wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2022 – 10:04 pm BST

PDB ID	:	7PLR
Title	:	Crystal structure of the N-terminal endonuclease domain of La Crosse virus L-protein bound to compound Baloxavir
Authors	:	Feracci, M.; Hernandez, S.; Vincentelli, R.; Ferron, F.; Reguera, J.; Canard, B.; Alvarez, K.
Deposited on	:	2021-09-01
Resolution	:	2.64 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

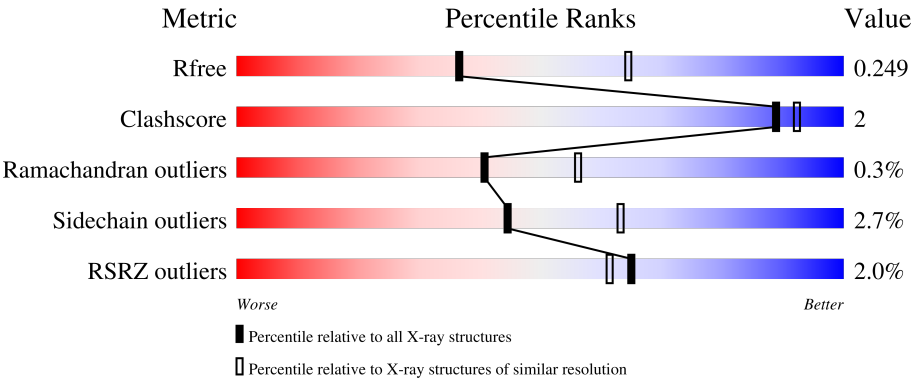
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	AAA	184	2% 92% 7%
1	BBB	184	% 93% 6%
1	DDD	184	2% 95% 5%
1	GGG	184	3% 96%

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	E4Z	AAA	201	X	-	-	-
2	E4Z	DDD	201	X	-	-	-
2	E4Z	GGG	201	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12568 atoms, of which 6177 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.

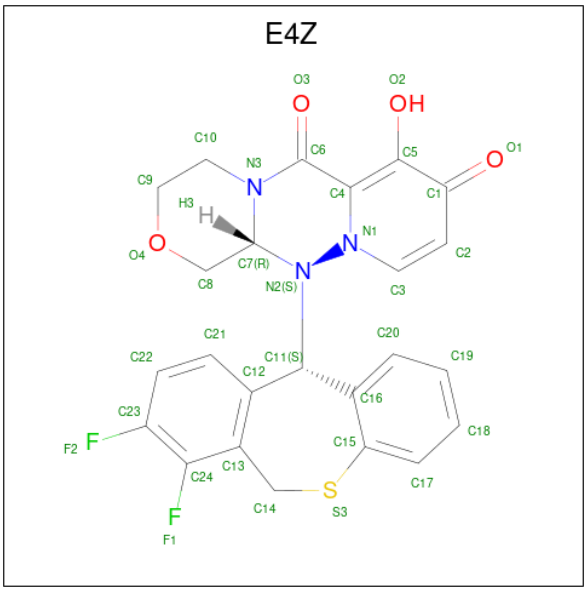
- Molecule 1 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	184	Total	C	H	N	O	S	35	1	0
			3052	990	1514	246	298	4			
1	BBB	184	Total	C	H	N	O	S	36	7	0
			3143	1017	1559	256	307	4			
1	DDD	184	Total	C	H	N	O	S	35	0	0
			3044	987	1511	246	296	4			
1	GGG	184	Total	C	H	N	O	S	36	2	0
			3063	993	1520	247	299	4			

There are 4 discrepancies between the modelled and reference sequences:

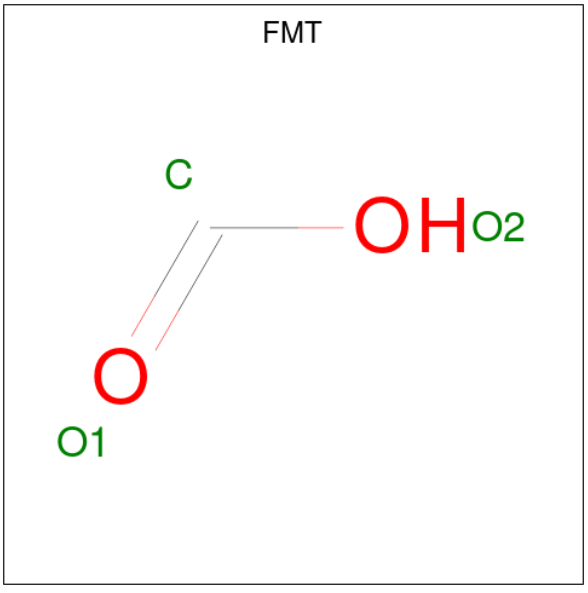
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	GLY	-	expression tag	UNP A5HC98
BBB	0	GLY	-	expression tag	UNP A5HC98
DDD	0	GLY	-	expression tag	UNP A5HC98
GGG	0	GLY	-	expression tag	UNP A5HC98

