



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2021 – 08:52 AM JST

PDB ID : 7E7R
Title : Crystal structure of RSL mutant in complex with Ligand
Authors : Li, L.; Chen, G.S.
Deposited on : 2021-02-27
Resolution : 1.82 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 : 2.18
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) : 2.18

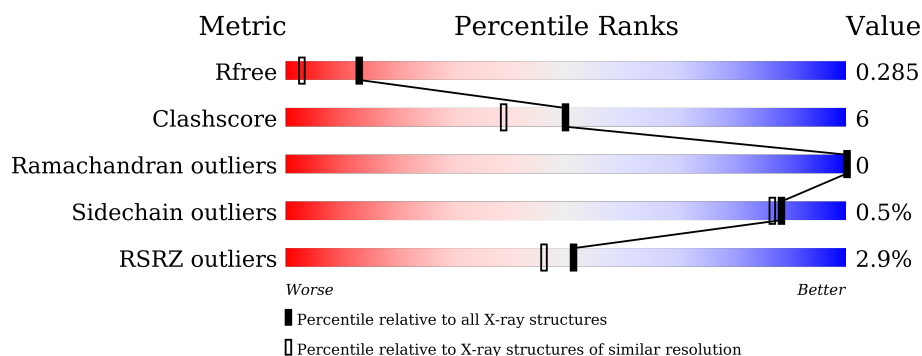
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	272	
1	B	272	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	R2F	A	301	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4641 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 Fucose-binding lectin protein,Fucose-binding lectin protein,Fucose-binding lectin protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1948	1230	327	385	6			
1	B	258	Total	C	N	O	S	0	0	0
			1962	1237	330	389	6			

There are 34 discrepancies between the modelled and reference sequences:

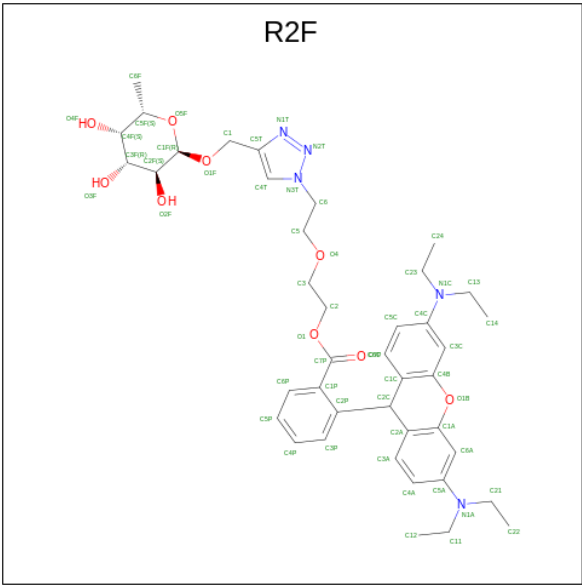
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	ARG	engineered mutation	UNP A0A0S4TLR1
A	88	SER	-	linker	UNP A0A0S4TLR1
A	89	SER	-	linker	UNP A0A0S4TLR1
A	90	THR	-	linker	UNP A0A0S4TLR1
A	91	VAL	-	linker	UNP A0A0S4TLR1
A	92	PRO	-	linker	UNP A0A0S4TLR1
A	93	GLY	-	linker	UNP A0A0S4TLR1
A	94	ASP	-	linker	UNP A0A0S4TLR1
A	108	ALA	ARG	engineered mutation	UNP A0A0S4TLR1
A	179	SER	-	linker	UNP A0A0S4TLR1
A	180	SER	-	linker	UNP A0A0S4TLR1
A	181	THR	-	linker	UNP A0A0S4TLR1
A	182	VAL	-	linker	UNP A0A0S4TLR1
A	183	PRO	-	linker	UNP A0A0S4TLR1
A	184	GLY	-	linker	UNP A0A0S4TLR1
A	185	ASP	-	linker	UNP A0A0S4TLR1
A	199	ALA	ARG	engineered mutation	UNP A0A0S4TLR1
B	17	ALA	ARG	engineered mutation	UNP A0A0S4TLR1
B	88	SER	-	linker	UNP A0A0S4TLR1
B	89	SER	-	linker	UNP A0A0S4TLR1
B	90	THR	-	linker	UNP A0A0S4TLR1
B	91	VAL	-	linker	UNP A0A0S4TLR1
B	92	PRO	-	linker	UNP A0A0S4TLR1
B	93	GLY	-	linker	UNP A0A0S4TLR1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	94	ASP	-	linker	UNP A0A0S4TLR1
B	108	ALA	ARG	engineered mutation	UNP A0A0S4TLR1
B	179	SER	-	linker	UNP A0A0S4TLR1
B	180	SER	-	linker	UNP A0A0S4TLR1
B	181	THR	-	linker	UNP A0A0S4TLR1
B	182	VAL	-	linker	UNP A0A0S4TLR1
B	183	PRO	-	linker	UNP A0A0S4TLR1
B	184	GLY	-	linker	UNP A0A0S4TLR1
B	185	ASP	-	linker	UNP A0A0S4TLR1
B	199	ALA	ARG	engineered mutation	UNP A0A0S4TLR1

- Molecule 2 is 2-[2-[4-[[[(2R,3S,4R,5S,6S)-6-methyl-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-1,2,3-triazol-1-yl]ethoxy]ethyl 2-[3,6-bis(diethylamino)-9H-xanthen-9-yl]benzoate (three-letter code: R2F) (formula: C₄₁H₅₃N₅O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			55	41	5	9		
2	A	1	Total	C	N	O	0	0
			55	41	5	9		
2	A	1	Total	C	N	O	0	0
			55	41	5	9		
2	B	1	Total	C	N	O	0	0
			55	41	5	9		
2	B	1	Total	C	N	O	0	0
			55	41	5	9		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			55	41	5	9		

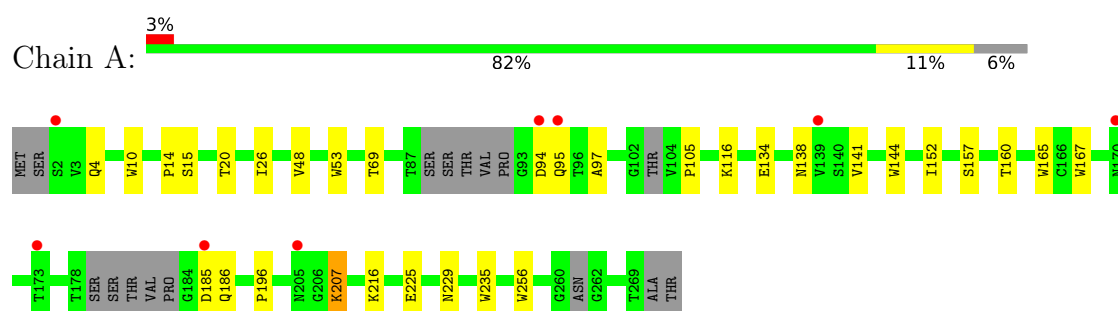
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	202	Total	O	0	0
			202	202		
3	B	199	Total	O	0	0
			199	199		

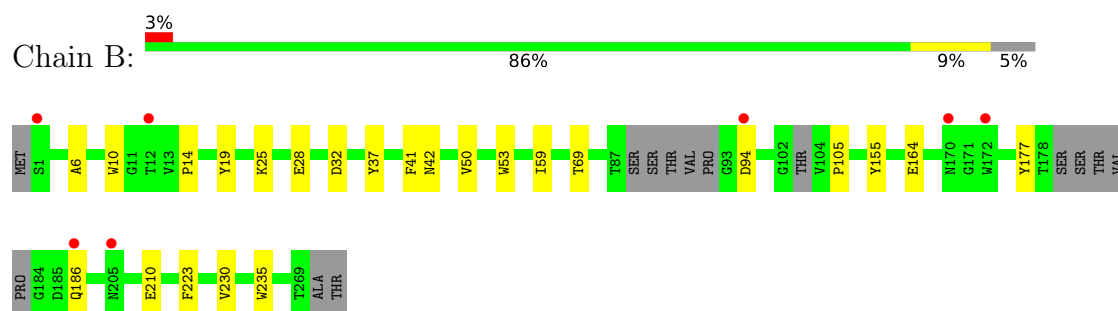
3 Residue-property plots [i](#)

