



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2021 – 12:17 PM JST

PDB ID : 7ECS  
Title : Crystal Structure of Aspergillus terreus Glutamate Dehydrogenase (AtGDH)  
Complexed With Malonate and NADPH  
Authors : Godsora, B.K.J.; Prakash, P.; Punekar, N.S.; Bhaumik, P.  
Deposited on : 2021-03-13  
Resolution : 1.74 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](mailto: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.

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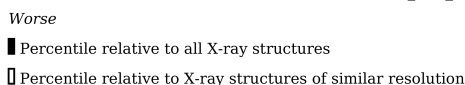
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

i

## X-RAY DIFFRACTION

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 <sub>free</sub>	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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  $\geq 3$ , 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	460	<div> <div></div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
1	B	460	<div> <div></div> <div>2%</div> <div>93%</div> <div>6%</div> </div>
1	C	460	<div> <div></div> <div>1%</div> <div>91%</div> <div>8%</div> </div>

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	GOL	A	503	-	-	X	-
2	GOL	A	504	-	-	X	-
2	GOL	C	507	-	X	-	-
3	MLI	A	508	-	-	X	-
3	MLI	B	511	-	-	X	-
3	MLI	C	510	-	-	X	-

## 2 Entry composition [i](#)

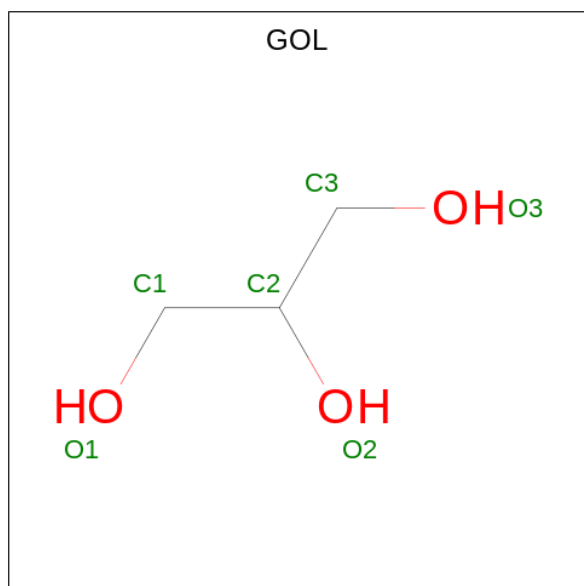
There are 5 unique types of molecules in this entry. The entry contains 12647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	12	0
			3527	2229	611	673	14			
1	B	460	Total	C	N	O	S	0	11	0
			3517	2222	609	672	14			
1	C	460	Total	C	N	O	S	0	13	0
			3531	2234	610	673	14			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



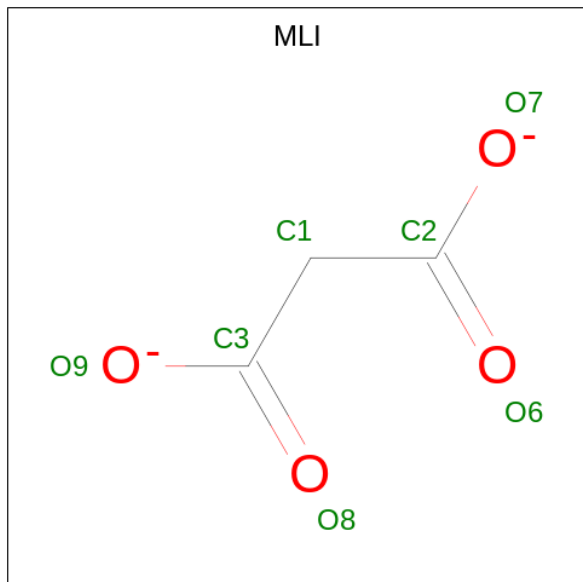
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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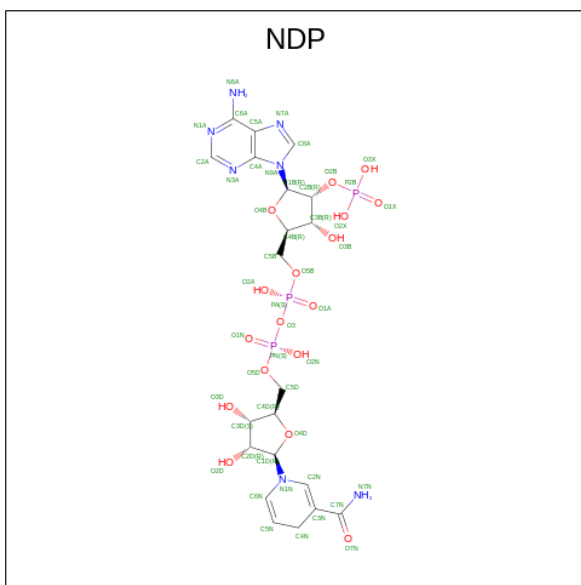
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	A	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	C	1	Total 48	C 21	N 7	O 17	P 3	0	0

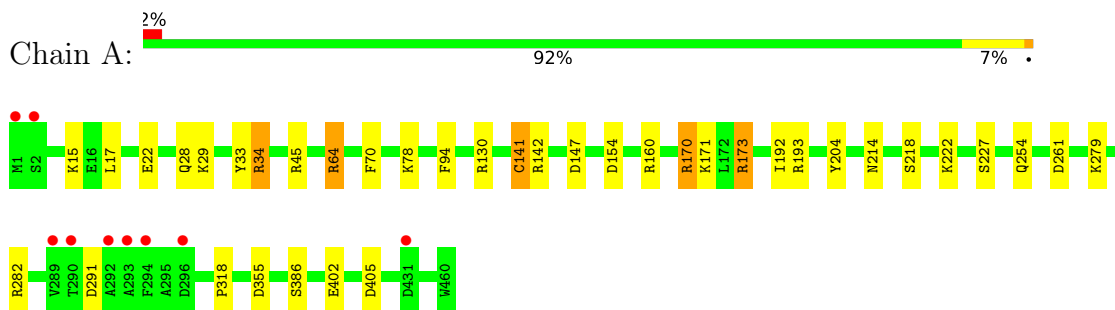
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	553	Total O 553 553	0	0
5	B	568	Total O 568 568	0	0
5	C	621	Total O 621 621	0	0

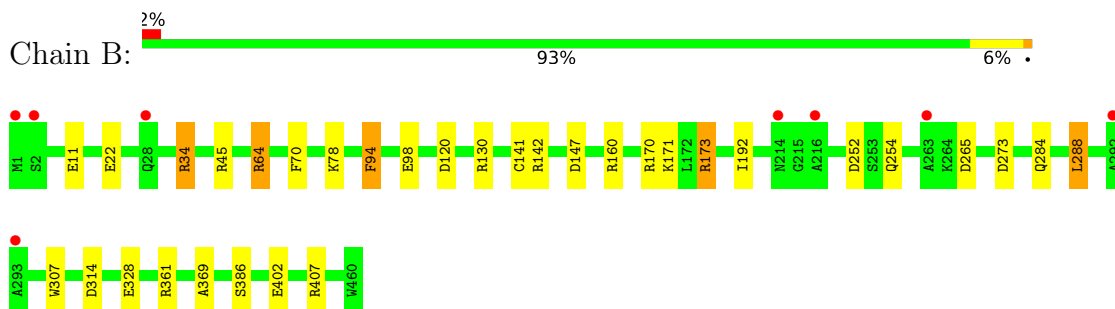
### 3 Residue-property plots [i](#)

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.

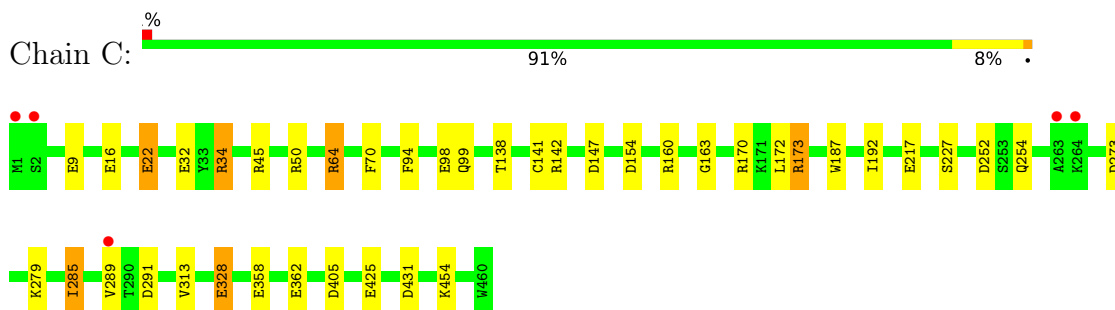
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.15Å 153.74Å 259.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.38 – 1.74 39.39 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.38-1.74) 99.9 (39.39-1.74)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.139 , 0.163 0.152 , 0.174	Depositor DCC
$R_{free}$ test set	12202 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NDP, GOL, MLI

