



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2022 – 10:29 AM EST

PDB ID : 7M0N
Title : The crystal structure of wild type PA endonuclease (2009/H1N1/CALIFORNIA) in complex with Raltegravir
Authors : Cuypers, M.G.; Slavish, P.J.; Yun, M.K.; Dubois, R.; Rankovic, Z.; White, S.W.
Deposited on : 2021-03-11
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
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) : 2.26

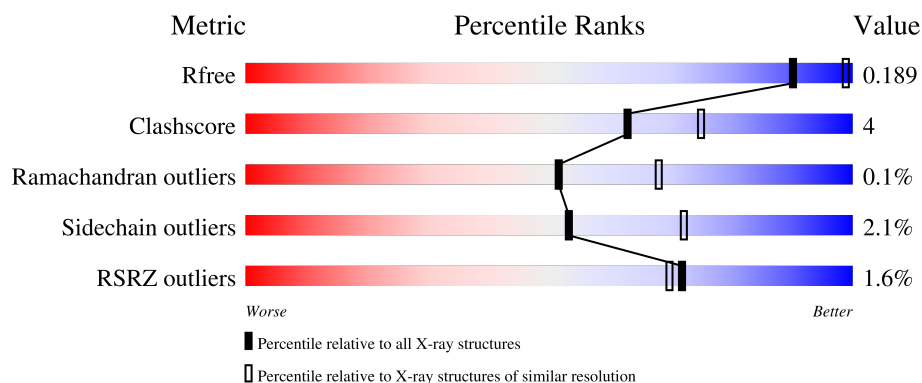
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	187	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	187	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
1	C	187	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
1	D	187	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6372 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein PA-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	1	0
			1498	945	259	283	11			
1	B	183	Total	C	N	O	S	0	0	0
			1487	935	257	284	11			
1	C	187	Total	C	N	O	S	0	1	0
			1511	956	261	283	11			
1	D	183	Total	C	N	O	S	0	0	0
			1481	934	254	282	11			

There are 60 discrepancies between the modelled and reference sequences:

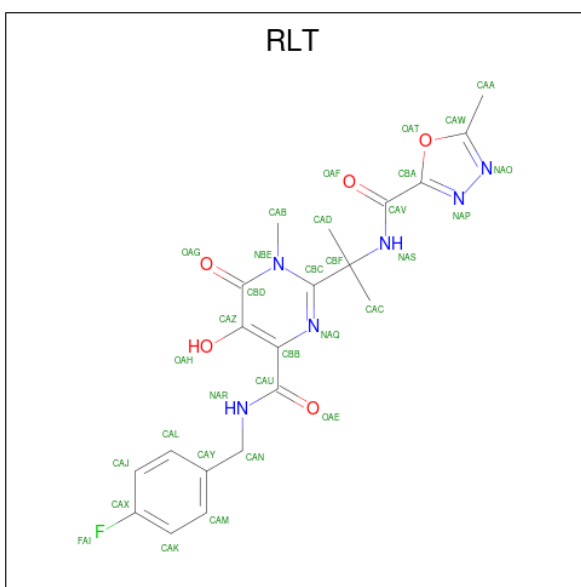
Chain	Residue	Modelled	Actual	Comment	Reference
A	50A	GLY	-	linker	UNP C6Y633
A	50B	GLY	-	linker	UNP C6Y633
A	50C	SER	-	linker	UNP C6Y633
A	129	THR	ILE	conflict	UNP C6Y633
A	142	GLU	LYS	conflict	UNP C6Y633
A	197	ALA	-	expression tag	UNP C6Y633
A	198	ALA	-	expression tag	UNP C6Y633
A	199	ALA	-	expression tag	UNP C6Y633
A	200	GLU	-	expression tag	UNP C6Y633
A	201	LEU	-	expression tag	UNP C6Y633
A	202	ALA	-	expression tag	UNP C6Y633
A	203	LEU	-	expression tag	UNP C6Y633
A	204	VAL	-	expression tag	UNP C6Y633
A	205	PRO	-	expression tag	UNP C6Y633
A	206	ARG	-	expression tag	UNP C6Y633
B	50A	GLY	-	linker	UNP C6Y633
B	50B	GLY	-	linker	UNP C6Y633
B	50C	SER	-	linker	UNP C6Y633
B	129	THR	ILE	conflict	UNP C6Y633
B	142	GLU	LYS	conflict	UNP C6Y633
B	197	ALA	-	expression tag	UNP C6Y633

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Chain	Residue	Modelled	Actual	Comment	Reference
B	198	ALA	-	expression tag	UNP C6Y633
B	199	ALA	-	expression tag	UNP C6Y633
B	200	GLU	-	expression tag	UNP C6Y633
B	201	LEU	-	expression tag	UNP C6Y633
B	202	ALA	-	expression tag	UNP C6Y633
B	203	LEU	-	expression tag	UNP C6Y633
B	204	VAL	-	expression tag	UNP C6Y633
B	205	PRO	-	expression tag	UNP C6Y633
B	206	ARG	-	expression tag	UNP C6Y633
C	50A	GLY	-	linker	UNP C6Y633
C	50B	GLY	-	linker	UNP C6Y633
C	50C	SER	-	linker	UNP C6Y633
C	129	THR	ILE	conflict	UNP C6Y633
C	142	GLU	LYS	conflict	UNP C6Y633
C	197	ALA	-	expression tag	UNP C6Y633
C	198	ALA	-	expression tag	UNP C6Y633
C	199	ALA	-	expression tag	UNP C6Y633
C	200	GLU	-	expression tag	UNP C6Y633
C	201	LEU	-	expression tag	UNP C6Y633
C	202	ALA	-	expression tag	UNP C6Y633
C	203	LEU	-	expression tag	UNP C6Y633
C	204	VAL	-	expression tag	UNP C6Y633
C	205	PRO	-	expression tag	UNP C6Y633
C	206	ARG	-	expression tag	UNP C6Y633
D	50A	GLY	-	linker	UNP C6Y633
D	50B	GLY	-	linker	UNP C6Y633
D	50C	SER	-	linker	UNP C6Y633
D	129	THR	ILE	conflict	UNP C6Y633
D	142	GLU	LYS	conflict	UNP C6Y633
D	197	ALA	-	expression tag	UNP C6Y633
D	198	ALA	-	expression tag	UNP C6Y633
D	199	ALA	-	expression tag	UNP C6Y633
D	200	GLU	-	expression tag	UNP C6Y633
D	201	LEU	-	expression tag	UNP C6Y633
D	202	ALA	-	expression tag	UNP C6Y633
D	203	LEU	-	expression tag	UNP C6Y633
D	204	VAL	-	expression tag	UNP C6Y633
D	205	PRO	-	expression tag	UNP C6Y633
D	206	ARG	-	expression tag	UNP C6Y633