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: Fucose-binding lectin protein,Fucose-binding lectin protein,Fucose-binding lectin protein



- Molecule 1: Fucose-binding lectin protein,Fucose-binding lectin protein,Fucose-binding lectin protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.43Å 81.96Å 97.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.64 – 1.82 62.64 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (62.64-1.82) 99.9 (62.64-1.82)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.250 , 0.285 0.250 , 0.285	Depositor DCC
R_{free} test set	2417 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4641	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.79 % 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 1.6747e-05. 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: R2F

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	0.42	0/2009	0.61	0/2759
1	B	0.44	0/2024	0.64	0/2781
All	All	0.43	0/4033	0.62	0/5540

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	1948	0	1777	25	0
1	B	1962	0	1792	19	0
2	A	165	0	0	0	0
2	B	165	0	0	1	0
3	A	202	0	0	3	0
3	B	199	0	0	0	0
All	All	4641	0	3569	45	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 6.

All (45) 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)
2:B:302:R2F:N2T	2:B:302:R2F:O4	2.07	0.87
1:B:186:GLN:HE22	1:B:230:VAL:HG12	1.40	0.85
1:A:4:GLN:HE22	1:A:48:VAL:H	1.27	0.79
1:B:186:GLN:NE2	1:B:230:VAL:HG12	1.97	0.79
1:A:207:LYS:HG2	3:A:573:HOH:O	1.89	0.71
1:A:116:LYS:NZ	3:A:401:HOH:O	2.27	0.68
1:A:4:GLN:NE2	1:A:48:VAL:H	1.93	0.67
1:A:95:GLN:OE1	1:A:138:ASN:ND2	2.30	0.64
1:B:186:GLN:NE2	1:B:230:VAL:H	1.97	0.61
1:B:186:GLN:HE22	1:B:230:VAL:H	1.52	0.57
1:A:4:GLN:HE22	1:A:48:VAL:N	2.00	0.57
1:B:186:GLN:HE22	1:B:230:VAL:N	2.03	0.56
1:B:186:GLN:NE2	1:B:230:VAL:N	2.54	0.56
1:B:69:THR:HA	1:B:94:ASP:OD2	2.07	0.54
1:B:53:TRP:CE2	1:B:105:PRO:HG3	2.46	0.51
1:A:95:GLN:OE1	1:A:138:ASN:HA	2.10	0.51
1:A:138:ASN:HB3	1:A:157:SER:HB2	1.93	0.50
1:B:14:PRO:HG3	1:B:235:TRP:CE2	2.47	0.49
1:A:4:GLN:HB2	1:A:229:ASN:ND2	2.28	0.48
1:A:152:ILE:HB	1:A:167:TRP:HB3	1.96	0.48
1:A:53:TRP:CE2	1:A:105:PRO:HG3	2.48	0.48
1:B:6:ALA:HB1	1:B:50:VAL:HG12	1.97	0.47
1:B:14:PRO:HG3	1:B:235:TRP:CZ2	2.50	0.47
1:B:164:GLU:HB2	1:B:177:TYR:HB3	1.96	0.47
1:A:160:THR:HA	1:A:185:ASP:OD2	2.16	0.46
1:B:19:TYR:CE2	1:B:28:GLU:HG3	2.52	0.45
1:B:25:LYS:HD2	1:B:42:ASN:OD1	2.17	0.45
1:A:4:GLN:NE2	1:A:48:VAL:N	2.63	0.45
1:A:186:GLN:OE1	1:A:229:ASN:HA	2.17	0.45
1:A:69:THR:HA	1:A:94:ASP:OD2	2.17	0.45
1:A:144:TRP:CE2	1:A:196:PRO:HG3	2.53	0.43
1:A:225:GLU:HG3	1:A:256:TRP:CE2	2.53	0.43
1:B:32:ASP:OD2	1:B:37:TYR:OH	2.31	0.43
1:B:28:GLU:HB2	1:B:41:PHE:HB3	2.00	0.43
1:A:97:ALA:HB1	1:A:141:VAL:HG12	2.01	0.42
1:A:134:GLU:HG3	1:A:165:TRP:CE2	2.54	0.42
1:A:4:GLN:NE2	1:A:48:VAL:HG12	2.35	0.42
1:B:10:TRP:CG	1:B:59:ILE:HD13	2.54	0.42
1:A:14:PRO:HG3	1:A:235:TRP:CE2	2.55	0.41
1:B:210:GLU:HB2	1:B:223:PHE:HB3	2.02	0.41
1:B:155:TYR:CE1	1:B:164:GLU:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TRP:CE2	1:A:15:SER:HB2	2.56	0.41
1:A:53:TRP:CZ2	1:A:105:PRO:HG3	2.56	0.41
1:A:20:THR:O	1:A:26:ILE:HA	2.21	0.41
1:A:207:LYS:CG	3:A:573:HOH:O	2.58	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	246/272 (90%)	241 (98%)	5 (2%)	0	100	100
1	B	250/272 (92%)	245 (98%)	5 (2%)	0	100	100
All	All	496/544 (91%)	486 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	197/212 (93%)	195 (99%)	2 (1%)	76	70
1	B	199/212 (94%)	199 (100%)	0	100	100
All	All	396/424 (93%)	394 (100%)	2 (0%)	88	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
1	A	216	LYS

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	4	GLN
1	B	186	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	R2F	B	303	-	60,60,60	1.84	8 (13%)	77,84,84	2.15	15 (19%)
2	R2F	B	302	-	60,60,60	1.64	7 (11%)	77,84,84	1.72	12 (15%)
2	R2F	B	301	-	60,60,60	1.70	8 (13%)	77,84,84	1.74	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	R2F	A	301	-	60,60,60	1.66	6 (10%)	77,84,84	1.74	10 (12%)
2	R2F	A	302	-	60,60,60	1.74	6 (10%)	77,84,84	1.96	17 (22%)
2	R2F	A	303	-	60,60,60	1.75	6 (10%)	77,84,84	1.88	14 (18%)