- Molecule 2 is Baloxavir acid (three-letter code: E4Z) (formula: $C_{24}H_{19}F_2N_3O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	AAA	1	Total	C	F	H	N	O	S	1	0
			53	24	2	19	3	4	1		
2	DDD	1	Total	C	F	H	N	O	S	1	0
			53	24	2	19	3	4	1		
2	GGG	1	Total	C	F	H	N	O	S	1	0
			53	24	2	19	3	4	1		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			5	1	2	2		

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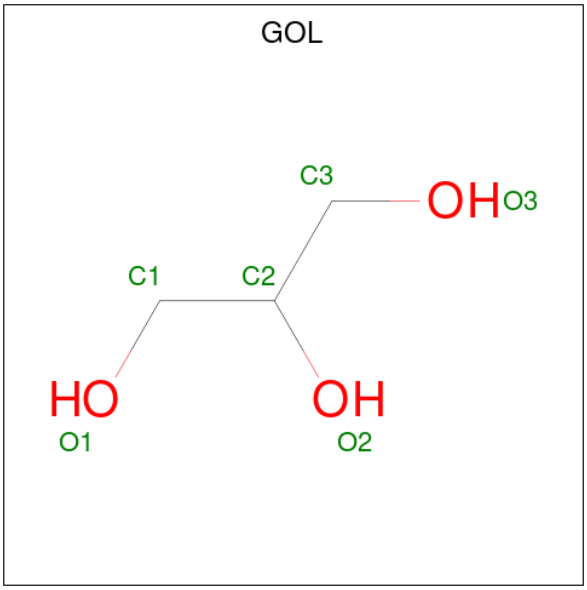
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C H O 5 1 2 2	1	0
3	DDD	1	Total C H O 5 1 2 2	1	0
3	GGG	1	Total C H O 5 1 2 2	1	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C H O 14 3 8 3	2	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	3	Total Mn 3 3	0	0
5	BBB	3	Total Mn 3 3	0	0
5	DDD	2	Total Mn 2 2	0	0
5	GGG	2	Total Mn 2 2	0	0

- Molecule 6 is water.

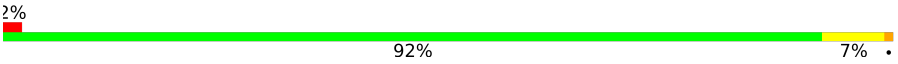
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	19	Total O 19 19	0	0
6	BBB	15	Total O 15 15	0	0
6	DDD	22	Total O 22 22	0	0
6	GGG	7	Total O 7 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

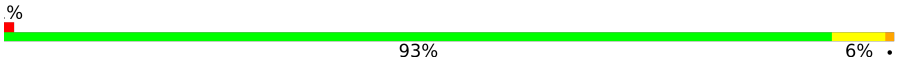
• Molecule 1: RNA-directed RNA polymerase L

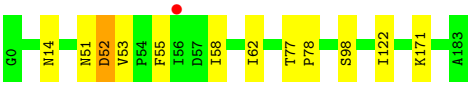
Chain AAA:



• Molecule 1: RNA-directed RNA polymerase L

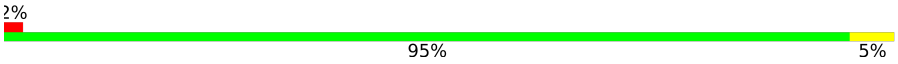
Chain BBB:

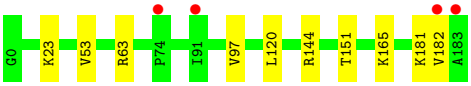




• Molecule 1: RNA-directed RNA polymerase L

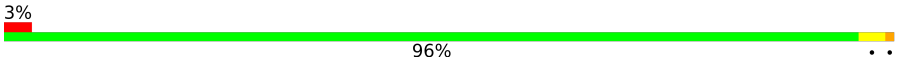
Chain DDD:

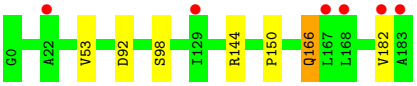




• Molecule 1: RNA-directed RNA polymerase L

Chain GGG:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.74Å 124.74Å 295.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	108.03 – 2.64 108.03 – 2.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (108.03-2.64) 100.0 (108.03-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.214 , 0.254 0.218 , 0.249	Depositor DCC
R_{free} test set	2047 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12568	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MN, FMT, E4Z

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	AAA	0.62	0/1573	0.70	0/2137
1	BBB	0.63	0/1623	0.68	0/2206
1	DDD	0.63	0/1565	0.70	0/2126
1	GGG	0.63	0/1581	0.69	0/2148
All	All	0.63	0/6342	0.69	0/8617