- Molecule 2 is N-(4-fluorobenzyl)-5-hydroxy-1-methyl-2-(1-methyl-1-[(5-methyl-1,3,4-oxadiazol-2-yl)carbonyl]amino)ethyl)-6-oxo-1,6-di hydropyrimidine-4-carboxamide (three-letter code: RLT) (formula: C₂₀H₂₁FN₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 32	C 20	F 1	N 6	O 5	0	0
2	B	1	Total 32	C 20	F 1	N 6	O 5	0	0
2	C	1	Total 32	C 20	F 1	N 6	O 5	0	0
2	D	1	Total 32	C 20	F 1	N 6	O 5	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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



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

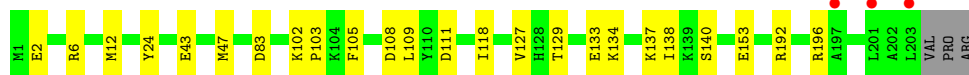
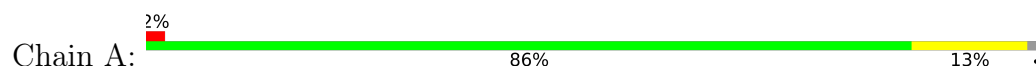
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	51	Total	O	0	0
			51	51		
6	C	52	Total	O	0	0
			52	52		
6	D	50	Total	O	0	0
			50	50		

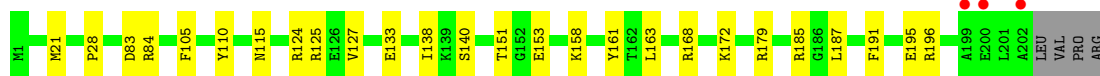
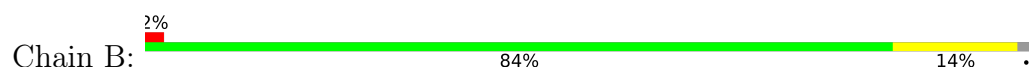
3 Residue-property plots [i](#)

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.

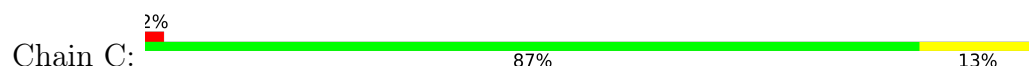
- Molecule 1: Protein PA-X



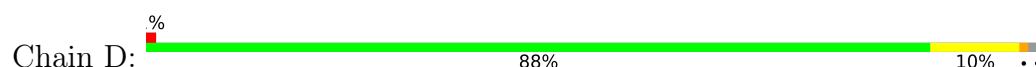
- Molecule 1: Protein PA-X



- Molecule 1: Protein PA-X



- Molecule 1: Protein PA-X



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	126.70Å 135.13Å 126.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.44 – 2.40 46.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.44-2.40) 99.4 (46.22-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.192 , 0.231 0.192 , 0.189	Depositor DCC
R_{free} test set	2152 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6372	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.8935e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, SO4, MN, RLT

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	0.25	0/1531	0.50	0/2059
1	B	0.25	0/1517	0.50	0/2041
1	C	0.27	0/1542	0.50	0/2077
1	D	0.25	0/1511	0.49	0/2035
All	All	0.26	0/6101	0.50	0/8212