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	R2F	B	303	-	-	16/36/70/70	0/6/6/6
2	R2F	B	302	-	-	16/36/70/70	0/6/6/6
2	R2F	B	301	-	-	17/36/70/70	0/6/6/6
2	R2F	A	301	-	-	22/36/70/70	0/6/6/6
2	R2F	A	302	-	-	20/36/70/70	0/6/6/6
2	R2F	A	303	-	-	15/36/70/70	0/6/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	R2F	C1C-C2C	-7.50	1.39	1.52
2	A	303	R2F	C1C-C2C	-7.34	1.39	1.52
2	B	303	R2F	C2A-C2C	-7.32	1.39	1.52
2	A	302	R2F	C2A-C2C	-7.22	1.39	1.52
2	A	302	R2F	C1C-C2C	-7.13	1.40	1.52
2	B	301	R2F	C1C-C2C	-7.09	1.40	1.52
2	A	303	R2F	C2A-C2C	-7.00	1.40	1.52
2	A	301	R2F	C2A-C2C	-6.87	1.40	1.52
2	B	302	R2F	C1C-C2C	-6.84	1.40	1.52
2	B	301	R2F	C2A-C2C	-6.83	1.40	1.52
2	A	301	R2F	C1C-C2C	-6.83	1.40	1.52
2	B	302	R2F	C2A-C2C	-6.69	1.40	1.52
2	A	301	R2F	O1-C7P	5.26	1.46	1.33
2	B	303	R2F	O1-C7P	5.17	1.46	1.33
2	A	303	R2F	O1-C7P	5.16	1.46	1.33
2	A	302	R2F	O1-C7P	5.09	1.46	1.33
2	B	301	R2F	O1-C7P	5.08	1.46	1.33
2	B	302	R2F	O1-C7P	4.98	1.46	1.33
2	A	303	R2F	N1T-N2T	4.10	1.41	1.34
2	A	302	R2F	N1T-N2T	3.74	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	R2F	N1T-N2T	3.61	1.40	1.34
2	B	301	R2F	N1T-N2T	3.50	1.40	1.34
2	B	302	R2F	N1T-N2T	3.31	1.40	1.34
2	B	303	R2F	O1F-C1F	3.31	1.45	1.40
2	A	303	R2F	N2T-N3T	3.30	1.40	1.34
2	B	303	R2F	C2P-C2C	-3.19	1.48	1.53
2	A	301	R2F	N1T-N2T	3.11	1.40	1.34
2	A	302	R2F	N2T-N3T	2.97	1.40	1.34
2	B	303	R2F	N2T-N3T	2.95	1.40	1.34
2	B	302	R2F	N2T-N3T	2.80	1.39	1.34
2	A	301	R2F	N2T-N3T	2.77	1.39	1.34
2	B	301	R2F	N2T-N3T	2.76	1.39	1.34
2	A	302	R2F	C2P-C2C	-2.60	1.49	1.53
2	B	301	R2F	C4T-N3T	-2.33	1.33	1.35
2	A	301	R2F	C4T-C5T	2.32	1.39	1.36
2	B	301	R2F	C2P-C2C	-2.30	1.50	1.53
2	B	302	R2F	C4T-C5T	2.25	1.39	1.36
2	B	301	R2F	C4T-C5T	2.22	1.39	1.36
2	A	303	R2F	C2P-C2C	-2.20	1.50	1.53
2	B	302	R2F	C4T-N3T	-2.18	1.33	1.35
2	B	303	R2F	C4T-C5T	2.16	1.39	1.36

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	303	R2F	C1C-C2C-C2A	9.54	120.05	105.83
2	A	302	R2F	C1C-C2C-C2A	9.44	119.91	105.83
2	B	301	R2F	C1C-C2C-C2A	9.03	119.29	105.83
2	A	303	R2F	C1C-C2C-C2A	8.89	119.09	105.83
2	B	302	R2F	C1C-C2C-C2A	8.75	118.89	105.83
2	A	301	R2F	C1C-C2C-C2A	8.64	118.71	105.83
2	B	303	R2F	O1F-C1F-C2F	7.99	120.77	108.30
2	A	301	R2F	O1-C7P-C1P	5.56	123.21	112.21
2	B	303	R2F	O1-C7P-C1P	4.94	121.99	112.21
2	A	302	R2F	O1-C7P-C1P	4.89	121.88	112.21
2	A	303	R2F	O1-C7P-C1P	4.67	121.44	112.21
2	A	303	R2F	C6C-C1C-C2C	-4.50	118.99	126.14
2	A	302	R2F	O1B-C4B-C3C	4.29	121.56	115.20
2	A	303	R2F	O1B-C4B-C3C	4.20	121.42	115.20
2	A	302	R2F	O1B-C1A-C6A	4.17	121.38	115.20
2	A	302	R2F	C6C-C1C-C2C	-4.14	119.56	126.14
2	B	303	R2F	C1-O1F-C1F	4.07	120.54	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	R2F	O1-C7P-C1P	4.05	120.22	112.21
2	B	302	R2F	O1B-C1A-C6A	3.91	120.99	115.20
2	B	301	R2F	C6C-C1C-C2C	-3.90	119.95	126.14
2	B	301	R2F	O1-C7P-C1P	3.83	119.78	112.21
2	A	302	R2F	N1T-N2T-N3T	-3.78	104.47	107.31
2	A	302	R2F	C3A-C2A-C2C	-3.74	120.21	126.14
2	A	303	R2F	N1T-N2T-N3T	-3.70	104.53	107.31
2	B	302	R2F	O1B-C4B-C3C	3.69	120.67	115.20
2	B	303	R2F	O1B-C4B-C3C	3.67	120.64	115.20
2	B	303	R2F	C3A-C2A-C2C	-3.67	120.32	126.14
2	B	303	R2F	C6C-C1C-C2C	-3.63	120.38	126.14
2	B	302	R2F	C3A-C2A-C2C	-3.61	120.41	126.14
2	B	301	R2F	O1B-C4B-C3C	3.58	120.50	115.20
2	B	302	R2F	C6C-C1C-C2C	-3.56	120.49	126.14
2	B	303	R2F	O1B-C1A-C6A	3.53	120.43	115.20
2	A	301	R2F	C3A-C2A-C2C	-3.51	120.57	126.14
2	A	301	R2F	C6C-C1C-C2C	-3.51	120.57	126.14
2	A	303	R2F	C3A-C2A-C2C	-3.44	120.69	126.14
2	B	301	R2F	C3A-C2A-C2C	-3.41	120.73	126.14
2	A	301	R2F	C2-O1-C7P	3.39	123.57	116.43
2	B	301	R2F	N1T-N2T-N3T	-3.33	104.81	107.31
2	A	303	R2F	O1B-C1A-C6A	3.32	120.12	115.20
2	B	301	R2F	O1B-C1A-C6A	3.29	120.07	115.20
2	A	301	R2F	O1B-C4B-C3C	3.24	119.99	115.20
2	A	301	R2F	O1B-C1A-C6A	3.17	119.90	115.20
2	A	301	R2F	N1T-N2T-N3T	-3.09	104.98	107.31
2	B	303	R2F	N1T-N2T-N3T	-3.04	105.02	107.31
2	A	303	R2F	C5C-C4C-N1C	-2.93	117.34	121.38
2	A	301	R2F	O1-C7P-O7P	-2.85	117.90	123.67
2	A	303	R2F	C2-O1-C7P	2.78	122.28	116.43
2	A	303	R2F	C2P-C2C-C2A	2.74	122.45	113.32
2	A	302	R2F	O1-C7P-O7P	-2.68	118.23	123.67
2	B	303	R2F	O1-C7P-O7P	-2.67	118.25	123.67
2	A	302	R2F	C1-C5T-C4T	-2.65	123.44	128.45
2	A	302	R2F	C5C-C4C-N1C	-2.62	117.77	121.38
2	B	301	R2F	C2P-C2C-C2A	2.56	121.85	113.32
2	B	301	R2F	C2-O1-C7P	2.51	121.72	116.43
2	A	301	R2F	C2P-C2C-C2A	2.49	121.59	113.32
2	A	303	R2F	C1-C5T-C4T	-2.48	123.77	128.45
2	A	303	R2F	O1-C7P-O7P	-2.45	118.70	123.67
2	A	302	R2F	O1B-C4B-C1C	-2.42	119.05	122.38
2	B	303	R2F	C2-O1-C7P	2.41	121.52	116.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	303	R2F	C2P-C2C-C2A	2.39	121.29	113.32
2	B	302	R2F	O1-C7P-O7P	-2.30	119.01	123.67
2	A	302	R2F	O5F-C5F-C6F	2.28	111.62	106.70
2	B	303	R2F	C6F-C5F-C4F	-2.26	108.90	113.07
2	B	302	R2F	C2P-C2C-C2A	2.25	120.81	113.32
2	B	303	R2F	C21-N1A-C5A	-2.24	118.09	121.39
2	B	302	R2F	C5C-C4C-N1C	-2.23	118.30	121.38
2	B	301	R2F	C1-C5T-C4T	-2.19	124.32	128.45
2	A	303	R2F	C6C-C1C-C4B	2.17	120.19	117.75
2	B	303	R2F	C6C-C1C-C4B	2.11	120.13	117.75
2	B	302	R2F	O1B-C1A-C2A	-2.11	119.48	122.38
2	B	302	R2F	C2P-C2C-C1C	2.10	120.31	113.32
2	A	302	R2F	C6C-C1C-C4B	2.09	120.11	117.75
2	A	302	R2F	C3A-C2A-C1A	2.07	120.09	117.75
2	A	303	R2F	O1B-C4B-C1C	-2.04	119.57	122.38
2	A	302	R2F	C2P-C2C-C2A	2.02	120.05	113.32
2	A	302	R2F	C2P-C2C-C1C	2.02	120.04	113.32
2	A	302	R2F	O1B-C1A-C2A	-2.01	119.61	122.38
2	B	302	R2F	N1T-N2T-N3T	-2.00	105.81	107.31

