



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2020 – 07:47 AM EST

PDB ID : 6NQT
Title : GalNac-T2 soaked with UDP-sugar
Authors : Fernandez, D.; Bertozzi, C.R.; Schumann, B.; Agbay, A.
Deposited on : 2019-01-21
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

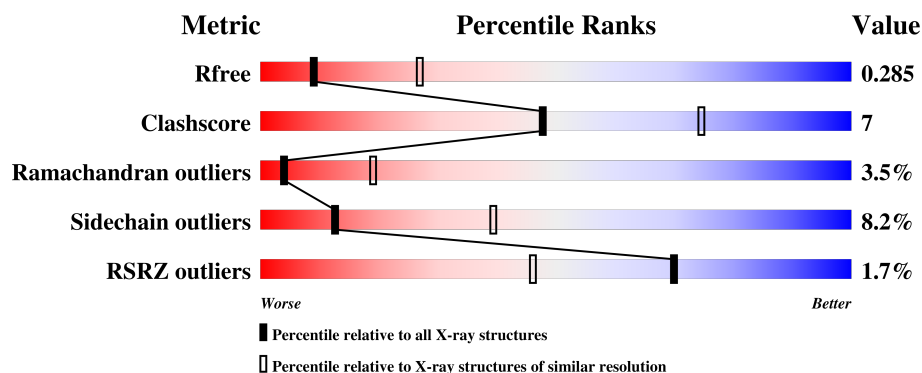
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	111664	1497 (3.10-3.02)
Clashscore	122126	1601 (3.10-3.02)
Ramachandran outliers	120053	1548 (3.10-3.02)
Sidechain outliers	120020	1547 (3.10-3.02)
RSRZ outliers	108989	1462 (3.10-3.02)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	571	<div> <div>66%</div> <div>17%</div> <div>•</div> <div>13%</div> </div>
1	B	571	<div> <div>68%</div> <div>14%</div> <div>• •</div> <div>13%</div> </div>
1	C	571	<div> <div>68%</div> <div>15%</div> <div>•</div> <div>14%</div> </div>
1	D	571	<div> <div>68%</div> <div>15%</div> <div>• •</div> <div>13%</div> </div>
1	E	571	<div> <div>66%</div> <div>15%</div> <div>•</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	571	

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
3	LR7	D	702	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23138 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 Polypeptide N-acetylgalactosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3954	2487	719	724	24			
1	B	494	Total	C	N	O	S	0	0	0
			3802	2388	687	704	23			
1	C	491	Total	C	N	O	S	0	0	0
			3796	2394	676	702	24			
1	D	495	Total	C	N	O	S	0	0	0
			3829	2409	689	707	24			
1	E	485	Total	C	N	O	S	0	0	0
			3700	2328	665	684	23			
1	F	483	Total	C	N	O	S	0	0	0
			3604	2264	644	673	23			

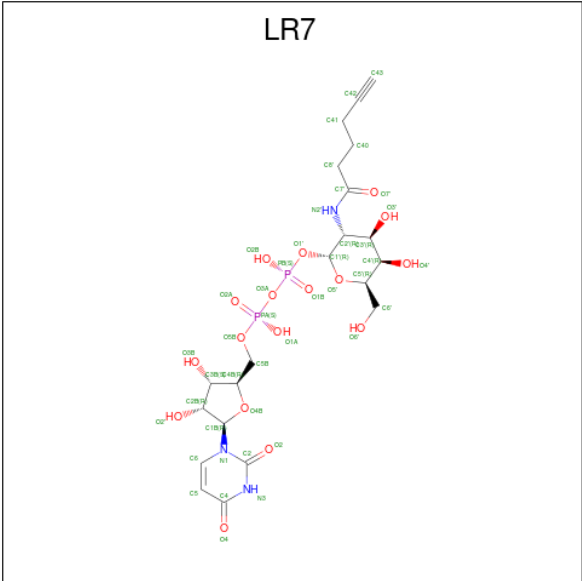
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	ALA	ILE	engineered mutation	UNP Q10471
A	310	ALA	LEU	engineered mutation	UNP Q10471
B	253	ALA	ILE	engineered mutation	UNP Q10471
B	310	ALA	LEU	engineered mutation	UNP Q10471
C	253	ALA	ILE	engineered mutation	UNP Q10471
C	310	ALA	LEU	engineered mutation	UNP Q10471
D	253	ALA	ILE	engineered mutation	UNP Q10471
D	310	ALA	LEU	engineered mutation	UNP Q10471
E	253	ALA	ILE	engineered mutation	UNP Q10471
E	310	ALA	LEU	engineered mutation	UNP Q10471
F	253	ALA	ILE	engineered mutation	UNP Q10471
F	310	ALA	LEU	engineered mutation	UNP Q10471

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is [[(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {R},4 {R},5 {R},6 {R})-3-(hex-5-ynoylamino)-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl] hydrogen phosphate (three-letter code: LR7) (formula: C₂₁H₃₁N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			43	21	3	17	2		
3	B	1	Total	C	N	O	P	0	0
			43	21	3	17	2		
3	C	1	Total	C	N	O	P	0	0
			43	21	3	17	2		
3	D	1	Total	C	N	O	P	0	0
			43	21	3	17	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			43	21	3	17	2		
3	F	1	Total	C	N	O	P	0	0
			43	21	3	17	2		

- Molecule 4 is water.

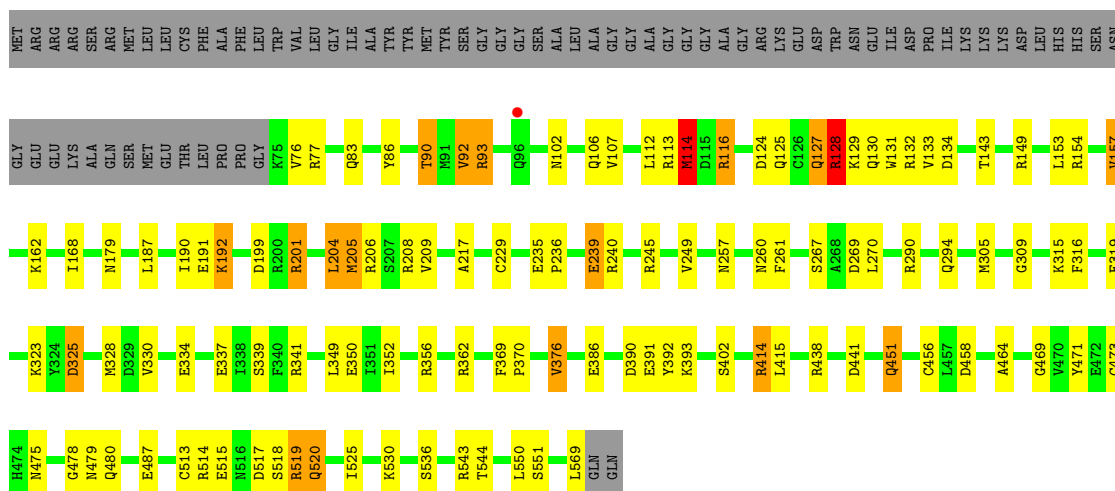
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	33	Total	O	0	0
			33	33		
4	C	27	Total	O	0	0
			27	27		
4	D	30	Total	O	0	0
			30	30		
4	E	17	Total	O	0	0
			17	17		
4	F	11	Total	O	0	0
			11	11		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