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	1.24	7/3630 (0.2%)	1.20	22/4907 (0.4%)
1	B	1.26	6/3620 (0.2%)	1.20	22/4895 (0.4%)
1	C	1.22	17/3637 (0.5%)	1.20	26/4918 (0.5%)
All	All	1.24	30/10887 (0.3%)	1.20	70/14720 (0.5%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	GLU	CD-OE1	10.49	1.37	1.25
1	C	217	GLU	CD-OE1	8.88	1.35	1.25
1	C	254	GLN	CG-CD	-7.79	1.33	1.51
1	B	402	GLU	CG-CD	7.29	1.62	1.51
1	C	217	GLU	CD-OE2	-7.29	1.17	1.25
1	A	193	ARG	CG-CD	6.74	1.68	1.51
1	A	170	ARG	NE-CZ	-6.62	1.24	1.33
1	C	32	GLU	CG-CD	6.61	1.61	1.51
1	C	98	GLU	CD-OE2	6.02	1.32	1.25
1	B	98	GLU	CD-OE2	5.78	1.32	1.25
1	C	358	GLU	CD-OE1	5.67	1.31	1.25
1	C	362	GLU	CD-OE1	-5.55	1.19	1.25
1	A	204	TYR	CE2-CZ	5.53	1.45	1.38
1	C	160	ARG	CZ-NH1	5.50	1.40	1.33
1	B	173	ARG	CZ-NH2	-5.49	1.25	1.33
1	B	307	TRP	CD2-CE2	5.46	1.47	1.41
1	A	141[A]	CYS	CB-SG	-5.42	1.73	1.81
1	A	141[B]	CYS	CB-SG	-5.42	1.73	1.81
1	C	16	GLU	CG-CD	5.41	1.60	1.51
1	C	328	GLU	CD-OE2	5.41	1.31	1.25
1	C	22	GLU	CD-OE2	-5.38	1.19	1.25
1	C	9	GLU	CD-OE2	5.34	1.31	1.25
1	C	227	SER	CA-CB	-5.31	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	362	GLU	CD-OE2	-5.28	1.19	1.25
1	C	313	VAL	CB-CG2	-5.20	1.42	1.52
1	A	402	GLU	CD-OE1	5.16	1.31	1.25
1	A	170	ARG	CG-CD	5.16	1.64	1.51
1	B	170	ARG	CZ-NH2	-5.12	1.26	1.33
1	C	425	GLU	CD-OE2	5.10	1.31	1.25
1	C	170	ARG	CZ-NH2	-5.06	1.26	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	ARG	NE-CZ-NH1	17.58	129.09	120.30
1	A	173	ARG	NE-CZ-NH1	16.84	128.72	120.30
1	B	173	ARG	NE-CZ-NH1	13.23	126.91	120.30
1	B	64[A]	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	B	64[B]	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	C	173	ARG	NE-CZ-NH2	-11.23	114.69	120.30
1	C	160	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	B	160	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	A	173	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	B	64[A]	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	64[B]	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	147	ASP	CB-CG-OD2	-9.66	109.61	118.30
1	A	64[A]	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	A	64[B]	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	C	34	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	C	64[A]	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	64[B]	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	273	ASP	CB-CG-OD1	8.37	125.83	118.30
1	C	291	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	34	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	C	142	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	B	273	ASP	CB-CG-OD1	7.95	125.45	118.30
1	C	160	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	170	ARG	NE-CZ-NH1	-7.83	116.38	120.30
1	A	64[A]	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	64[B]	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	C	50	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	142	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	C	147	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	B	170	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	B	252	ASP	CB-CG-OD2	-7.07	111.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	170	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	A	33	TYR	CB-CG-CD1	6.81	125.09	121.00
1	A	147	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	279	LYS	CD-CE-NZ	-6.68	96.33	111.70
1	C	173	ARG	CD-NE-CZ	6.66	132.93	123.60
1	B	314	ASP	CB-CG-OD1	-6.66	112.31	118.30
1	A	34	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	405	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	279	LYS	CD-CE-NZ	-6.36	97.08	111.70
1	C	289	VAL	CB-CA-C	-6.32	99.40	111.40
1	A	142	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	C	291	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	B	98	GLU	OE1-CD-OE2	6.25	130.80	123.30
1	A	45	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	454	LYS	CD-CE-NZ	-6.08	97.72	111.70
1	C	50	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	265	ASP	CB-CG-OD2	-6.00	112.89	118.30
1	C	217	GLU	CG-CD-OE1	5.86	130.02	118.30
1	A	160	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	120	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	261	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	355	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	C	405	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	407	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	173	ARG	CD-NE-CZ	5.56	131.39	123.60
1	C	45	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	142	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	130	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	170	ARG	CA-CB-CG	5.27	124.99	113.40
1	A	282	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	170	ARG	CG-CD-NE	-5.25	100.78	111.80
1	C	170	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	B	98	GLU	CG-CD-OE1	-5.16	107.98	118.30
1	B	173	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	C	252	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	C	431	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	130	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	130	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	A	3527	0	3501	20	0
1	B	3517	0	3487	16	0
1	C	3531	0	3510	14	0
2	A	42	0	56	7	0
2	B	54	0	72	1	0
2	C	48	0	64	0	0
3	A	14	0	4	3	0
3	B	14	0	4	2	0
3	C	14	0	4	3	0
4	A	48	0	26	2	0
4	B	48	0	26	2	0
4	C	48	0	26	2	0
5	A	553	0	0	15	0
5	B	568	0	0	4	0
5	C	621	0	0	8	0
All	All	12647	0	10780	66	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 3.

All (66) 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:A:503:GOL:O3	2:A:504:GOL:H31	1.47	1.10
2:A:503:GOL:O3	2:A:504:GOL:C3	1.99	1.09
2:A:503:GOL:H32	2:A:504:GOL:H32	1.32	1.09
2:A:503:GOL:C3	2:A:504:GOL:H32	1.90	0.99
5:A:663:HOH:O	1:B:171:LYS:HD2	1.68	0.93
1:B:11:GLU:HG2	5:B:1115:HOH:O	1.75	0.85
2:A:503:GOL:C3	2:A:504:GOL:C3	2.58	0.79
1:B:141[B]:CYS:SG	1:B:173:ARG:HG3	2.27	0.73
1:A:171[B]:LYS:HG3	5:C:760:HOH:O	1.93	0.69
1:A:28:GLN:HG2	5:A:631:HOH:O	1.95	0.66
1:B:141[B]:CYS:SG	1:B:173:ARG:CG	2.84	0.66
1:C:141[B]:CYS:SG	1:C:173:ARG:HG2	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64[A]:ARG:NH1	5:C:602:HOH:O	2.17	0.61
1:C:141[B]:CYS:SG	1:C:173:ARG:HD3	2.40	0.60
3:C:510:MLI:O6	5:C:601:HOH:O	2.16	0.60
1:C:141[B]:CYS:SG	1:C:173:ARG:CG	2.90	0.60
1:A:141[A]:CYS:SG	1:A:173:ARG:HG2	2.41	0.60
1:A:141[A]:CYS:SG	1:A:173:ARG:CG	2.92	0.58
1:B:22:GLU:OE2	1:B:34:ARG:NH1	2.27	0.58
2:A:503:GOL:HO3	2:A:504:GOL:H31	1.68	0.57
3:A:508:MLI:O9	5:A:601:HOH:O	2.18	0.55
1:B:328:GLU:HG2	5:B:1081:HOH:O	2.06	0.55
2:A:503:GOL:H2	5:A:913:HOH:O	2.07	0.54
1:A:78:LYS:HE3	1:A:386[B]:SER:OG	2.08	0.54
5:A:780:HOH:O	1:B:171:LYS:HG3	2.07	0.54
5:A:663:HOH:O	1:B:171:LYS:CD	2.43	0.53
1:C:328:GLU:HG2	5:C:1120:HOH:O	2.09	0.52
1:A:254[A]:GLN:NE2	5:A:612:HOH:O	2.43	0.51
1:A:28:GLN:CG	5:A:631:HOH:O	2.57	0.49
3:B:511:MLI:H12	4:B:512:NDP:H41N	1.94	0.48
3:C:510:MLI:C1	4:C:511:NDP:H41N	2.43	0.48
3:B:511:MLI:C1	4:B:512:NDP:H41N	2.43	0.48
1:A:141[A]:CYS:SG	1:A:173:ARG:HD3	2.54	0.48
1:A:171[B]:LYS:CE	5:C:760:HOH:O	2.61	0.48
1:C:22:GLU:OE2	1:C:34:ARG:NH1	2.28	0.47
3:A:508:MLI:H12	4:A:510:NDP:H41N	1.96	0.46
1:A:171[B]:LYS:HE3	5:C:760:HOH:O	2.16	0.46
1:B:361:ARG:HA	1:B:369:ALA:HB1	1.98	0.45
1:C:34:ARG:HD2	5:C:896:HOH:O	2.15	0.45
3:A:508:MLI:C1	4:A:510:NDP:H41N	2.47	0.45
1:A:64[A]:ARG:HD2	5:A:616:HOH:O	2.15	0.45
1:A:173:ARG:NH2	5:A:622:HOH:O	2.49	0.45
1:B:64[B]:ARG:NH1	5:B:617:HOH:O	2.46	0.44
1:C:163:GLY:HA2	1:C:187:TRP:CH2	2.53	0.44
1:B:78:LYS:HE3	1:B:386[B]:SER:OG	2.17	0.44
1:B:141[B]:CYS:HG	1:B:173:ARG:HG3	1.83	0.44
2:B:502:GOL:H32	5:B:861:HOH:O	2.17	0.44
1:B:94:PHE:CD1	1:B:94:PHE:C	2.90	0.43
1:C:99:GLN:NE2	5:C:623:HOH:O	2.52	0.43
1:C:141[B]:CYS:SG	1:C:173:ARG:CD	3.07	0.42
1:A:15:LYS:NZ	5:A:621:HOH:O	2.51	0.42
1:A:29:LYS:HD2	5:A:989:HOH:O	2.18	0.42
1:A:64[B]:ARG:NH1	5:A:611:HOH:O	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:O	1:A:222:LYS:HE2	2.20	0.41
1:A:254[B]:GLN:NE2	5:A:608:HOH:O	2.36	0.41
1:B:141[B]:CYS:SG	1:B:173:ARG:HG2	2.57	0.41
1:B:288:LEU:HD12	1:B:288:LEU:C	2.41	0.41
1:C:138:THR:HA	1:C:172:LEU:HD11	2.02	0.41
1:A:291:ASP:HB3	5:A:797:HOH:O	2.20	0.41
1:A:22:GLU:OE1	1:A:34:ARG:NH1	2.32	0.41
1:A:227:SER:OG	1:A:318:PRO:HA	2.21	0.40
3:C:510:MLI:C3	4:C:511:NDP:H41N	2.52	0.40
1:B:254[B]:GLN:OE1	1:B:284:GLN:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/460 (102%)	461 (98%)	7 (2%)	2 (0%)	34	17
1	B	469/460 (102%)	458 (98%)	10 (2%)	1 (0%)	47	29
1	C	471/460 (102%)	463 (98%)	6 (1%)	2 (0%)	34	17
All	All	1410/1380 (102%)	1382 (98%)	23 (2%)	5 (0%)	34	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ILE
1	B	192	ILE
1	C	192	ILE
1	A	154	ASP
1	C	154	ASP

### 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	363/351 (103%)	358 (99%)	5 (1%)	67	50
1	B	362/351 (103%)	359 (99%)	3 (1%)	81	72
1	C	364/351 (104%)	360 (99%)	4 (1%)	73	59
All	All	1089/1053 (103%)	1077 (99%)	12 (1%)	76	59

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	70	PHE
1	A	94	PHE
1	A	170	ARG
1	A	214	ASN
1	B	70	PHE
1	B	94	PHE
1	B	288	LEU
1	C	70	PHE
1	C	94	PHE
1	C	285[A]	ILE
1	C	285[B]	ILE

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

Mol	Chain	Res	Type
1	B	61	GLN
1	C	99	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