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	R2F	C5-C6-N3T-N2T
2	A	303	R2F	C5-C6-N3T-C4T
2	B	301	R2F	C1P-C7P-O1-C2
2	B	301	R2F	O4-C5-C6-N3T
2	B	302	R2F	O4-C5-C6-N3T
2	B	302	R2F	C5-C6-N3T-N2T
2	B	303	R2F	C5-C6-N3T-N2T
2	B	303	R2F	C2F-C1F-O1F-C1
2	A	301	R2F	C3C-C4C-N1C-C13
2	A	303	R2F	C3C-C4C-N1C-C13
2	A	303	R2F	C5C-C4C-N1C-C23
2	B	301	R2F	C4A-C5A-N1A-C21
2	B	301	R2F	C4A-C5A-N1A-C11
2	B	301	R2F	C6A-C5A-N1A-C11
2	A	301	R2F	O7P-C7P-O1-C2
2	B	301	R2F	O7P-C7P-O1-C2
2	B	302	R2F	O7P-C7P-O1-C2
2	A	303	R2F	C5C-C4C-N1C-C13

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Mol	Chain	Res	Type	Atoms
2	B	301	R2F	C6A-C5A-N1A-C21
2	A	301	R2F	C1P-C7P-O1-C2
2	B	302	R2F	C1P-C7P-O1-C2
2	A	301	R2F	C3C-C4C-N1C-C23
2	A	301	R2F	C5C-C4C-N1C-C23
2	A	301	R2F	C5C-C4C-N1C-C13
2	A	302	R2F	C3C-C4C-N1C-C23
2	A	302	R2F	C3C-C4C-N1C-C13
2	A	302	R2F	C5C-C4C-N1C-C23
2	A	302	R2F	C5C-C4C-N1C-C13
2	A	303	R2F	C3C-C4C-N1C-C23
2	B	301	R2F	C5C-C4C-N1C-C23
2	B	302	R2F	C3C-C4C-N1C-C23
2	B	302	R2F	C3C-C4C-N1C-C13
2	B	302	R2F	C5C-C4C-N1C-C23
2	B	302	R2F	C5C-C4C-N1C-C13
2	A	303	R2F	C14-C13-N1C-C4C
2	B	301	R2F	C3C-C4C-N1C-C23
2	B	301	R2F	C3C-C4C-N1C-C13
2	B	301	R2F	C5C-C4C-N1C-C13
2	A	301	R2F	C4A-C5A-N1A-C21
2	A	301	R2F	C6A-C5A-N1A-C11
2	B	303	R2F	C6-C5-O4-C3
2	A	301	R2F	C14-C13-N1C-C4C
2	A	301	R2F	C6A-C5A-N1A-C21
2	A	301	R2F	C4A-C5A-N1A-C11
2	B	303	R2F	C4A-C5A-N1A-C21
2	B	303	R2F	C6A-C5A-N1A-C11
2	A	302	R2F	O1-C2-C3-O4
2	A	302	R2F	C22-C21-N1A-C11
2	A	303	R2F	C14-C13-N1C-C23
2	B	302	R2F	C12-C11-N1A-C21
2	B	303	R2F	C4A-C5A-N1A-C11
2	B	303	R2F	C22-C21-N1A-C11
2	A	301	R2F	C14-C13-N1C-C23
2	B	303	R2F	C6A-C5A-N1A-C21
2	A	303	R2F	C1P-C7P-O1-C2
2	B	302	R2F	O1-C2-C3-O4
2	B	301	R2F	O1-C2-C3-O4
2	B	301	R2F	C12-C11-N1A-C21
2	A	301	R2F	C6-C5-O4-C3
2	B	303	R2F	C1P-C7P-O1-C2

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Mol	Chain	Res	Type	Atoms
2	A	301	R2F	C22-C21-N1A-C5A
2	A	302	R2F	C1P-C7P-O1-C2
2	A	303	R2F	O7P-C7P-O1-C2
2	A	302	R2F	C24-C23-N1C-C4C
2	B	302	R2F	C24-C23-N1C-C4C
2	B	302	R2F	C2-C3-O4-C5
2	B	303	R2F	C22-C21-N1A-C5A
2	A	302	R2F	C22-C21-N1A-C5A
2	B	303	R2F	O5F-C1F-O1F-C1
2	A	302	R2F	O7P-C7P-O1-C2
2	A	302	R2F	O4-C5-C6-N3T
2	B	302	R2F	C24-C23-N1C-C13
2	B	301	R2F	C12-C11-N1A-C5A
2	B	302	R2F	C12-C11-N1A-C5A
2	A	301	R2F	C22-C21-N1A-C11
2	A	302	R2F	C24-C23-N1C-C13
2	B	303	R2F	O7P-C7P-O1-C2
2	A	302	R2F	C4A-C5A-N1A-C21
2	A	302	R2F	C6A-C5A-N1A-C11
2	A	302	R2F	C6A-C5A-N1A-C21
2	A	302	R2F	C4A-C5A-N1A-C11
2	A	302	R2F	C14-C13-N1C-C4C
2	B	301	R2F	C5-C6-N3T-C4T
2	B	302	R2F	C5-C6-N3T-C4T
2	B	303	R2F	C5-C6-N3T-C4T
2	A	301	R2F	C6P-C1P-C7P-O1
2	B	303	R2F	C2A-C2C-C2P-C1P
2	A	303	R2F	O1-C2-C3-O4
2	A	302	R2F	C6-C5-O4-C3
2	A	302	R2F	C14-C13-N1C-C23
2	A	301	R2F	C2P-C1P-C7P-O1
2	B	302	R2F	C6-C5-O4-C3
2	A	301	R2F	C5-C6-N3T-C4T
2	A	303	R2F	C6-C5-O4-C3
2	B	303	R2F	C2-C3-O4-C5
2	A	302	R2F	C2-C3-O4-C5
2	A	301	R2F	C5-C6-N3T-N2T
2	B	303	R2F	C2A-C2C-C2P-C3P
2	B	301	R2F	C1C-C2C-C2P-C1P
2	A	301	R2F	O1-C2-C3-O4
2	A	303	R2F	C6A-C5A-N1A-C21
2	A	301	R2F	C6P-C1P-C7P-O7P