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

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	AAA	1538	1514	1512	4	0
1	BBB	1584	1559	1557	7	0
1	DDD	1533	1511	1508	2	1
1	GGG	1543	1520	1519	1	0
2	AAA	34	19	0	3	0
2	DDD	34	19	0	3	0
2	GGG	34	19	0	3	0
3	AAA	6	4	2	0	0
3	DDD	3	2	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	GGG	3	2	1	0	0
4	AAA	6	8	8	0	0
5	AAA	3	0	0	0	0
5	BBB	3	0	0	0	0
5	DDD	2	0	0	0	0
5	GGG	2	0	0	0	0
6	AAA	19	0	0	0	0
6	BBB	15	0	0	0	0
6	DDD	22	0	0	0	0
6	GGG	7	0	0	0	0
All	All	6391	6177	6108	23	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 23 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:DDD:63:ARG:NH2	1:DDD:120:LEU:O	2.28	0.66
2:DDD:201:E4Z:C16	2:DDD:201:E4Z:C3	2.82	0.58
1:AAA:63:ARG:NH2	1:AAA:120:LEU:O	2.38	0.56
1:AAA:84:ILE:HG21	1:AAA:148:LEU:HD11	1.88	0.55
2:AAA:201:E4Z:C3	2:AAA:201:E4Z:C16	2.87	0.53

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:97:VAL:O	1:DDD:165:LYS:HZ2[10_554]	1.56	0.04

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	AAA	183/184 (100%)	179 (98%)	4 (2%)	0	100 100
1	BBB	189/184 (103%)	183 (97%)	4 (2%)	2 (1%)	14 20
1	DDD	182/184 (99%)	179 (98%)	3 (2%)	0	100 100
1	GGG	184/184 (100%)	180 (98%)	3 (2%)	1 (0%)	29 43
All	All	738/736 (100%)	721 (98%)	14 (2%)	3 (0%)	41 48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	GGG	150	PRO
1	BBB	52[A]	ASP
1	BBB	52[B]	ASP

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	AAA	175/174 (101%)	166 (95%)	9 (5%)	24 37
1	BBB	181/174 (104%)	180 (99%)	1 (1%)	86 93
1	DDD	174/174 (100%)	170 (98%)	4 (2%)	50 68
1	GGG	176/174 (101%)	169 (96%)	7 (4%)	31 47
All	All	706/696 (101%)	685 (97%)	21 (3%)	44 59

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	GGG	53	VAL
1	GGG	98	SER
1	GGG	182	VAL
1	GGG	144	ARG
1	GGG	92[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	FMT	GGG	202	-	2,2,2	0.26	0	1,1,1	0.17	0
3	FMT	AAA	204	-	2,2,2	0.26	0	1,1,1	0.19	0
2	E4Z	AAA	201	5	36,39,39	0.94	2 (5%)	37,59,59	1.44	5 (13%)
2	E4Z	DDD	201	5	36,39,39	0.90	1 (2%)	37,59,59	1.41	5 (13%)
3	FMT	AAA	202	-	2,2,2	0.33	0	1,1,1	0.13	0
4	GOL	AAA	203	-	5,5,5	0.10	0	5,5,5	0.26	0
2	E4Z	GGG	201	5	36,39,39	0.86	1 (2%)	37,59,59	1.30	4 (10%)
3	FMT	DDD	202	-	2,2,2	0.20	0	1,1,1	0.23	0

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	E4Z	AAA	201	5	1/1/5/5	0/0/44/44	0/4/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E4Z	GGG	201	5	1/1/5/5	0/0/44/44	0/4/6/6
2	E4Z	DDD	201	5	1/1/5/5	0/0/44/44	0/4/6/6
4	GOL	AAA	203	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	201	E4Z	C4-C5	3.45	1.41	1.36
2	AAA	201	E4Z	C4-C5	3.44	1.41	1.36
2	GGG	201	E4Z	C4-C5	3.32	1.41	1.36
2	AAA	201	E4Z	C14-S3	2.29	1.84	1.82

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	GGG	201	E4Z	C2-C1-C5	4.67	119.79	115.04
2	AAA	201	E4Z	C2-C1-C5	4.57	119.69	115.04
2	AAA	201	E4Z	C8-C7-N3	4.55	111.66	109.01
2	DDD	201	E4Z	C2-C1-C5	4.42	119.54	115.04
2	DDD	201	E4Z	C8-C7-N3	4.07	111.38	109.01

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AAA	201	E4Z	C11
2	DDD	201	E4Z	C11
2	GGG	201	E4Z	C11

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	203	GOL	O1-C1-C2-C3
4	AAA	203	GOL	O1-C1-C2-O2

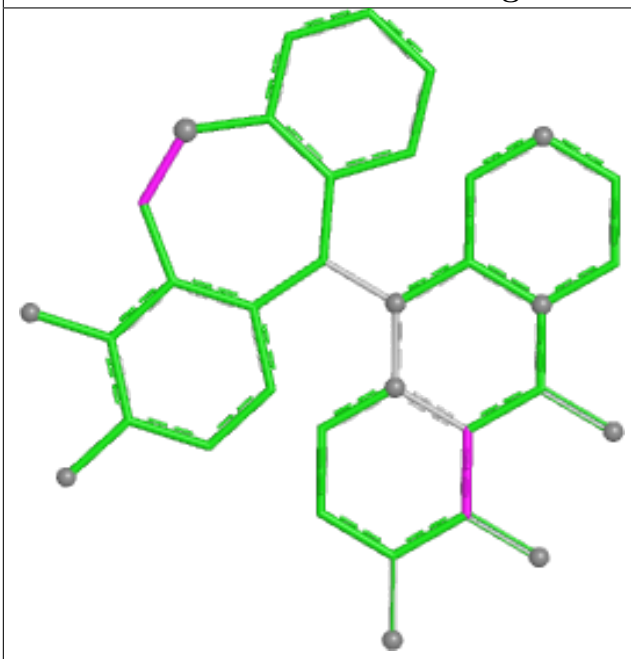
There are no ring outliers.

