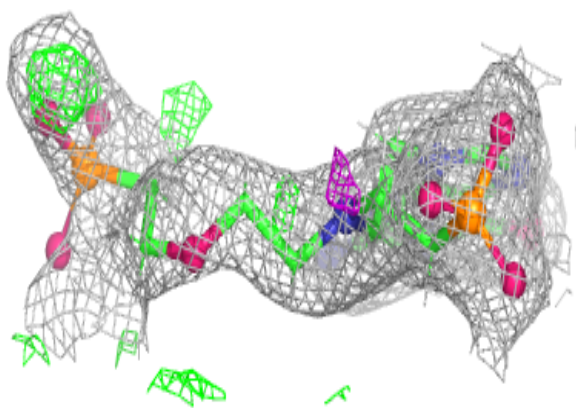
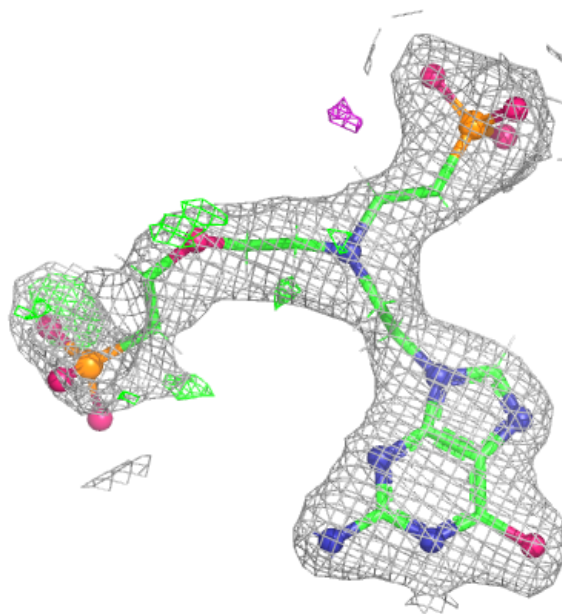
Electron density around 3L5 H 301 (A):

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



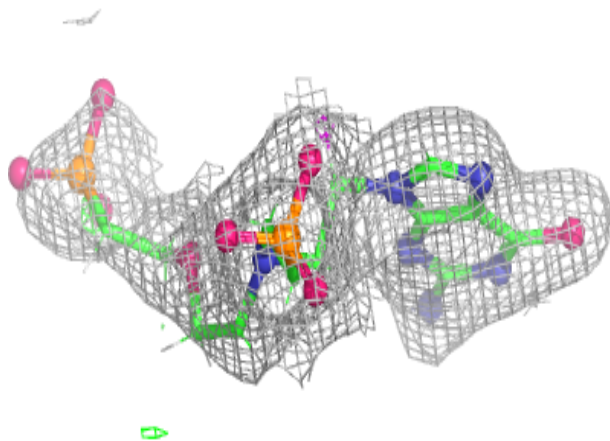
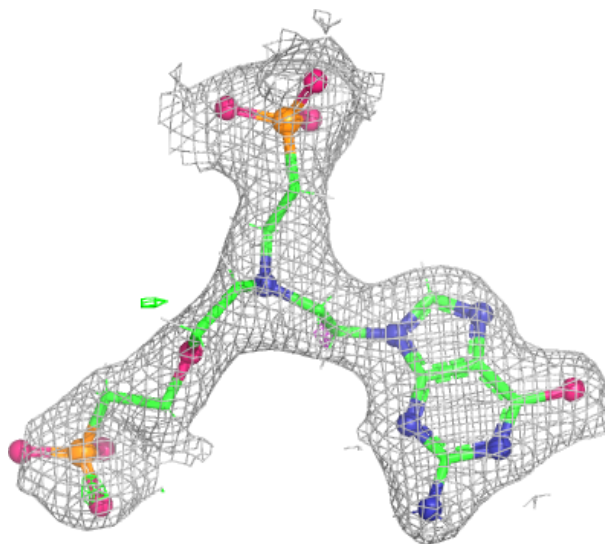
Electron density around 3L5 H 301 (B):

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



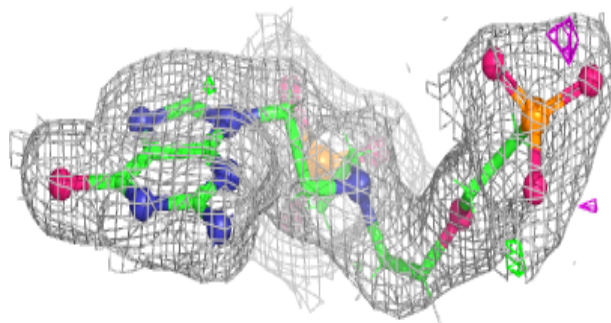
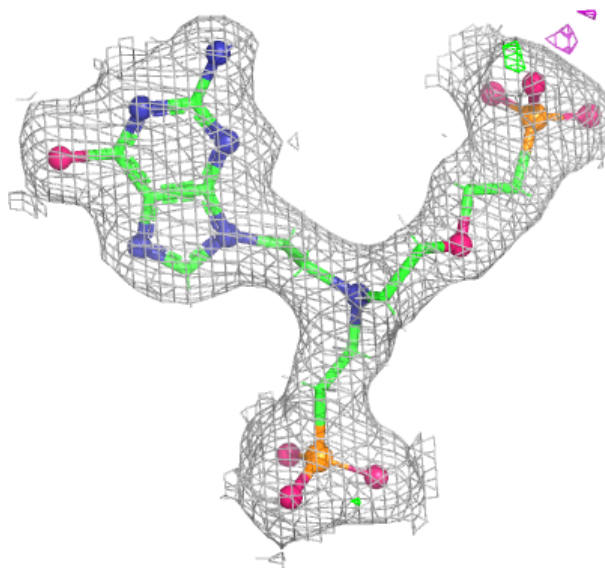
Electron density around 3L5 B 301:

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



Electron density around 3L5 F 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 ⓘ

There are no such residues in this entry.