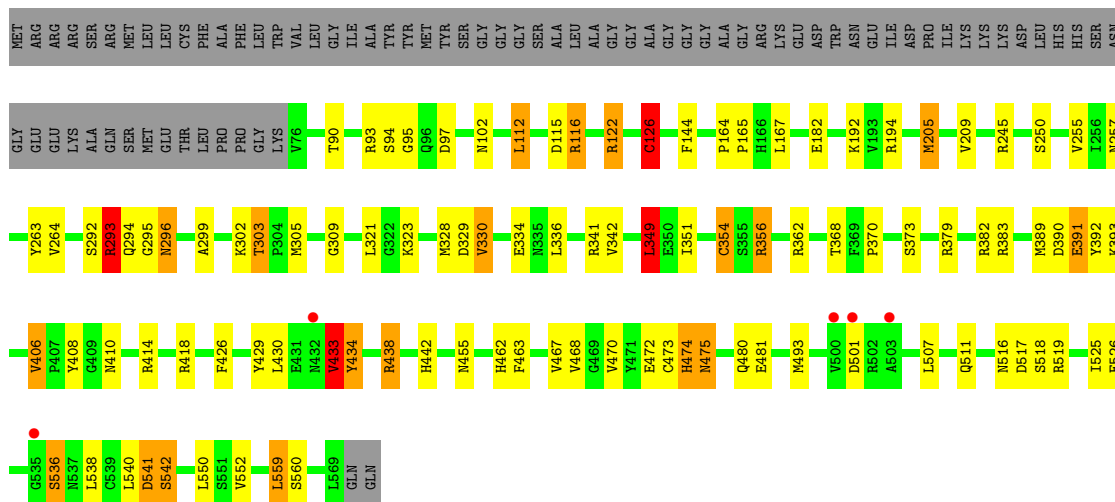
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

Chain A: 

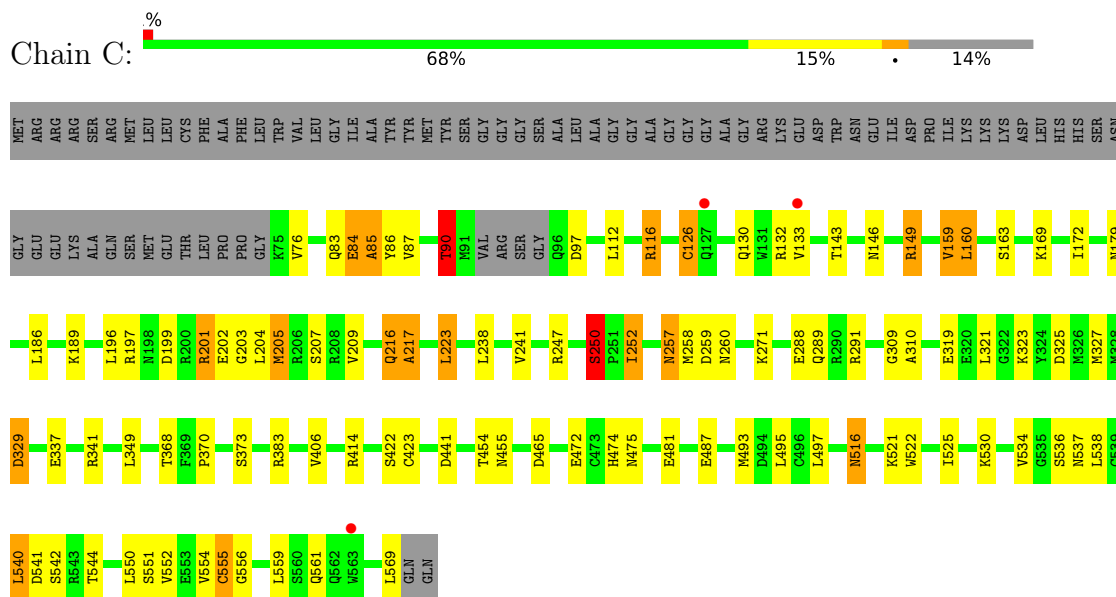


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

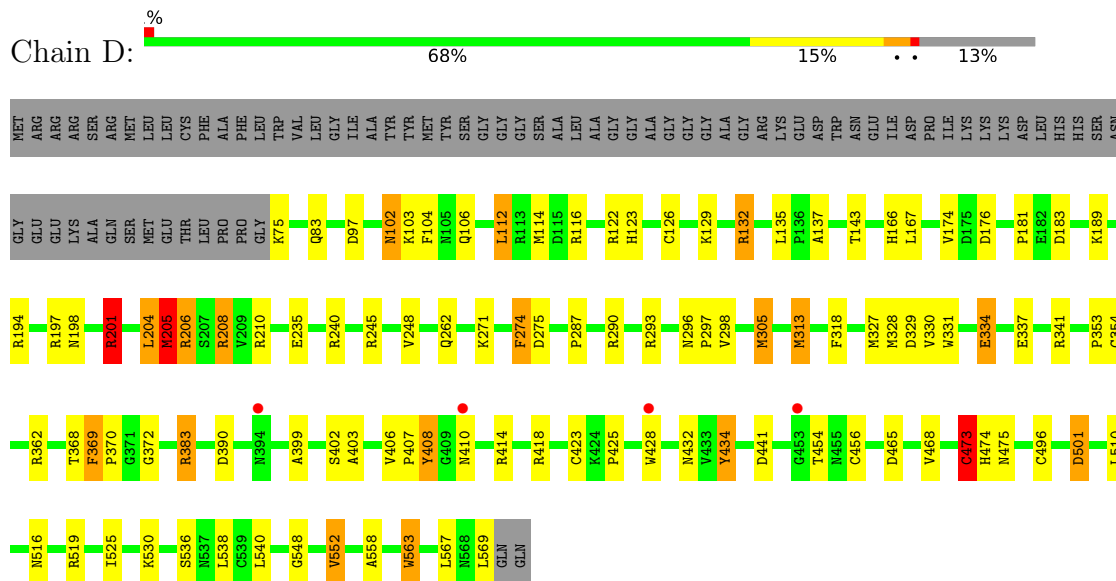
Chain B: 



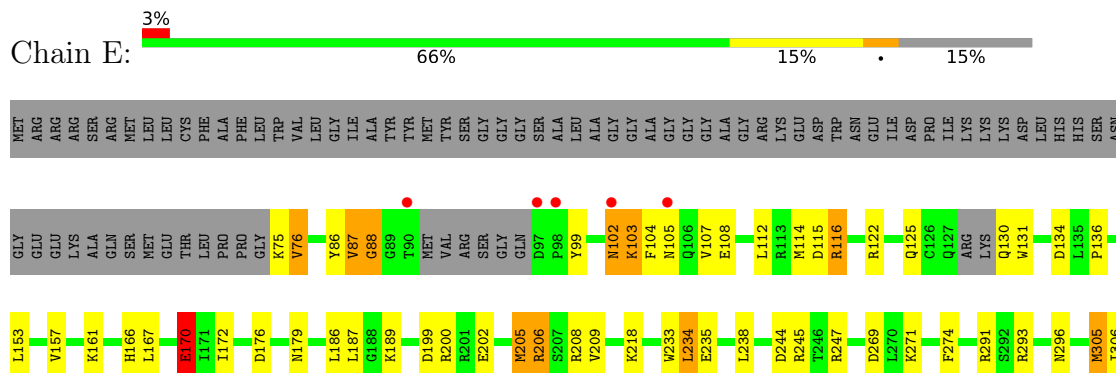
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