33 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	$\# Z  > 2$
3	MLI	C	509	-	0,6,6	-	-	0,7,7	-	-
2	GOL	C	508	-	5,5,5	0.68	0	5,5,5	0.67	0
2	GOL	A	503	-	5,5,5	0.60	0	5,5,5	1.40	1 (20%)
2	GOL	C	503	-	5,5,5	0.87	0	5,5,5	1.26	1 (20%)
2	GOL	B	502	-	5,5,5	0.73	0	5,5,5	0.74	0
2	GOL	A	506	-	5,5,5	0.84	0	5,5,5	1.25	1 (20%)
4	NDP	C	511	-	45,52,52	1.20	4 (8%)	53,80,80	1.32	7 (13%)
2	GOL	B	508	-	5,5,5	0.91	0	5,5,5	0.55	0
2	GOL	B	503	-	5,5,5	0.91	0	5,5,5	1.31	1 (20%)
2	GOL	A	504	-	5,5,5	0.81	0	5,5,5	1.08	0
4	NDP	A	510	-	45,52,52	1.05	3 (6%)	53,80,80	1.15	5 (9%)
2	GOL	A	502	-	5,5,5	0.65	0	5,5,5	1.22	0
2	GOL	B	509	-	5,5,5	1.29	0	5,5,5	1.00	0
2	GOL	C	504	-	5,5,5	1.13	1 (20%)	5,5,5	1.78	2 (40%)
2	GOL	C	502	-	5,5,5	0.75	0	5,5,5	1.37	1 (20%)
3	MLI	A	509	-	0,6,6	-	-	0,7,7	-	-
2	GOL	A	507	-	5,5,5	0.97	0	5,5,5	1.59	1 (20%)
2	GOL	C	506	-	5,5,5	1.05	0	5,5,5	0.99	0
3	MLI	A	508	-	0,6,6	-	-	0,7,7	-	-
2	GOL	B	504	-	5,5,5	1.31	1 (20%)	5,5,5	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	506	-	5,5,5	0.87	0	5,5,5	1.53	1 (20%)
2	GOL	C	507	-	5,5,5	1.80	1 (20%)	5,5,5	2.75	3 (60%)
3	MLI	B	511	-	0,6,6	-	-	0,7,7	-	-
2	GOL	A	505	-	5,5,5	0.98	0	5,5,5	1.43	1 (20%)
3	MLI	C	510	-	0,6,6	-	-	0,7,7	-	-
2	GOL	B	507	-	5,5,5	0.96	0	5,5,5	1.40	1 (20%)
2	GOL	C	501	-	5,5,5	0.91	0	5,5,5	1.32	0
3	MLI	B	510	-	0,6,6	-	-	0,7,7	-	-
2	GOL	C	505	-	5,5,5	1.04	0	5,5,5	2.86	3 (60%)
4	NDP	B	512	-	45,52,52	1.36	7 (15%)	53,80,80	1.19	4 (7%)
2	GOL	B	505	-	5,5,5	0.24	0	5,5,5	1.61	1 (20%)
2	GOL	B	501	-	5,5,5	0.81	0	5,5,5	3.28	2 (40%)
2	GOL	A	501	-	5,5,5	0.68	0	5,5,5	1.04	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
3	MLI	C	509	-	-	0/0/4/4	-
2	GOL	C	508	-	-	4/4/4/4	-
2	GOL	A	503	-	-	3/4/4/4	-
2	GOL	C	503	-	-	0/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	A	506	-	-	2/4/4/4	-
4	NDP	C	511	-	-	5/30/77/77	0/5/5/5
2	GOL	B	508	-	-	0/4/4/4	-
2	GOL	B	503	-	-	4/4/4/4	-
2	GOL	A	504	-	-	4/4/4/4	-
4	NDP	A	510	-	-	7/30/77/77	0/5/5/5
2	GOL	A	502	-	-	3/4/4/4	-
2	GOL	B	509	-	-	1/4/4/4	-
2	GOL	C	504	-	-	0/4/4/4	-
2	GOL	C	502	-	-	4/4/4/4	-
3	MLI	A	509	-	-	0/0/4/4	-
2	GOL	A	507	-	-	2/4/4/4	-
2	GOL	C	506	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLI	A	508	-	-	0/0/4/4	-
2	GOL	B	504	-	-	0/4/4/4	-
2	GOL	B	506	-	-	0/4/4/4	-
2	GOL	C	507	-	-	2/4/4/4	-
3	MLI	B	511	-	-	0/0/4/4	-
2	GOL	A	505	-	-	3/4/4/4	-
3	MLI	C	510	-	-	0/0/4/4	-
2	GOL	B	507	-	-	2/4/4/4	-
2	GOL	C	501	-	-	2/4/4/4	-
3	MLI	B	510	-	-	0/0/4/4	-
2	GOL	C	505	-	-	2/4/4/4	-
4	NDP	B	512	-	-	7/30/77/77	0/5/5/5
2	GOL	B	505	-	-	4/4/4/4	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	A	501	-	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	NDP	C2A-N3A	3.54	1.37	1.32
4	B	512	NDP	C2A-N3A	3.21	1.37	1.32
4	C	511	NDP	P2B-O3X	-3.12	1.42	1.54
4	C	511	NDP	P2B-O2B	2.93	1.64	1.59
2	C	507	GOL	C3-C2	2.85	1.63	1.51
4	B	512	NDP	C6N-C5N	2.69	1.38	1.33
4	A	510	NDP	C6N-C5N	2.66	1.38	1.33
4	B	512	NDP	C4A-N3A	-2.62	1.32	1.35
2	C	504	GOL	O1-C1	2.43	1.52	1.42
4	B	512	NDP	C4N-C5N	-2.43	1.42	1.48
4	B	512	NDP	PA-O2A	-2.36	1.44	1.55
4	B	512	NDP	C2A-N1A	2.33	1.38	1.33
4	C	511	NDP	C2A-N3A	2.33	1.35	1.32
4	C	511	NDP	C4A-N3A	-2.24	1.32	1.35
2	B	504	GOL	O1-C1	2.16	1.51	1.42
4	B	512	NDP	O4D-C1D	2.14	1.47	1.42
4	A	510	NDP	C3B-C2B	-2.09	1.48	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GOL	C3-C2-C1	-6.42	86.75	111.70
2	C	505	GOL	C3-C2-C1	-4.13	95.66	111.70
2	C	505	GOL	O2-C2-C3	4.12	127.25	109.12
2	C	507	GOL	O3-C3-C2	4.11	129.92	110.20
4	A	510	NDP	N3A-C2A-N1A	-3.64	122.98	128.68
2	C	507	GOL	O1-C1-C2	-3.47	93.57	110.20
4	C	511	NDP	N6A-C6A-N1A	3.43	125.69	118.57
2	A	507	GOL	O3-C3-C2	3.06	124.89	110.20
2	C	504	GOL	C3-C2-C1	2.93	123.10	111.70
4	C	511	NDP	O2B-P2B-O1X	-2.87	98.30	109.39
2	B	501	GOL	O1-C1-C2	-2.69	97.32	110.20
2	B	506	GOL	O3-C3-C2	2.67	122.98	110.20
4	A	510	NDP	O3X-P2B-O2X	2.66	117.79	107.64
4	C	511	NDP	O3B-C3B-C4B	-2.65	103.40	111.05
4	A	510	NDP	C3D-C2D-C1D	-2.61	96.47	101.43
2	A	505	GOL	C3-C2-C1	2.56	121.67	111.70
2	C	507	GOL	O2-C2-C3	2.48	120.05	109.12
2	C	505	GOL	O1-C1-C2	-2.47	98.35	110.20
4	C	511	NDP	O2X-P2B-O2B	-2.45	95.01	105.99
2	A	506	GOL	O1-C1-C2	2.44	121.89	110.20
2	A	503	GOL	O2-C2-C1	2.41	119.72	109.12
4	B	512	NDP	C3N-C2N-N1N	-2.37	119.71	123.10
4	C	511	NDP	O2X-P2B-O1X	2.32	119.77	110.68
2	B	507	GOL	O3-C3-C2	2.30	121.22	110.20
4	C	511	NDP	C5A-C6A-N6A	-2.29	116.87	120.35
2	C	504	GOL	O2-C2-C3	-2.24	99.27	109.12
4	B	512	NDP	O2B-C2B-C3B	2.20	119.67	111.68
4	A	510	NDP	C2A-N1A-C6A	2.20	122.51	118.75
2	B	505	GOL	O1-C1-C2	-2.16	99.84	110.20
2	C	502	GOL	O1-C1-C2	2.15	120.51	110.20
2	B	503	GOL	O1-C1-C2	2.14	120.46	110.20
4	B	512	NDP	O3B-C3B-C4B	-2.13	104.88	111.05
4	C	511	NDP	O3X-P2B-O1X	2.12	119.00	110.68
4	A	510	NDP	N6A-C6A-N1A	2.05	122.83	118.57
4	B	512	NDP	C2D-C1D-N1N	2.05	118.44	113.30
2	C	503	GOL	C3-C2-C1	2.01	119.52	111.70

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	O1-C1-C2-C3
2	A	504	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	505	GOL	O1-C1-C2-C3
2	A	506	GOL	C1-C2-C3-O3
2	A	507	GOL	C1-C2-C3-O3
2	A	507	GOL	O2-C2-C3-O3
2	B	501	GOL	O1-C1-C2-C3
2	B	502	GOL	C1-C2-C3-O3
2	B	503	GOL	O1-C1-C2-C3
2	B	503	GOL	C1-C2-C3-O3
2	B	505	GOL	O1-C1-C2-C3
2	B	507	GOL	C1-C2-C3-O3
2	C	501	GOL	C1-C2-C3-O3
2	C	502	GOL	O1-C1-C2-C3
2	C	505	GOL	O1-C1-C2-C3
2	C	507	GOL	O1-C1-C2-C3
2	A	503	GOL	O1-C1-C2-O2
2	C	502	GOL	O1-C1-C2-O2
4	A	510	NDP	C3B-C2B-O2B-P2B
4	B	512	NDP	C3B-C2B-O2B-P2B
2	A	502	GOL	C1-C2-C3-O3
2	B	505	GOL	C1-C2-C3-O3
2	C	505	GOL	C1-C2-C3-O3
2	C	508	GOL	O1-C1-C2-C3
2	A	504	GOL	O2-C2-C3-O3
2	A	505	GOL	O1-C1-C2-O2
2	A	506	GOL	O2-C2-C3-O3
2	B	501	GOL	O1-C1-C2-O2
2	B	503	GOL	O1-C1-C2-O2
2	B	503	GOL	O2-C2-C3-O3
2	C	507	GOL	O1-C1-C2-O2
2	A	503	GOL	O2-C2-C3-O3
2	B	502	GOL	O2-C2-C3-O3
2	B	507	GOL	O2-C2-C3-O3
2	C	501	GOL	O2-C2-C3-O3
4	A	510	NDP	C1B-C2B-O2B-P2B
4	B	512	NDP	C1B-C2B-O2B-P2B
2	A	504	GOL	O1-C1-C2-O2
2	A	505	GOL	O2-C2-C3-O3
2	C	508	GOL	O2-C2-C3-O3
2	C	502	GOL	O2-C2-C3-O3
2	A	502	GOL	O1-C1-C2-C3
2	A	504	GOL	O1-C1-C2-C3
4	A	510	NDP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
4	A	510	NDP	C2D-C1D-N1N-C6N
2	A	502	GOL	O2-C2-C3-O3
2	B	505	GOL	O1-C1-C2-O2
2	B	509	GOL	O2-C2-C3-O3
4	A	510	NDP	O4D-C1D-N1N-C6N
4	B	512	NDP	O4D-C1D-N1N-C6N
4	B	512	NDP	C2D-C1D-N1N-C6N
4	C	511	NDP	O4D-C1D-N1N-C6N
2	B	505	GOL	O2-C2-C3-O3
2	C	508	GOL	O1-C1-C2-O2
4	C	511	NDP	C2D-C1D-N1N-C6N
2	C	508	GOL	C1-C2-C3-O3
4	A	510	NDP	C5D-O5D-PN-O3
4	B	512	NDP	C5D-O5D-PN-O3
4	C	511	NDP	C5D-O5D-PN-O3
4	B	512	NDP	O4B-C4B-C5B-O5B
2	C	502	GOL	C1-C2-C3-O3
4	B	512	NDP	C5D-O5D-PN-O1N
4	A	510	NDP	O4B-C4B-C5B-O5B
4	C	511	NDP	O4B-C4B-C5B-O5B
4	C	511	NDP	C3B-C2B-O2B-P2B

