



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:14 PM UTC

PDB ID : 8RP0 / pdb_00008rp0
Title : Aminodeoxychorismate synthase complex from Escherichia coli, with glutamine and chorismate added
Authors : Sung, S.; Funke, F.J.; Schlee, S.; Sterner, R.; Wilmanns, M.
Deposited on : 2024-01-12
Resolution : 1.64 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 ⓘ 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

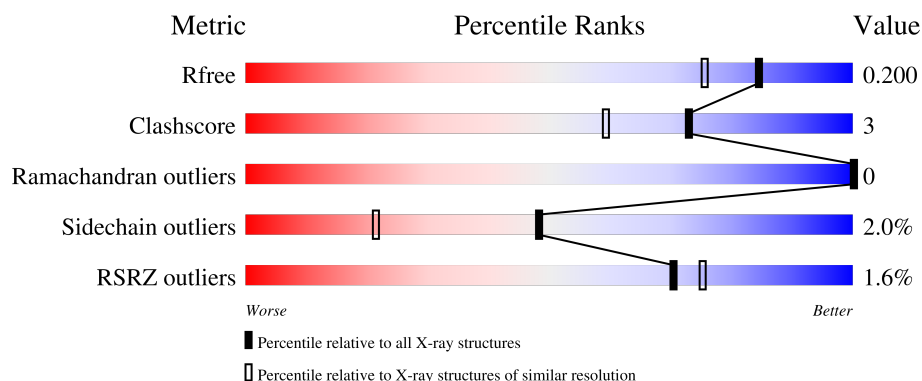
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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}	180053	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	AAA	189	% 94% 5% ..
1	BBB	189	4% 89% 11% .
2	CCC	455	% 93% 5% .
2	DDD	455	% 93% 6% .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21430 atoms, of which 10113 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 Aminodeoxychorismate synthase component 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	188	Total	C	H	N	O	S	73	0	0
			2929	934	1462	259	266	8			
1	BBB	189	Total	C	H	N	O	S	73	0	0
			2937	936	1467	260	266	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	GLY	-	expression tag	UNP P00903
AAA	0	GLY	-	expression tag	UNP P00903
BBB	-1	GLY	-	expression tag	UNP P00903
BBB	0	GLY	-	expression tag	UNP P00903

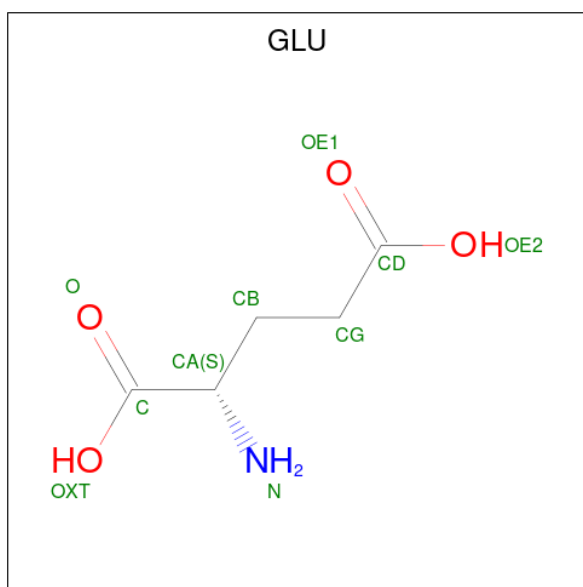
- Molecule 2 is a protein called Aminodeoxychorismate synthase component 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	CCC	454	Total	C	H	N	O	S	192	1	0
			7147	2277	3535	632	689	14			
2	DDD	455	Total	C	H	N	O	S	192	2	0
			7180	2285	3553	637	691	14			

There are 4 discrepancies between the modelled and reference sequences:

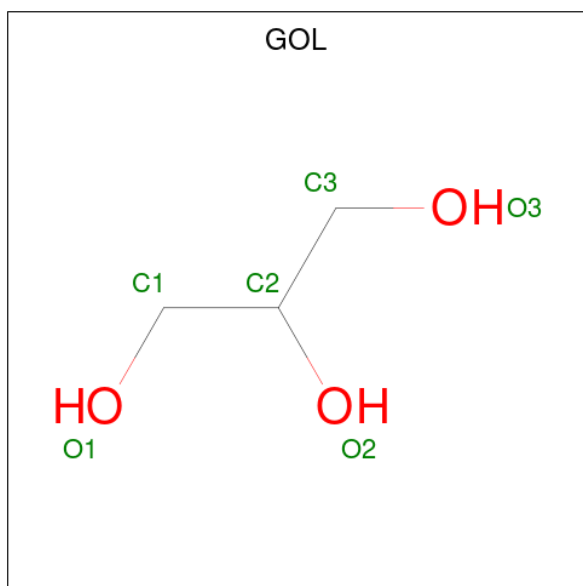
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-1	GLY	-	expression tag	UNP P05041
CCC	0	HIS	-	expression tag	UNP P05041
DDD	-1	GLY	-	expression tag	UNP P05041
DDD	0	HIS	-	expression tag	UNP P05041

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	0	0
			17	5	8	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