3 monomers are involved in 9 short contacts:

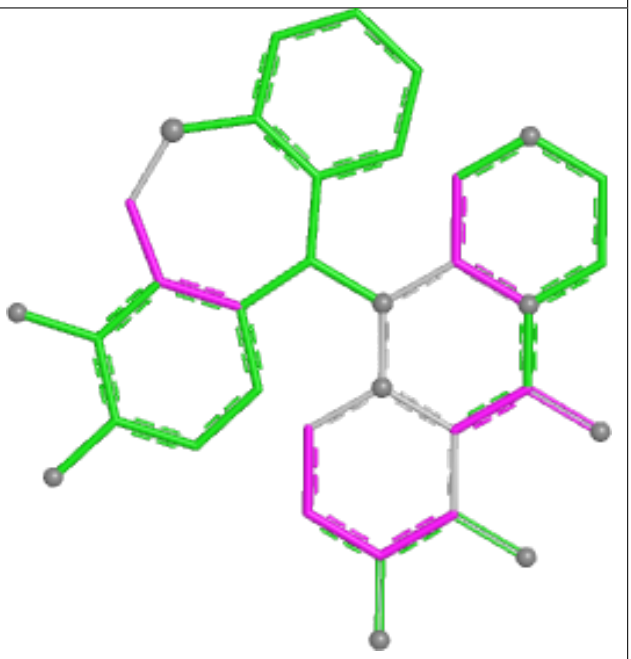
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	201	E4Z	3	0
2	DDD	201	E4Z	3	0
2	GGG	201	E4Z	3	0

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 then 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.