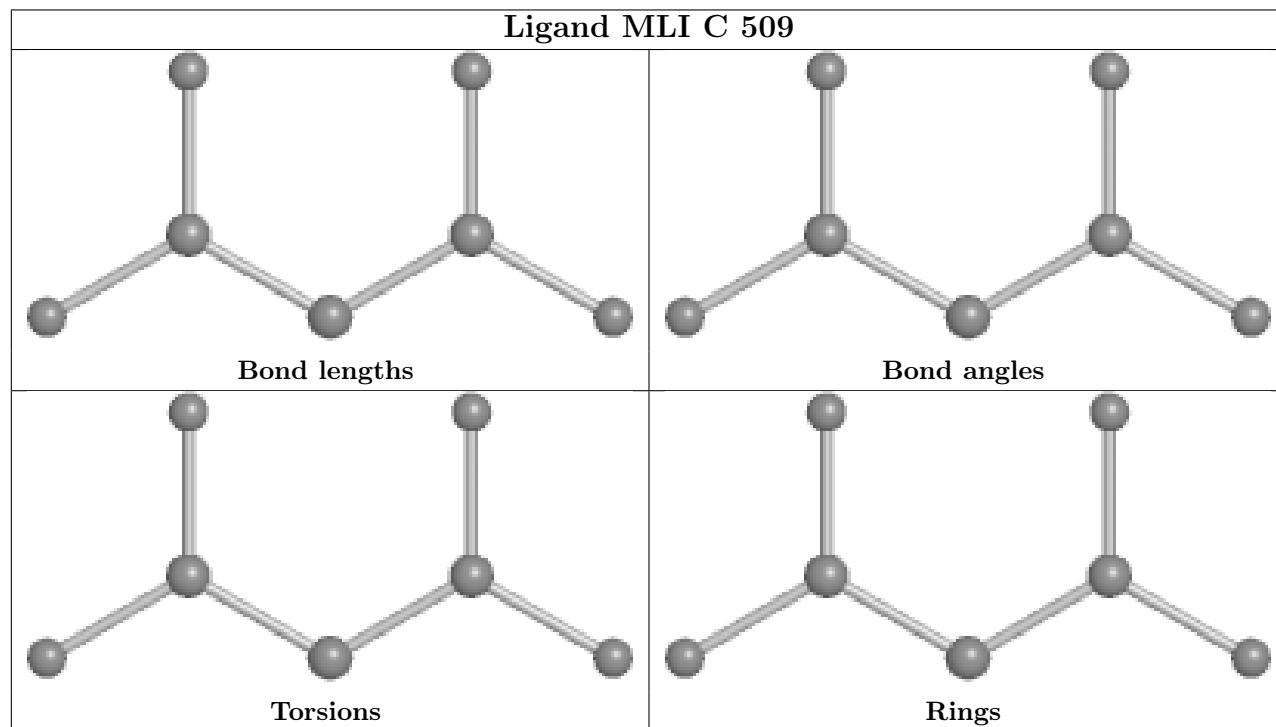
There are no ring outliers.

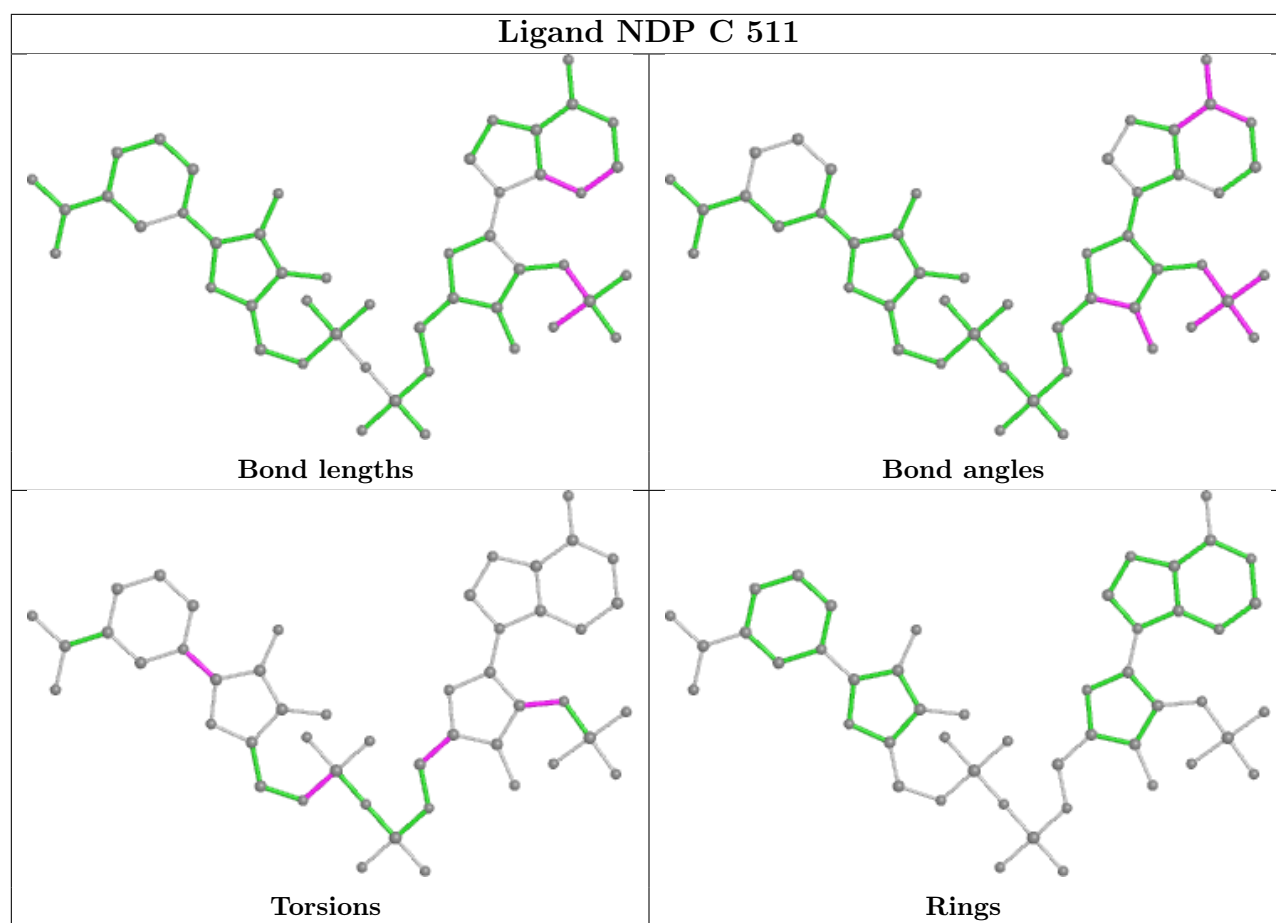
9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	GOL	7	0
2	B	502	GOL	1	0
4	C	511	NDP	2	0
2	A	504	GOL	6	0
4	A	510	NDP	2	0
3	A	508	MLI	3	0
3	B	511	MLI	2	0
3	C	510	MLI	3	0
4	B	512	NDP	2	0