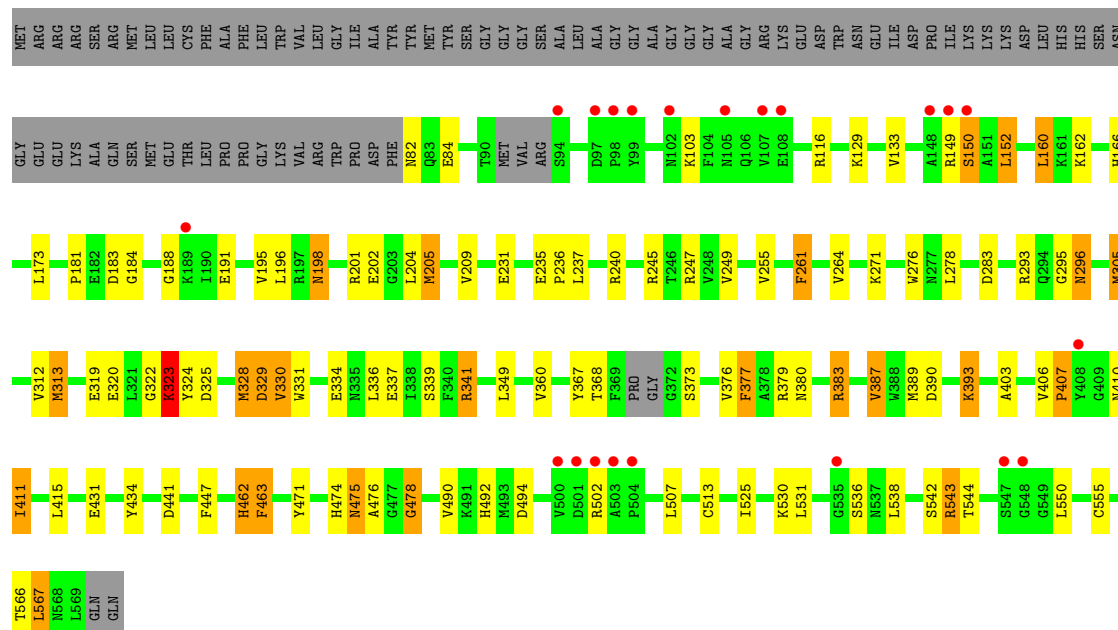


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2



• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.58Å 120.13Å 247.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.70 – 3.05 38.87 – 3.05	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.70-3.05) 96.6 (38.87-3.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.231 , 0.286 0.234 , 0.285	Depositor DCC
R_{free} test set	3349 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23138	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, LR7

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	0.76	0/4046	1.02	22/5473 (0.4%)
1	B	0.80	1/3890 (0.0%)	1.07	20/5287 (0.4%)
1	C	0.76	1/3885 (0.0%)	1.04	15/5277 (0.3%)
1	D	0.81	2/3920 (0.1%)	1.11	28/5325 (0.5%)
1	E	0.82	0/3784	1.14	25/5141 (0.5%)
1	F	0.86	1/3684 (0.0%)	1.13	27/5015 (0.5%)
All	All	0.80	5/23209 (0.0%)	1.09	137/31518 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	GLU	CD-OE1	8.13	1.34	1.25
1	B	536	SER	CB-OG	-7.09	1.33	1.42
1	C	250	SER	CB-OG	-5.24	1.35	1.42
1	F	320	GLU	CD-OE2	-5.16	1.20	1.25
1	D	337	GLU	CD-OE1	-5.14	1.20	1.25

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	541	ASP	CB-CG-OD1	-15.16	104.66	118.30
1	E	541	ASP	CB-CG-OD2	14.25	131.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	341	ARG	NE-CZ-NH2	11.95	126.27	120.30
1	E	341	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	F	293	ARG	NE-CZ-NH2	9.54	125.07	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	137	ALA	Mainchain
1	D	407	PRO	Peptide

5.2 Too-close contacts

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	3954	0	3867	58	0
1	B	3802	0	3592	47	0
1	C	3796	0	3604	52	0
1	D	3829	0	3627	48	0
1	E	3700	0	3446	46	0
1	F	3604	0	3310	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	43	0	0	5	0
3	B	43	0	0	4	0
3	C	43	0	0	3	0
3	D	43	0	0	8	0
3	E	43	0	0	0	0
3	F	43	0	0	1	0
4	A	71	0	0	4	0
4	B	33	0	0	1	0
4	C	27	0	0	1	0
4	D	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	17	0	0	0	0
4	F	11	0	0	0	0
All	All	23138	0	21446	293	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 7.

The worst 5 of 293 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:D:298:VAL:HG21	1:D:354:CYS:SG	1.88	1.14
1:B:293:ARG:O	1:B:295:GLY:N	1.86	1.06
1:D:456:CYS:SG	1:D:473:CYS:HB2	1.97	1.05
1:E:75:LYS:O	1:E:189:LYS:O	1.77	1.01
1:B:255:VAL:O	1:B:263:TYR:O	1.78	1.01

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	493/571 (86%)	455 (92%)	28 (6%)	10 (2%)	8	30
1	B	492/571 (86%)	435 (88%)	38 (8%)	19 (4%)	3	17
1	C	487/571 (85%)	439 (90%)	34 (7%)	14 (3%)	5	23
1	D	493/571 (86%)	449 (91%)	32 (6%)	12 (2%)	6	26
1	E	477/571 (84%)	417 (87%)	38 (8%)	22 (5%)	2	14
1	F	477/571 (84%)	406 (85%)	45 (9%)	26 (6%)	2	10
All	All	2919/3426 (85%)	2601 (89%)	215 (7%)	103 (4%)	4	19

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	A	128	ARG
1	A	191	GLU
1	A	475	ASN
1	B	94	SER

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	424/483 (88%)	389 (92%)	35 (8%)	12	39
1	B	389/483 (80%)	358 (92%)	31 (8%)	13	41
1	C	392/483 (81%)	356 (91%)	36 (9%)	10	33
1	D	395/483 (82%)	361 (91%)	34 (9%)	11	38
1	E	371/483 (77%)	345 (93%)	26 (7%)	16	46
1	F	353/483 (73%)	324 (92%)	29 (8%)	12	39
All	All	2324/2898 (80%)	2133 (92%)	191 (8%)	12	39

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	257	ASN
1	D	112	LEU
1	F	376	VAL
1	C	291	ARG
1	C	487	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	257	ASN
1	C	480	GLN