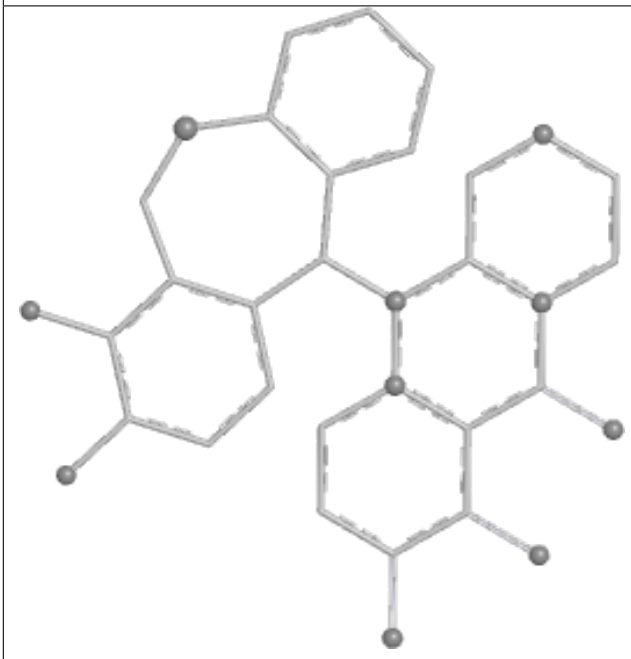
Ligand E4Z AAA 201



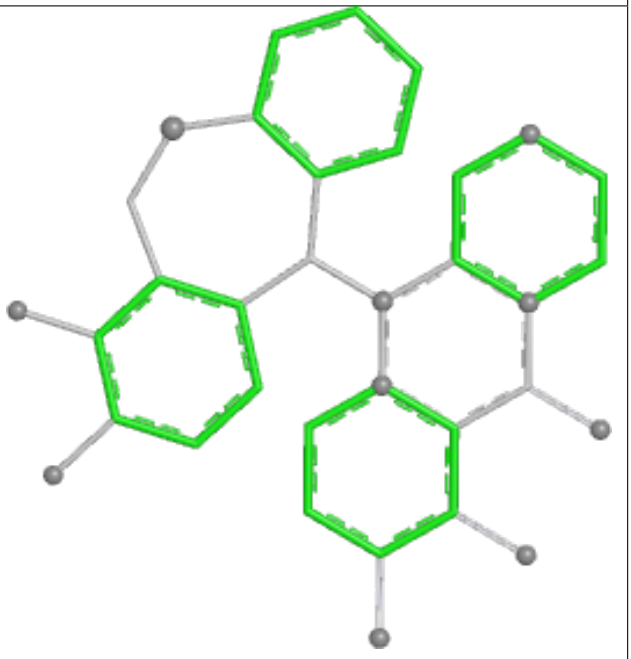
Bond lengths



Bond angles

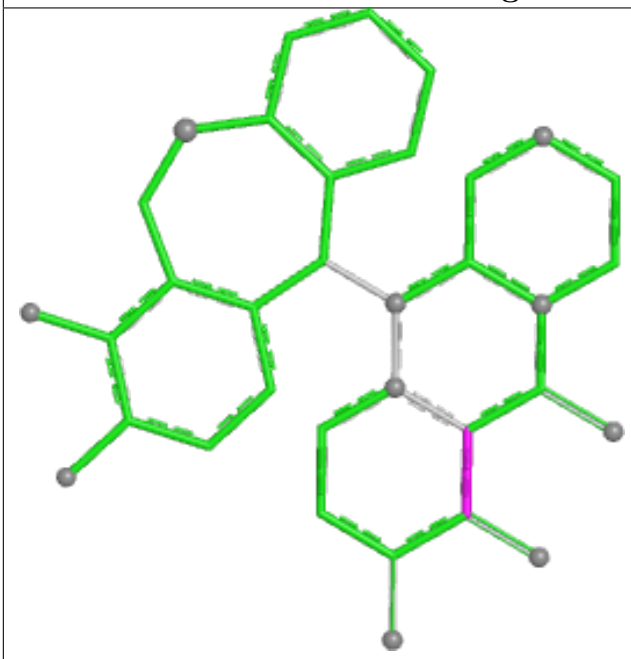


Torsions

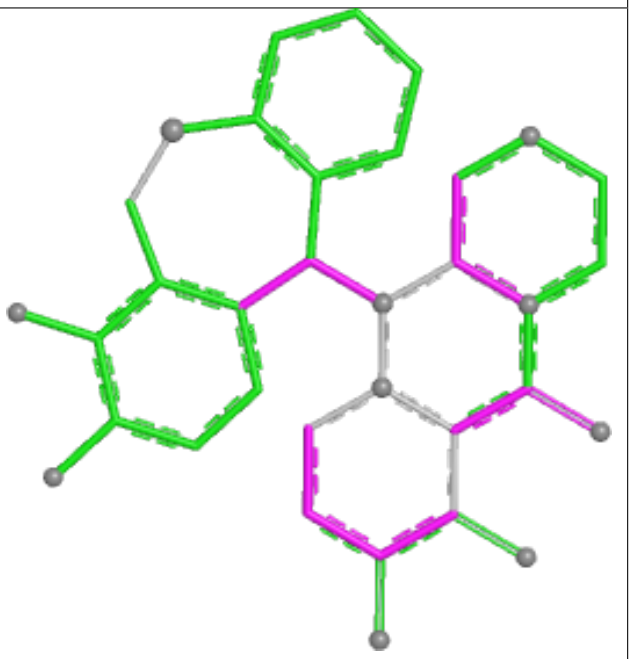


Rings

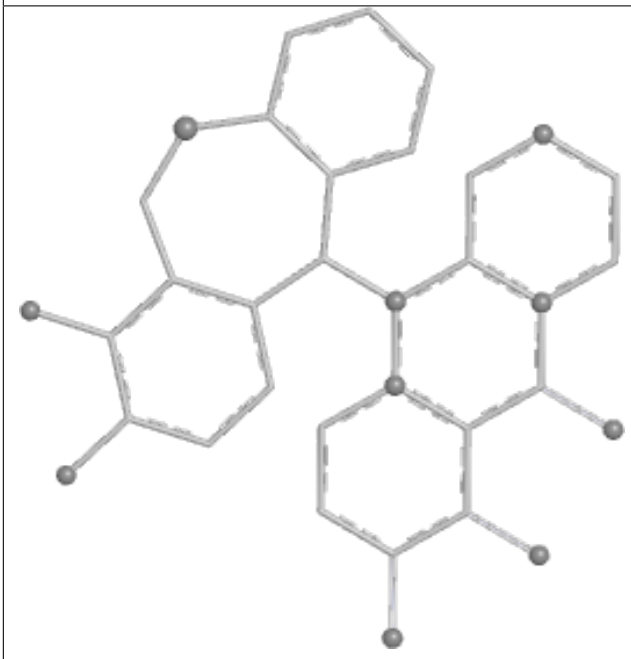
Ligand E4Z DDD 201



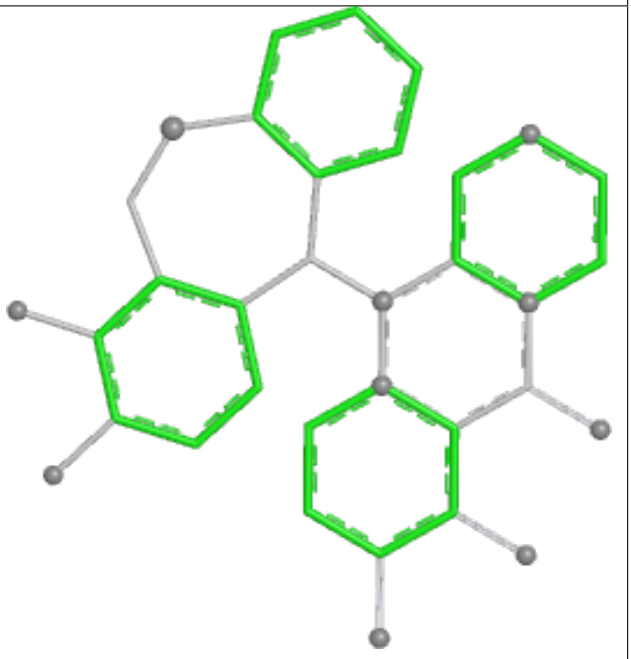
Bond lengths



Bond angles

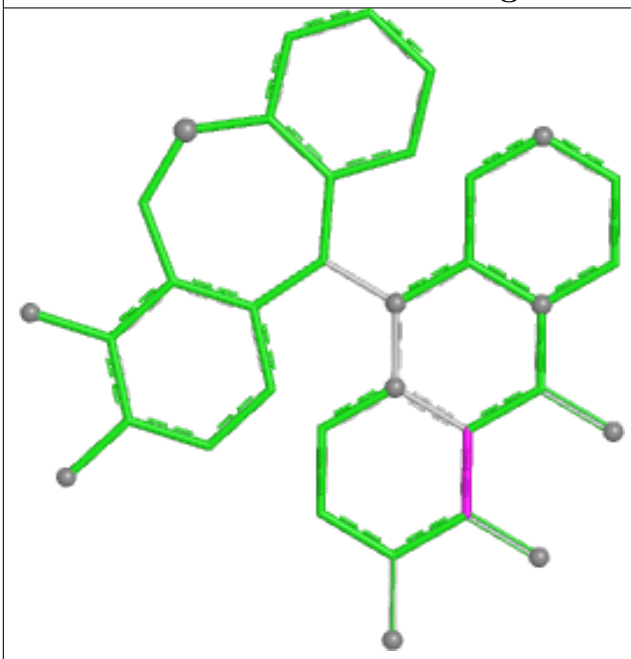


Torsions

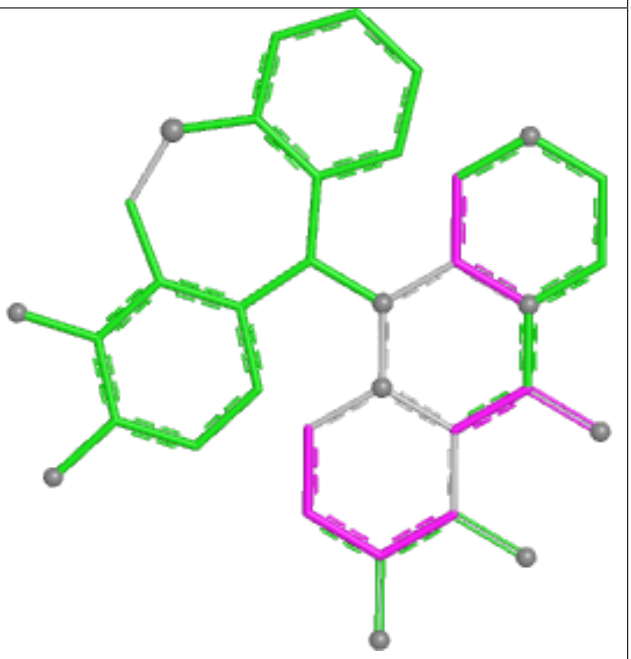


Rings

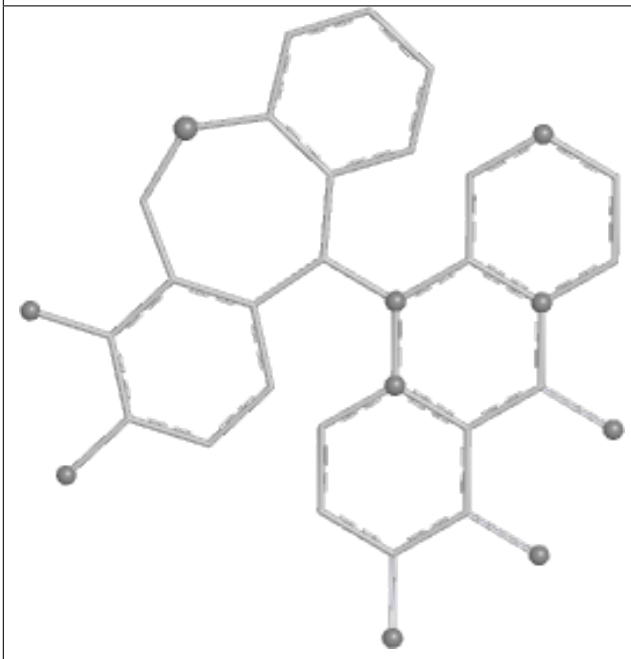
Ligand E4Z GGG 201



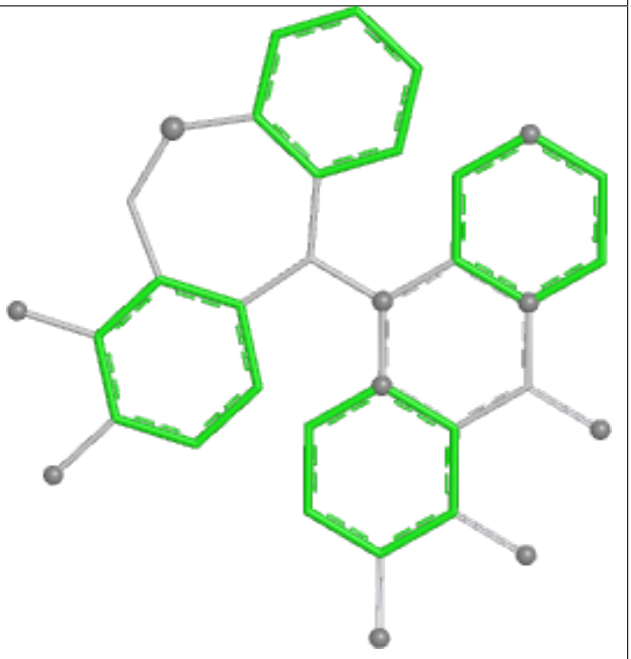
Bond lengths



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	AAA	184/184 (100%)	0.64	4 (2%)	62	58	43, 54, 75, 94	0