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	1498	0	1453	14	0
1	B	1487	0	1431	18	0
1	C	1511	0	1451	10	0
1	D	1481	0	1417	11	0
2	A	32	0	20	4	0
2	B	32	0	20	6	0
2	C	32	0	20	0	0
2	D	32	0	20	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	1	0
5	B	12	0	16	0	0
5	D	18	0	24	1	0
6	A	36	0	0	2	0
6	B	51	0	0	1	0
6	C	52	0	0	0	0
6	D	50	0	0	0	0
All	All	6372	0	5872	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PHE:HB3	2:B:301:RLT:HAK	1.68	0.75
1:A:105:PHE:HB3	2:A:301:RLT:HAK	1.72	0.71
1:C:43:GLU:O	1:C:47:MET:HG3	1.99	0.62
1:A:43:GLU:O	1:A:47:MET:HG3	2.00	0.62
1:D:46:PHE:HB3	5:D:304:GOL:H11	1.83	0.61
1:D:30:ILE:HD12	1:D:31:GLU:HG3	1.84	0.60
1:A:129:THR:O	1:A:133:GLU:HG3	2.04	0.58
1:A:192:ARG:NH1	6:A:403:HOH:O	2.36	0.57
1:B:138:ILE:HG22	1:B:140:SER:H	1.70	0.56
1:A:134[B]:LYS:NZ	2:A:301:RLT:OAT	2.38	0.56
1:C:170:ARG:HD2	1:D:74:HIS:HB3	1.89	0.55
1:D:104:LYS:HD2	1:D:104:LYS:H	1.72	0.55
1:C:86:MET:O	1:C:90:VAL:HG23	2.07	0.54
1:B:125:ARG:NH1	6:B:402:HOH:O	2.38	0.53
1:A:127:VAL:HG21	1:A:153:GLU:HG2	1.90	0.53
1:C:138:ILE:HD12	1:C:140:SER:HB3	1.92	0.52
1:D:86:MET:O	1:D:90:VAL:HG23	2.10	0.51
1:D:75:ARG:NH1	4:D:308:SO4:O2	2.32	0.51
1:B:133:GLU:HB3	2:B:301:RLT:HAAA	1.92	0.51
1:B:151:THR:HG22	1:B:179:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:NZ	6:A:404:HOH:O	2.44	0.50
1:D:161:TYR:O	1:D:163:LEU:N	2.45	0.49
1:B:110:TYR:OH	1:B:115:ASN:OD1	2.28	0.48
1:A:133:GLU:HB2	2:A:301:RLT:HAAA	1.95	0.48
1:B:84:ARG:HH12	2:B:301:RLT:CAL	2.26	0.48
1:A:24:TYR:OH	2:A:301:RLT:HAL	2.13	0.48
1:B:168:ARG:O	1:B:172:LYS:HG3	2.14	0.47
1:B:185:ARG:HB2	1:B:187:LEU:CD2	2.45	0.46
1:D:27:ASP:HB3	1:D:30:ILE:HG13	1.97	0.46
1:D:77:GLU:HG2	1:D:94:ILE:HD11	1.98	0.46
1:A:108:ASP:O	1:A:109:LEU:HD23	2.16	0.46
1:B:158:LYS:N	1:B:158:LYS:HD3	2.31	0.46
1:C:108:ASP:O	1:C:109:LEU:HD23	2.16	0.45
1:B:161:TYR:O	1:B:163:LEU:N	2.47	0.45
1:B:21:MET:HE1	1:B:28:PRO:HA	1.97	0.45
1:B:84:ARG:HH12	2:B:301:RLT:HAL	1.83	0.44
1:B:124:ARG:CZ	1:B:195:GLU:HB2	2.47	0.44
1:C:84:ARG:NH1	1:C:88:TRP:HE1	2.16	0.44
1:D:124:ARG:CZ	1:D:195:GLU:HB2	2.48	0.43
1:A:111:ASP:HB2	1:A:118:ILE:HD11	2.00	0.43
1:D:157:THR:HG22	1:D:158:LYS:HG3	2.00	0.42
1:B:84:ARG:HH12	2:B:301:RLT:CAJ	2.33	0.42
1:A:138:ILE:C	1:A:140:SER:H	2.23	0.41
1:B:124:ARG:HD3	1:B:191:PHE:CE2	2.55	0.41
1:B:127:VAL:HG11	1:B:153:GLU:HB2	2.02	0.41
1:C:201:LEU:HD23	1:C:201:LEU:HA	1.83	0.41
1:C:34:LYS:O	1:C:38:ILE:HG12	2.20	0.41
1:B:84:ARG:NH1	2:B:301:RLT:HAL	2.36	0.41
1:C:124:ARG:CZ	1:C:195:GLU:HB2	2.51	0.41
1:C:179:ARG:HG3	1:C:188:TRP:CH2	2.56	0.41
1:A:102:LYS:HA	1:A:103:PRO:HD3	1.98	0.40
1:A:2:GLU:O	1:A:6:ARG:HG3	2.20	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	183/187 (98%)	176 (96%)	7 (4%)	0	100	100
1	B	181/187 (97%)	176 (97%)	5 (3%)	0	100	100
1	C	186/187 (100%)	182 (98%)	3 (2%)	1 (0%)	29	41
1	D	181/187 (97%)	177 (98%)	4 (2%)	0	100	100
All	All	731/748 (98%)	711 (97%)	19 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	73	LYS

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	158/165 (96%)	155 (98%)	3 (2%)	57	75
1	B	157/165 (95%)	155 (99%)	2 (1%)	69	84
1	C	156/165 (94%)	151 (97%)	5 (3%)	39	59
1	D	154/165 (93%)	151 (98%)	3 (2%)	57	75
All	All	625/660 (95%)	612 (98%)	13 (2%)	53	72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	83	ASP
1	A	196	ARG
1	B	83	ASP
1	B	196	ARG

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Mol	Chain	Res	Type
1	C	1	MET
1	C	134	LYS
1	C	184	SER
1	C	194	SER
1	C	196	ARG
1	D	104	LYS
1	D	184	SER
1	D	194	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	D	180	GLN

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 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	RLT	A	301	3	29,34,34	0.87	2 (6%)	31,50,50	1.05	1 (3%)
5	GOL	D	304	-	5,5,5	0.90	0	5,5,5	1.02	0
4	SO4	D	307	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	A	305	-	4,4,4	0.13	0	6,6,6	0.07	0
2	RLT	C	301	3	29,34,34	0.86	2 (6%)	31,50,50	1.06	1 (3%)
4	SO4	B	307	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	C	304	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.04	0
5	GOL	B	303	-	5,5,5	0.89	0	5,5,5	1.05	0
4	SO4	B	306	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	308	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.04	0
5	GOL	D	302	-	5,5,5	0.90	0	5,5,5	1.02	0
2	RLT	B	301	3	29,34,34	0.87	2 (6%)	31,50,50	1.03	1 (3%)
5	GOL	B	302	-	5,5,5	0.88	0	5,5,5	1.03	0
5	GOL	D	303	-	5,5,5	0.91	0	5,5,5	0.99	0
2	RLT	D	301	3	29,34,34	0.86	2 (6%)	31,50,50	1.02	1 (3%)