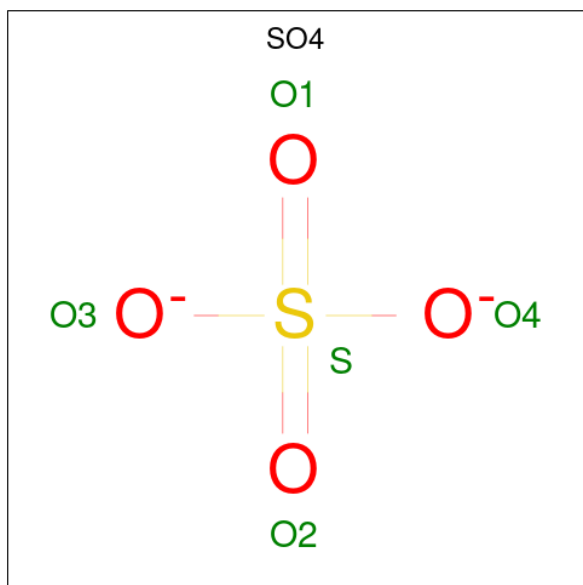
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
4	CCC	1	Total	C	H	O	2	0
			14	3	8	3		
4	CCC	1	Total	C	H	O	2	0
			14	3	8	3		

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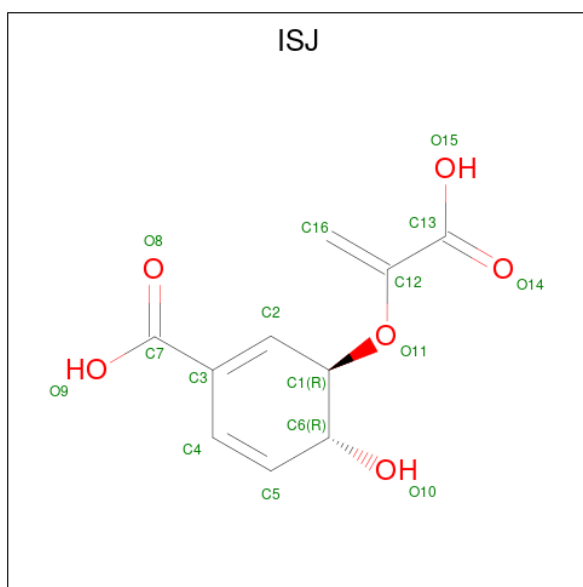
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	CCC	1	Total	C	H	O	2	0
			14	3	8	3		
4	DDD	1	Total	C	H	O	2	0
			14	3	8	3		
4	DDD	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



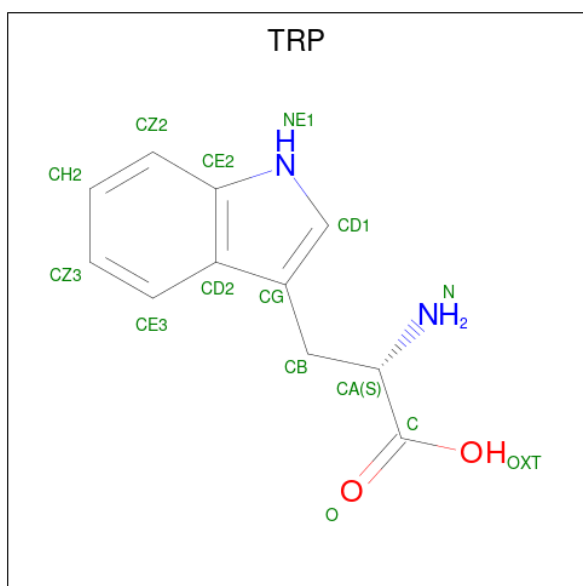
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	DDD	1	Total	O	S	0	0
			5	4	1		
5	DDD	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (3R,4R)-3-[(1-carboxyethenyl)oxy]-4-hydroxycyclohexa-1,5-diene-1-carboxylic acid (CCD ID: ISJ) (formula: C₁₀H₁₀O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	CCC	1	Total	C	H	O	1	0
			24	10	8	6		
6	DDD	1	Total	C	H	O	1	0
			24	10	8	6		

- Molecule 7 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	CCC	1	Total	C	H	N	O	0	0
			27	11	12	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	DDD	1	Total	C	H	N	O	0	0
			27	11	12	2	2		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	CCC	1	Total	Mg	0	0
			1	1		
8	DDD	2	Total	Mg	0	0
			2	2		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	CCC	5	Total	Cl	0	0
			5	5		
9	DDD	2	Total	Cl	0	0
			2	2		

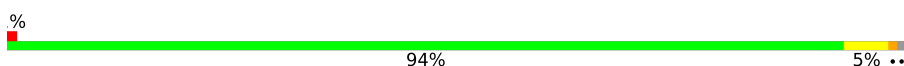
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	139	Total	O	0	0
			139	139		
10	BBB	66	Total	O	0	0
			66	66		
10	CCC	405	Total	O	0	0
			405	405		
10	DDD	389	Total	O	0	0
			389	389		

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.