1	BBB	184/184 (100%)	0.50	1 (0%)	91	90	44, 56, 78, 93	0
1	DDD	184/184 (100%)	0.64	4 (2%)	62	58	46, 57, 72, 84	0
1	GGG	184/184 (100%)	0.61	6 (3%)	46	43	46, 61, 88, 104	0
All	All	736/736 (100%)	0.60	15 (2%)	65	61	43, 57, 79, 104	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	183	ALA	4.4
1	GGG	183	ALA	4.4
1	DDD	183	ALA	3.6
1	DDD	182	VAL	3.2
1	GGG	182	VAL	3.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

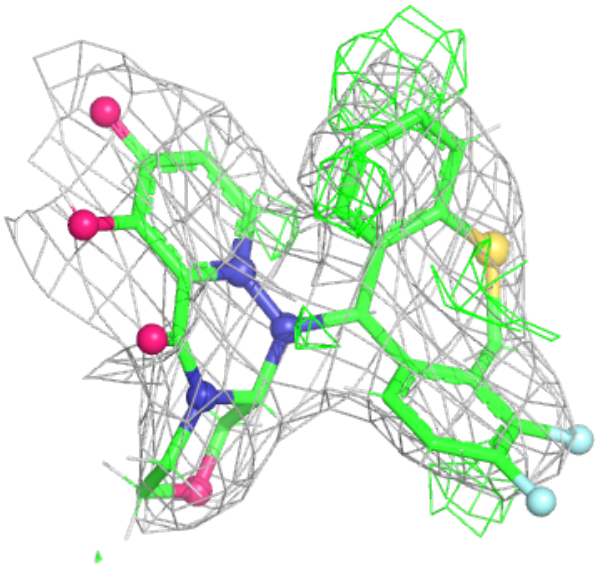
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

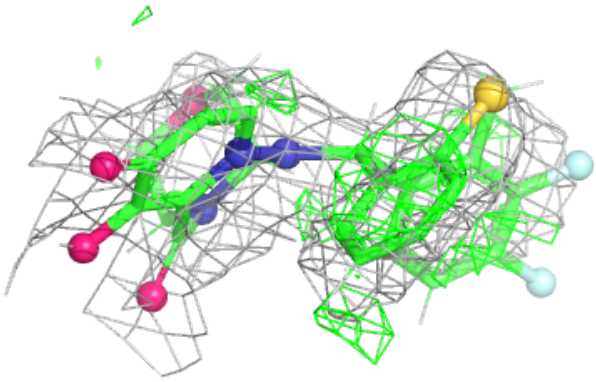
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MN	BBB	203	1/1	0.60	0.10	111,111,111,111	0
4	GOL	AAA	203	6/6	0.62	0.36	72,73,74,75	2