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	RLT	A	301	3	-	0/17/24/24	0/3/3/3
5	GOL	D	304	-	-	2/4/4/4	-
2	RLT	C	301	3	-	0/17/24/24	0/3/3/3
5	GOL	B	303	-	-	0/4/4/4	-
5	GOL	D	302	-	-	0/4/4/4	-
2	RLT	B	301	3	-	0/17/24/24	0/3/3/3
5	GOL	B	302	-	-	0/4/4/4	-
5	GOL	D	303	-	-	2/4/4/4	-
2	RLT	D	301	3	-	0/17/24/24	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RLT	CBA-CAV	-2.63	1.46	1.50
2	B	301	RLT	CBA-CAV	-2.61	1.46	1.50
2	C	301	RLT	CBA-CAV	-2.53	1.46	1.50
2	D	301	RLT	CBA-CAV	-2.45	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RLT	CAA-CAW	-2.17	1.47	1.49
2	C	301	RLT	CAA-CAW	-2.16	1.47	1.49
2	D	301	RLT	CAA-CAW	-2.15	1.47	1.49
2	B	301	RLT	CAA-CAW	-2.14	1.47	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	RLT	CAA-CAW-NAO	4.99	130.62	119.65
2	B	301	RLT	CAA-CAW-NAO	4.96	130.54	119.65
2	A	301	RLT	CAA-CAW-NAO	4.95	130.52	119.65
2	D	301	RLT	CAA-CAW-NAO	4.91	130.44	119.65

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	303	GOL	C1-C2-C3-O3
5	D	304	GOL	C1-C2-C3-O3
5	D	303	GOL	O2-C2-C3-O3
5	D	304	GOL	O2-C2-C3-O3

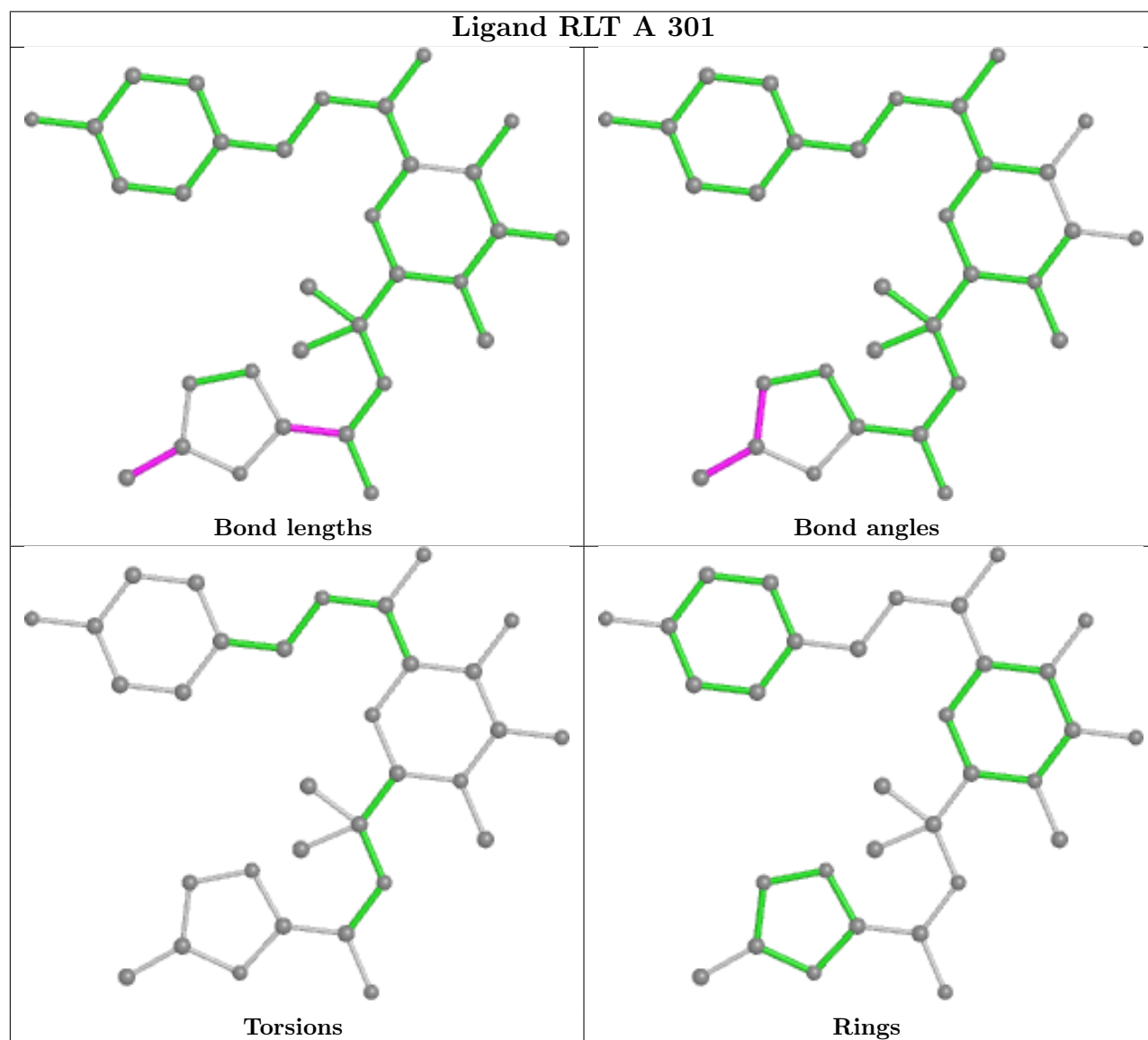
There are no ring outliers.