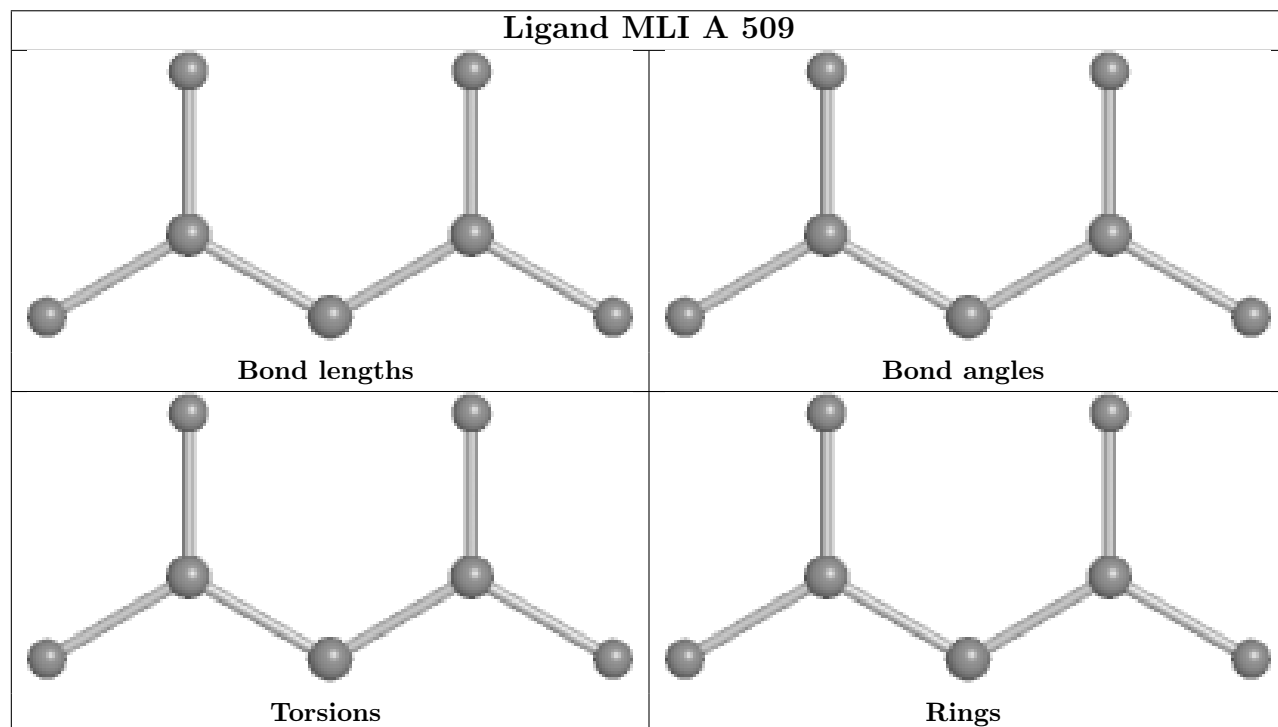
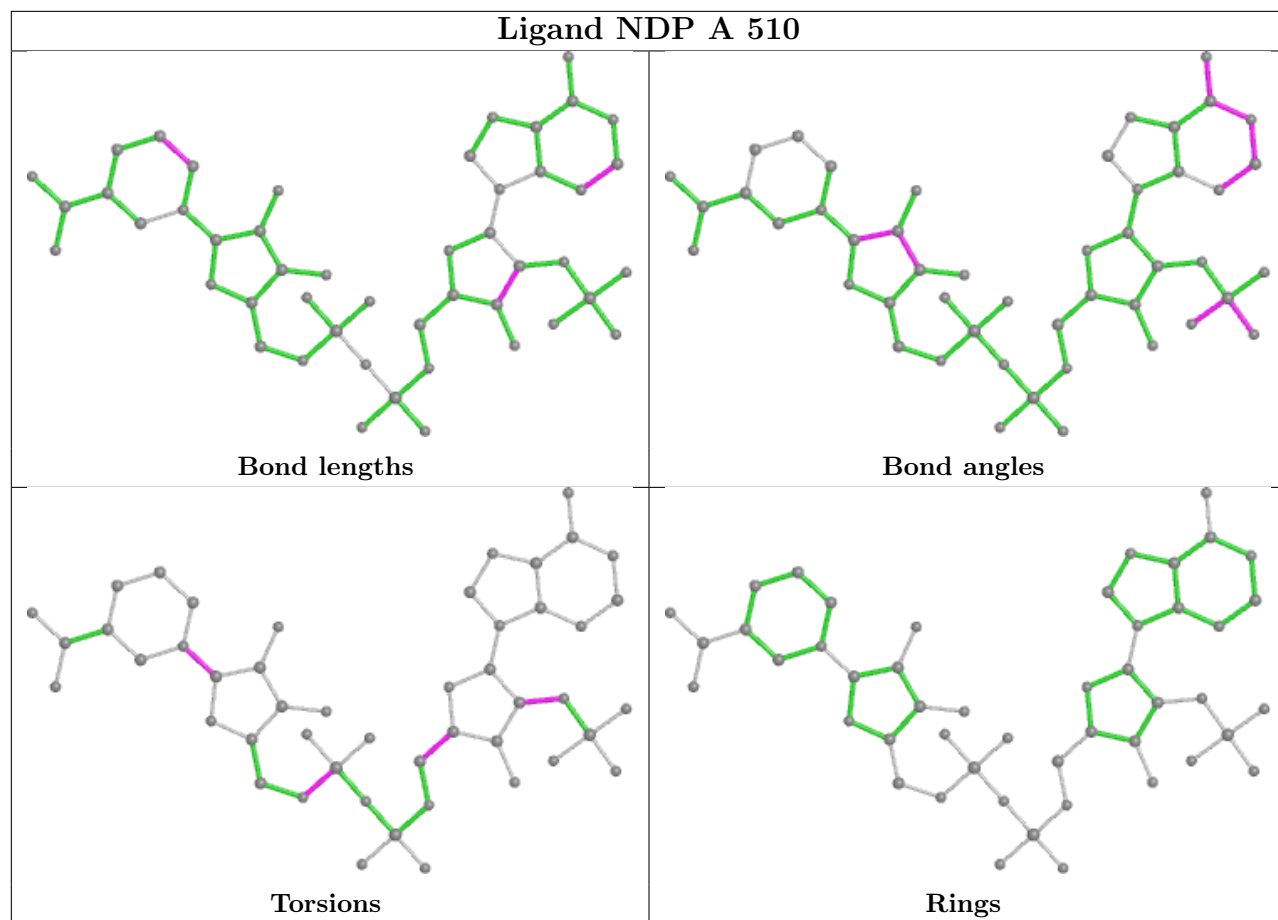
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

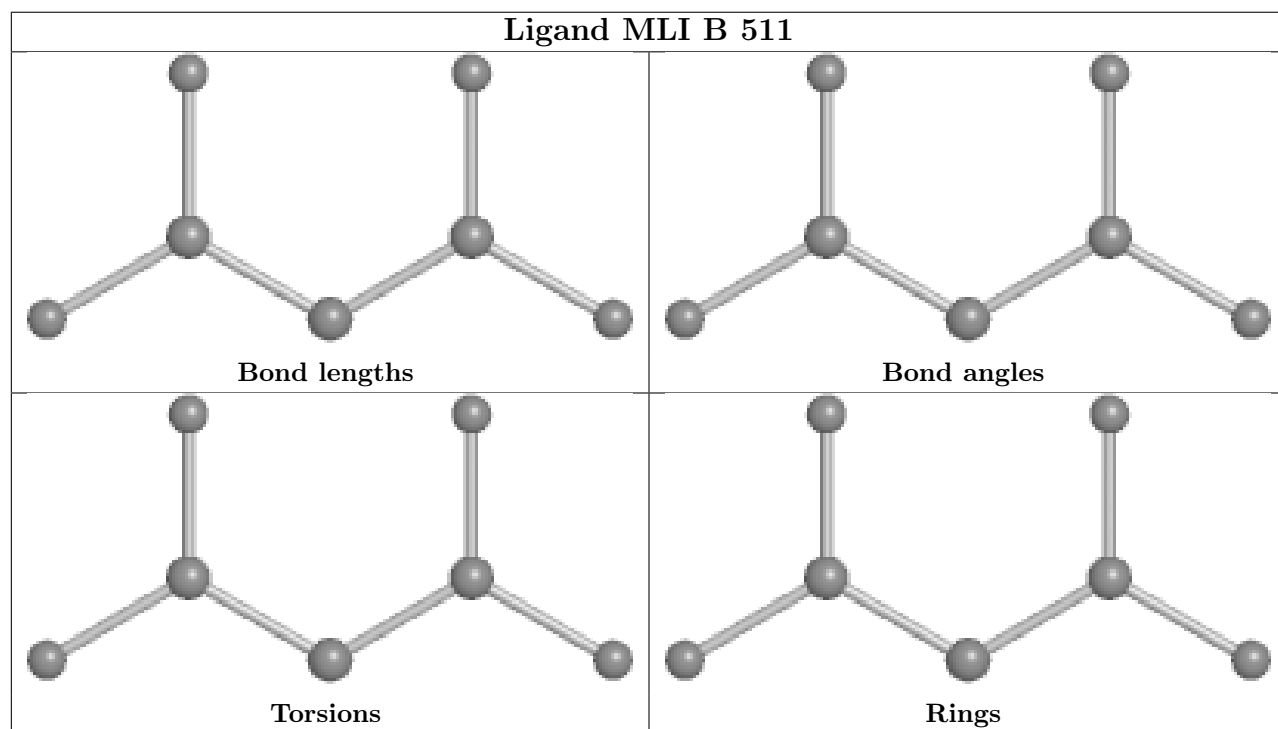
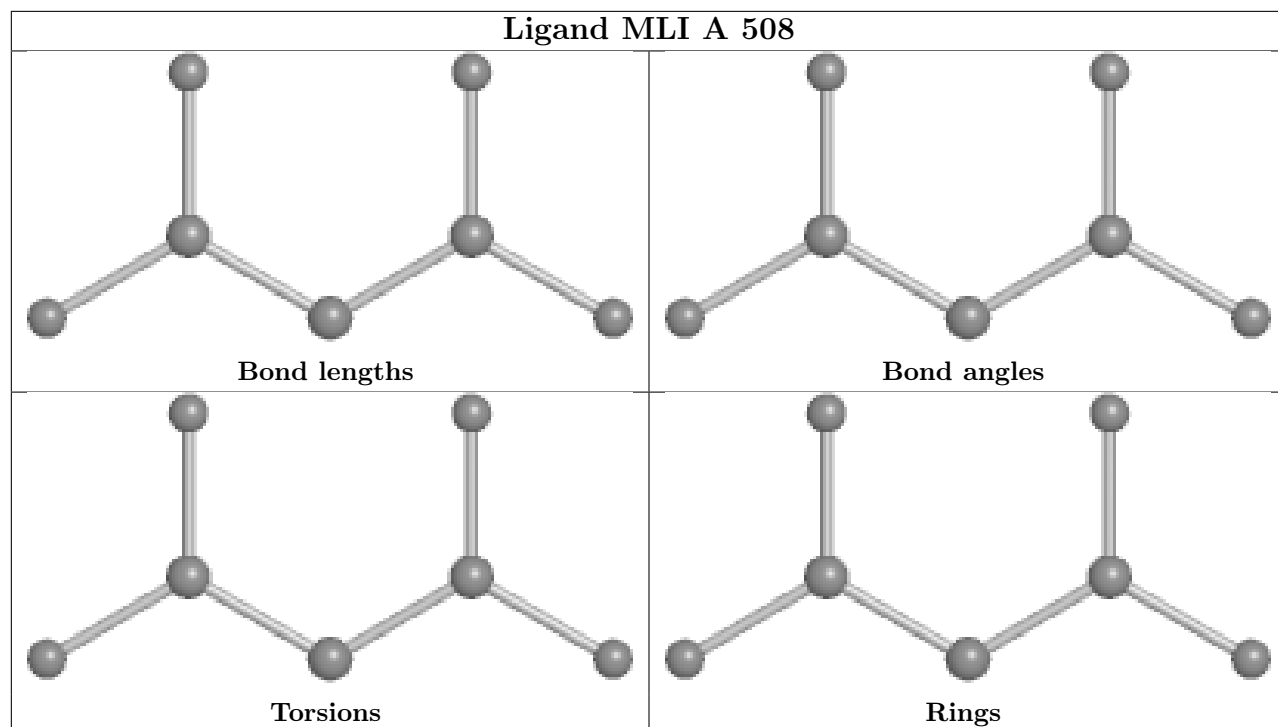
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