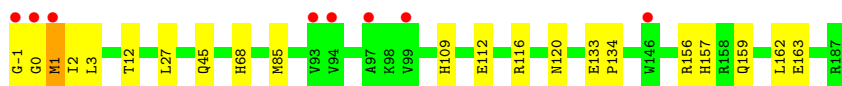
- Molecule 1: Aminodeoxychorismate synthase component 2

Chain AAA: 

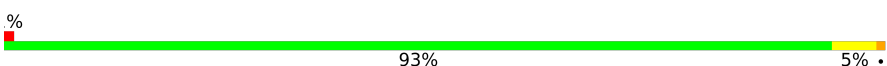


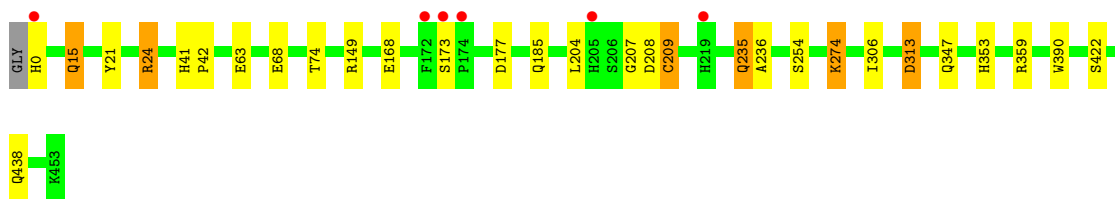
- Molecule 1: Aminodeoxychorismate synthase component 2

Chain BBB: 

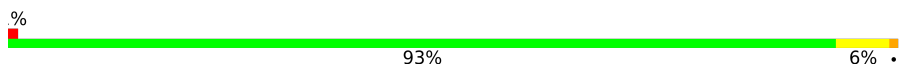


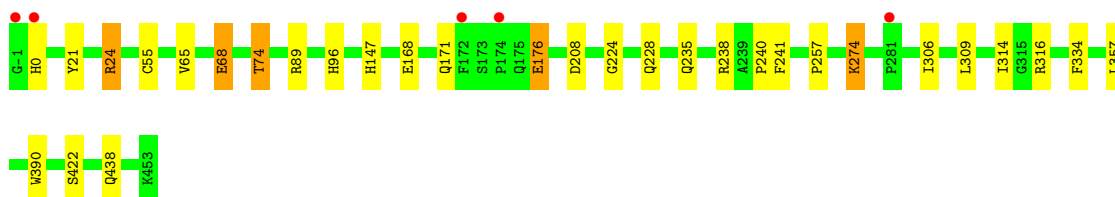
- Molecule 2: Aminodeoxychorismate synthase component 1

Chain CCC: 



- Molecule 2: Aminodeoxychorismate synthase component 1

Chain DDD: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.18Å 109.95Å 175.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.64 – 1.64 46.64 – 1.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.64-1.64) 100.0 (46.64-1.64)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.170 , 0.199 0.170 , 0.200	Depositor DCC
R_{free} test set	9423 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21430	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: MG, CL, SO4, GOL, ISJ

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	1.10	0/1503	1.20	3/2042 (0.1%)
1	BBB	1.09	0/1506	1.20	5/2047 (0.2%)
2	CCC	1.08	1/3694 (0.0%)	1.21	6/5018 (0.1%)
2	DDD	1.07	2/3709 (0.1%)	1.17	2/5037 (0.0%)
All	All	1.08	3/10412 (0.0%)	1.19	16/14144 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BBB	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	147	HIS	CE1-NE2	5.64	1.38	1.32
2	CCC	254	SER	CA-CB	-5.33	1.45	1.53
2	DDD	334	PHE	N-CA	5.18	1.49	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	1	MET	N-CA-C	-9.34	101.08	111.07
2	CCC	208	ASP	CA-CB-CG	7.21	119.81	112.60
1	AAA	170	GLU	CB-CG-CD	6.35	123.40	112.60
1	BBB	1	MET	CA-C-O	-6.25	114.26	120.82
2	CCC	207	GLY	CA-C-N	6.10	128.46	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	0	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1467	1462	1454	8	0
1	BBB	1470	1467	1458	12	0
2	CCC	3612	3535	3522	17	1
2	DDD	3627	3553	3537	25	0
3	AAA	9	8	5	0	0
4	AAA	6	8	8	0	0
4	CCC	18	24	24	1	0
4	DDD	12	16	16	1	0
5	AAA	5	0	0	0	0
5	BBB	5	0	0	0	0
5	CCC	5	0	0	0	0
5	DDD	10	0	0	1	0
6	CCC	16	8	8	3	0
6	DDD	16	8	8	2	0
7	CCC	15	12	9	0	0
7	DDD	15	12	9	0	0
8	CCC	1	0	0	0	0
8	DDD	2	0	0	0	1
9	CCC	5	0	0	0	0
9	DDD	2	0	0	0	0
10	AAA	139	0	0	2	0
10	BBB	66	0	0	0	0
10	CCC	405	0	0	8	0
10	DDD	389	0	0	13	0
All	All	11317	10113	10058	65	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 3.