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Mol	Chain	Res	Type
1	F	432	ASN
1	C	344	GLN
1	C	452	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
3	LR7	A	702	2	37,45,45	0.85	1 (2%)	48,66,66	1.64	7 (14%)
3	LR7	B	702	2	37,45,45	0.81	1 (2%)	48,66,66	2.11	12 (25%)
3	LR7	C	702	2	37,45,45	0.80	1 (2%)	48,66,66	1.59	7 (14%)
3	LR7	D	702	2	37,45,45	1.05	2 (5%)	48,66,66	3.95	13 (27%)
3	LR7	E	702	2	37,45,45	0.83	1 (2%)	48,66,66	2.14	13 (27%)
3	LR7	F	702	2	37,45,45	0.80	1 (2%)	48,66,66	1.52	6 (12%)

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
3	LR7	A	702	2	-	8/26/68/68	0/3/3/3
3	LR7	B	702	2	-	12/26/68/68	0/3/3/3
3	LR7	C	702	2	-	6/26/68/68	0/3/3/3
3	LR7	D	702	2	1/1/12/13	8/26/68/68	0/3/3/3
3	LR7	E	702	2	-	9/26/68/68	0/3/3/3
3	LR7	F	702	2	-	7/26/68/68	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	LR7	C4-N3	3.36	1.38	1.33
3	B	702	LR7	C4-N3	3.32	1.38	1.33
3	E	702	LR7	C4-N3	3.25	1.38	1.33
3	F	702	LR7	C4-N3	3.18	1.38	1.33
3	D	702	LR7	C4-N3	3.11	1.38	1.33

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	LR7	O5'-C1'-O1'	16.10	132.41	111.36
3	D	702	LR7	C1'-C2'-N2'	-14.69	85.15	110.96
3	D	702	LR7	C3'-C2'-N2'	-12.02	87.62	110.58
3	E	702	LR7	O5'-C1'-O1'	6.63	120.03	111.36
3	E	702	LR7	O5'-C1'-C2'	-6.50	97.70	110.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	702	LR7	C1'

5 of 50 torsion outliers are listed below:

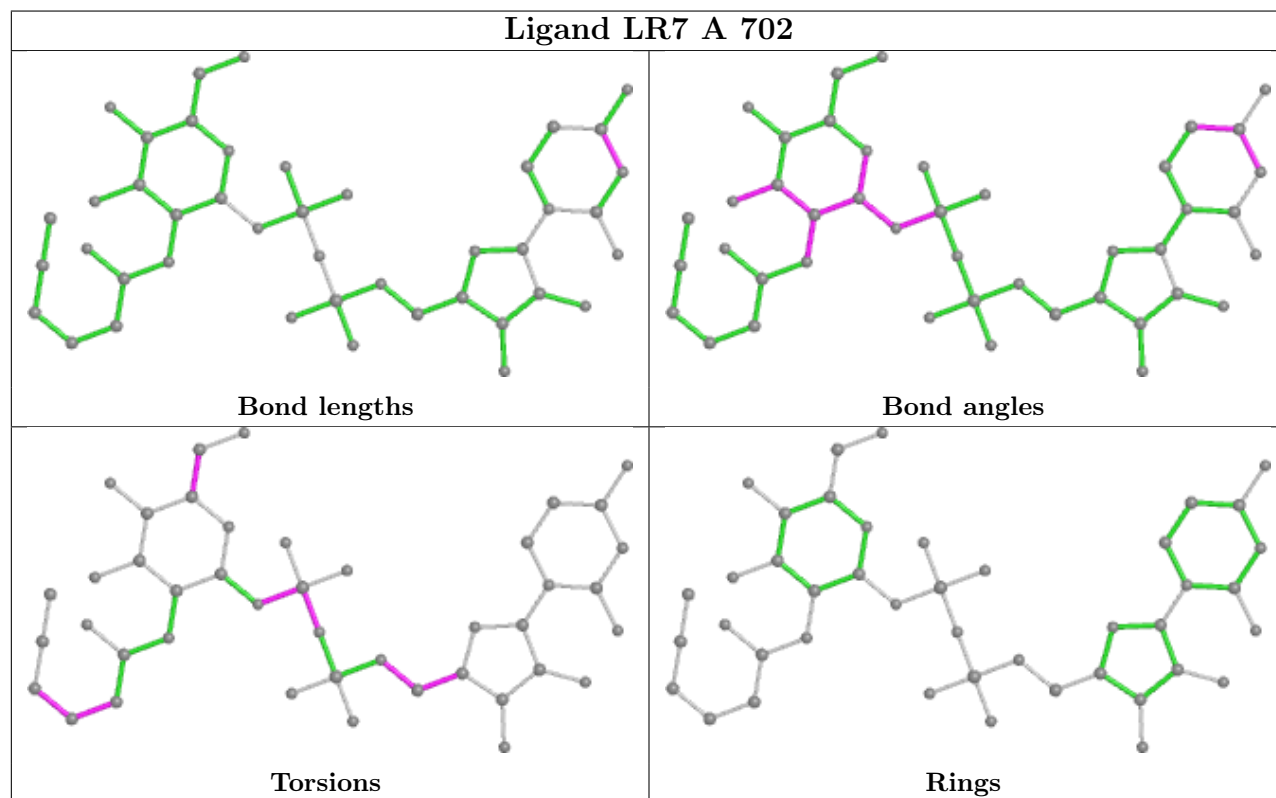
Mol	Chain	Res	Type	Atoms
3	B	702	LR7	C5B-O5B-PA-O2A
3	F	702	LR7	C1'-O1'-PB-O2B
3	F	702	LR7	O5'-C1'-O1'-PB
3	D	702	LR7	O4B-C4B-C5B-O5B
3	D	702	LR7	C5B-O5B-PA-O1A

There are no ring outliers.