4 monomers are involved in 12 short contacts:

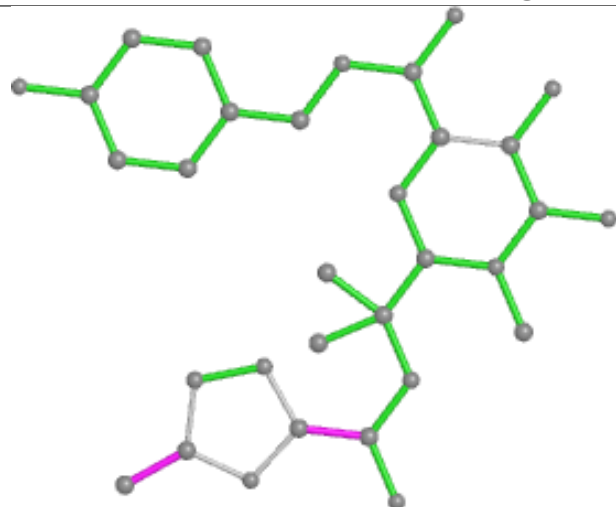
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RLT	4	0
5	D	304	GOL	1	0
4	D	308	SO4	1	0
2	B	301	RLT	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

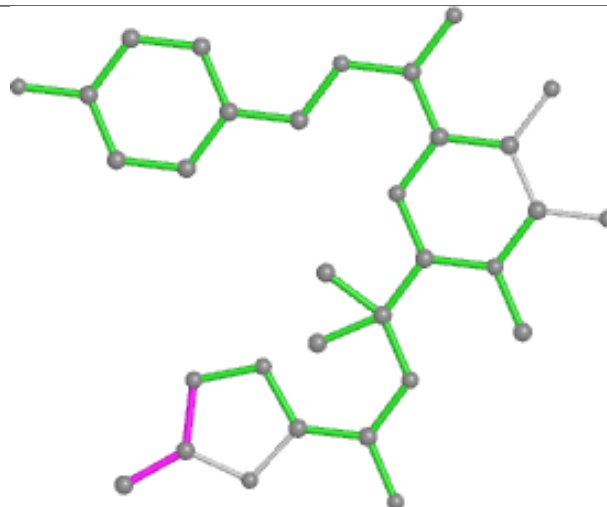
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



