



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:06 PM UTC

PDB ID : 7ECS / pdb_00007ecs
Title : Crystal Structure of Aspergillus terreus Glutamate Dehydrogenase (AtGDH)
Complexed With Malonate and NADPH
Authors : Godsora, B.K.J.; Prakash, P.; Puneekar, 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

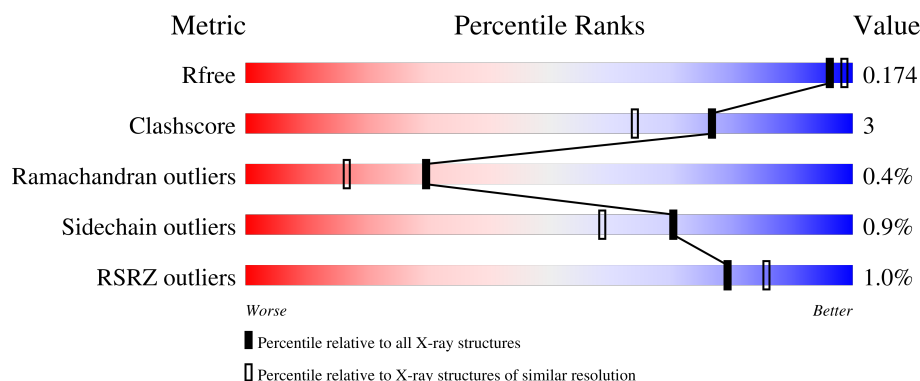
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	460	87% 12% .
1	B	460	91% 8% .
1	C	460	92% 7% .

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	C	507	-	X	-	-
3	MLI	A	508	-	-	X	-
3	MLI	A	509	-	X	-	-
3	MLI	B	511	-	-	X	-
3	MLI	C	510	-	X	X	-

2 Entry composition [i](#)

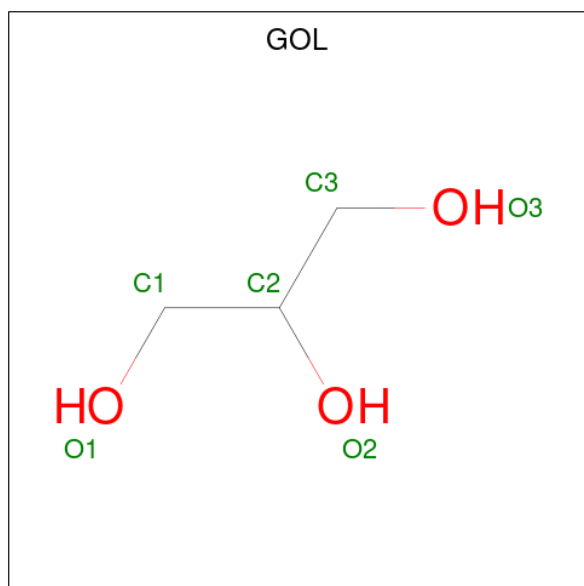
There are 5 unique types of molecules in this entry. The entry contains 12647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



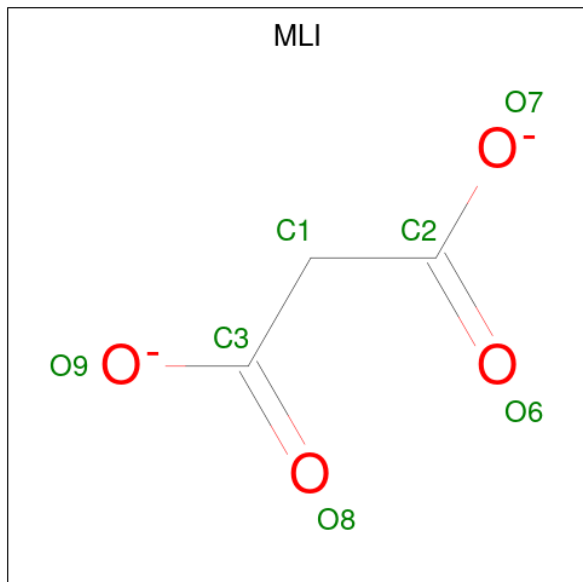
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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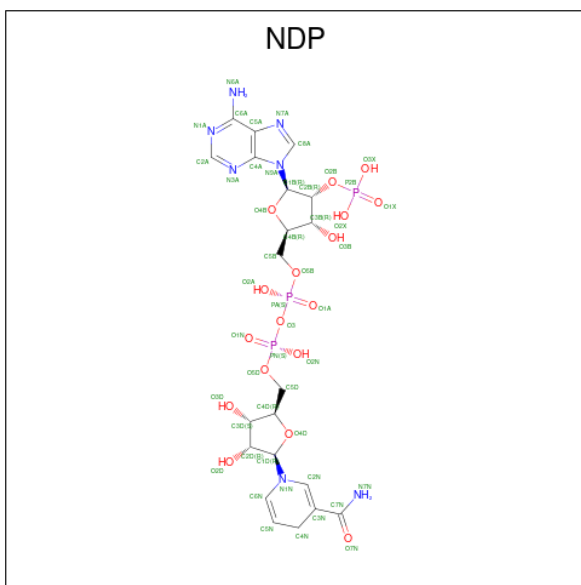
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total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

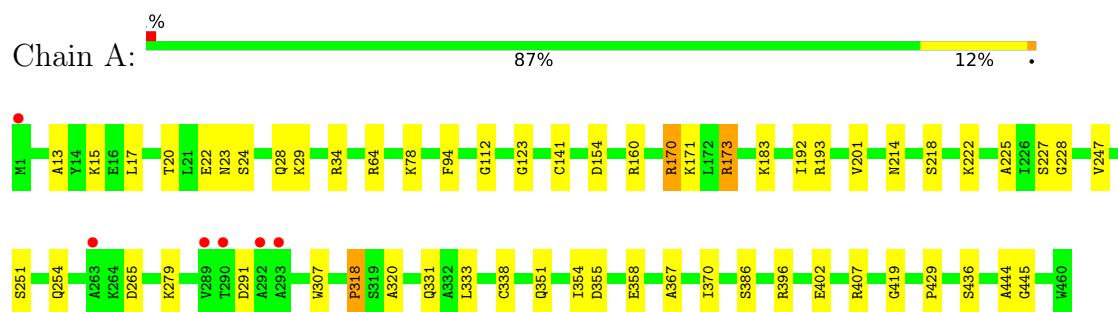
- Molecule 5 is water.

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

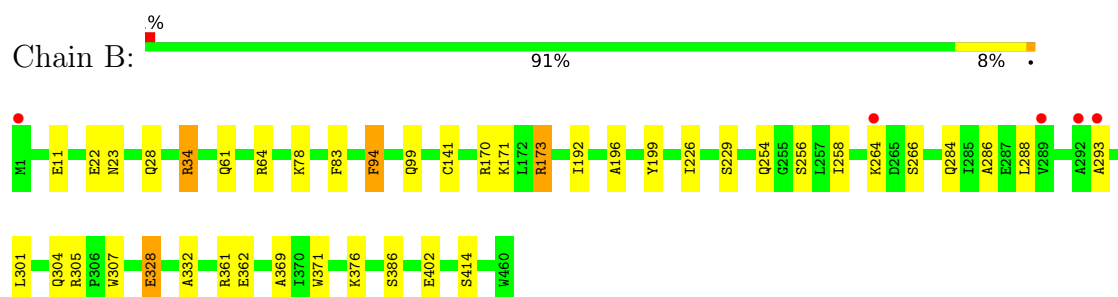
3 Residue-property plots

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.