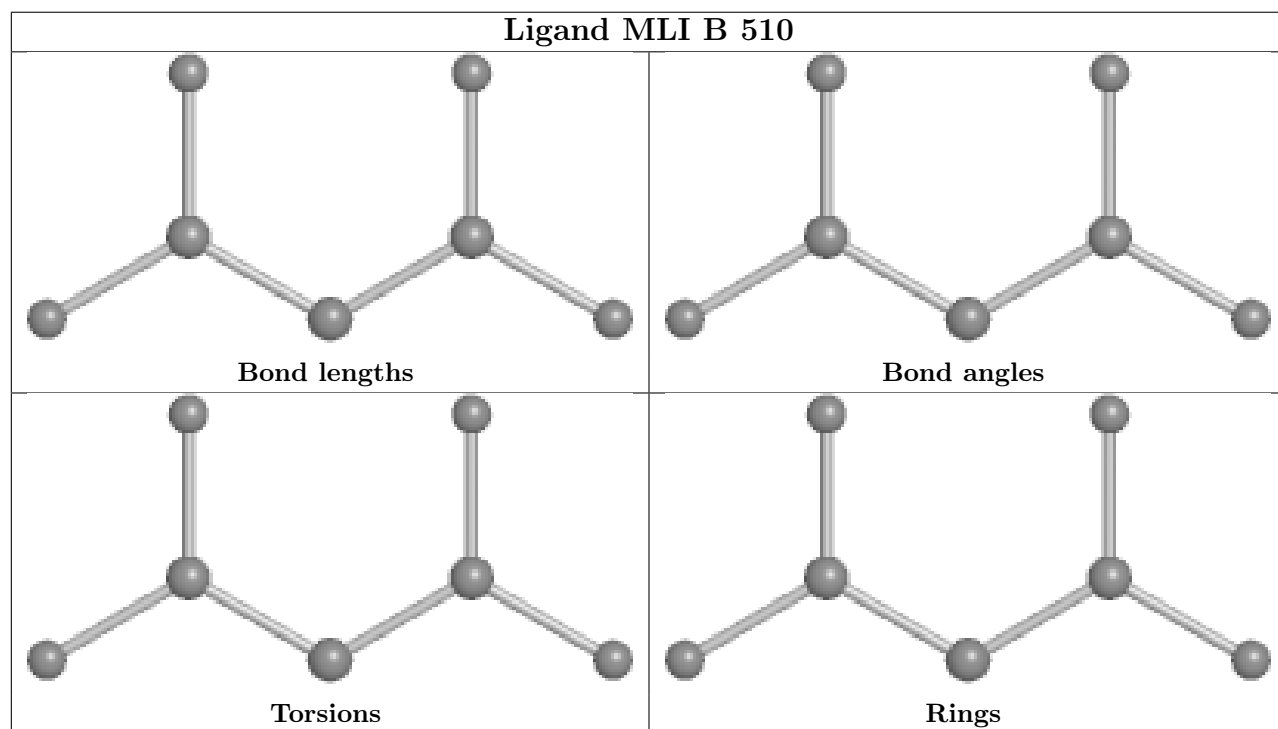
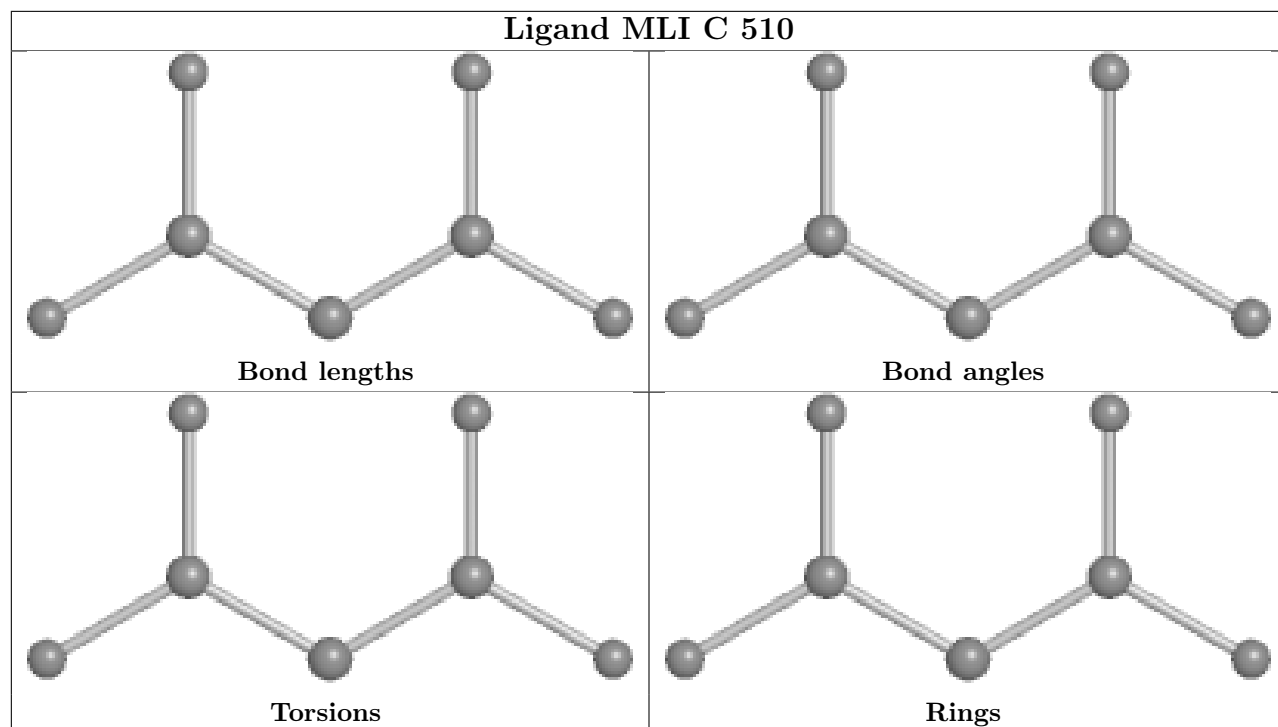


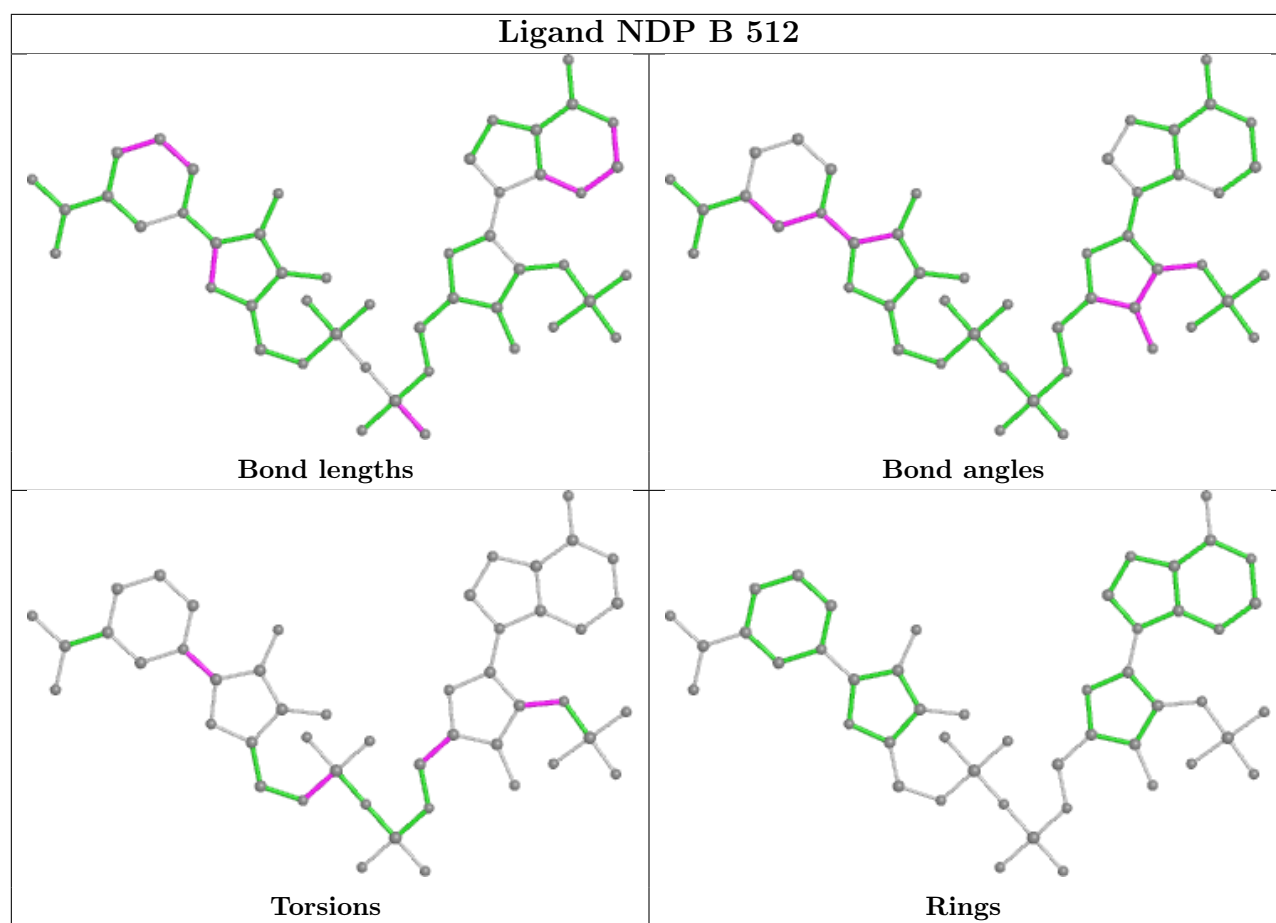












## 5.7 Other polymers [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	460/460 (100%)	-0.36	9 (1%) 65 71	13, 18, 34, 55	2 (0%)
1	B	460/460 (100%)	-0.29	8 (1%) 70 76	12, 18, 33, 58	4 (0%)
1	C	460/460 (100%)	-0.48	5 (1%) 80 85	12, 16, 29, 52	3 (0%)
All	All	1380/1380 (100%)	-0.38	22 (1%) 72 78	12, 17, 32, 58	9 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	ALA	5.6
1	B	293	ALA	4.3
1	A	292	ALA	3.9
1	A	290	THR	3.7
1	B	1	MET	3.6
1	A	289	VAL	3.5
1	A	2	SER	3.5
1	B	292	ALA	3.2
1	A	1	MET	3.2
1	C	263	ALA	3.1
1	C	289	VAL	3.0
1	B	2	SER	2.8
1	A	431	ASP	2.6
1	B	263	ALA	2.6
1	C	1	MET	2.4
1	C	2	SER	2.4
1	B	28	GLN	2.3
1	A	294	PHE	2.3
1	C	264	LYS	2.2
1	B	214[A]	ASN	2.1
1	B	216	ALA	2.0
1	A	296	ASP	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