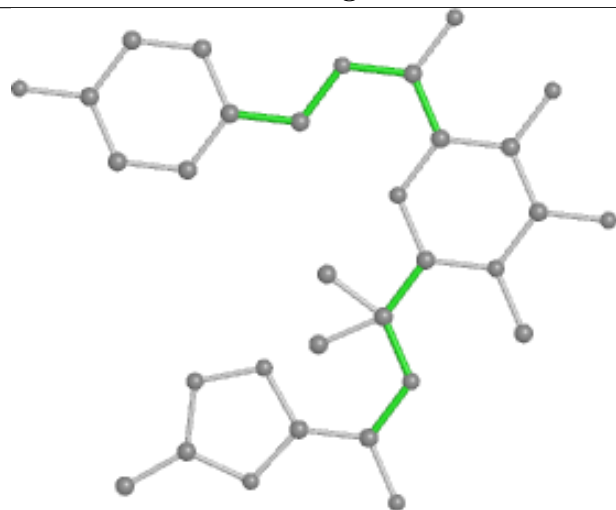
Ligand RLT C 301



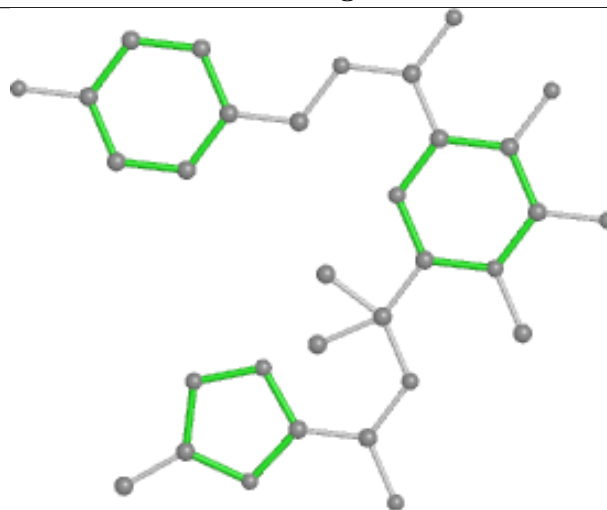
Bond lengths



Bond angles

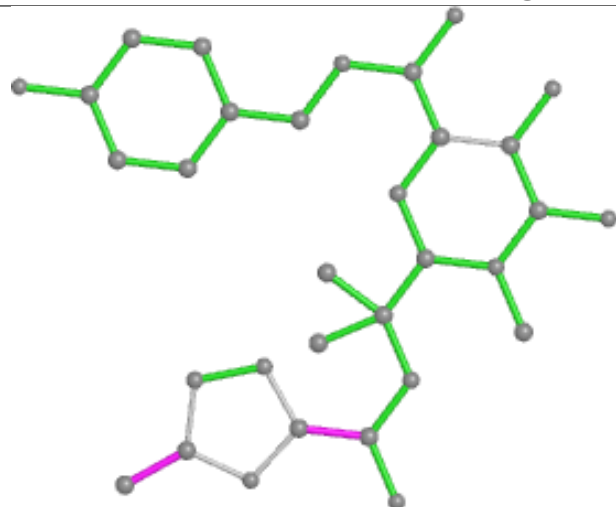


Torsions

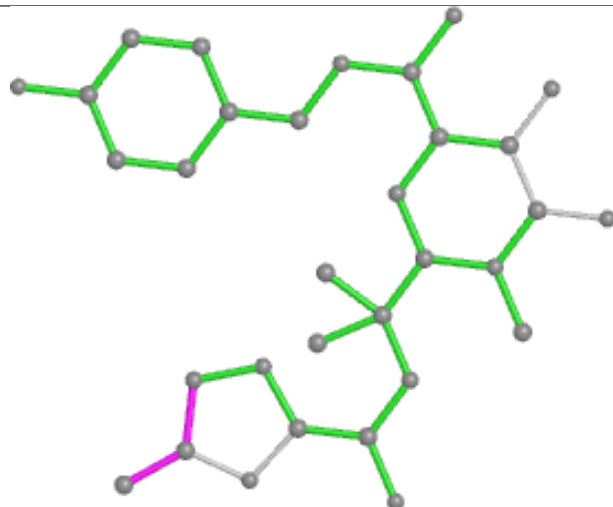


Rings

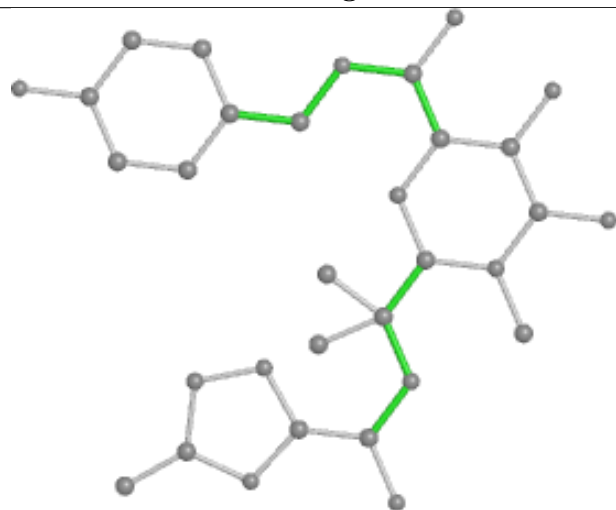
Ligand RLT B 301



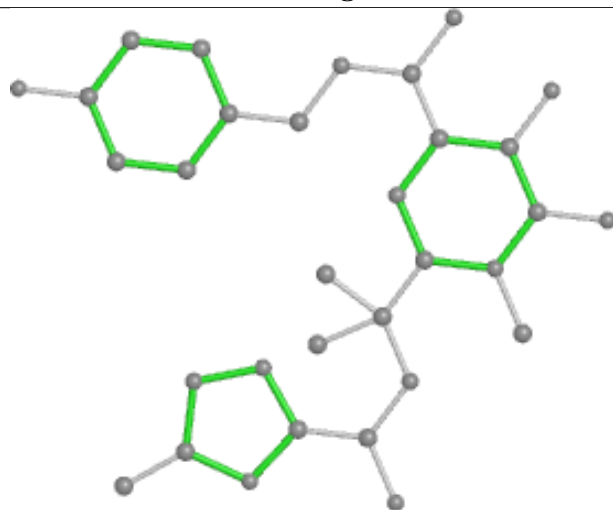
Bond lengths



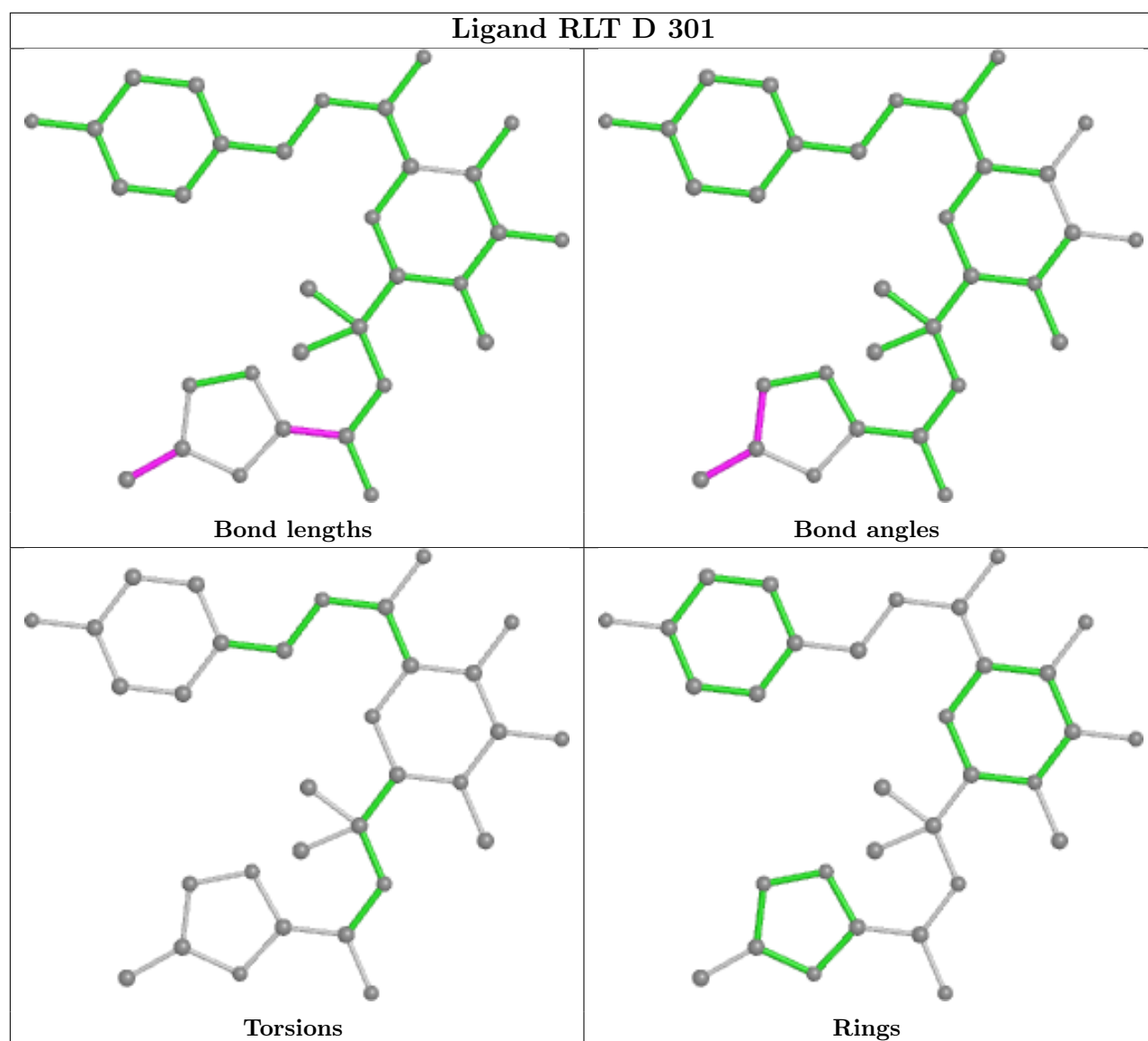
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	184/187 (98%)	0.04	3 (1%) 72 70	49, 67, 119, 169	0
1	B	183/187 (97%)	0.05	3 (1%) 72 70	47, 66, 121, 179	0
1	C	187/187 (100%)	-0.02	4 (2%) 63 61	44, 65, 115, 173	0
1	D	183/187 (97%)	-0.06	2 (1%) 80 79	45, 66, 117, 178	0
All	All	737/748 (98%)	0.00	12 (1%) 72 70	44, 66, 123, 179	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	LEU	4.8
1	B	199	ALA	4.3
1	C	205	PRO	4.3
1	C	203	LEU	3.8
1	C	206	ARG	3.6
1	A	197	ALA	3.1
1	B	202	ALA	3.0
1	B	200	GLU	2.8
1	D	199	ALA	2.7
1	D	24	TYR	2.6
1	C	204	VAL	2.1
1	A	203	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