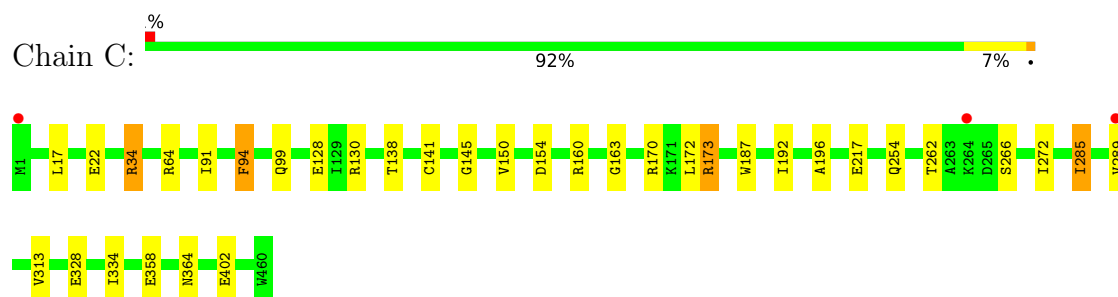
• Molecule 1: Glutamate dehydrogenase



• 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, α , β , γ	120.15Å 153.74Å 259.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.38 – 1.74 39.38 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.38-1.74) 99.8 (39.38-1.74)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	18.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NDP, 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	1.59	31/3630 (0.9%)	1.27	7/4907 (0.1%)
1	B	1.58	26/3620 (0.7%)	1.26	6/4895 (0.1%)
1	C	1.48	16/3637 (0.4%)	1.24	12/4918 (0.2%)
All	All	1.55	73/10887 (0.7%)	1.26	25/14720 (0.2%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	VAL	CA-CB	-8.13	1.44	1.54
1	A	354	ILE	N-CA	-8.08	1.36	1.46
1	B	293	ALA	CA-C	7.92	1.64	1.52
1	A	170	ARG	NE-CZ	-7.83	1.24	1.33
1	C	254	GLN	CG-CD	-7.57	1.33	1.52
1	A	331	GLN	N-CA	7.24	1.55	1.46
1	A	320	ALA	CA-C	7.08	1.58	1.52
1	A	247	VAL	CA-CB	6.90	1.61	1.53
1	A	24	SER	N-CA	-6.71	1.38	1.46
1	B	301	LEU	N-CA	-6.66	1.39	1.46
1	C	145	GLY	N-CA	6.59	1.52	1.45
1	B	256	SER	C-O	6.49	1.31	1.23
1	B	376	LYS	N-CA	6.45	1.54	1.46
1	B	286	ALA	N-CA	6.38	1.54	1.46
1	A	436	SER	CA-C	6.37	1.61	1.52
1	B	264	LYS	CA-C	6.36	1.61	1.52
1	C	266	SER	N-CA	6.31	1.53	1.45
1	C	358	GLU	CA-C	6.27	1.60	1.52
1	B	402	GLU	CD-OE1	6.23	1.37	1.25
1	C	91	ILE	N-CA	-6.10	1.39	1.46
1	B	83	PHE	C-O	6.02	1.30	1.23
1	A	367	ALA	CA-C	-6.01	1.44	1.52
1	C	128	GLU	N-CA	-6.00	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GLY	N-CA	5.98	1.53	1.45
1	A	23	ASN	CA-C	-5.97	1.46	1.53
1	B	23	ASN	CA-C	-5.97	1.46	1.53
1	A	429	PRO	CA-C	5.93	1.59	1.52
1	A	338	CYS	N-CA	5.91	1.53	1.46
1	B	305	ARG	N-CA	5.89	1.52	1.46
1	A	444	ALA	CA-C	5.88	1.60	1.52
1	B	307	TRP	CA-C	5.83	1.60	1.52
1	B	226	ILE	N-CA	5.83	1.53	1.46
1	B	173	ARG	CZ-NH2	-5.80	1.25	1.33
1	A	225	ALA	N-CA	-5.80	1.39	1.46
1	A	370	ILE	CA-CB	-5.74	1.47	1.54
1	B	199	TYR	CA-C	-5.71	1.45	1.52
1	A	307	TRP	CA-C	5.67	1.60	1.52
1	A	318	PRO	CA-C	5.64	1.59	1.52
1	B	266	SER	CA-C	-5.62	1.45	1.52
1	A	160	ARG	C-O	5.60	1.30	1.24
1	B	258	ILE	CA-CB	-5.60	1.47	1.54
1	C	150	VAL	C-O	5.53	1.29	1.23
1	C	262	THR	N-CA	5.53	1.53	1.46
1	B	170	ARG	CD-NE	-5.52	1.38	1.46
1	B	229	SER	CA-C	-5.52	1.46	1.53
1	B	61	GLN	CD-NE2	-5.46	1.21	1.33
1	A	193	ARG	CG-CD	5.45	1.68	1.52
1	B	170	ARG	CZ-NH2	-5.42	1.26	1.33
1	A	20	THR	CA-C	-5.40	1.45	1.52
1	C	170	ARG	CZ-NH2	-5.37	1.26	1.33
1	A	358	GLU	CA-C	5.37	1.59	1.52
1	C	160	ARG	CZ-NH1	5.32	1.40	1.32
1	C	217	GLU	CD-OE1	5.30	1.35	1.25
1	B	304	GLN	CA-C	5.29	1.59	1.52
1	A	112	GLY	CA-C	-5.26	1.48	1.52
1	A	396	ARG	CZ-NH2	-5.26	1.26	1.33
1	A	355	ASP	CA-C	5.22	1.59	1.52
1	A	419	GLY	CA-C	5.18	1.57	1.52
1	B	99	GLN	CA-CB	5.16	1.61	1.53
1	A	13	ALA	CA-C	-5.13	1.46	1.52
1	C	364	ASN	CA-C	-5.12	1.46	1.52
1	A	351	GLN	CA-C	5.09	1.59	1.52
1	A	123	GLY	C-O	-5.08	1.17	1.24
1	B	414	SER	CA-C	-5.08	1.45	1.52
1	B	362	GLU	C-O	-5.07	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	ASP	CA-C	5.07	1.59	1.53
1	A	333	LEU	CA-CB	5.07	1.61	1.53
1	C	334	ILE	C-O	5.06	1.29	1.24
1	C	17	LEU	CA-C	5.04	1.59	1.52
1	C	130	ARG	C-O	5.03	1.29	1.24
1	B	28	GLN	C-O	-5.02	1.18	1.24
1	C	34	ARG	NE-CZ	-5.01	1.27	1.33
1	B	328	GLU	CA-C	-5.00	1.46	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	ALA	N-CA-C	8.45	121.25	111.11
1	C	289	VAL	CB-CA-C	-7.94	99.40	112.26
1	C	173	ARG	NE-CZ-NH1	7.59	129.09	121.50
1	A	183	LYS	CA-C-N	7.29	126.92	119.92
1	A	183	LYS	C-N-CA	7.29	126.92	119.92
1	A	173	ARG	NE-CZ-NH1	7.22	128.72	121.50
1	B	196	ALA	N-CA-C	6.96	118.52	111.07
1	B	332	ALA	N-CA-C	6.23	118.07	111.28
1	C	173	ARG	CD-NE-CZ	6.09	132.93	124.40
1	A	279	LYS	N-CA-C	5.85	118.61	111.82
1	C	313	VAL	N-CA-CB	-5.76	101.70	112.36
1	C	34	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	B	371	TRP	O-C-N	5.50	129.76	123.27
1	A	170	ARG	CA-CB-CG	5.45	124.99	114.10
1	B	173	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	C	289	VAL	CA-C-O	-5.38	114.66	120.47
1	B	34	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	C	289	VAL	O-C-N	5.31	127.80	121.80
1	B	170	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	A	170	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	A	170	ARG	CG-CD-NE	-5.10	100.78	112.00
1	C	217	GLU	CG-CD-OE1	5.05	130.02	118.40
1	C	272	ILE	N-CA-C	-5.05	105.47	110.62
1	C	173	ARG	NE-CZ-NH2	-5.02	114.69	119.20
1	C	170	ARG	NE-CZ-NH2	5.01	123.71	119.20

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	22	0
1	B	3517	0	3487	16	0
1	C	3531	0	3510	14	0
2	A	42	0	56	1	0
2	B	54	0	72	2	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	62	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 (62) 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)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:94:PHE:CD1	1:B:94:PHE:C	2.90	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:288:LEU:HD12	1:B:288:LEU:C	2.41	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:94:PHE:CD1	1:C:94:PHE:C	2.95	0.44
1:C:163:GLY:HA2	1:C:187:TRP:CH2	2.53	0.44
1:B:141[B]:CYS:HG	1:B:173:ARG:HG3	1.83	0.44
1:B:78:LYS:HE3	1:B:386[B]:SER:OG	2.17	0.44
2:B:502:GOL:H32	5:B:861:HOH:O	2.17	0.44
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
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:C:138:THR:HA	1:C:172:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:407:ARG:HH12	2:B:503:GOL:HO3	1.69	0.41
1:A:227:SER:OG	1:A:318:PRO:HA	2.21	0.40
1:A:228:GLY:C	1:A:251:SER:O	2.64	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 [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	470/460 (102%)	461 (98%)	7 (2%)	2 (0%)	30	16
1	B	469/460 (102%)	458 (98%)	10 (2%)	1 (0%)	43	29
1	C	471/460 (102%)	463 (98%)	6 (1%)	2 (0%)	30	16
All	All	1410/1380 (102%)	1382 (98%)	23 (2%)	5 (0%)	30	16

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%)	59	41
1	B	362/351 (103%)	361 (100%)	1 (0%)	86	82
1	C	364/351 (104%)	360 (99%)	4 (1%)	65	50
All	All	1089/1053 (103%)	1079 (99%)	10 (1%)	70	59

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	94	PHE
1	A	170	ARG
1	A	214	ASN
1	A	402	GLU
1	B	94	PHE
1	C	94	PHE
1	C	285[A]	ILE
1	C	285[B]	ILE
1	C	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
1	B	28	GLN
1	B	61	GLN
1	B	174	ASN
1	B	304	GLN
1	C	99	GLN
1	C	254	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
2	GOL	B	504	-	5,5,5	1.32	1 (20%)	5,5,5	0.93	0
2	GOL	B	502	-	5,5,5	0.76	0	5,5,5	0.77	0
2	GOL	C	504	-	5,5,5	1.14	1 (20%)	5,5,5	1.88	2 (40%)
2	GOL	C	507	-	5,5,5	1.89	1 (20%)	5,5,5	2.93	3 (60%)
2	GOL	B	505	-	5,5,5	0.25	0	5,5,5	1.73	1 (20%)
2	GOL	C	505	-	5,5,5	1.09	0	5,5,5	3.05	3 (60%)
2	GOL	B	508	-	5,5,5	0.92	0	5,5,5	0.60	0
2	GOL	C	508	-	5,5,5	0.70	0	5,5,5	0.70	0
2	GOL	B	501	-	5,5,5	0.86	0	5,5,5	3.49	2 (40%)
2	GOL	C	502	-	5,5,5	0.80	0	5,5,5	1.43	1 (20%)
3	MLI	B	510	-	6,6,6	1.86	2 (33%)	7,7,7	1.30	1 (14%)
2	GOL	B	507	-	5,5,5	0.97	0	5,5,5	1.49	2 (40%)
2	GOL	A	502	-	5,5,5	0.65	0	5,5,5	1.30	0
2	GOL	A	504	-	5,5,5	0.83	0	5,5,5	1.16	0
4	NDP	C	511	-	51,52,52	1.31	4 (7%)	71,80,80	1.47	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	506	-	5,5,5	0.90	0	5,5,5	1.61	1 (20%)
2	GOL	A	505	-	5,5,5	0.99	0	5,5,5	1.50	1 (20%)
2	GOL	A	503	-	5,5,5	0.61	0	5,5,5	1.47	1 (20%)
2	GOL	C	503	-	5,5,5	0.88	0	5,5,5	1.35	1 (20%)
2	GOL	A	506	-	5,5,5	0.85	0	5,5,5	1.31	1 (20%)
2	GOL	B	509	-	5,5,5	1.32	0	5,5,5	1.07	0
3	MLI	C	509	-	6,6,6	1.88	2 (33%)	7,7,7	1.80	2 (28%)
2	GOL	C	506	-	5,5,5	1.06	0	5,5,5	1.05	0
3	MLI	C	510	-	6,6,6	1.73	1 (16%)	7,7,7	4.15	5 (71%)
4	NDP	B	512	-	51,52,52	1.61	8 (15%)	71,80,80	1.43	13 (18%)
2	GOL	A	501	-	5,5,5	0.74	0	5,5,5	1.13	0
2	GOL	B	503	-	5,5,5	0.94	0	5,5,5	1.37	1 (20%)
2	GOL	C	501	-	5,5,5	0.93	0	5,5,5	1.39	1 (20%)
3	MLI	A	509	-	6,6,6	2.22	3 (50%)	7,7,7	0.29	0
4	NDP	A	510	-	51,52,52	1.17	7 (13%)	71,80,80	1.29	10 (14%)
3	MLI	A	508	-	6,6,6	1.34	1 (16%)	7,7,7	2.67	3 (42%)
3	MLI	B	511	-	6,6,6	1.41	1 (16%)	7,7,7	1.86	2 (28%)
2	GOL	A	507	-	5,5,5	0.99	0	5,5,5	1.68	1 (20%)