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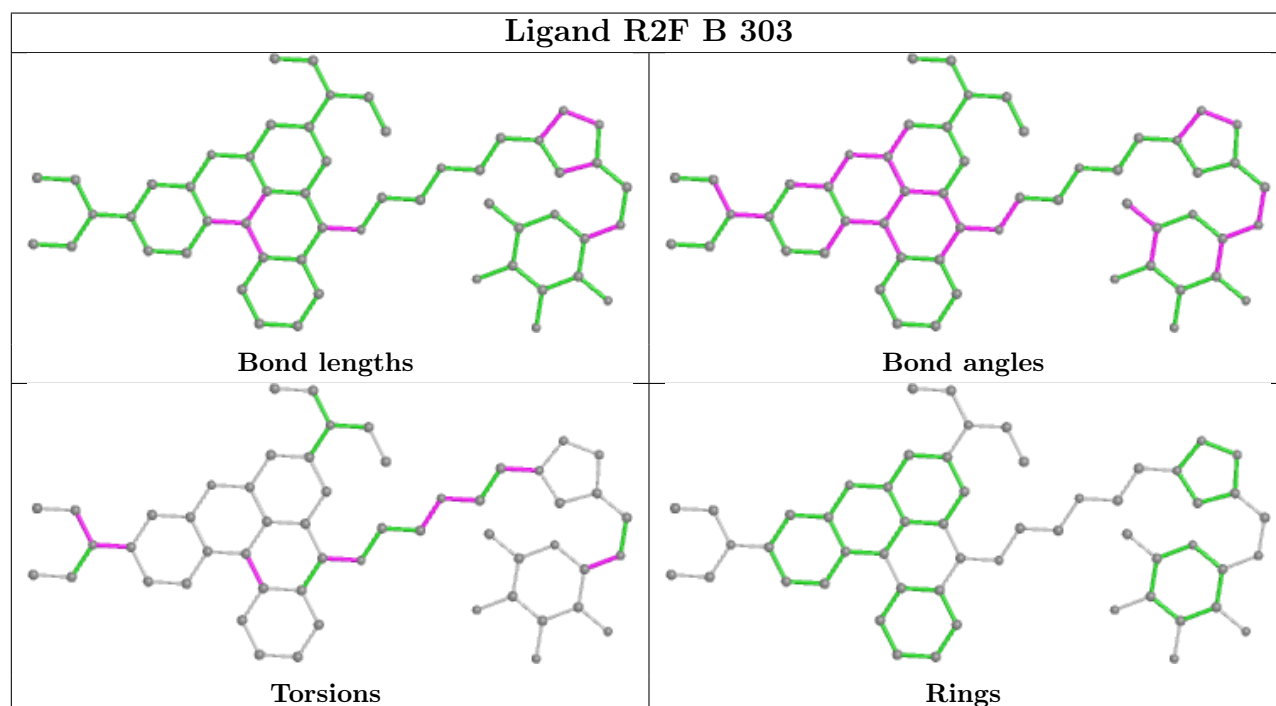
Mol	Chain	Res	Type	Atoms
2	A	303	R2F	C4A-C5A-N1A-C21
2	A	301	R2F	C2-C3-O4-C5
2	A	303	R2F	C6A-C5A-N1A-C11
2	B	301	R2F	C6P-C1P-C7P-O1

There are no ring outliers.

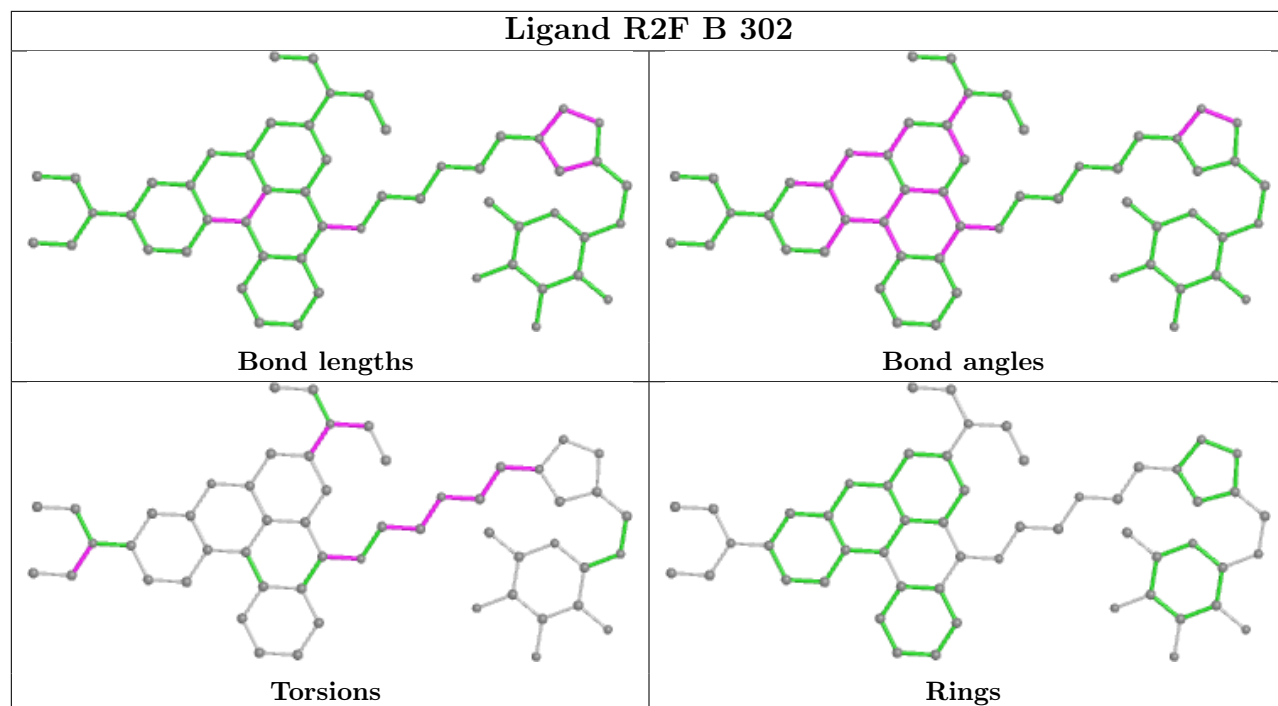
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	R2F	1	0

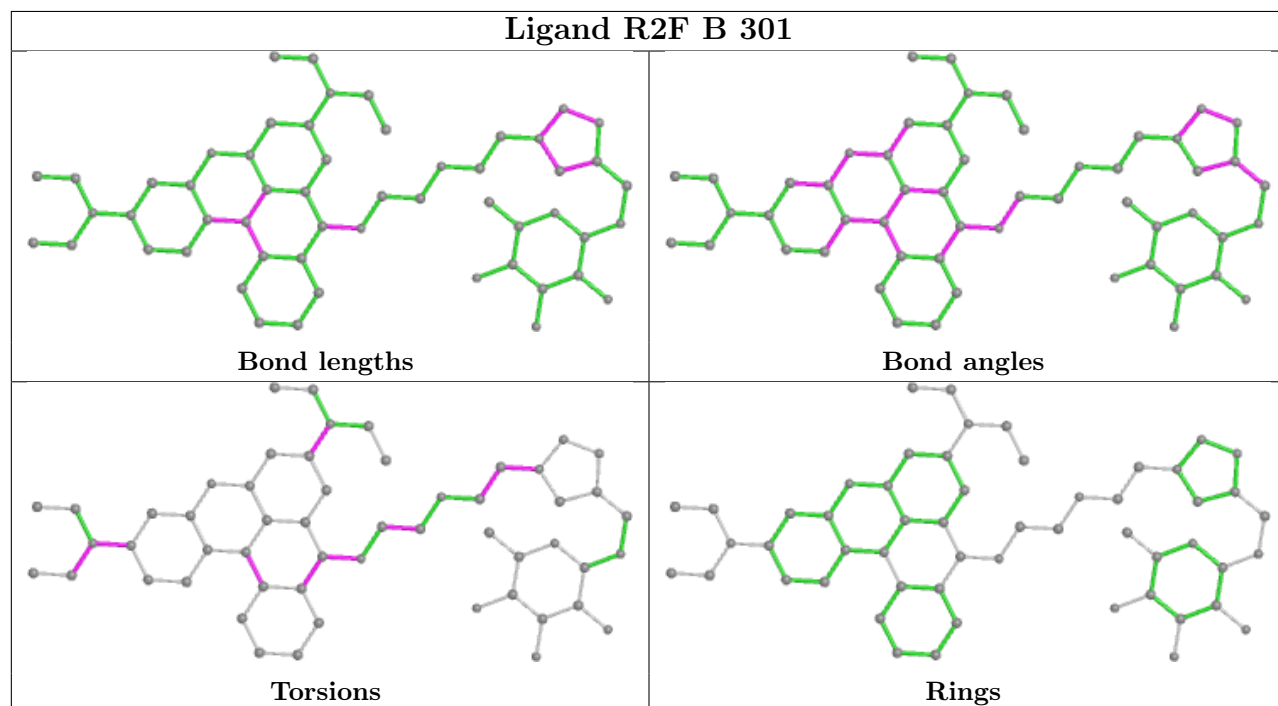
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