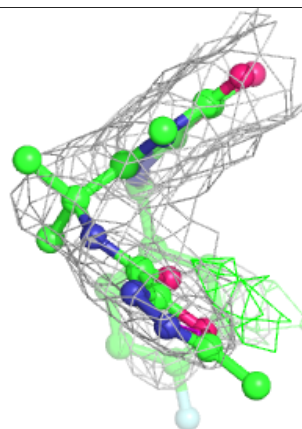
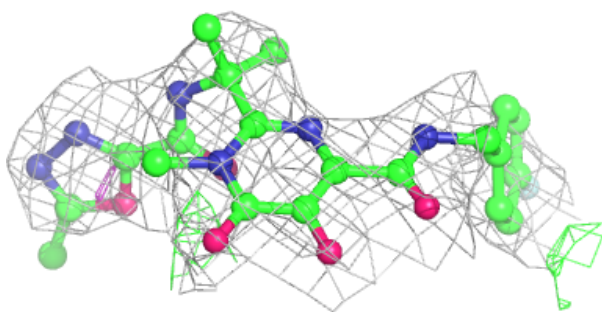
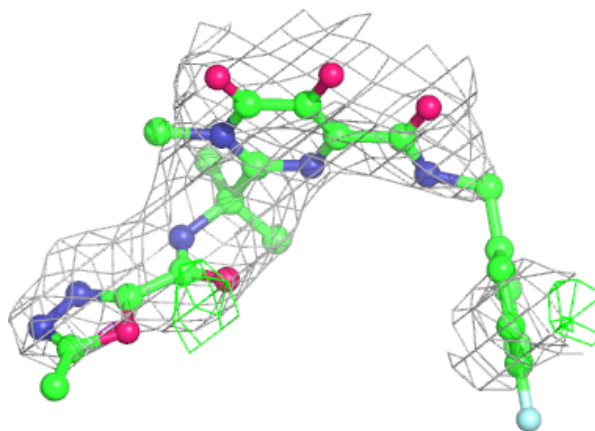
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	303	6/6	0.73	0.21	84,100,107,109	0
4	SO4	A	305	5/5	0.79	0.20	84,106,115,122	0
5	GOL	D	304	6/6	0.86	0.29	95,109,117,146	0
4	SO4	B	307	5/5	0.87	0.14	87,102,109,121	0
5	GOL	B	302	6/6	0.87	0.15	72,83,85,90	0
2	RLT	C	301	32/32	0.88	0.23	72,113,133,138	0
2	RLT	D	301	32/32	0.89	0.24	88,121,135,143	0
2	RLT	A	301	32/32	0.90	0.26	98,139,149,155	0
4	SO4	D	308	5/5	0.91	0.14	100,101,120,121	0
5	GOL	D	303	6/6	0.91	0.24	71,78,83,119	0
2	RLT	B	301	32/32	0.91	0.24	77,116,131,136	0
5	GOL	D	302	6/6	0.92	0.14	86,93,113,114	0
4	SO4	D	307	5/5	0.92	0.23	92,102,131,134	0
4	SO4	C	305	5/5	0.92	0.17	78,100,111,117	0
4	SO4	A	304	5/5	0.93	0.22	85,89,106,127	0
4	SO4	B	306	5/5	0.94	0.20	85,91,116,119	0
3	MN	A	303	1/1	0.95	0.06	81,81,81,81	0
4	SO4	C	304	5/5	0.96	0.19	82,86,109,120	0
3	MN	D	305	1/1	0.97	0.07	82,82,82,82	0
3	MN	D	306	1/1	0.98	0.13	62,62,62,62	0
3	MN	A	302	1/1	0.98	0.09	64,64,64,64	0
3	MN	B	304	1/1	0.99	0.05	79,79,79,79	0
3	MN	B	305	1/1	0.99	0.14	61,61,61,61	0
3	MN	C	302	1/1	0.99	0.13	60,60,60,60	0
3	MN	C	303	1/1	1.00	0.07	77,77,77,77	0