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	GOL	B	504	-	-	0/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	C	504	-	-	0/4/4/4	-
2	GOL	C	507	-	-	2/4/4/4	-
2	GOL	B	505	-	-	4/4/4/4	-
2	GOL	C	505	-	-	2/4/4/4	-
2	GOL	B	508	-	-	0/4/4/4	-
2	GOL	C	508	-	-	3/4/4/4	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	C	502	-	-	3/4/4/4	-
3	MLI	B	510	-	-	0/4/4/4	-
2	GOL	B	507	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	502	-	-	3/4/4/4	-
2	GOL	A	504	-	-	4/4/4/4	-
4	NDP	C	511	-	-	3/34/77/77	0/5/5/5
2	GOL	B	506	-	-	0/4/4/4	-
2	GOL	A	505	-	-	3/4/4/4	-
2	GOL	A	503	-	-	3/4/4/4	-
2	GOL	C	503	-	-	0/4/4/4	-
2	GOL	A	506	-	-	2/4/4/4	-
2	GOL	B	509	-	-	1/4/4/4	-
3	MLI	C	509	-	-	0/4/4/4	-
2	GOL	C	506	-	-	0/4/4/4	-
3	MLI	C	510	-	-	1/4/4/4	-
4	NDP	B	512	-	-	5/34/77/77	0/5/5/5
2	GOL	A	501	-	-	0/4/4/4	-
2	GOL	B	503	-	-	4/4/4/4	-
2	GOL	C	501	-	-	2/4/4/4	-
3	MLI	A	509	-	-	4/4/4/4	-
4	NDP	A	510	-	-	5/34/77/77	0/5/5/5
3	MLI	A	508	-	-	2/4/4/4	-
3	MLI	B	511	-	-	2/4/4/4	-
2	GOL	A	507	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	512	NDP	PN-O3	6.93	1.67	1.59
4	A	510	NDP	C5A-C4A	3.68	1.45	1.39
3	A	509	MLI	C1-C3	3.55	1.56	1.51
4	C	511	NDP	C4A-N9A	-3.54	1.30	1.37
3	C	510	MLI	C1-C2	-3.26	1.46	1.51
4	C	511	NDP	P2B-O3X	-3.22	1.42	1.54
4	B	512	NDP	C5A-C4A	3.19	1.44	1.39
3	B	510	MLI	C1-C3	3.14	1.55	1.51
2	C	507	GOL	C3-C2	3.06	1.63	1.51
4	C	511	NDP	P2B-O2B	3.03	1.64	1.59
3	C	509	MLI	C1-C3	2.86	1.55	1.51
3	A	509	MLI	O8-C3	2.65	1.30	1.22
4	A	510	NDP	PN-O3	2.64	1.62	1.59
4	B	512	NDP	C4A-N9A	-2.58	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	512	NDP	C4N-C5N	-2.49	1.42	1.49
4	C	511	NDP	C5A-C4A	2.49	1.43	1.39
2	C	504	GOL	O1-C1	2.44	1.52	1.42
3	A	508	MLI	O8-C3	2.43	1.30	1.22
4	B	512	NDP	C2A-N1A	2.43	1.38	1.33
4	B	512	NDP	PA-O2A	-2.39	1.44	1.55
3	A	509	MLI	O6-C2	2.31	1.29	1.22
3	B	511	MLI	O7-C2	-2.25	1.23	1.30
4	A	510	NDP	C5A-N7A	-2.22	1.35	1.39
4	B	512	NDP	O4D-C1D	2.19	1.47	1.42
4	A	510	NDP	C2A-N3A	2.17	1.37	1.33
3	B	510	MLI	C1-C2	2.17	1.54	1.51
2	B	504	GOL	O1-C1	2.17	1.51	1.42
4	A	510	NDP	C8A-N7A	2.16	1.35	1.31
4	A	510	NDP	C3B-C2B	-2.15	1.48	1.53
3	C	509	MLI	O8-C3	2.14	1.29	1.22
4	B	512	NDP	C5A-N7A	-2.13	1.35	1.39
4	A	510	NDP	C4A-N9A	-2.08	1.33	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GOL	C3-C2-C1	-6.83	86.75	111.80
3	C	510	MLI	O6-C2-C1	-6.05	104.86	122.11
3	C	510	MLI	O8-C3-C1	-5.96	105.14	122.11
3	C	510	MLI	O7-C2-O6	5.50	137.49	123.33
3	A	508	MLI	O8-C3-C1	-4.71	108.69	122.11
2	C	505	GOL	C3-C2-C1	-4.40	95.66	111.80
2	C	505	GOL	O2-C2-C3	4.36	127.25	109.18
2	C	507	GOL	O3-C3-C2	4.34	129.92	110.38
3	A	508	MLI	O9-C3-O8	4.28	134.33	123.33
4	B	512	NDP	C5A-C4A-N3A	-3.95	121.27	126.72
2	C	507	GOL	O1-C1-C2	-3.73	93.57	110.38
4	A	510	NDP	N3A-C2A-N1A	-3.70	122.98	128.58
4	C	511	NDP	C5A-C4A-N3A	-3.67	121.66	126.72
3	C	509	MLI	O8-C3-C1	-3.55	112.00	122.11
4	C	511	NDP	C4A-N9A-C8A	3.49	109.41	105.74
4	C	511	NDP	N6A-C6A-N1A	3.29	125.69	118.38
2	A	507	GOL	O3-C3-C2	3.22	124.89	110.38
3	C	510	MLI	O9-C3-C1	3.18	124.36	114.51
4	C	511	NDP	N9A-C8A-N7A	-3.11	109.52	113.94
4	C	511	NDP	O2B-P2B-O1X	-3.09	98.30	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	504	GOL	C3-C2-C1	3.08	123.10	111.80
3	B	511	MLI	O8-C3-C1	-3.05	113.43	122.11
4	B	512	NDP	O2A-PA-O3	3.01	115.41	107.27
2	B	501	GOL	O1-C1-C2	-2.90	97.32	110.38
3	C	509	MLI	O9-C3-C1	2.86	123.37	114.51
2	B	506	GOL	O3-C3-C2	2.80	122.98	110.38
4	C	511	NDP	O2X-P2B-O2B	-2.78	95.01	105.85
3	C	510	MLI	O9-C3-O8	2.78	130.48	123.33
4	A	510	NDP	C5A-C4A-N3A	-2.77	122.91	126.72
4	C	511	NDP	N3A-C4A-N9A	2.72	131.79	127.17
4	B	512	NDP	C4A-C5A-N7A	-2.72	107.47	110.58
2	A	505	GOL	C3-C2-C1	2.69	121.67	111.80
4	C	511	NDP	O3B-C3B-C4B	-2.67	103.40	111.08
2	C	505	GOL	O1-C1-C2	-2.67	98.35	110.38
4	A	510	NDP	O3X-P2B-O2X	2.66	117.79	107.80
4	B	512	NDP	N3A-C4A-N9A	2.64	131.66	127.17
4	A	510	NDP	C3D-C2D-C1D	-2.64	96.47	101.46
2	C	507	GOL	O2-C2-C3	2.63	120.05	109.18
4	C	511	NDP	C5A-C6A-N6A	-2.59	116.87	123.29
3	B	511	MLI	O9-C3-O8	2.59	129.99	123.33
2	A	506	GOL	O1-C1-C2	2.56	121.89	110.38
2	A	503	GOL	O2-C2-C1	2.55	119.72	109.18
4	A	510	NDP	N3A-C4A-N9A	2.52	131.45	127.17
4	B	512	NDP	O3-PA-O1A	-2.50	103.18	110.70
4	B	512	NDP	C5A-N7A-C8A	2.50	107.38	103.45
3	A	508	MLI	O7-C2-O6	2.48	129.70	123.33
4	B	512	NDP	C6A-C5A-C4A	2.41	120.47	117.18
2	B	507	GOL	O3-C3-C2	2.41	121.22	110.38
2	C	504	GOL	O2-C2-C3	-2.39	99.27	109.18
4	B	512	NDP	C3N-C2N-N1N	-2.38	119.71	123.20
2	B	505	GOL	O1-C1-C2	-2.34	99.84	110.38
4	A	510	NDP	N9A-C8A-N7A	-2.33	110.64	113.94
4	B	512	NDP	P2B-O2B-C2B	-2.32	117.23	123.43
3	B	510	MLI	O9-C3-C1	2.32	121.69	114.51
4	A	510	NDP	C2A-N1A-C6A	2.30	122.51	118.73
4	C	511	NDP	O2X-P2B-O1X	2.29	119.77	110.83
4	A	510	NDP	C4A-N9A-C8A	2.29	108.14	105.74
2	C	502	GOL	O1-C1-C2	2.25	120.51	110.38
2	B	503	GOL	O1-C1-C2	2.24	120.46	110.38
4	B	512	NDP	O2B-C2B-C3B	2.23	119.67	111.68
4	B	512	NDP	O3B-C3B-C4B	-2.16	104.88	111.08
2	B	507	GOL	O1-C1-C2	-2.11	100.88	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	GOL	C3-C2-C1	2.10	119.52	111.80
4	B	512	NDP	N9A-C8A-N7A	-2.10	110.96	113.94
4	C	511	NDP	O3X-P2B-O1X	2.09	119.00	110.83
4	B	512	NDP	C2D-C1D-N1N	2.09	118.44	113.31
4	A	510	NDP	C5A-C6A-N6A	-2.04	118.24	123.29
2	C	501	GOL	O1-C1-C2	2.03	119.53	110.38
4	A	510	NDP	N6A-C6A-N1A	2.00	122.83	118.38

There are no chirality outliers.

All (66) 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
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
4	A	510	NDP	C5D-O5D-PN-O1N
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

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Mol	Chain	Res	Type	Atoms
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
3	A	508	MLI	C2-C1-C3-O8
3	A	509	MLI	C2-C1-C3-O9
2	A	502	GOL	O1-C1-C2-C3
3	B	511	MLI	C2-C1-C3-O9
3	C	510	MLI	C3-C1-C2-O7
2	A	502	GOL	O2-C2-C3-O3
2	B	505	GOL	O1-C1-C2-O2
2	B	509	GOL	O2-C2-C3-O3
3	A	508	MLI	C2-C1-C3-O9
4	B	512	NDP	C5D-O5D-PN-O1N
2	B	505	GOL	O2-C2-C3-O3
2	C	508	GOL	O1-C1-C2-O2
4	A	510	NDP	C2D-C1D-N1N-C6N
4	A	510	NDP	O4D-C1D-N1N-C6N
4	B	512	NDP	O4D-C1D-N1N-C6N
4	C	511	NDP	O4D-C1D-N1N-C6N
4	B	512	NDP	C2D-C1D-N1N-C6N
3	A	509	MLI	C2-C1-C3-O8
4	C	511	NDP	C2D-C1D-N1N-C6N
3	A	509	MLI	C3-C1-C2-O6
3	B	511	MLI	C2-C1-C3-O8
2	A	504	GOL	O1-C1-C2-C3
3	A	509	MLI	C3-C1-C2-O7
4	C	511	NDP	C3B-C2B-O2B-P2B

There are no ring outliers.