The worst 5 of 65 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:DDD:55:CYS:HB2	10:DDD:911:HOH:O	1.31	1.31
2:DDD:316:ARG:NH2	10:DDD:602:HOH:O	1.71	1.21
5:DDD:509:SO4:O2	10:DDD:601:HOH:O	1.61	1.13
2:DDD:89:ARG:HD3	10:DDD:613:HOH:O	1.45	1.13
1:BBB:1:GLY:HA3	1:BBB:3:LEU:HB2	1.29	1.08

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)
2:CCC:353:HIS:HE2	8:DDD:504:MG:MG[3_454]	1.31	0.29

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	AAA	186/189 (98%)	182 (98%)	4 (2%)	0	100	100
1	BBB	187/189 (99%)	182 (97%)	5 (3%)	0	100	100
2	CCC	453/455 (100%)	442 (98%)	11 (2%)	0	100	100
2	DDD	455/455 (100%)	441 (97%)	14 (3%)	0	100	100
All	All	1281/1288 (100%)	1247 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	157/157 (100%)	155 (99%)	2 (1%)	61	38
1	BBB	157/157 (100%)	154 (98%)	3 (2%)	50	23
2	CCC	392/391 (100%)	383 (98%)	9 (2%)	44	17
2	DDD	393/391 (100%)	385 (98%)	8 (2%)	48	21
All	All	1099/1096 (100%)	1077 (98%)	22 (2%)	48	21

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	DDD	0	HIS
2	DDD	168	GLU
2	DDD	68	GLU
2	DDD	171	GLN
2	CCC	15	GLN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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
4	GOL	CCC	510	-	5,5,5	0.19	0	5,5,5	0.54	0
4	GOL	DDD	508	-	5,5,5	0.14	0	5,5,5	0.51	0
5	SO4	AAA	203	-	4,4,4	0.19	0	6,6,6	0.12	0
5	SO4	DDD	510	-	4,4,4	0.17	0	6,6,6	0.24	0
6	ISJ	DDD	501	8	16,16,16	2.58	5 (31%)	13,22,22	2.81	6 (46%)
5	SO4	BBB	1101	-	4,4,4	0.27	0	6,6,6	0.37	0
5	SO4	CCC	512	-	4,4,4	0.26	0	6,6,6	0.12	0
3	GLU	AAA	201	-	6,8,9	0.93	0	6,9,11	0.81	0
4	GOL	AAA	202	-	5,5,5	0.20	0	5,5,5	0.66	0
4	GOL	DDD	507	-	5,5,5	0.13	0	5,5,5	0.40	0
5	SO4	DDD	509	-	4,4,4	0.32	0	6,6,6	0.11	0
6	ISJ	CCC	501	8	16,16,16	2.58	5 (31%)	13,22,22	2.65	8 (61%)
7	TRP	CCC	502	-	15,16,16	0.69	0	18,22,22	0.60	0
4	GOL	CCC	511	-	5,5,5	0.13	0	5,5,5	0.37	0
7	TRP	DDD	502	-	15,16,16	0.82	1 (6%)	18,22,22	0.61	0
4	GOL	CCC	509	-	5,5,5	0.20	0	5,5,5	0.49	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
4	GOL	CCC	510	-	-	4/4/4/4	-
4	GOL	DDD	508	-	-	3/4/4/4	-
6	ISJ	DDD	501	8	-	4/10/25/25	0/1/1/1
3	GLU	AAA	201	-	-	1/8/8/9	-
4	GOL	AAA	202	-	-	3/4/4/4	-
4	GOL	DDD	507	-	-	3/4/4/4	-
6	ISJ	CCC	501	8	-	4/10/25/25	0/1/1/1
7	TRP	CCC	502	-	-	0/8/8/8	0/2/2/2
4	GOL	CCC	511	-	-	2/4/4/4	-
7	TRP	DDD	502	-	-	0/8/8/8	0/2/2/2
4	GOL	CCC	509	-	-	2/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CCC	501	ISJ	C12-C13	-6.86	1.42	1.49
6	DDD	501	ISJ	C12-C13	-6.25	1.43	1.49
6	DDD	501	ISJ	C2-C3	5.47	1.47	1.35
6	CCC	501	ISJ	C2-C3	4.50	1.45	1.35
6	DDD	501	ISJ	O11-C1	3.05	1.51	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	DDD	501	ISJ	C1-O11-C12	5.57	125.65	117.03
6	CCC	501	ISJ	O15-C13-C12	4.56	121.68	113.91
6	DDD	501	ISJ	C16-C12-C13	-4.00	115.33	122.73
6	CCC	501	ISJ	C1-O11-C12	3.96	123.17	117.03
6	CCC	501	ISJ	C16-C12-C13	-3.77	115.76	122.73

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201	GLU	OE1-CD-CG-CB
4	CCC	509	GOL	O1-C1-C2-C3
4	CCC	510	GOL	O1-C1-C2-O2
4	CCC	510	GOL	O1-C1-C2-C3
4	CCC	510	GOL	C1-C2-C3-O3