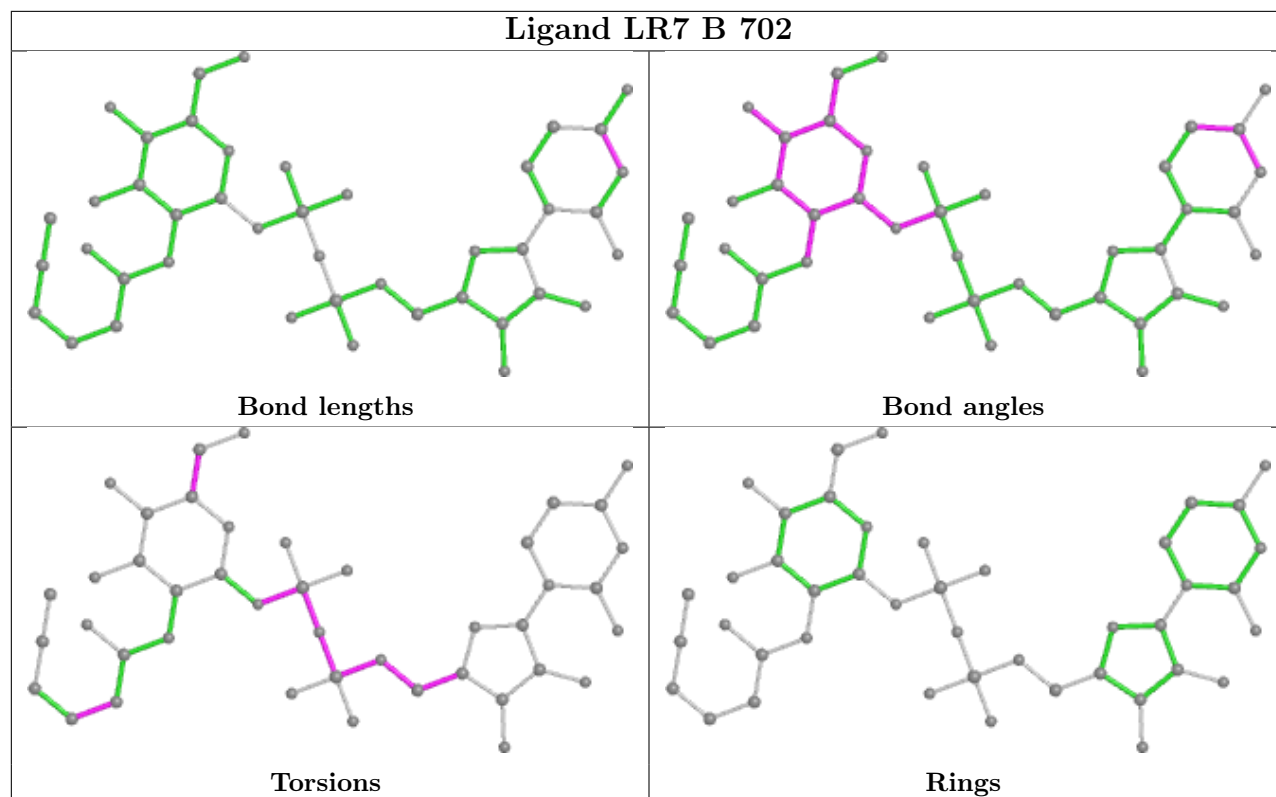
5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	LR7	5	0
3	B	702	LR7	4	0
3	C	702	LR7	3	0
3	D	702	LR7	8	0
3	F	702	LR7	1	0

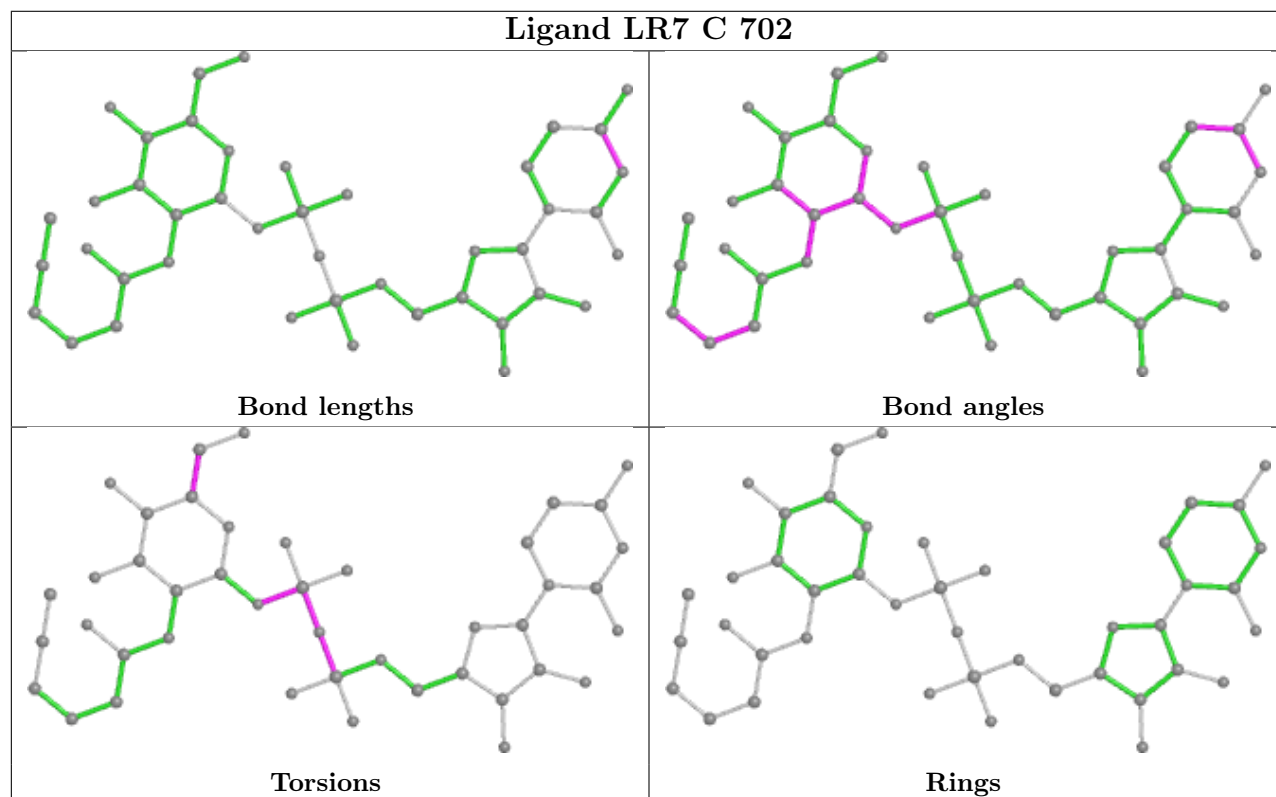
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