9 monomers are involved in 11 short contacts:

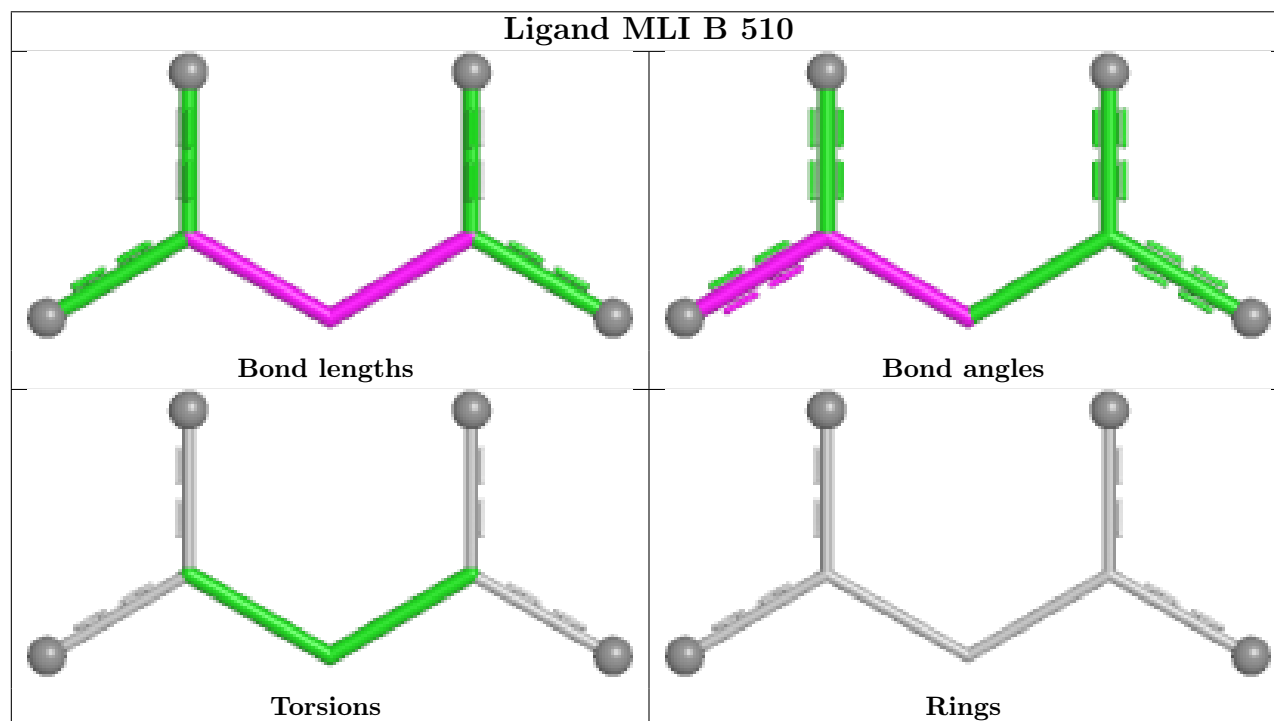
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	GOL	1	0