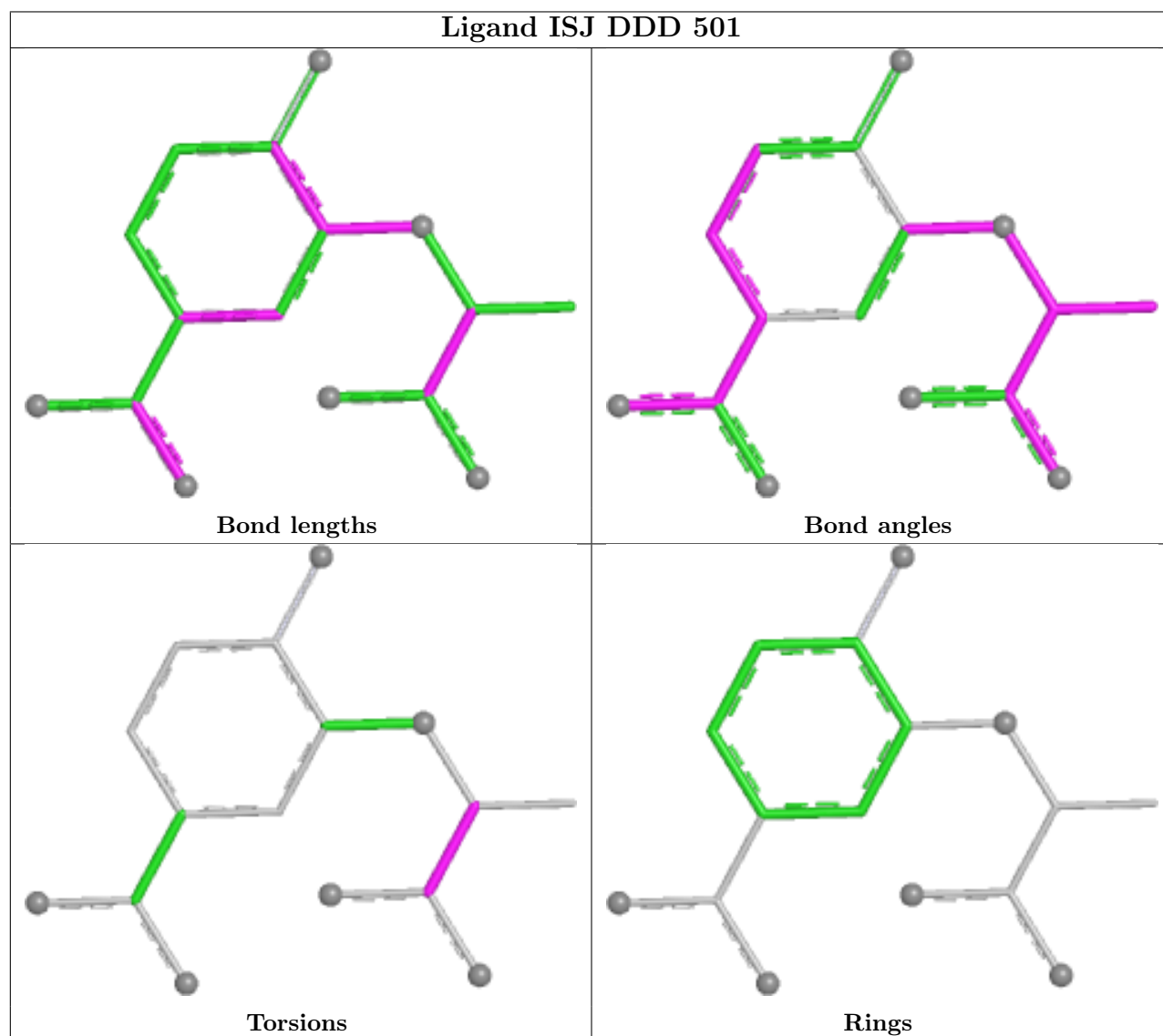
There are no ring outliers.

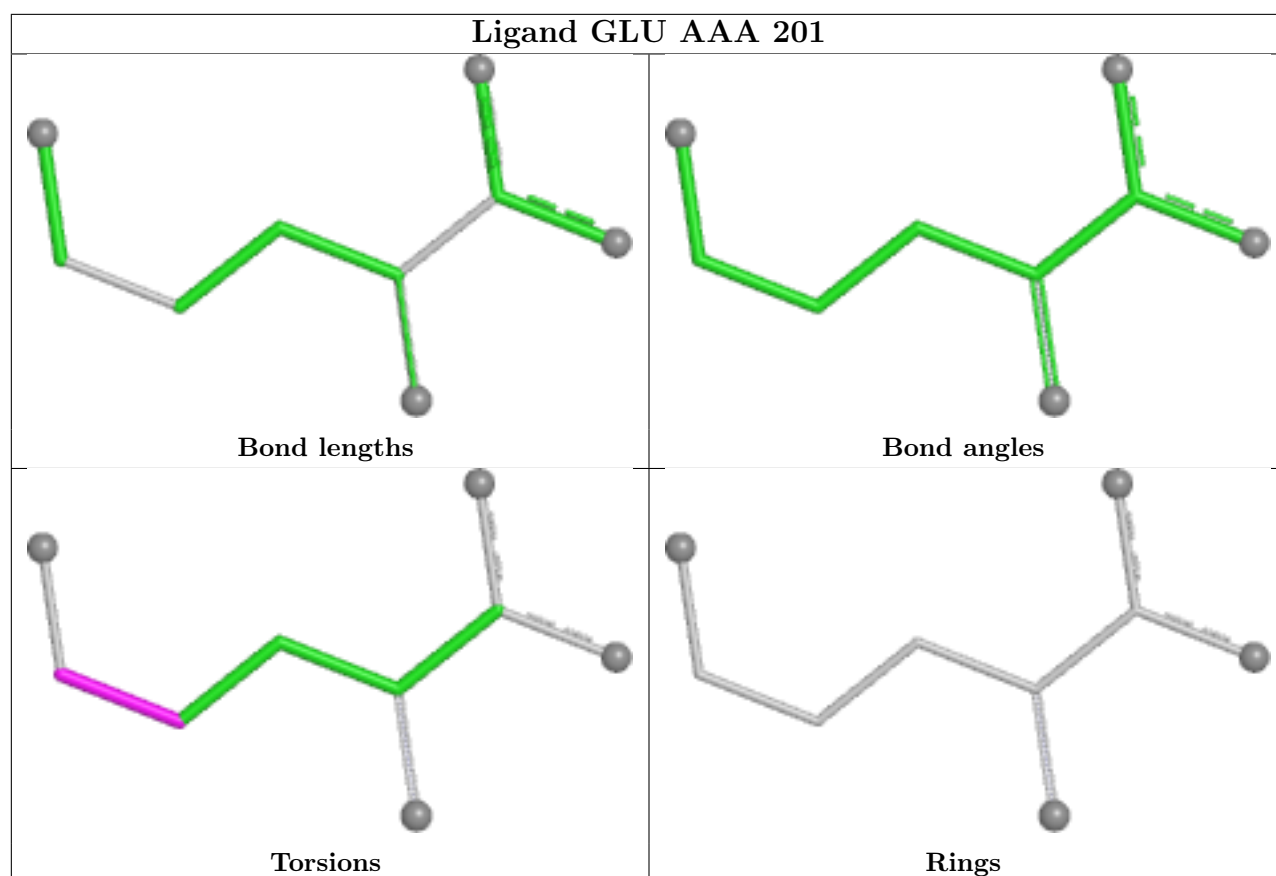
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	510	GOL	1	0
6	DDD	501	ISJ	2	0
4	DDD	507	GOL	1	0
5	DDD	509	SO4	1	0
6	CCC	501	ISJ	3	0