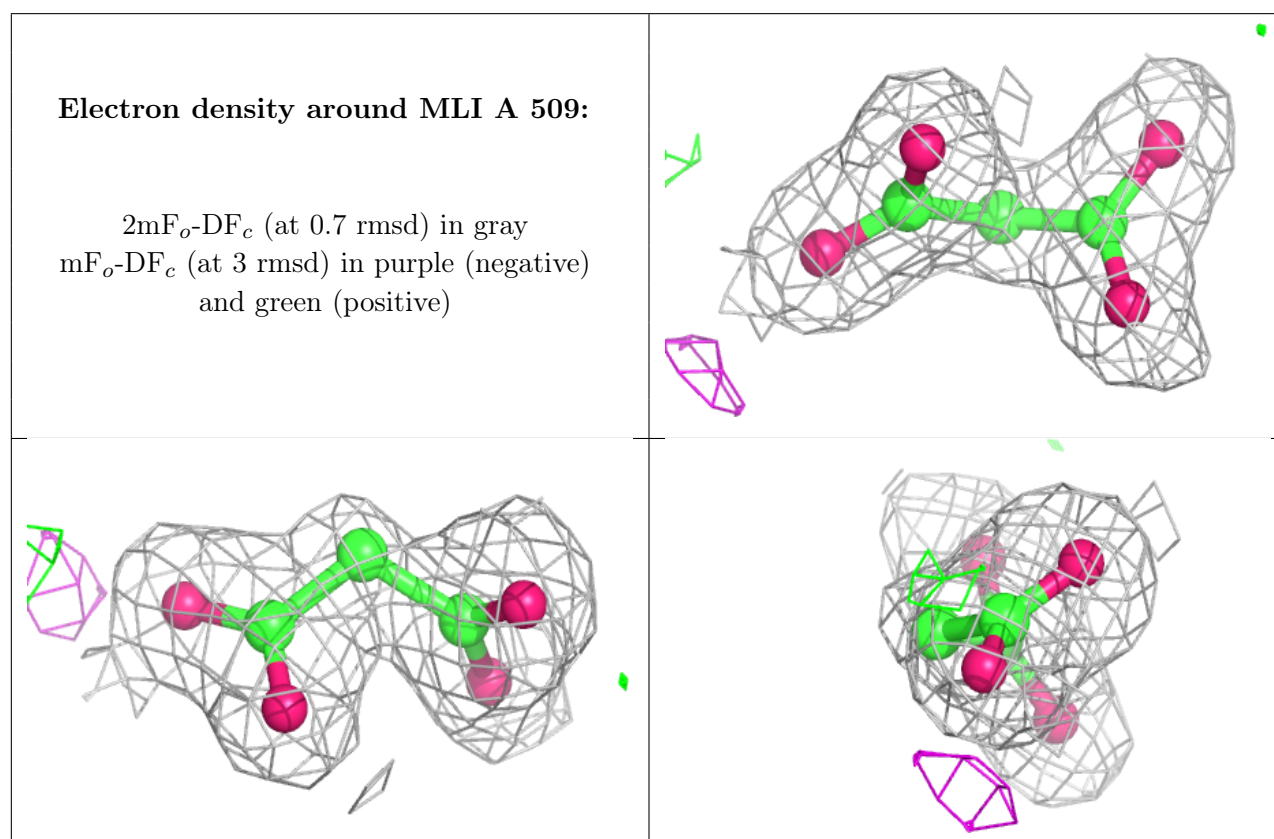
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	508	6/6	0.76	0.25	36,40,53,61	6
2	GOL	A	507	6/6	0.82	0.19	38,49,54,58	0
2	GOL	B	506	6/6	0.85	0.22	37,49,54,62	0
2	GOL	B	504	6/6	0.87	0.10	29,37,38,39	0
2	GOL	A	503	6/6	0.89	0.28	13,17,18,20	6
2	GOL	C	502	6/6	0.89	0.16	31,37,38,41	0
2	GOL	B	505	6/6	0.89	0.26	47,57,63,64	0
2	GOL	C	506	6/6	0.90	0.11	40,43,55,59	0
2	GOL	C	505	6/6	0.90	0.13	26,41,43,45	0
2	GOL	C	507	6/6	0.92	0.17	21,46,54,73	0
2	GOL	A	506	6/6	0.93	0.16	23,44,55,58	0
2	GOL	C	504	6/6	0.93	0.18	18,43,50,59	0
2	GOL	B	509	6/6	0.93	0.10	29,37,44,46	0
2	GOL	B	508	6/6	0.94	0.10	20,33,43,50	0
2	GOL	A	502	6/6	0.94	0.16	32,34,42,47	0
2	GOL	A	505	6/6	0.94	0.09	21,39,44,56	0
2	GOL	B	503	6/6	0.94	0.17	33,36,39,42	0
3	MLI	A	509	7/7	0.94	0.16	29,33,38,39	0
2	GOL	B	507	6/6	0.95	0.20	22,36,49,53	0
2	GOL	B	501	6/6	0.95	0.10	23,34,41,45	0
2	GOL	B	502	6/6	0.96	0.14	27,32,38,40	0
2	GOL	C	503	6/6	0.96	0.08	19,33,40,45	0
2	GOL	A	504	6/6	0.96	0.11	19,27,29,30	6
2	GOL	C	501	6/6	0.96	0.14	27,32,34,41	0
3	MLI	B	510	7/7	0.96	0.19	27,29,34,34	0
2	GOL	A	501	6/6	0.97	0.10	28,33,40,42	0
3	MLI	B	511	7/7	0.97	0.07	17,23,25,25	0

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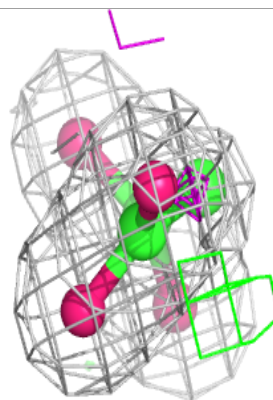
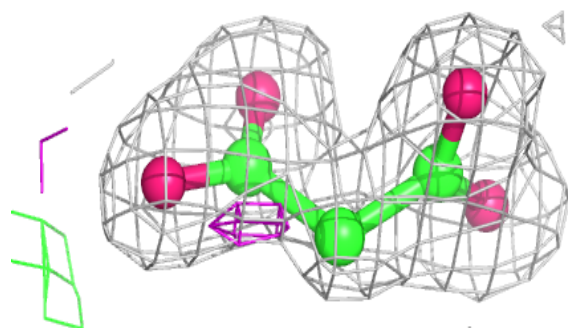
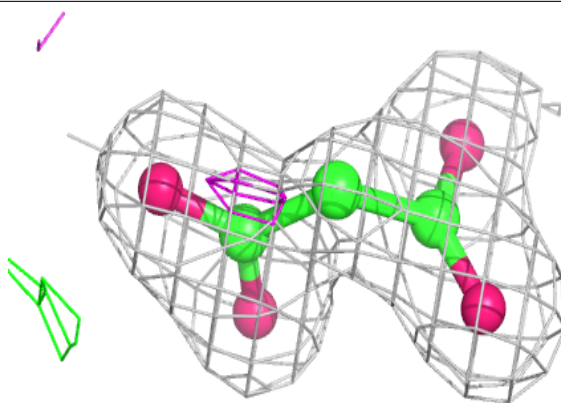
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MLI	C	509	7/7	0.97	0.14	22,27,29,31	0
3	MLI	C	510	7/7	0.97	0.07	16,24,29,30	0
3	MLI	A	508	7/7	0.98	0.06	18,23,24,27	0
4	NDP	A	510	48/48	0.98	0.07	12,16,24,24	0
4	NDP	B	512	48/48	0.98	0.07	13,17,23,26	0
4	NDP	C	511	48/48	0.99	0.06	12,15,22,25	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 MLI B 510:**

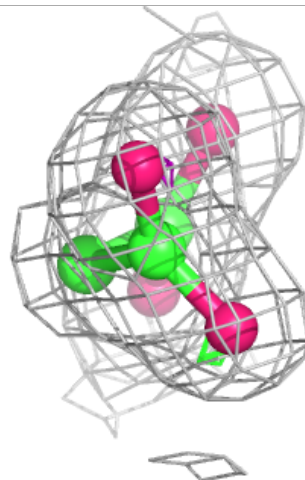
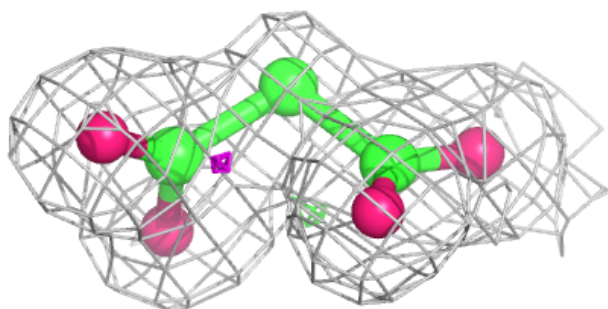
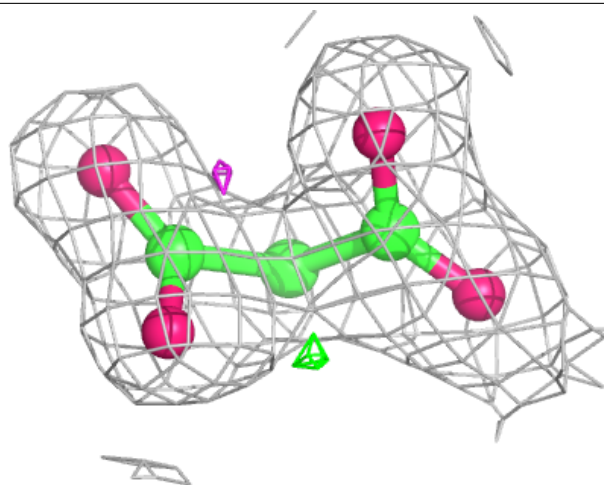
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





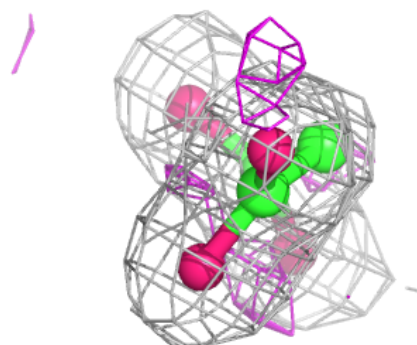
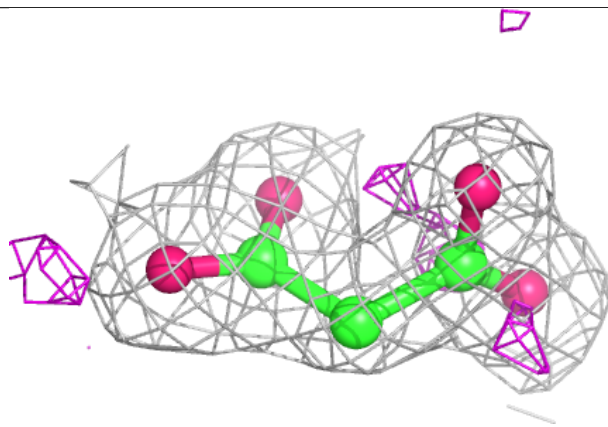
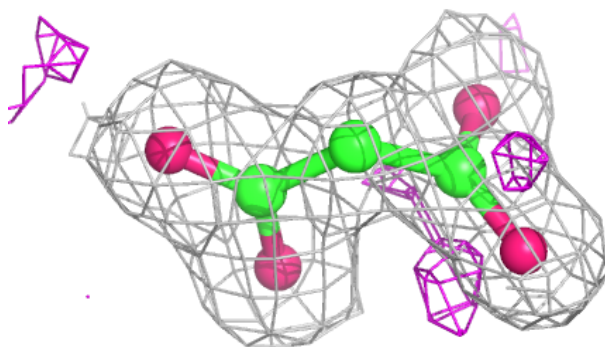
**Electron density around MLI B 511:**