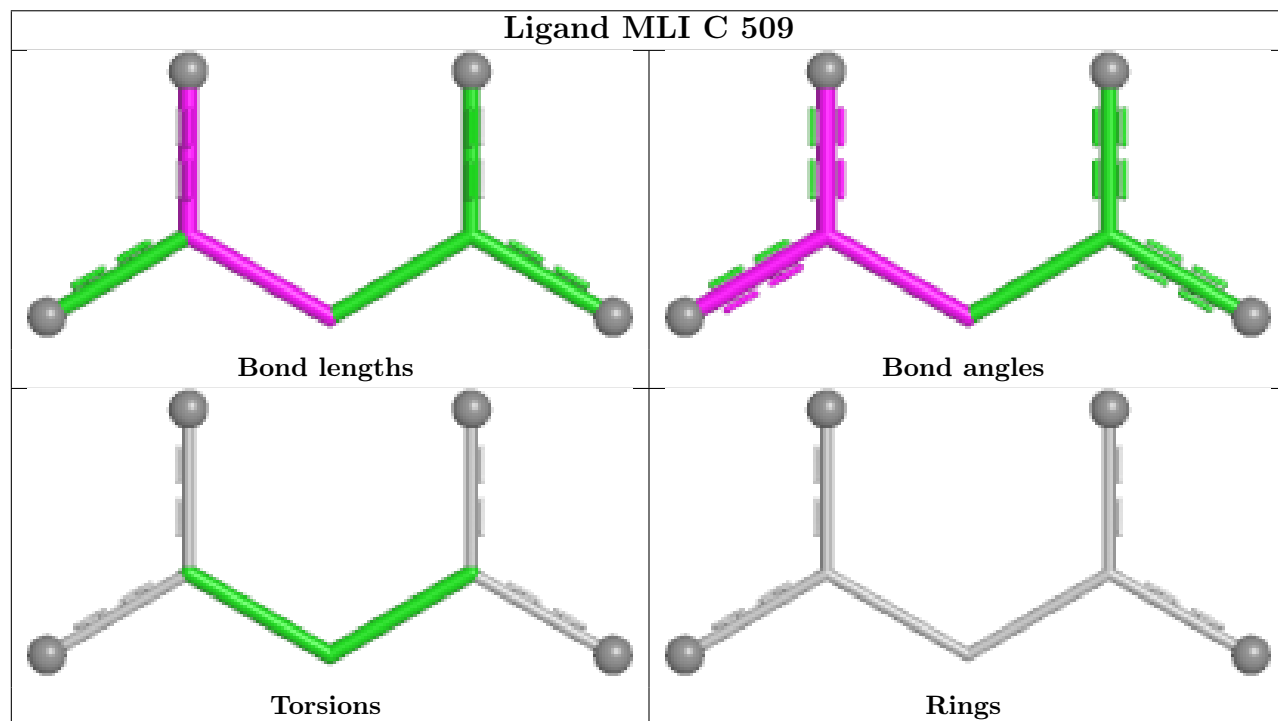
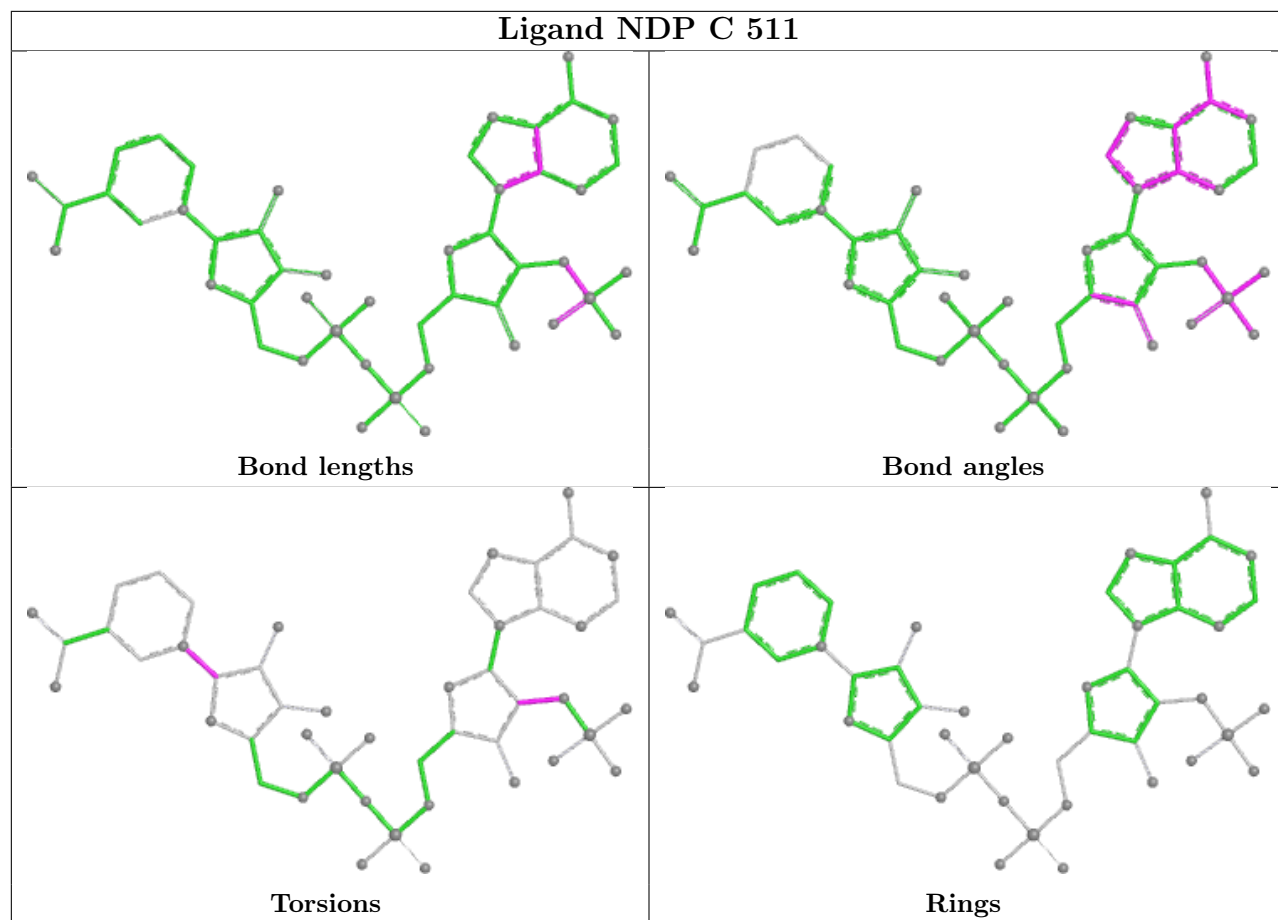
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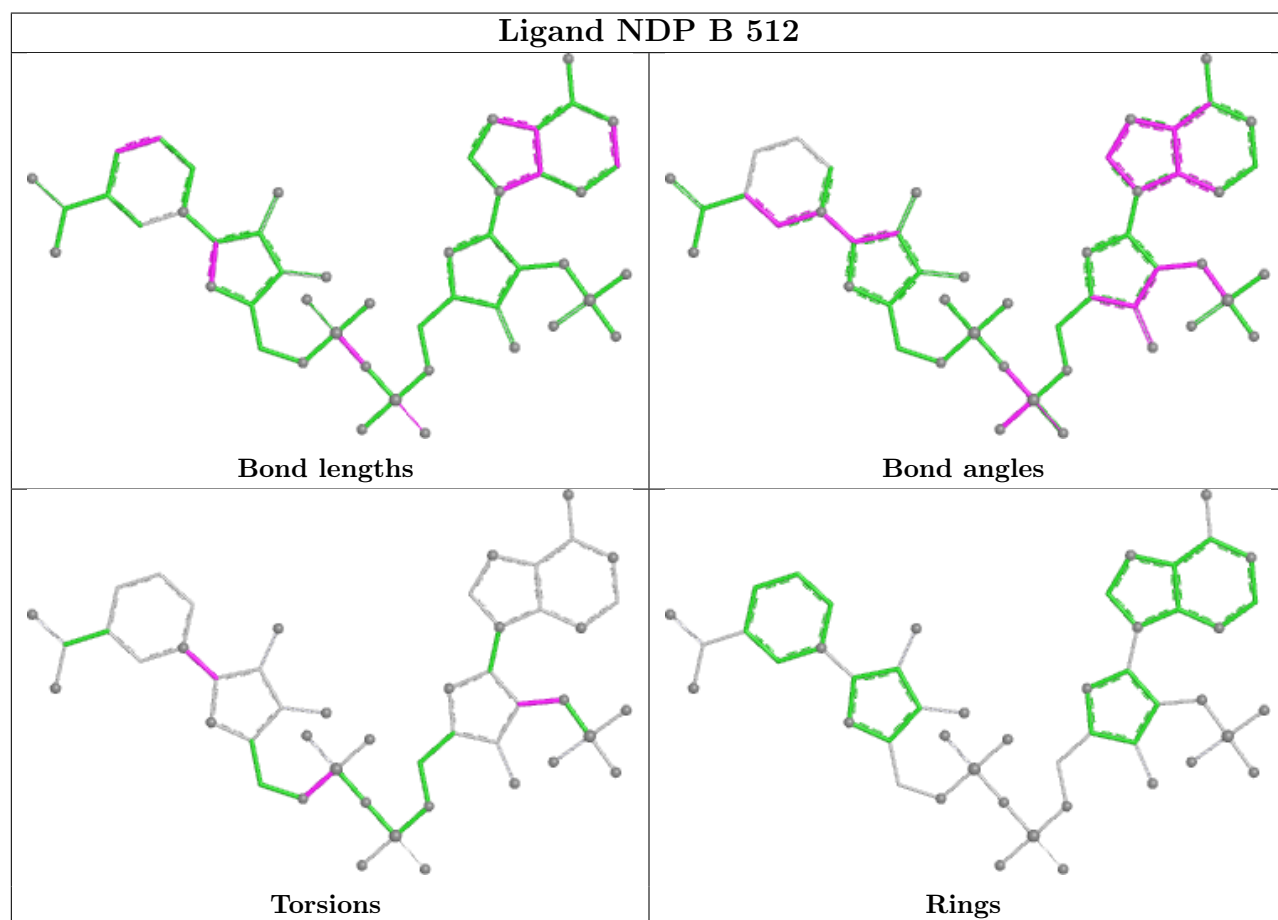
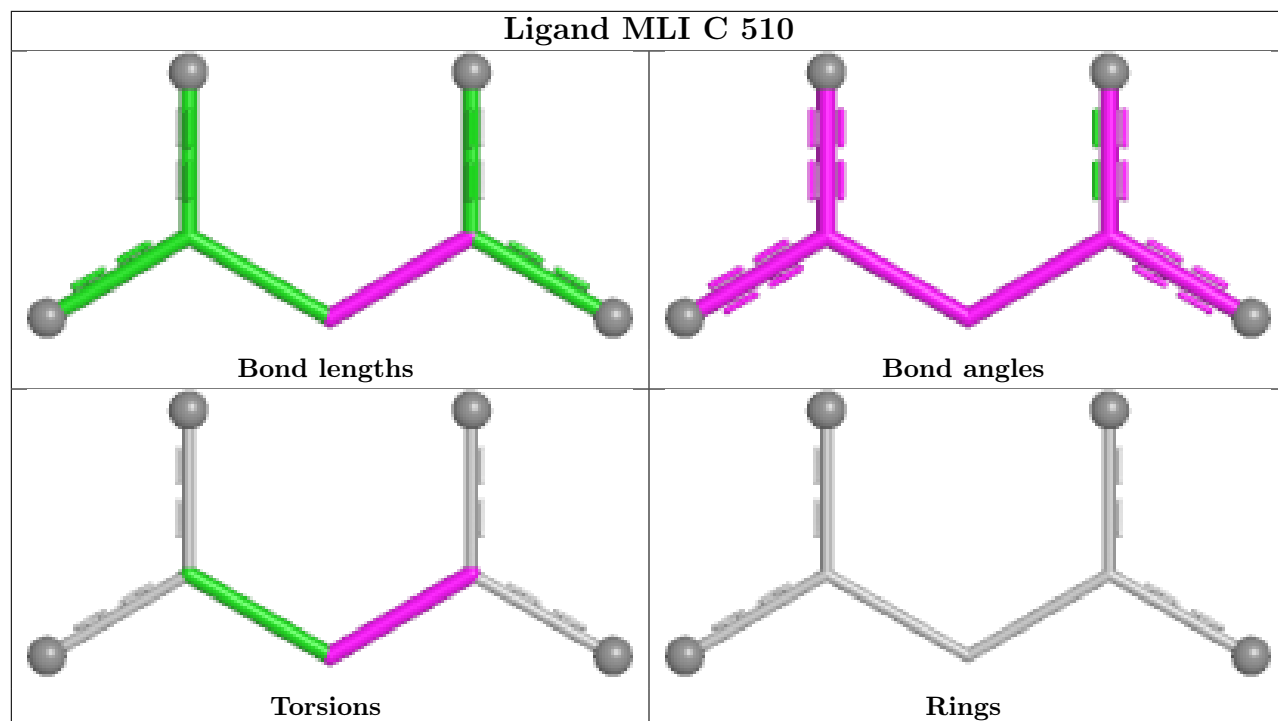
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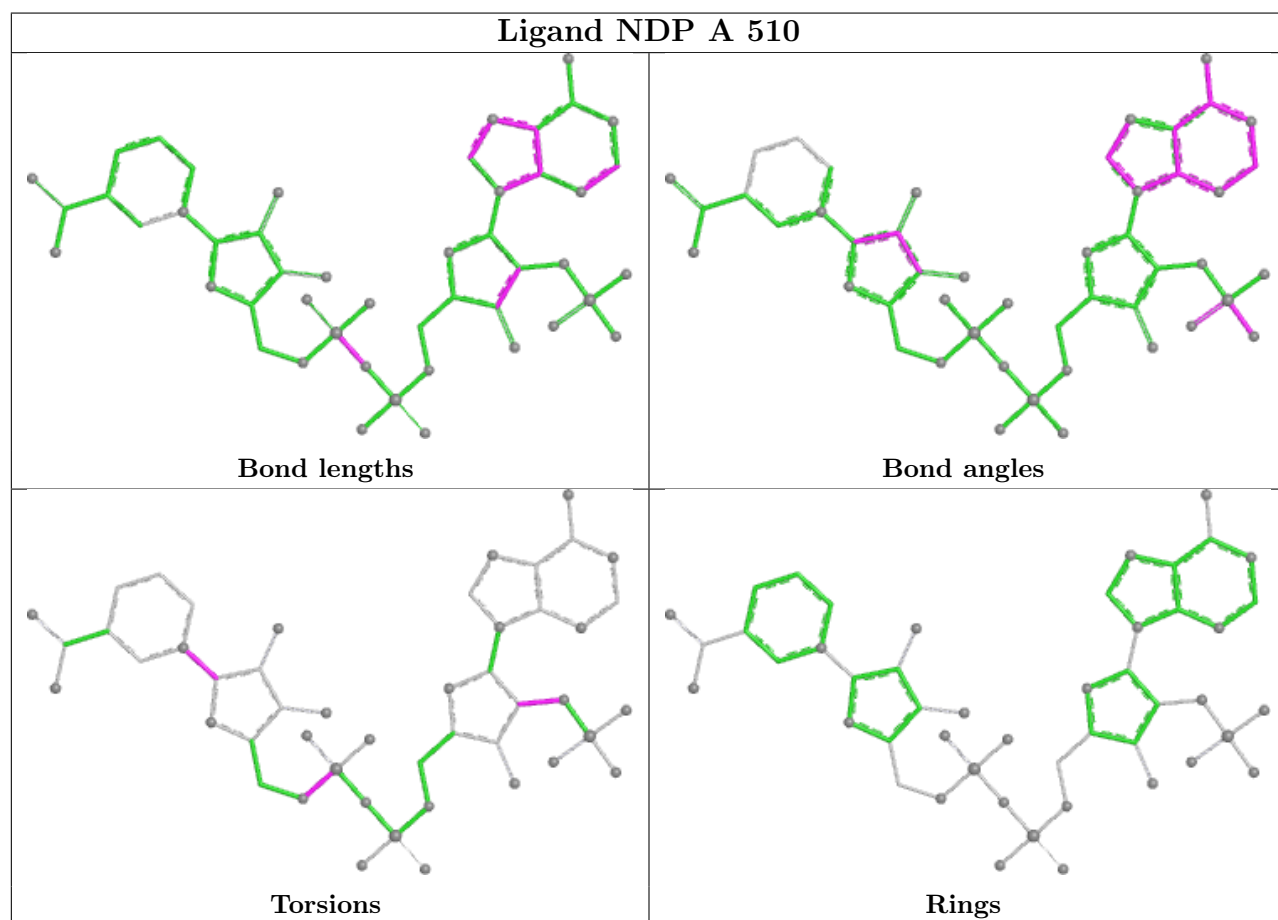
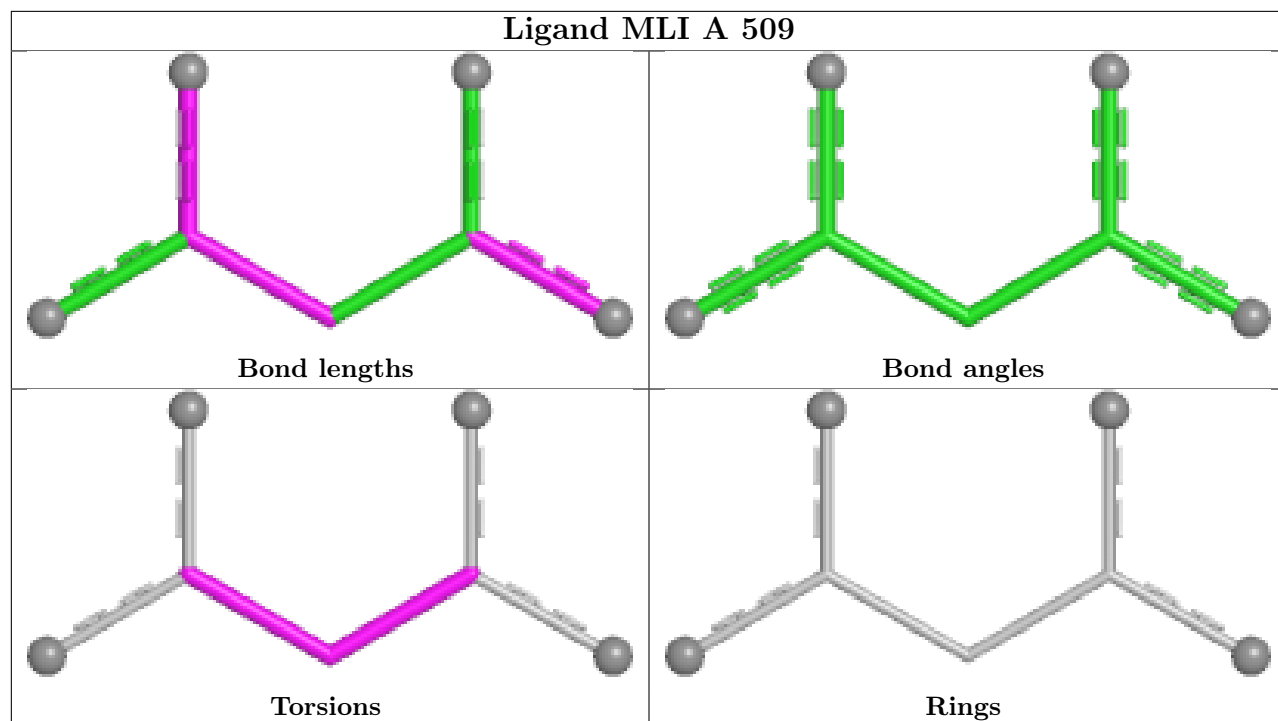
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	511	NDP	2	0
2	A	503	GOL	1	0
3	C	510	MLI	3	0
4	B	512	NDP	2	0
2	B	503	GOL	1	0
4	A	510	NDP	2	0
3	A	508	MLI	3	0
3	B	511	MLI	2	0