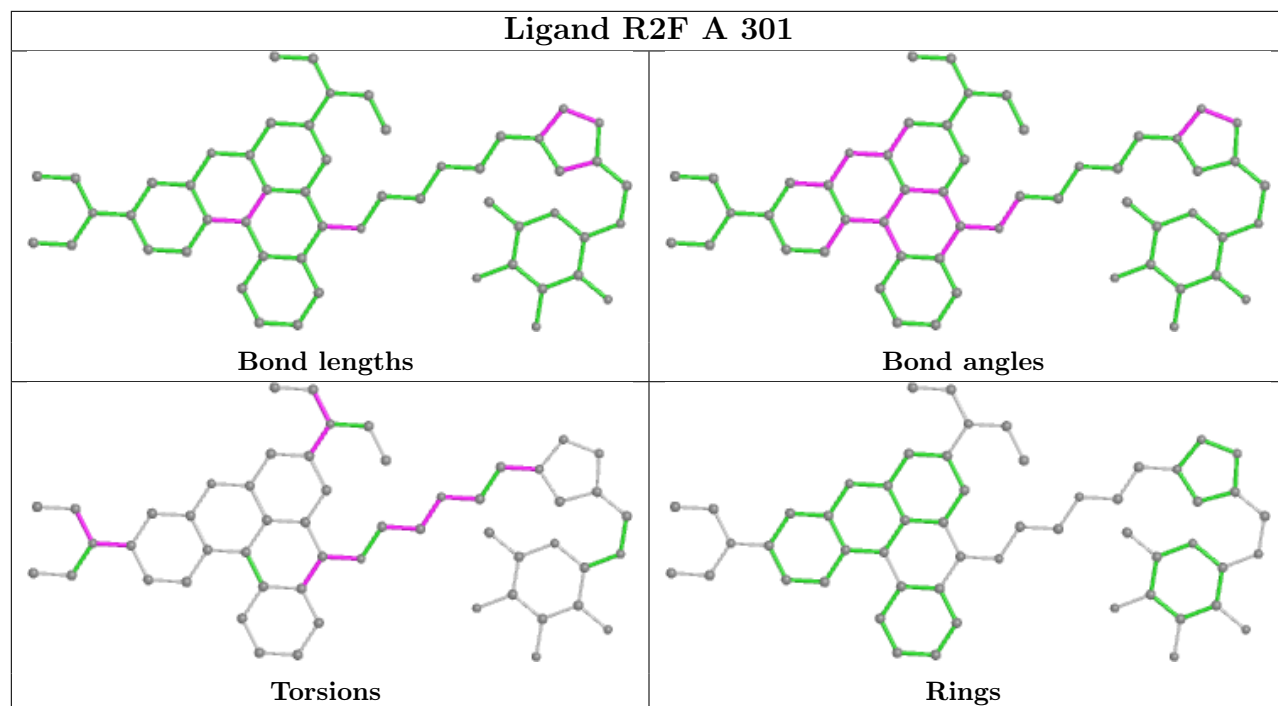
Ligand R2F B 302



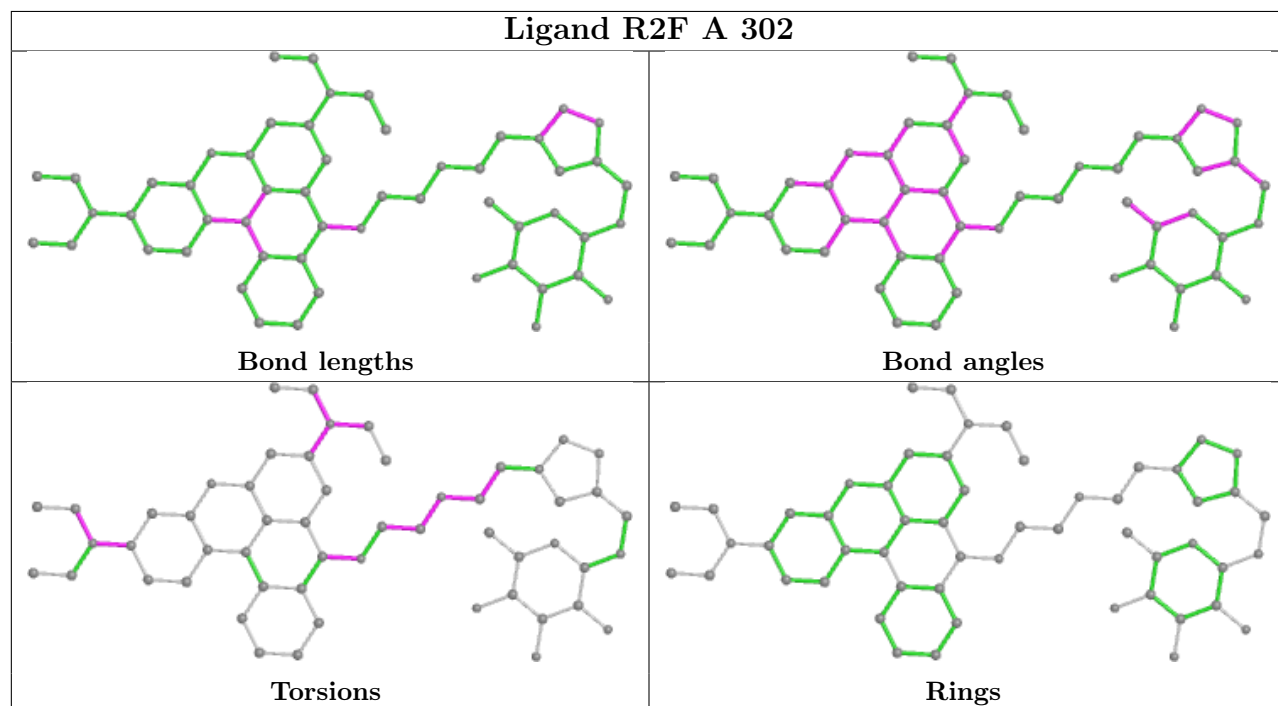
Ligand R2F B 301

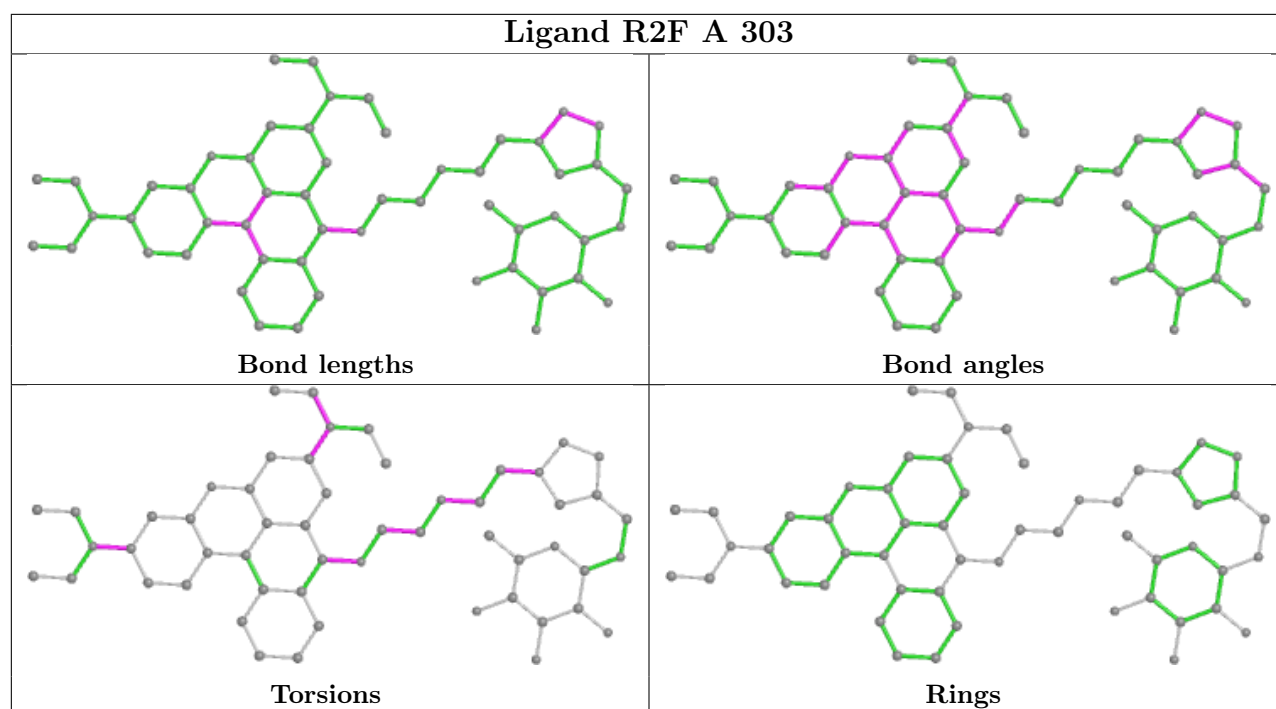


Ligand R2F A 301



Ligand R2F A 302





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	256/272 (94%)	0.38	8 (3%)	49	43	16, 23, 41, 58	0
1	B	258/272 (94%)	0.32	7 (2%)	54	49	14, 22, 38, 59	0
All	All	514/544 (94%)	0.35	15 (2%)	51	46	14, 22, 39, 59	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ASN	4.1
1	B	170	ASN	3.2
1	A	185	ASP	3.1
1	A	94	ASP	2.8
1	B	12	THR	2.7
1	B	94	ASP	2.6
1	B	172	TRP	2.6
1	A	205	ASN	2.4
1	A	2	SER	2.3
1	B	186	GLN	2.3
1	B	1	SER	2.3
1	A	173	THR	2.2
1	B	205	ASN	2.2
1	A	95	GLN	2.1