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



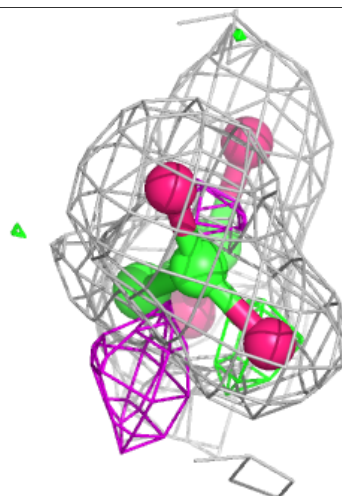
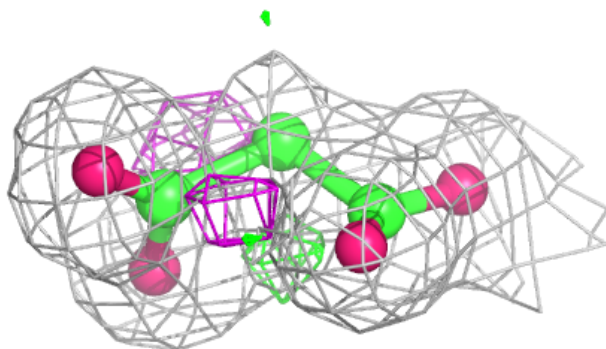
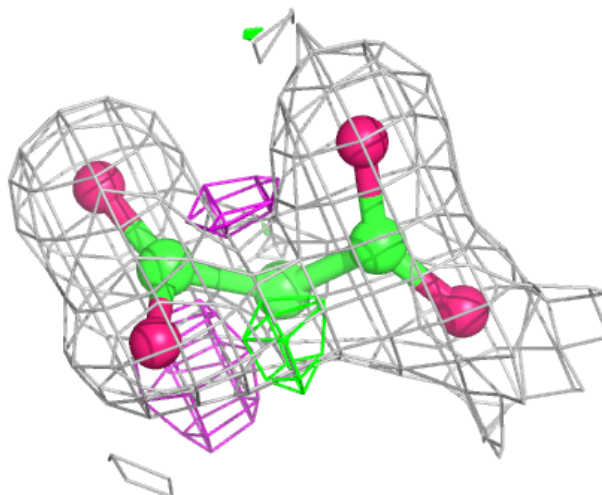
**Electron density around MLI C 509:**

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and green (positive)



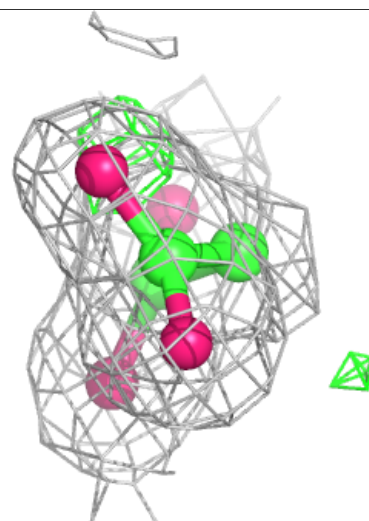
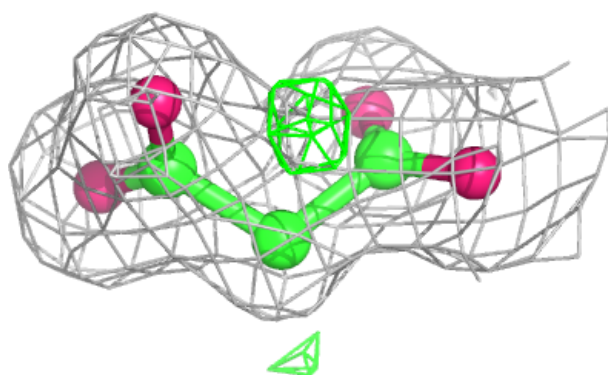
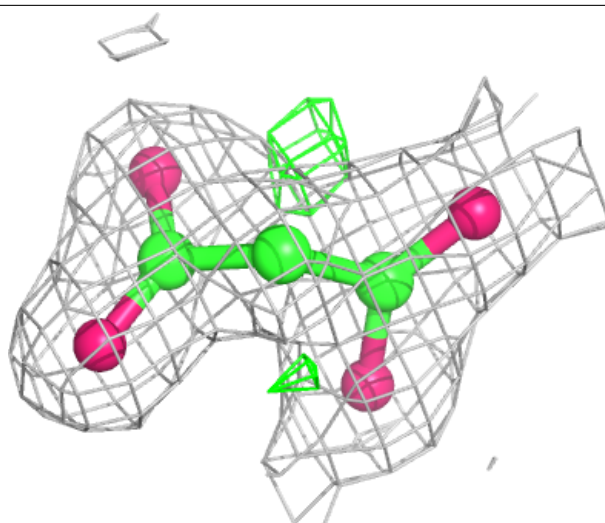
**Electron density around MLI C 510:**

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



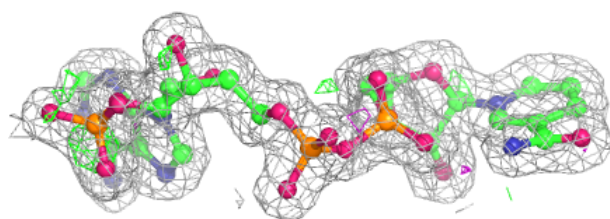
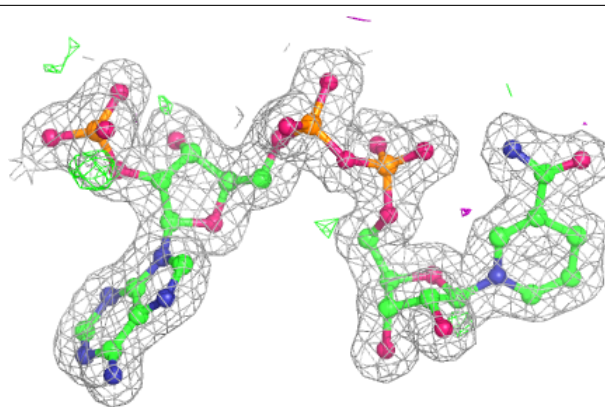
**Electron density around MLI A 508:**

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and green (positive)

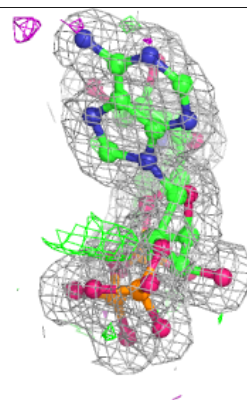
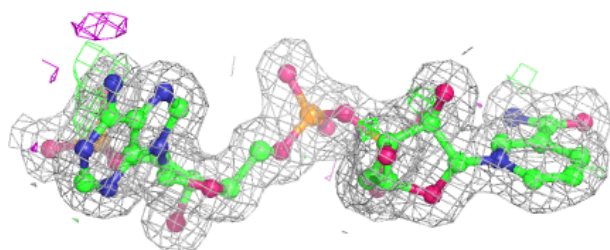
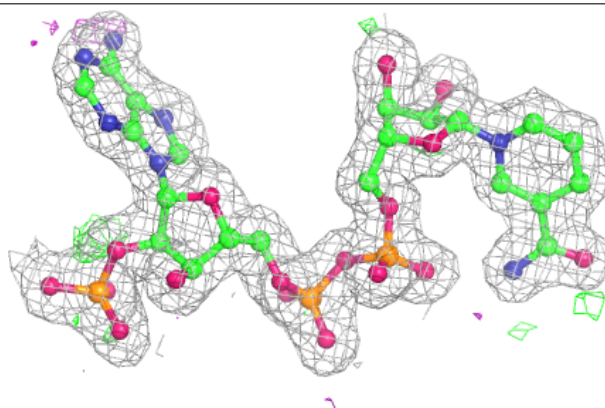


**Electron density around NDP A 510:**

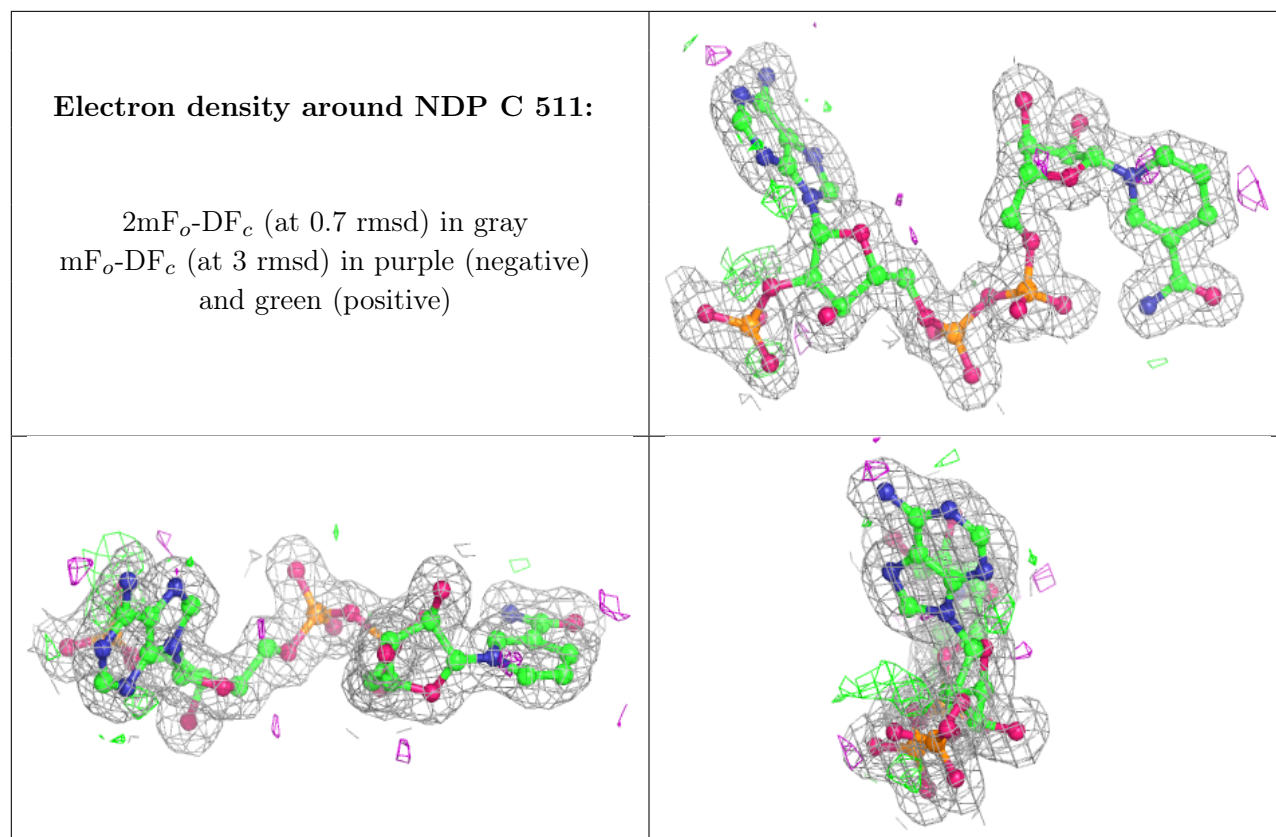
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NDP B 512:**

$2mF_o-DF_c$  (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.