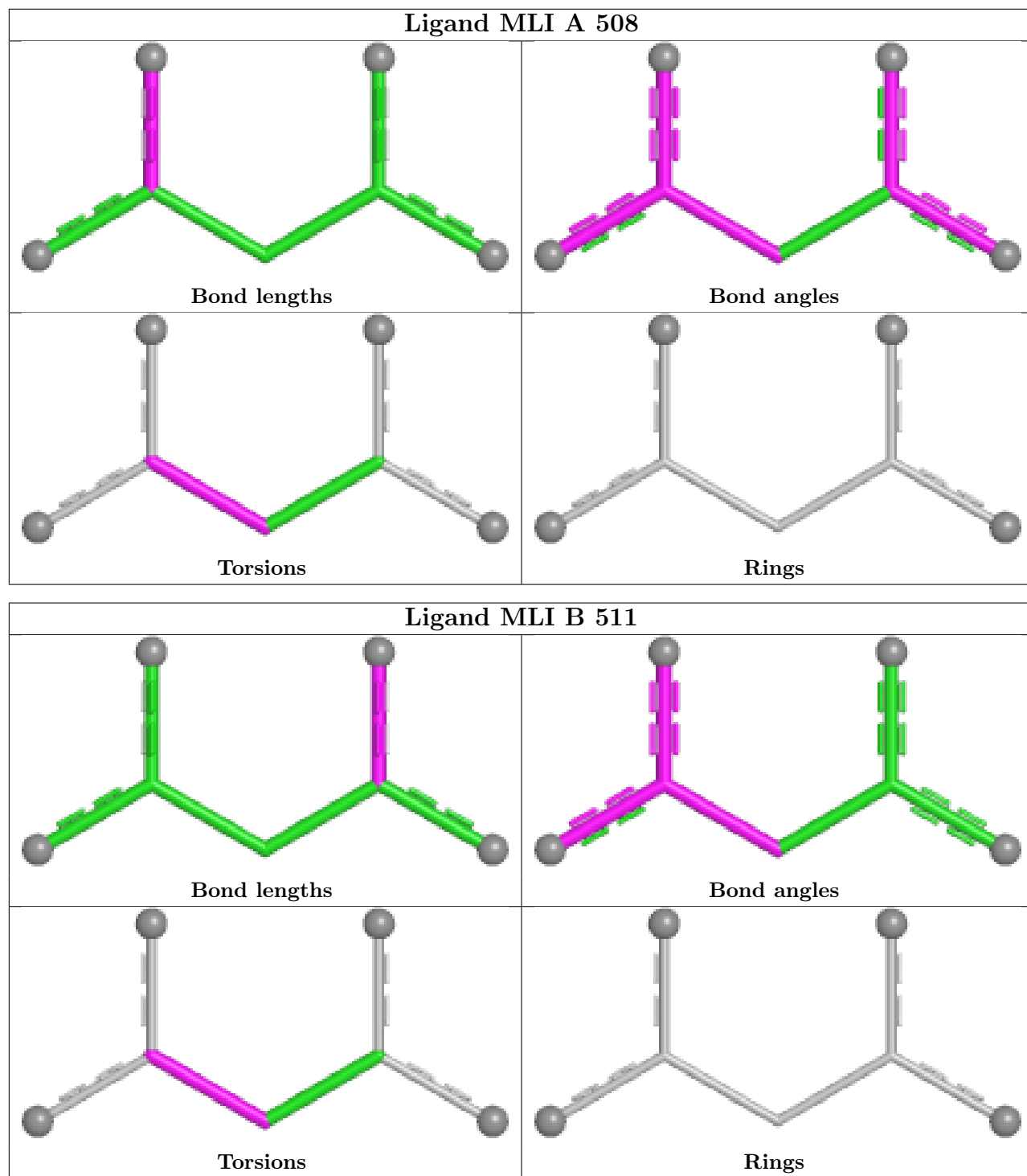
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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, 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	460/460 (100%)	-0.39	6 (1%) 75 82	9, 18, 34, 55	14 (3%)
1	B	460/460 (100%)	-0.38	5 (1%) 78 84	9, 18, 32, 58	14 (3%)
1	C	460/460 (100%)	-0.61	3 (0%) 84 89	8, 16, 28, 52	15 (3%)
All	All	1380/1380 (100%)	-0.46	14 (1%) 79 86	8, 17, 32, 58	43 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	289	VAL	5.2
1	B	293	ALA	4.5
1	A	293	ALA	4.5
1	B	292	ALA	3.9
1	B	264	LYS	3.3
1	A	1	MET	3.2
1	B	289	VAL	2.9
1	A	289	VAL	2.8
1	C	1	MET	2.8
1	A	292	ALA	2.5
1	B	1	MET	2.5
1	A	290	THR	2.4
1	A	263	ALA	2.2
1	C	264	LYS	2.1

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 [i](#)

There are no oligosaccharides 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, 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.

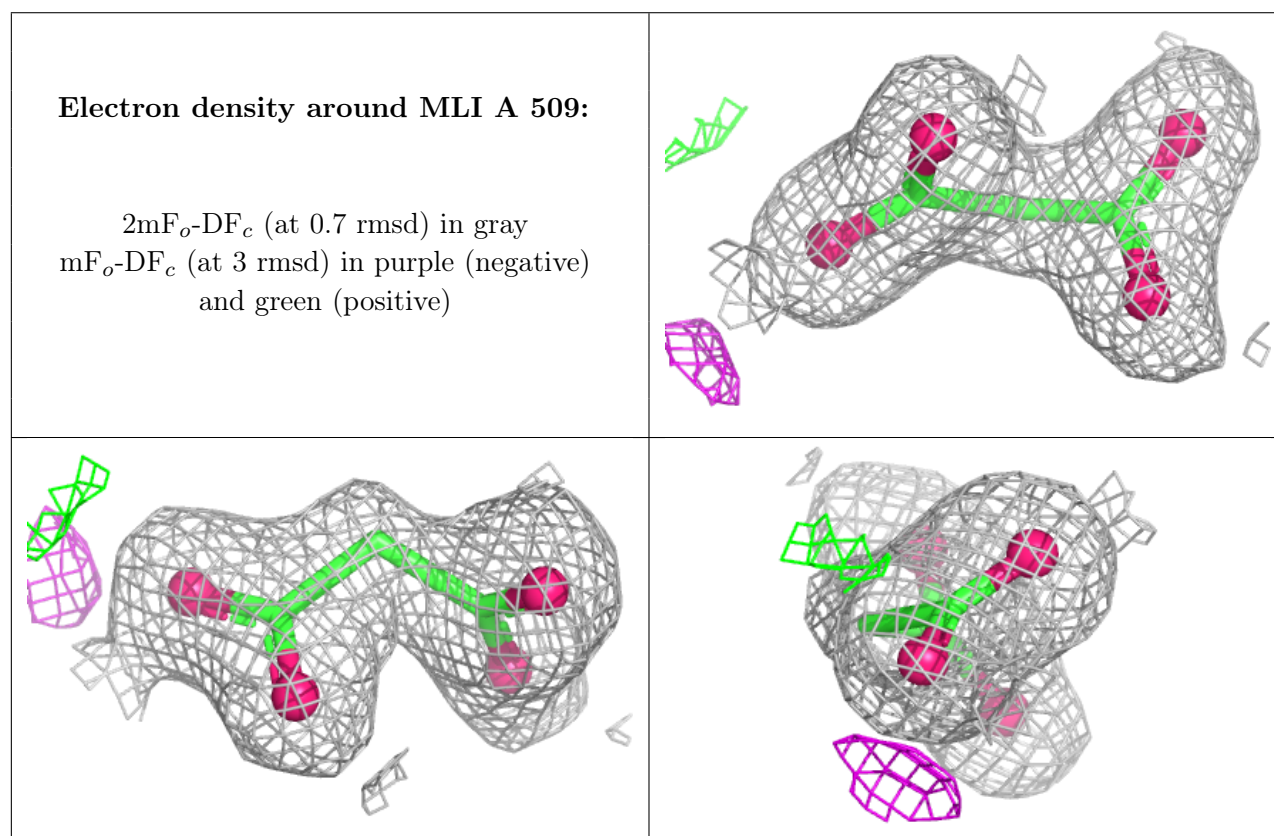
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	507	6/6	0.82	0.16	38,49,54,58	0
2	GOL	C	507	6/6	0.84	0.21	21,46,54,73	0
2	GOL	B	505	6/6	0.85	0.19	47,57,63,64	0
2	GOL	A	503	6/6	0.85	0.22	13,17,18,20	6
2	GOL	B	506	6/6	0.87	0.17	37,49,54,62	0
2	GOL	C	505	6/6	0.88	0.15	26,41,43,45	0
2	GOL	C	508	6/6	0.88	0.19	36,40,53,61	6
2	GOL	B	504	6/6	0.89	0.12	29,37,38,39	0
2	GOL	C	506	6/6	0.89	0.17	40,43,55,59	0
2	GOL	A	506	6/6	0.92	0.14	23,44,55,58	0
2	GOL	B	509	6/6	0.93	0.10	29,37,44,46	0
2	GOL	C	504	6/6	0.93	0.14	18,43,50,59	0
2	GOL	B	507	6/6	0.93	0.11	22,36,49,53	0
2	GOL	B	502	6/6	0.94	0.09	27,32,38,40	0
2	GOL	B	508	6/6	0.94	0.11	20,33,43,50	0
2	GOL	A	505	6/6	0.94	0.11	21,39,44,56	0
2	GOL	C	501	6/6	0.94	0.09	27,32,34,41	0
2	GOL	C	502	6/6	0.94	0.10	31,37,38,41	0
2	GOL	A	502	6/6	0.95	0.09	32,34,42,47	0
2	GOL	B	501	6/6	0.95	0.10	23,34,41,45	0
2	GOL	C	503	6/6	0.95	0.09	19,33,40,45	0
2	GOL	A	501	6/6	0.95	0.08	28,33,40,42	0
3	MLI	A	509	7/7	0.95	0.07	29,33,38,39	0
2	GOL	B	503	6/6	0.96	0.07	33,36,39,42	0
2	GOL	A	504	6/6	0.96	0.09	19,27,29,30	6
3	MLI	B	510	7/7	0.96	0.07	27,29,34,34	0
3	MLI	C	509	7/7	0.96	0.06	22,27,29,31	0
3	MLI	A	508	7/7	0.97	0.08	18,23,24,27	0
3	MLI	C	510	7/7	0.97	0.10	16,24,29,30	0
3	MLI	B	511	7/7	0.98	0.08	17,23,25,25	0
4	NDP	A	510	48/48	0.99	0.04	12,16,24,24	0
4	NDP	B	512	48/48	0.99	0.04	13,17,23,26	0