3	FMT	GGG	202	3/3	0.70	0.20	20,80,83,86	1
3	FMT	DDD	202	3/3	0.78	0.17	68,68,69,69	1
3	FMT	AAA	204	3/3	0.87	0.23	76,77,79,80	1
2	E4Z	GGG	201	34/34	0.88	0.22	69,73,83,86	53
2	E4Z	DDD	201	34/34	0.92	0.19	61,74,83,84	1
2	E4Z	AAA	201	34/34	0.93	0.21	72,82,86,89	1
5	MN	BBB	202	1/1	0.95	0.24	92,92,92,92	0
3	FMT	AAA	202	3/3	0.95	0.26	56,58,58,59	1
5	MN	AAA	205	1/1	0.96	0.14	83,83,83,83	0
5	MN	GGG	204	1/1	0.96	0.18	86,86,86,86	0
5	MN	AAA	207	1/1	0.98	0.17	65,65,65,65	0
5	MN	BBB	201	1/1	0.99	0.29	52,52,52,52	0
5	MN	DDD	203	1/1	0.99	0.25	50,50,50,50	0
5	MN	DDD	204	1/1	0.99	0.19	74,74,74,74	0
5	MN	GGG	203	1/1	0.99	0.26	57,57,57,57	0
5	MN	AAA	206	1/1	0.99	0.24	50,50,50,50	0