1	A	139	VAL	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 ⓘ

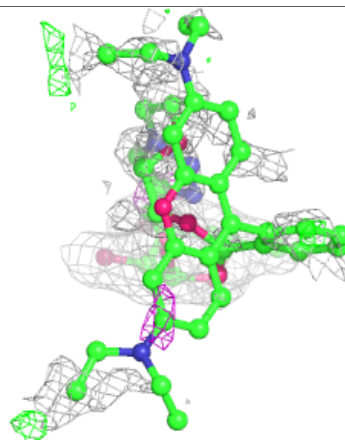
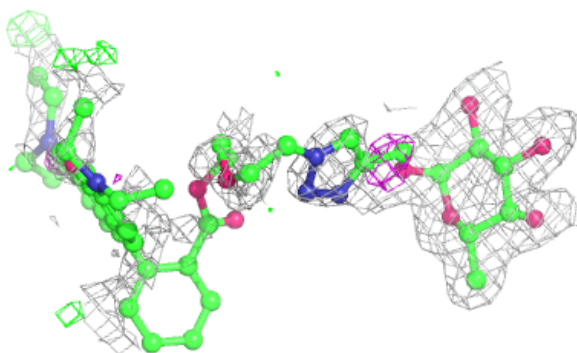
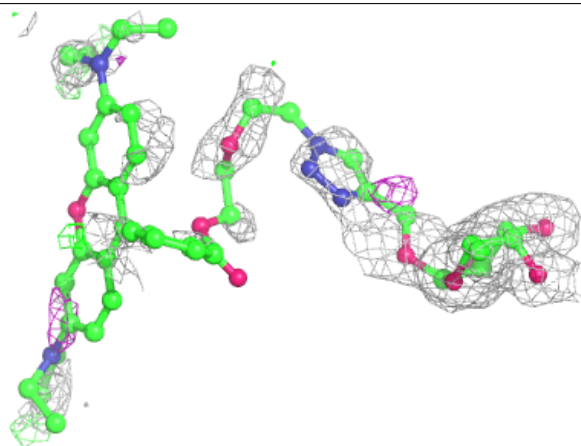
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	R2F	B	303	55/55	0.77	0.35	21,67,78,80	0
2	R2F	A	302	55/55	0.78	0.38	22,81,84,85	0
2	R2F	A	303	55/55	0.79	0.40	21,70,79,81	0
2	R2F	A	301	55/55	0.79	0.41	20,71,81,81	0
2	R2F	B	302	55/55	0.81	0.42	19,77,85,87	0
2	R2F	B	301	55/55	0.82	0.43	18,72,88,89	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.

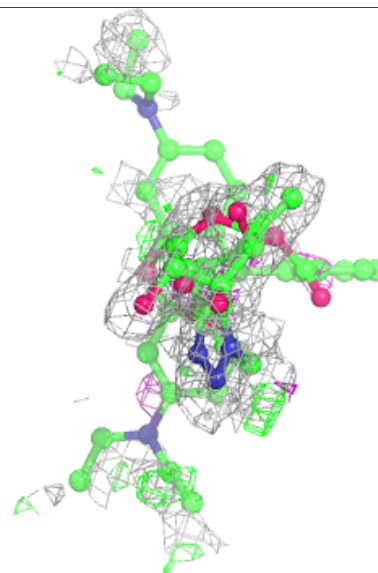
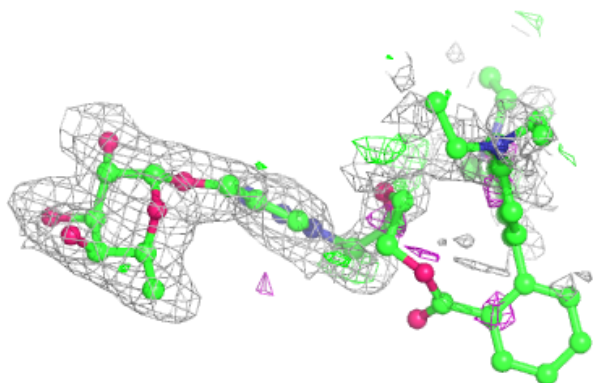
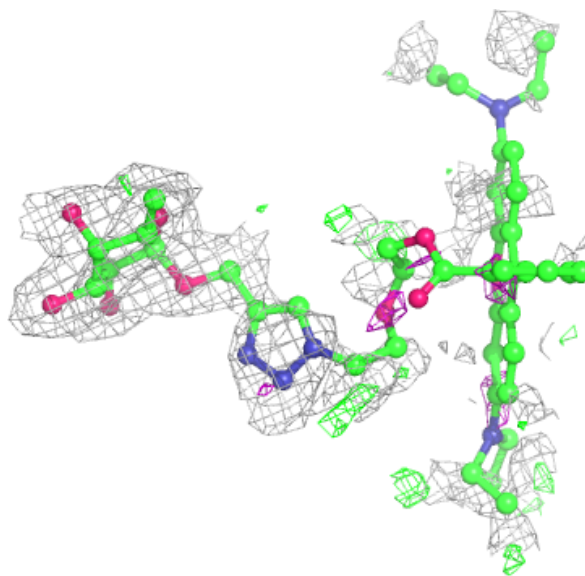
Electron density around R2F B 303:

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



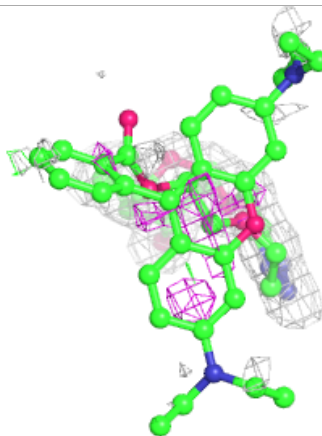
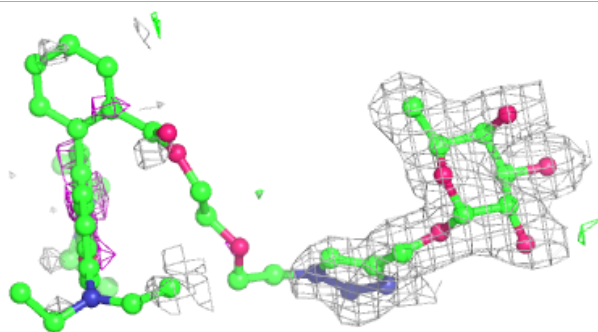
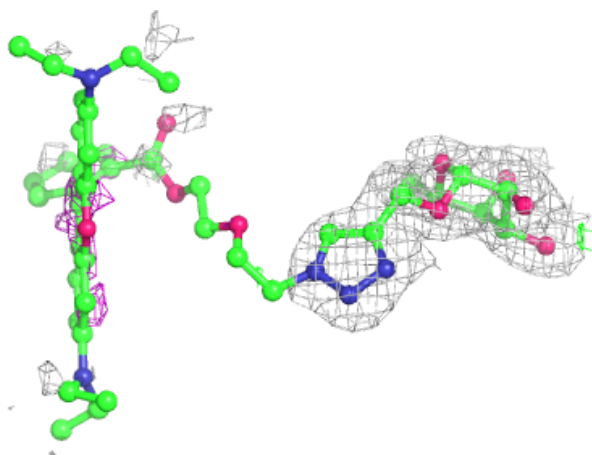
Electron density around R2F A 302:

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



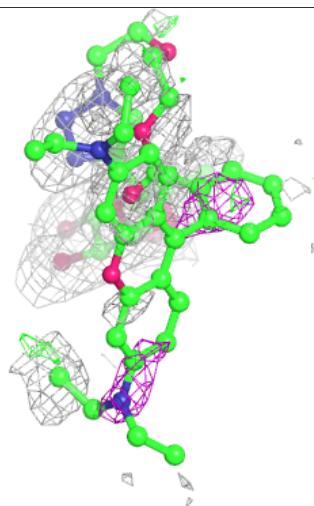
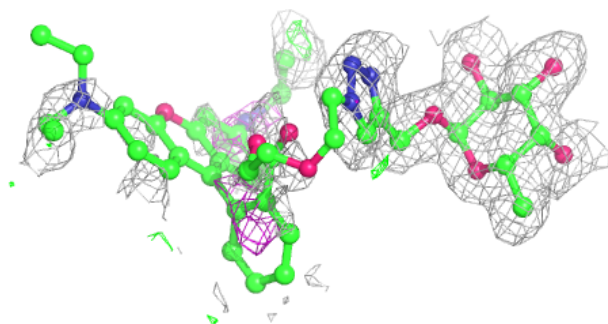
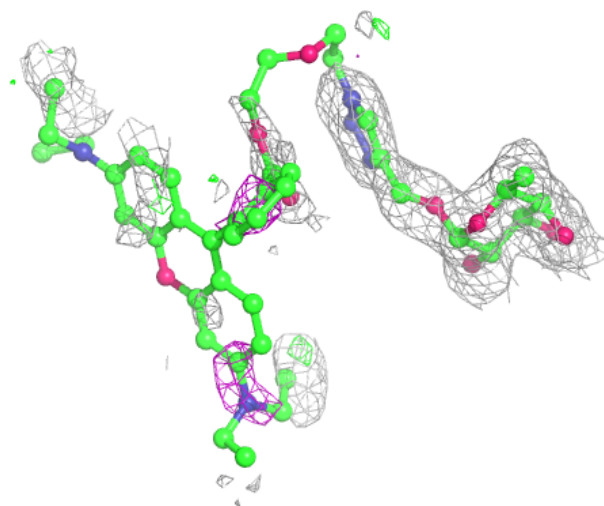
Electron density around R2F A 303:

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



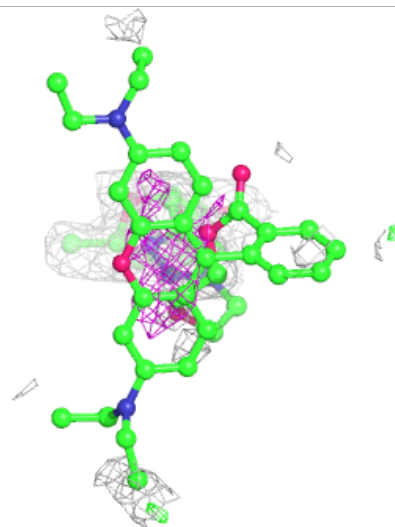
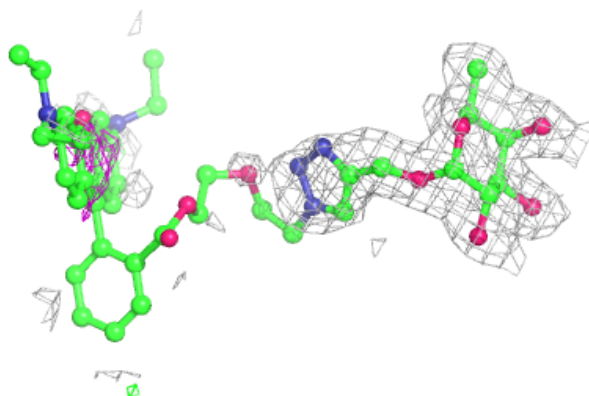
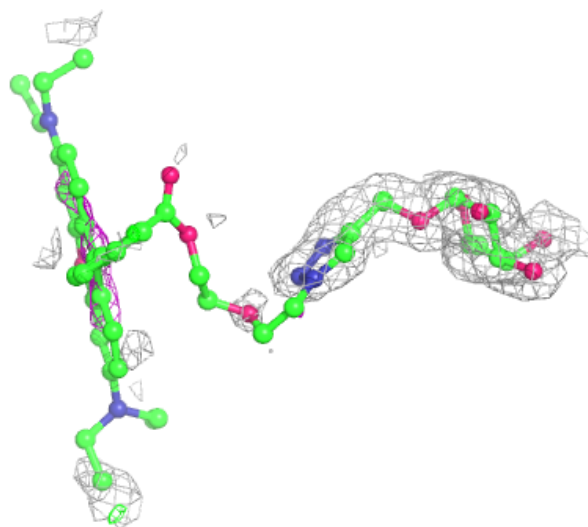
Electron density around R2F A 301:

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



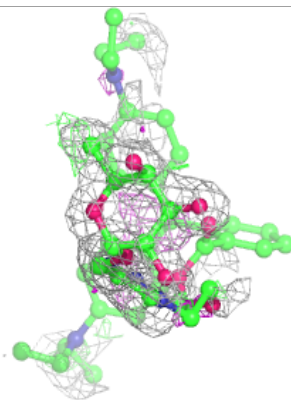
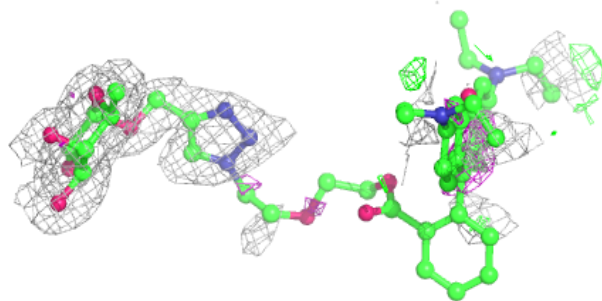
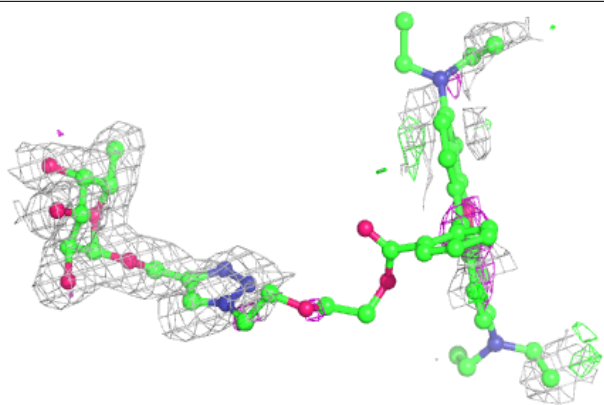
Electron density around R2F B 302:

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



Electron density around R2F 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.