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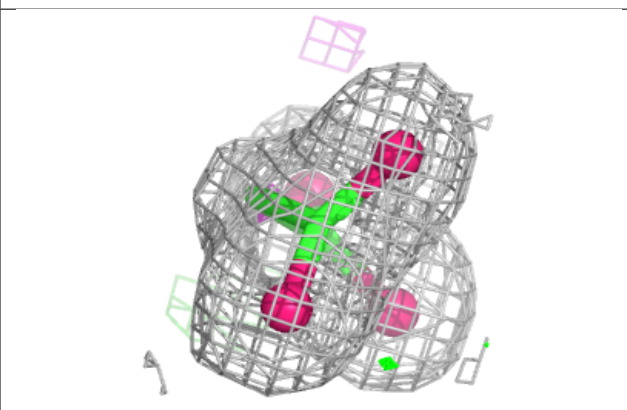
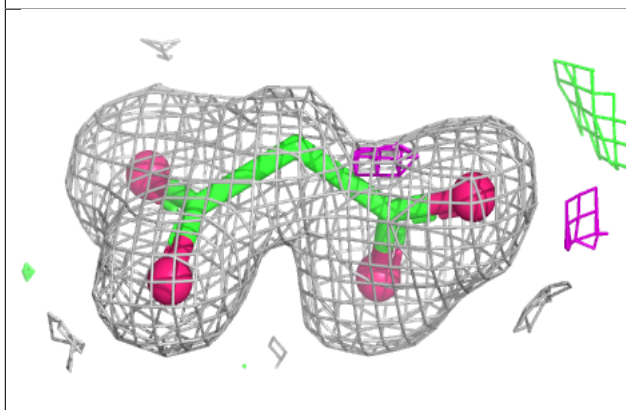
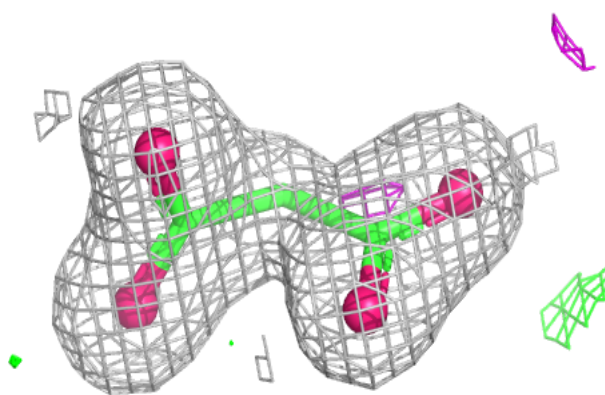
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NDP	C	511	48/48	0.99	0.04	12,15,22,25	0

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.

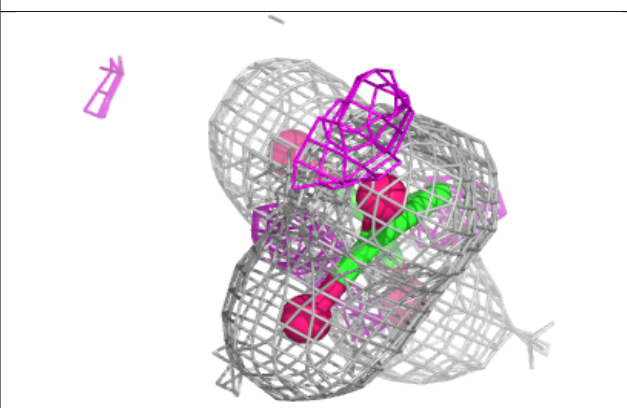
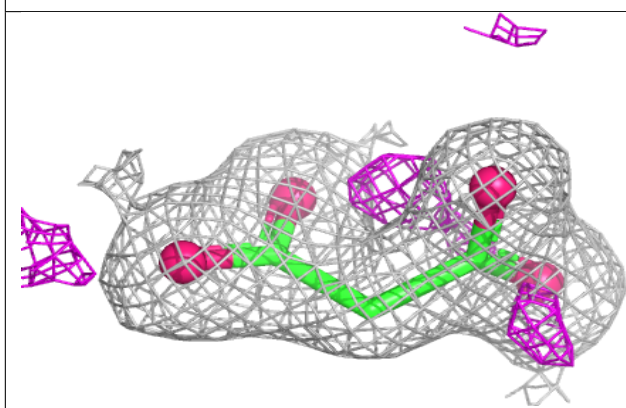
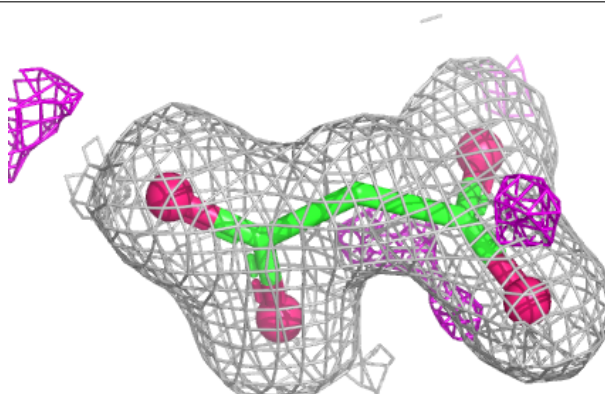


Electron density around MLI B 510:

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

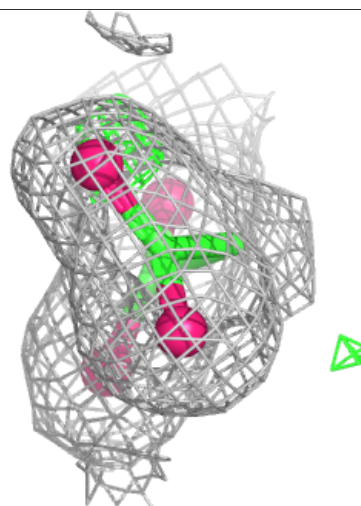
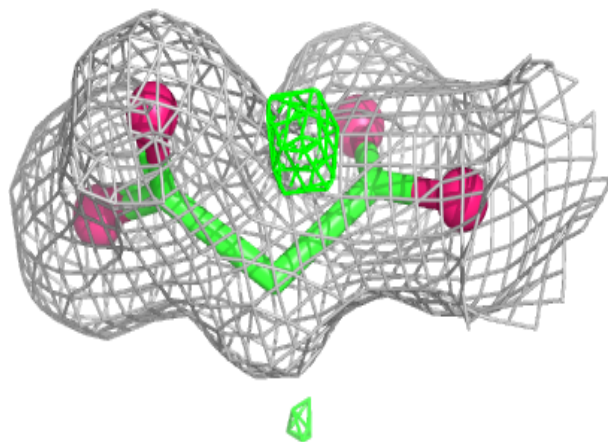
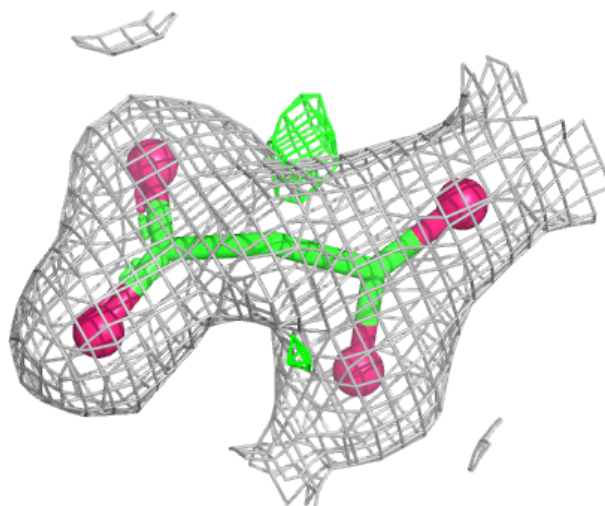
**Electron density around MLI C 509:**