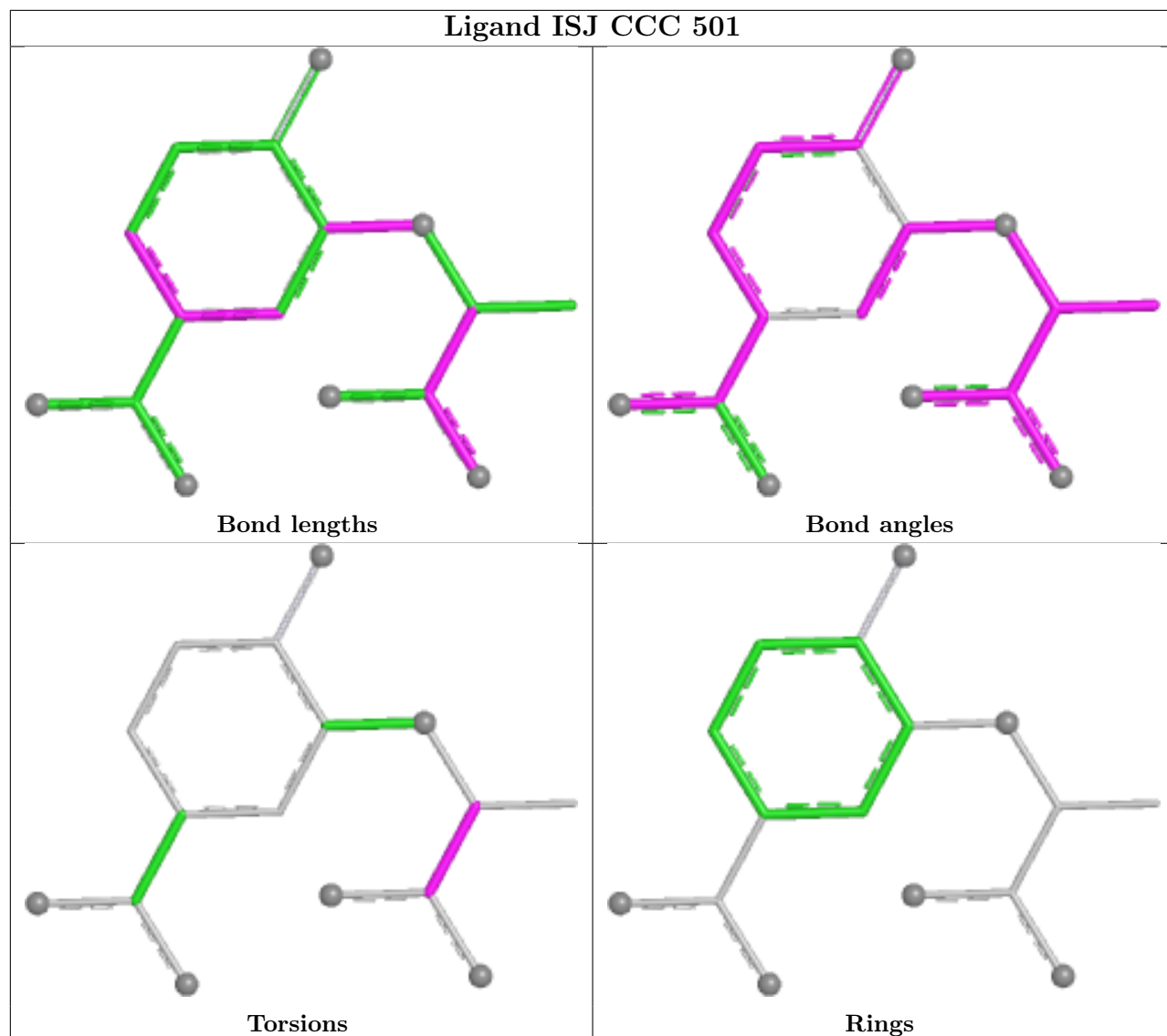
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