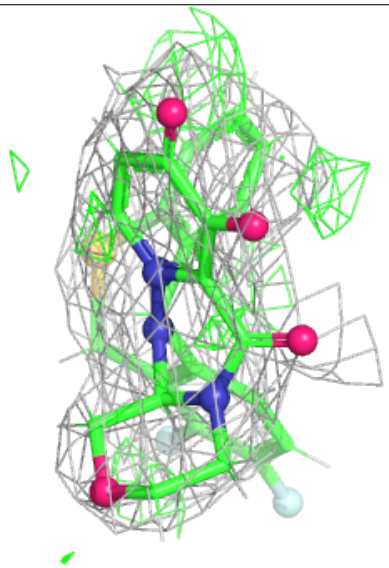
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around E4Z GGG 201:

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

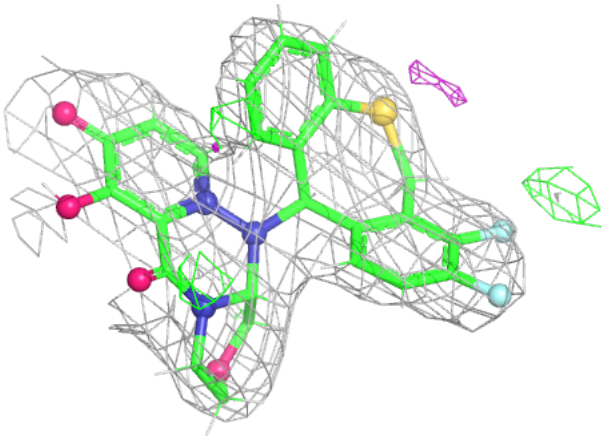


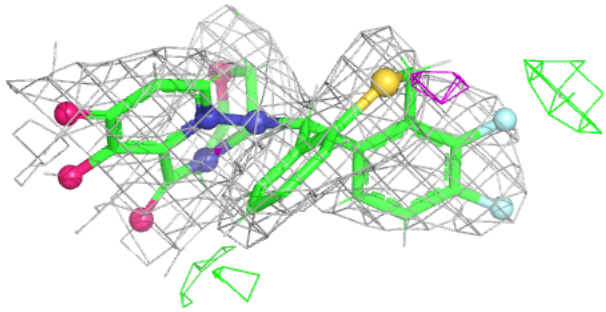


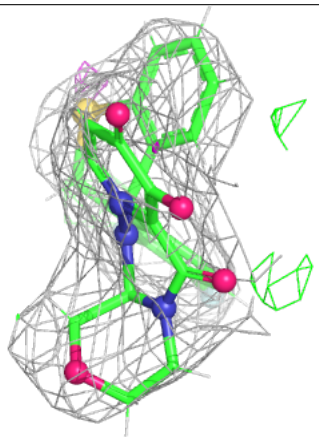


Electron density around E4Z DDD 201:

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







Electron density around E4Z AAA 201:

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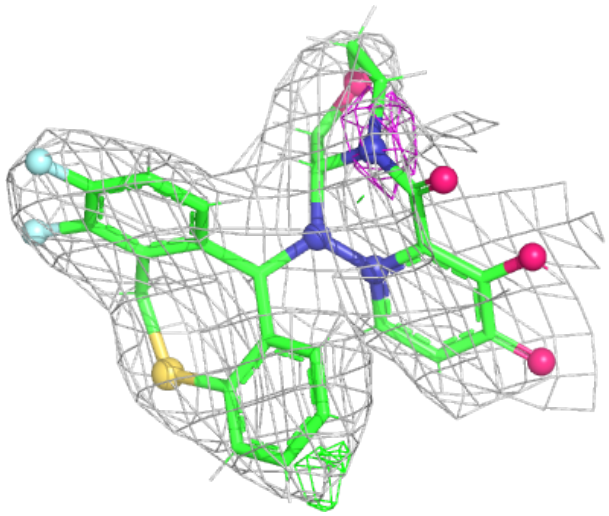
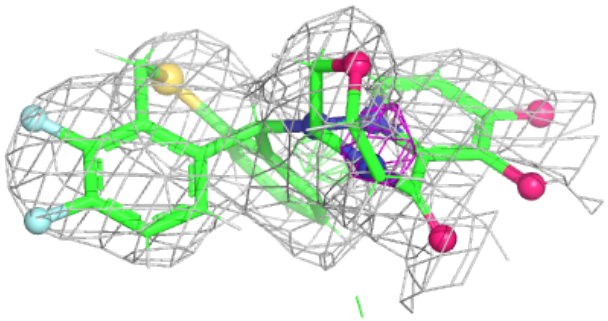
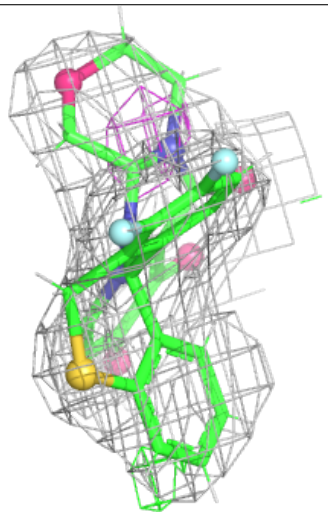
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.