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



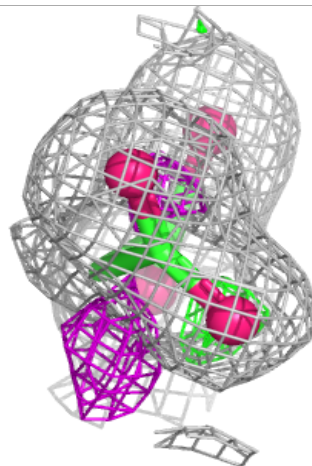
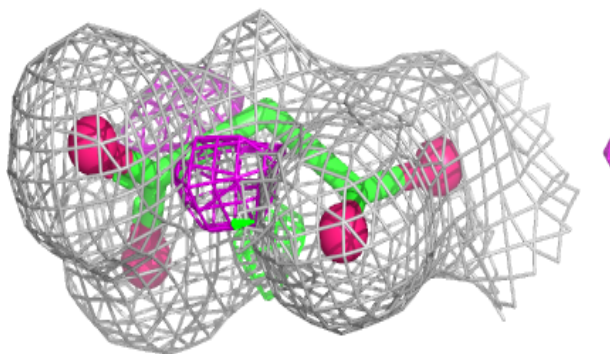
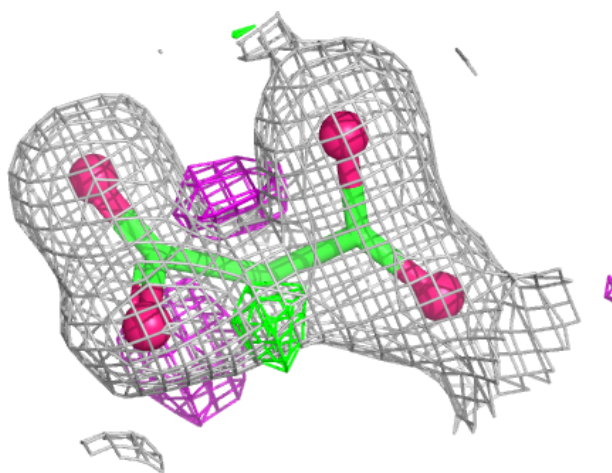
Electron density around MLI A 508:

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



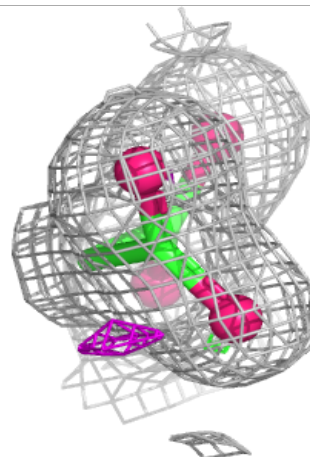
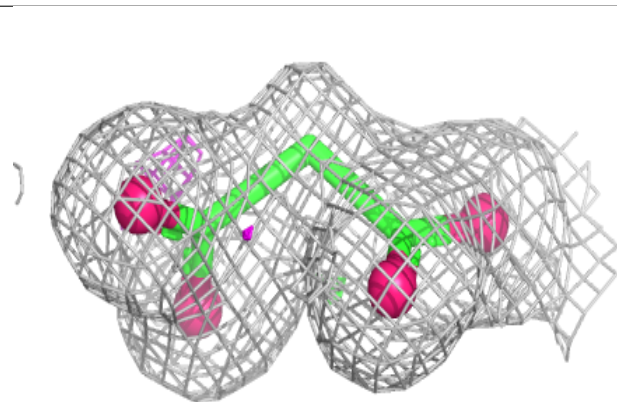
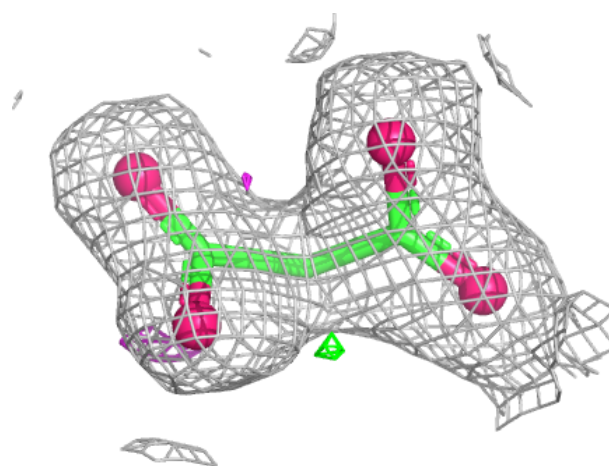
Electron density around MLI C 510:

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



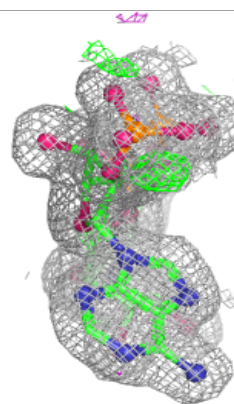
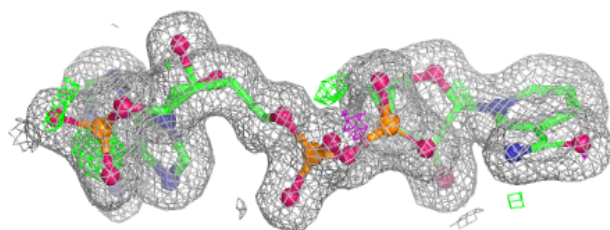
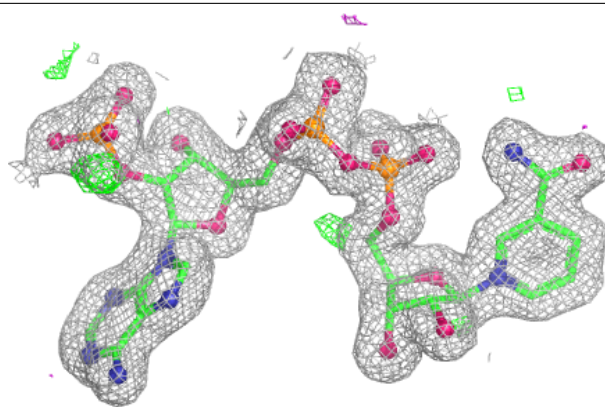
Electron density around MLI B 511:

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

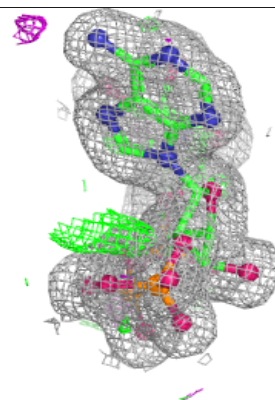
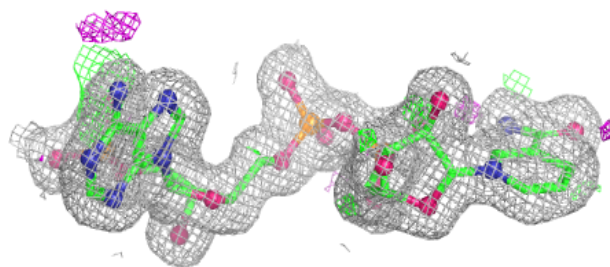
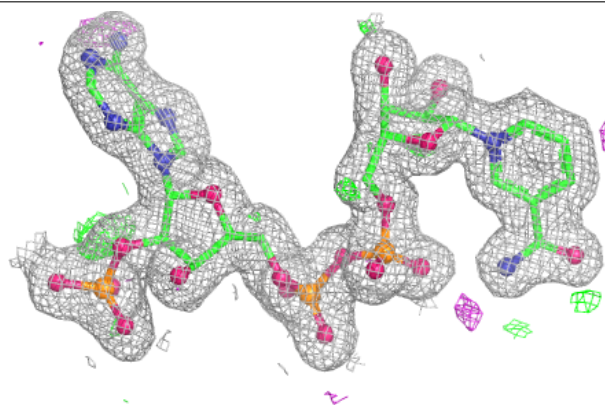


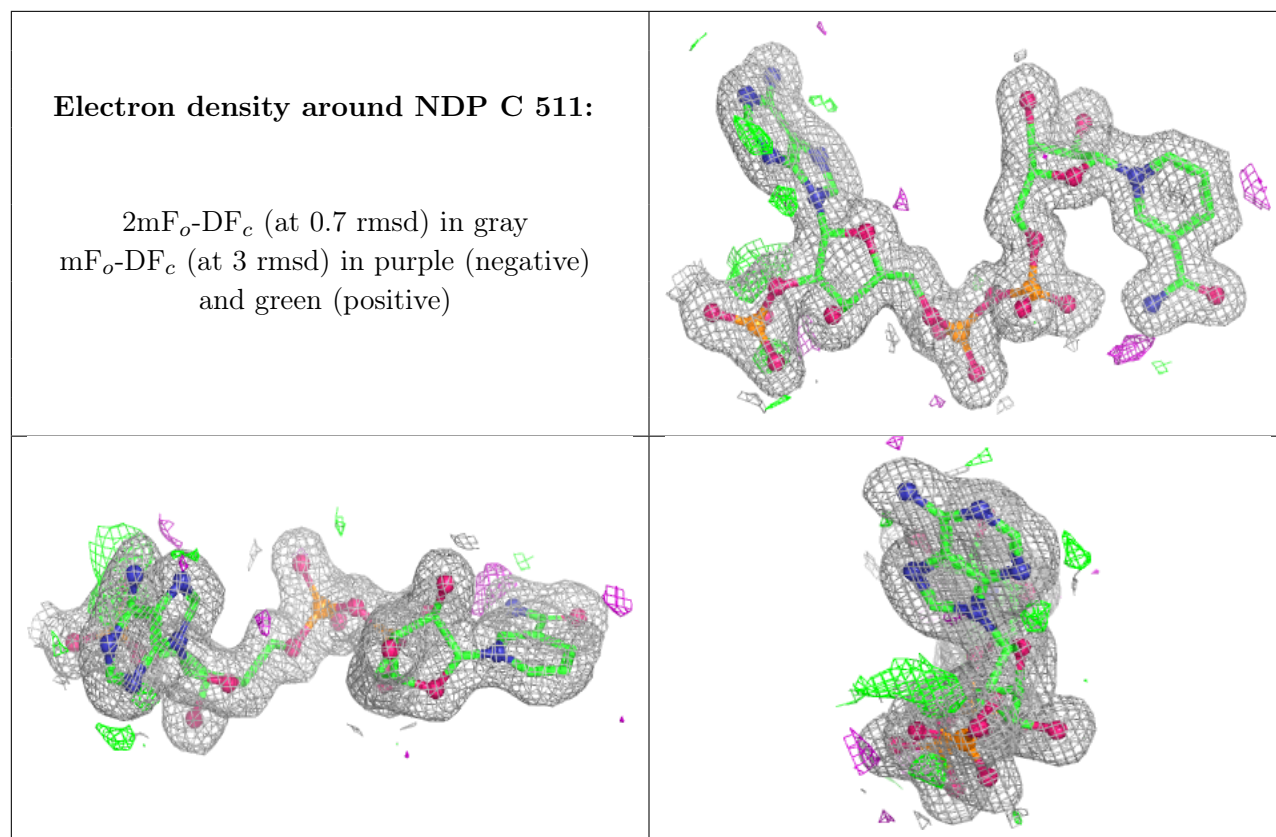
Electron density around NDP A 510:

$2mF_o-DF_c$ (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.