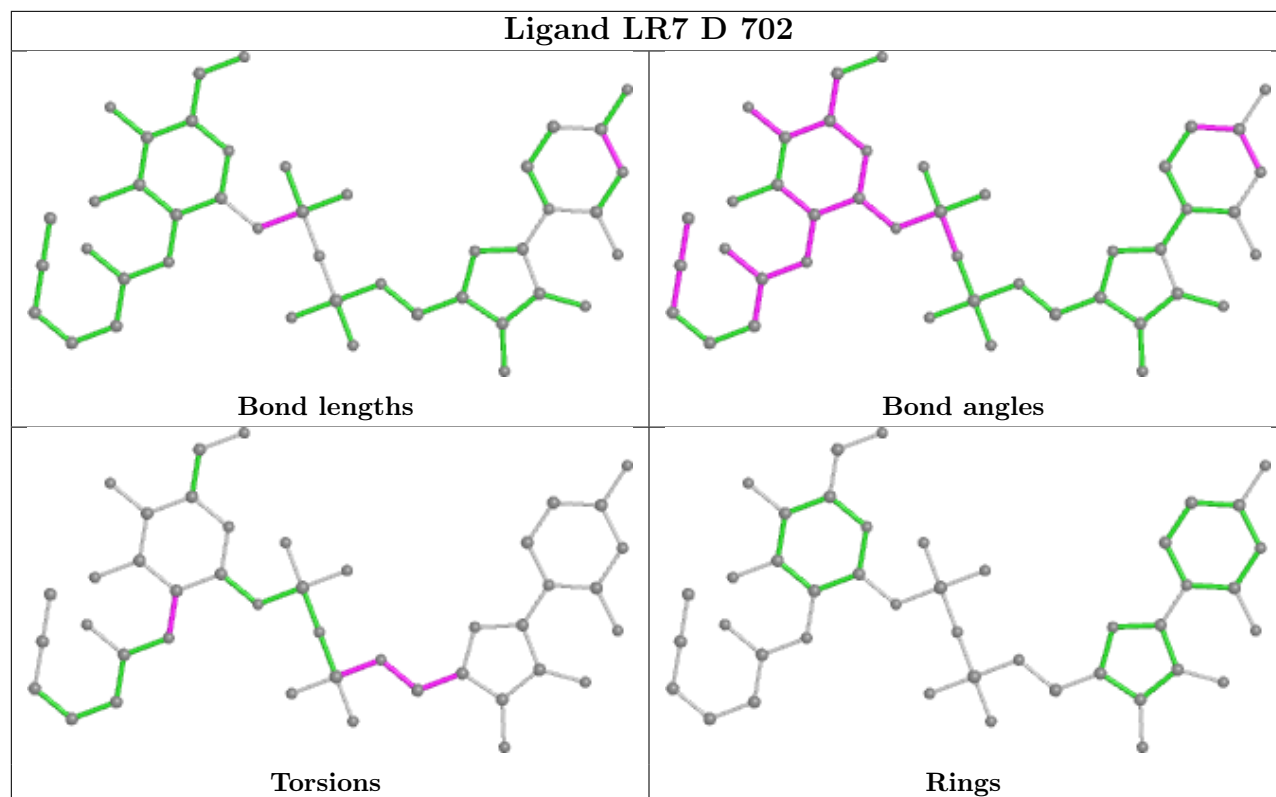
Ligand LR7 B 702



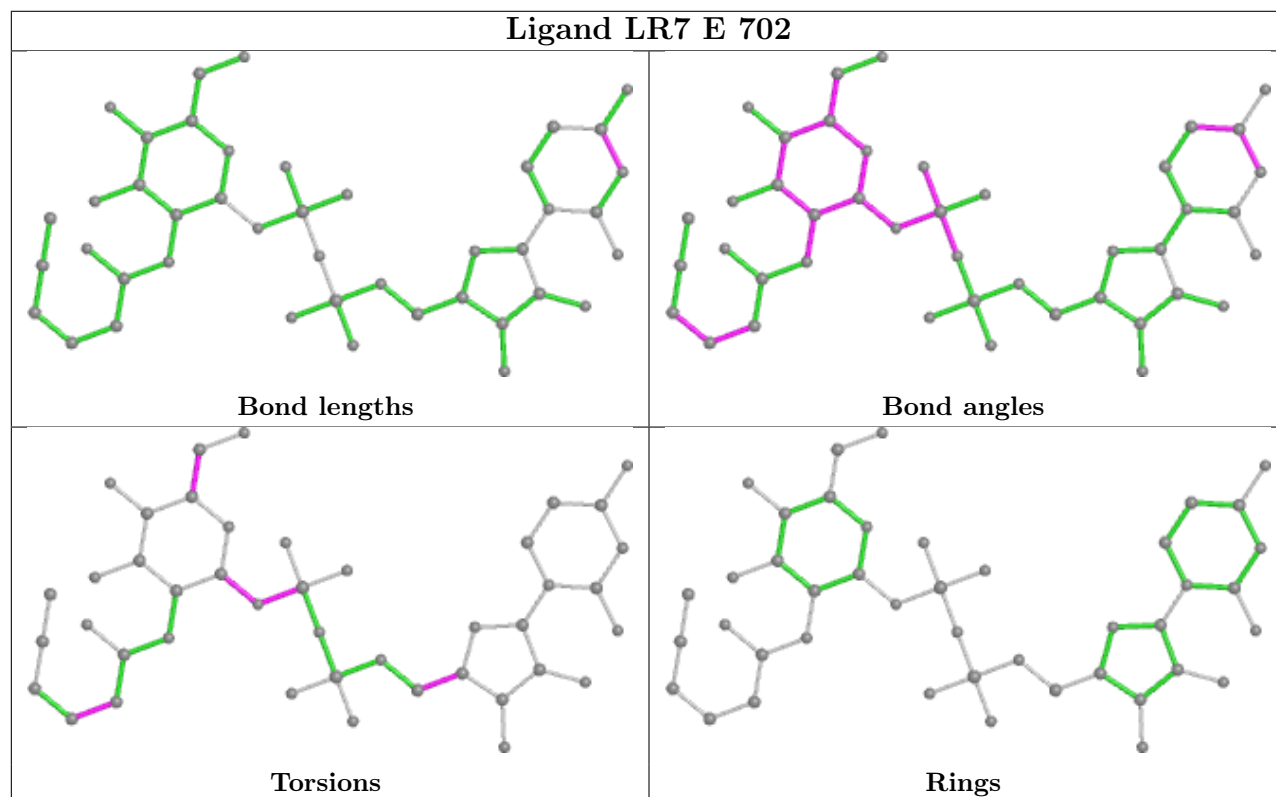
Ligand LR7 C 702

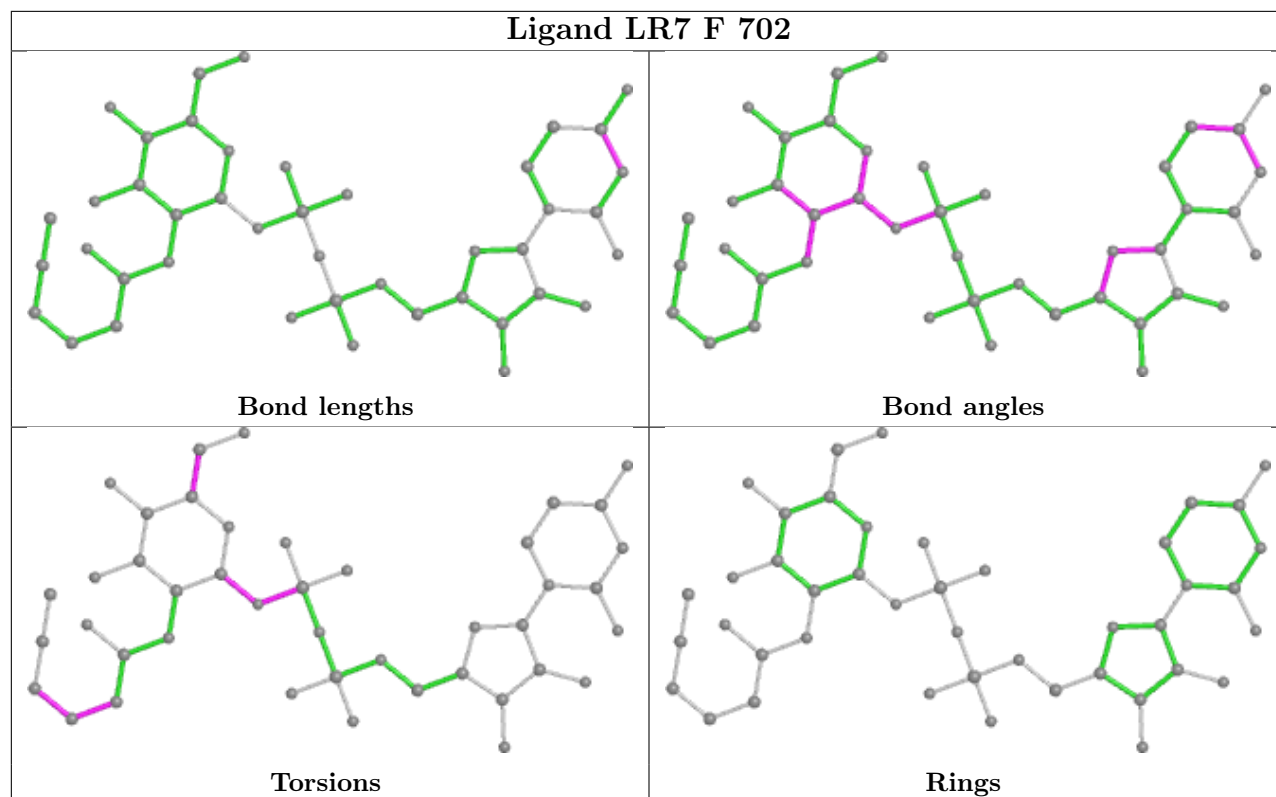


Ligand LR7 D 702



Ligand LR7 E 702





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	495/571 (86%)	-0.24	1 (0%) 94 88	30, 52, 73, 89	0
1	B	494/571 (86%)	-0.02	5 (1%) 82 64	32, 63, 95, 117	0
1	C	491/571 (85%)	-0.05	3 (0%) 89 76	34, 60, 88, 118	0
1	D	495/571 (86%)	-0.10	4 (0%) 86 69	33, 62, 85, 124	0
1	E	485/571 (84%)	0.11	16 (3%) 46 23	42, 73, 108, 131	0
1	F	483/571 (84%)	0.25	21 (4%) 35 17	40, 82, 111, 133	0
All	All	2943/3426 (85%)	-0.01	50 (1%) 70 46	30, 64, 101, 133	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	98	PRO	4.3
1	F	547	SER	3.9
1	E	407	PRO	3.7
1	B	500	VAL	3.6
1	E	504	PRO	3.6

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 carbohydrates in this entry.