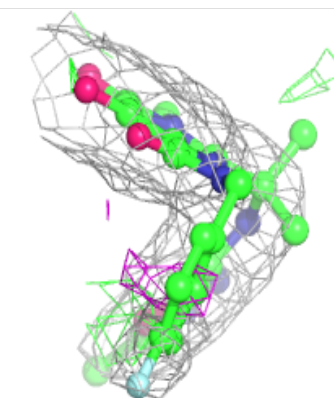
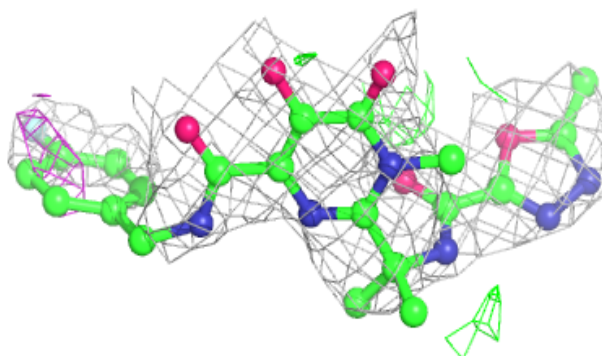
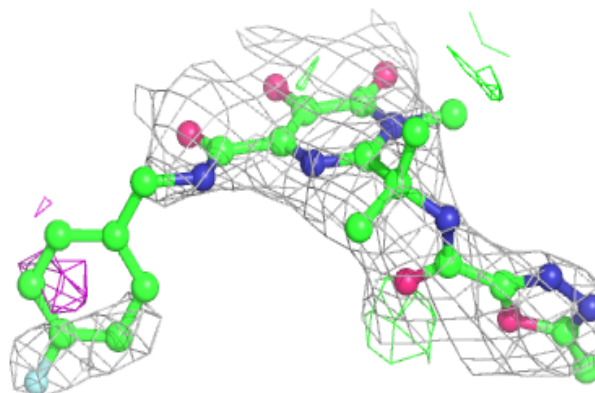
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RLT C 301:

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

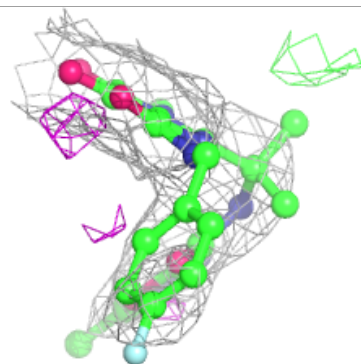
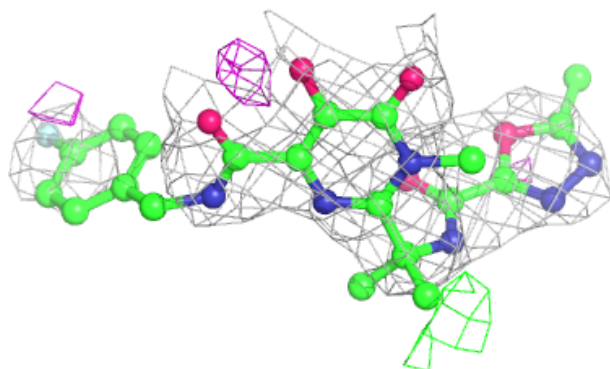
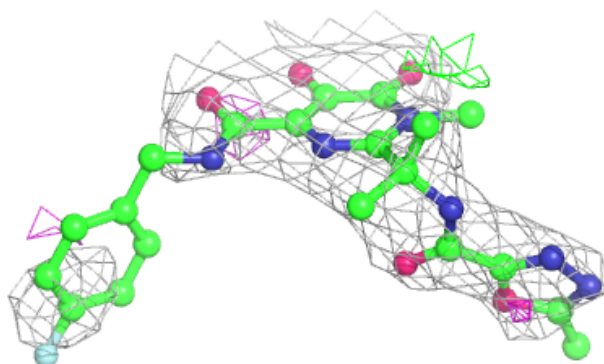
**Electron density around RLT D 301:**

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

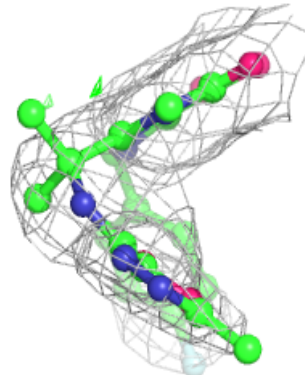
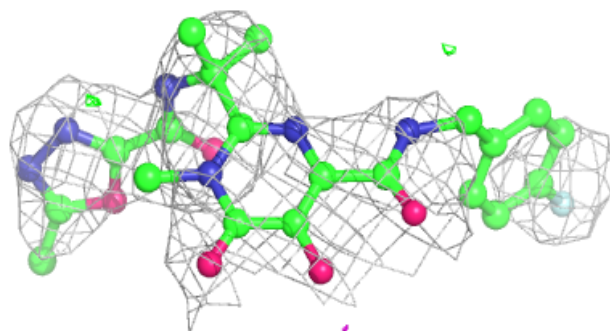
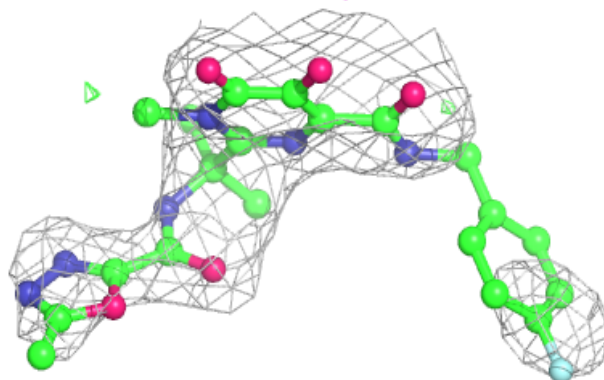


Electron density around RLT A 301:

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

**Electron density around RLT 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.