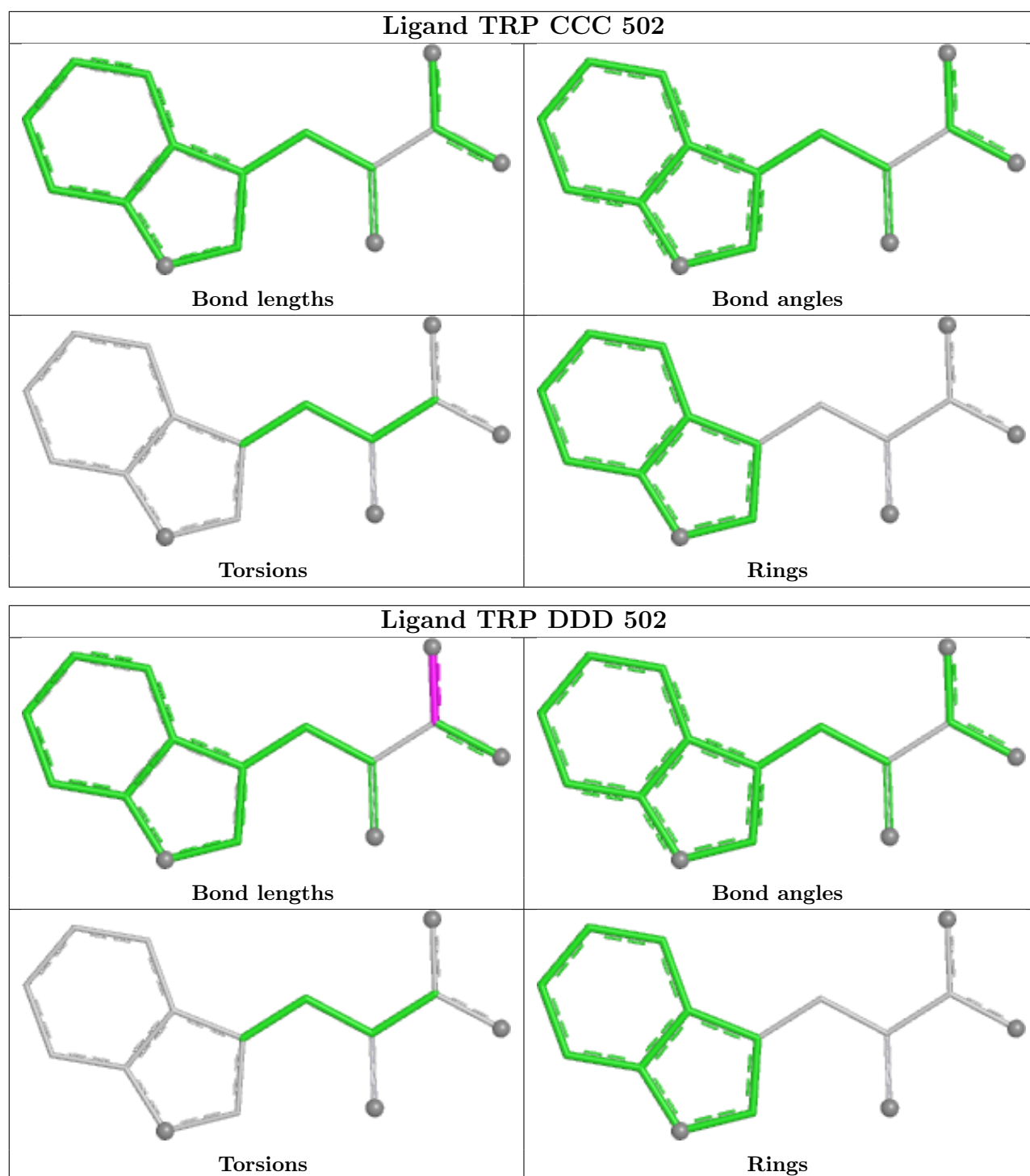
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand ISJ CCC 501





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	188/189 (99%)	-0.09	2 (1%) 78 83	21, 31, 51, 70	0
1	BBB	189/189 (100%)	0.49	8 (4%) 40 45	23, 41, 68, 90	0
2	CCC	454/455 (99%)	-0.23	6 (1%) 75 80	15, 30, 51, 100	1 (0%)
2	DDD	455/455 (100%)	-0.17	5 (1%) 78 83	12, 30, 52, 101	2 (0%)
All	All	1286/1288 (99%)	-0.08	21 (1%) 70 75	12, 31, 54, 101	3 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	-1	GLY	9.0
2	CCC	173	SER	4.2
2	CCC	205	HIS	3.9
2	CCC	172	PHE	3.9
1	AAA	0	GLY	3.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