6.4 Ligands

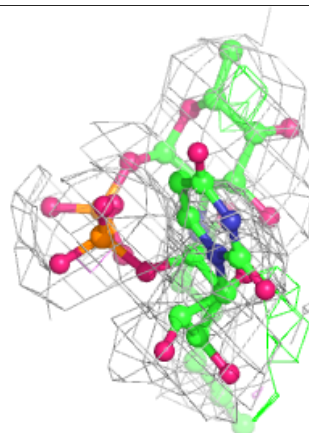
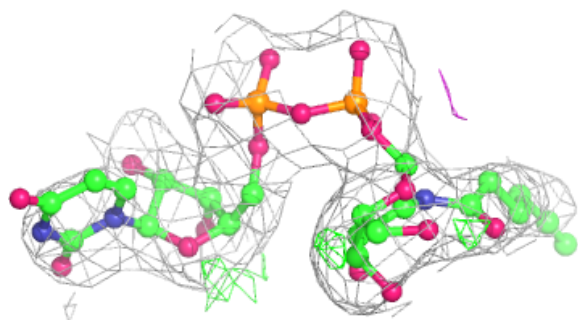
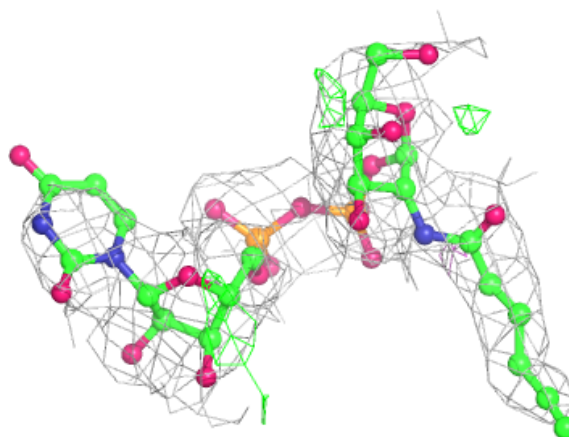
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LR7	E	702	43/43	0.91	0.27	52,69,97,108	0
3	LR7	F	702	43/43	0.92	0.21	64,76,94,96	0
3	LR7	D	702	43/43	0.93	0.25	41,54,78,82	0
3	LR7	A	702	43/43	0.94	0.21	41,48,61,72	0
3	LR7	B	702	43/43	0.95	0.21	41,57,85,97	0
3	LR7	C	702	43/43	0.95	0.23	47,54,67,72	0
2	MN	D	701	1/1	0.97	0.14	50,50,50,50	0
2	MN	F	701	1/1	0.98	0.15	73,73,73,73	0
2	MN	A	701	1/1	0.98	0.19	49,49,49,49	0
2	MN	C	701	1/1	0.99	0.20	48,48,48,48	0
2	MN	E	701	1/1	0.99	0.19	47,47,47,47	0
2	MN	B	701	1/1	1.00	0.14	30,30,30,30	0

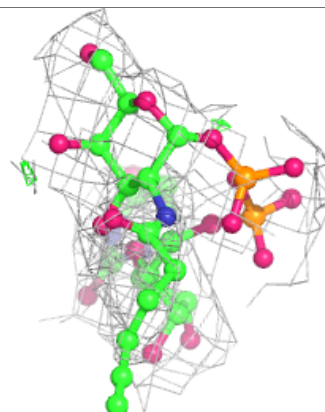
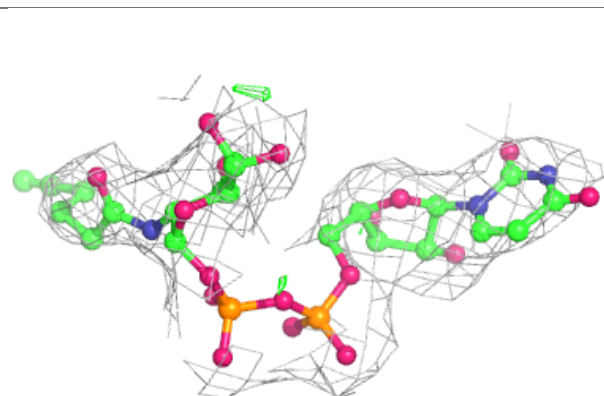
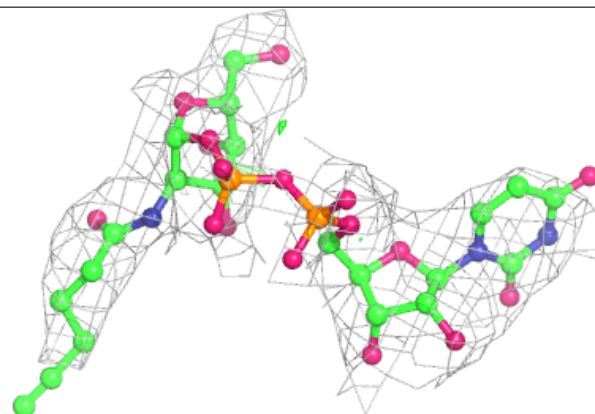
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LR7 E 702:

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

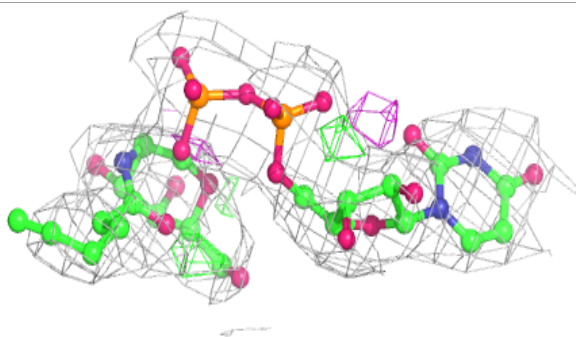
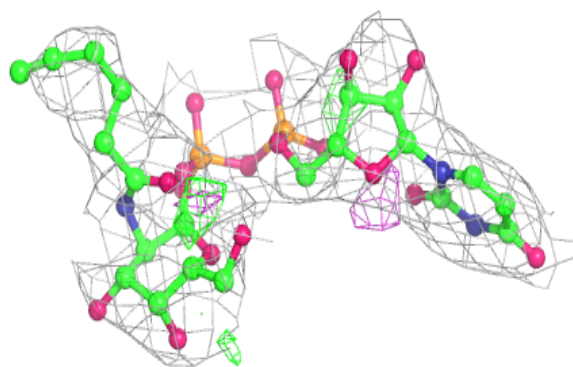
**Electron density around LR7 F 702:**

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

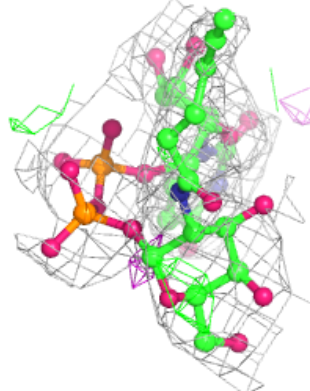
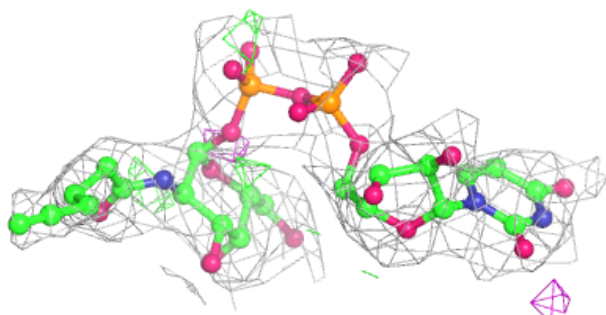
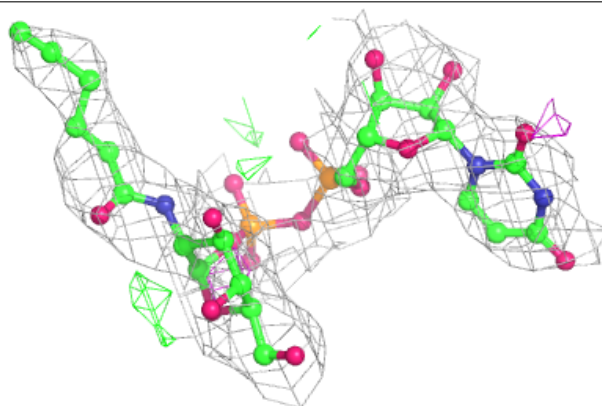


Electron density around LR7 D 702:

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

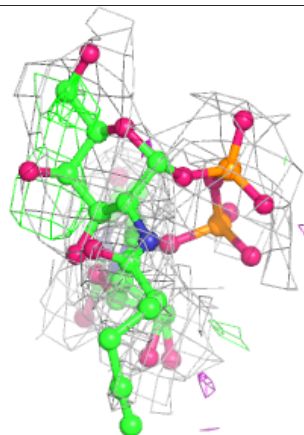
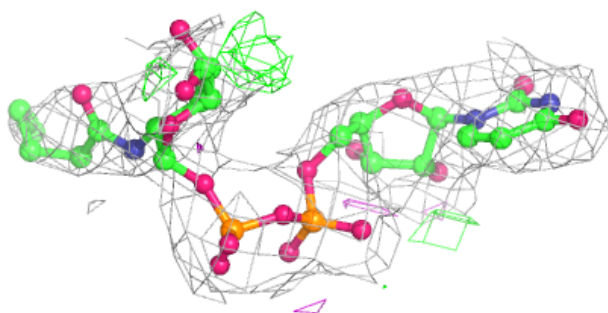
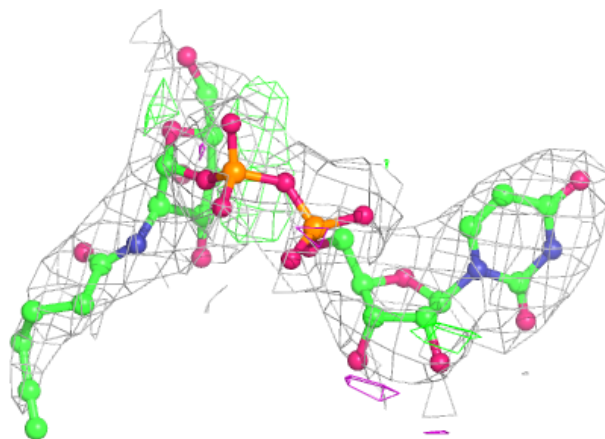
**Electron density around LR7 A 702:**

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

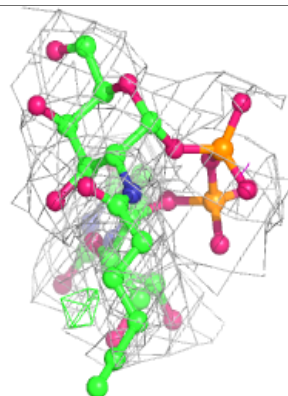
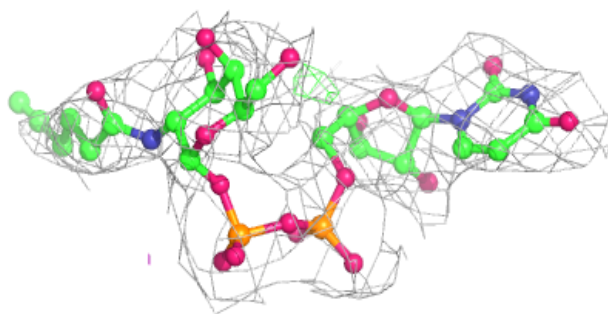
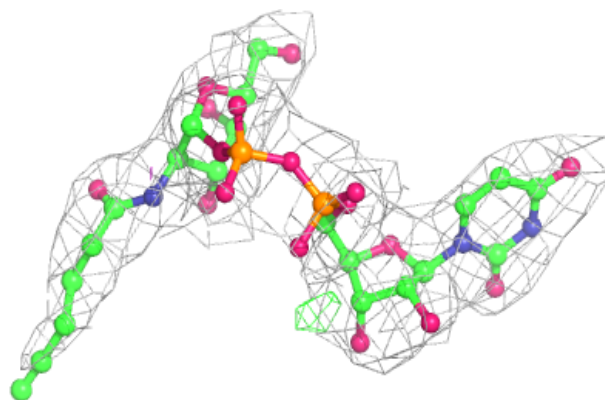


Electron density around LR7 B 702:

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

**Electron density around LR7 C 702:**

$2mF_o-DF_c$ (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.