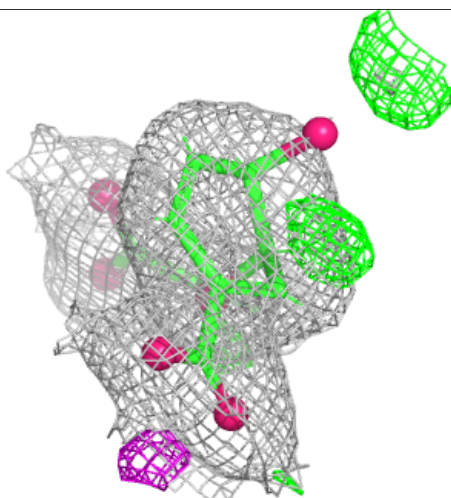
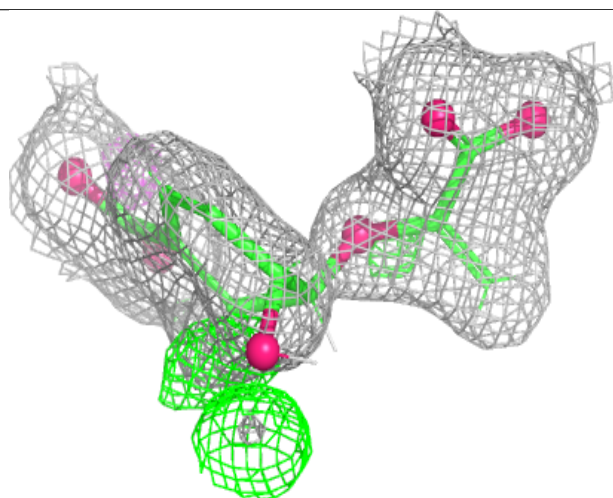
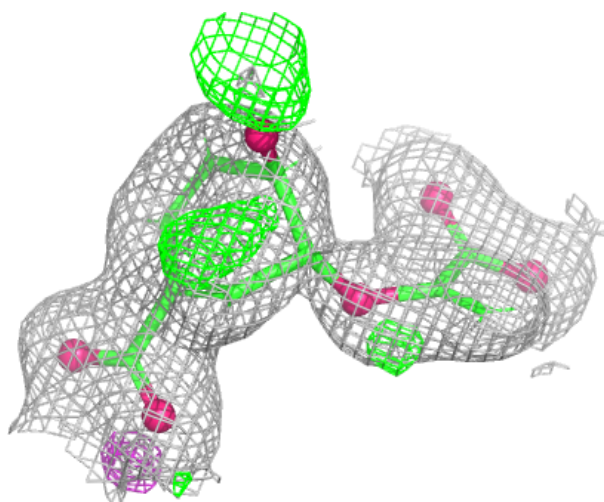
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	GOL	CCC	509	6/6	0.68	0.19	6,61,64,73	2
5	SO4	CCC	512	5/5	0.70	0.15	92,95,102,109	0
4	GOL	AAA	202	6/6	0.77	0.14	6,49,67,73	2
4	GOL	CCC	510	6/6	0.79	0.13	6,59,64,78	2
9	CL	CCC	508	1/1	0.80	0.17	62,62,62,62	0
5	SO4	BBB	1101	5/5	0.82	0.10	46,54,72,79	0
5	SO4	DDD	509	5/5	0.83	0.12	52,55,67,68	2
4	GOL	CCC	511	6/6	0.84	0.17	56,62,64,71	2
5	SO4	AAA	203	5/5	0.84	0.10	48,72,81,83	0
9	CL	CCC	505	1/1	0.85	0.14	81,81,81,81	0
4	GOL	DDD	508	6/6	0.87	0.15	53,56,78,79	2
5	SO4	DDD	510	5/5	0.88	0.09	48,49,51,59	1
9	CL	CCC	506	1/1	0.89	0.13	57,57,57,57	0
4	GOL	DDD	507	6/6	0.89	0.13	62,70,75,77	2
9	CL	CCC	504	1/1	0.90	0.18	63,63,63,63	0
9	CL	DDD	506	1/1	0.91	0.15	64,64,64,64	0
6	ISJ	DDD	501	16/16	0.94	0.09	27,33,39,59	5
9	CL	CCC	507	1/1	0.94	0.12	75,75,75,75	0
6	ISJ	CCC	501	16/16	0.95	0.09	25,32,40,69	5
3	GLU	AAA	201	9/10	0.95	0.07	31,32,34,35	1
9	CL	DDD	505	1/1	0.96	0.18	61,61,61,61	0
8	MG	DDD	503	1/1	0.97	0.05	31,31,31,31	0
7	TRP	CCC	502	15/15	0.97	0.05	20,23,26,27	0
8	MG	DDD	504	1/1	0.99	0.04	24,24,24,24	0
7	TRP	DDD	502	15/15	0.99	0.04	22,24,26,29	0
8	MG	CCC	503	1/1	1.00	0.01	29,29,29,29	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.

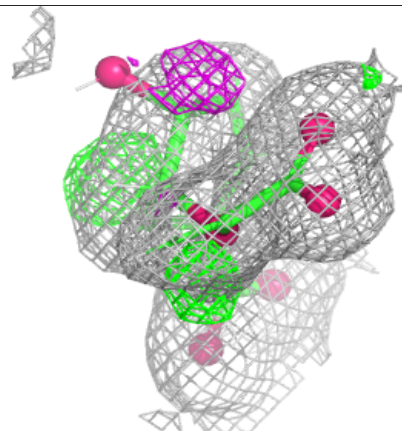
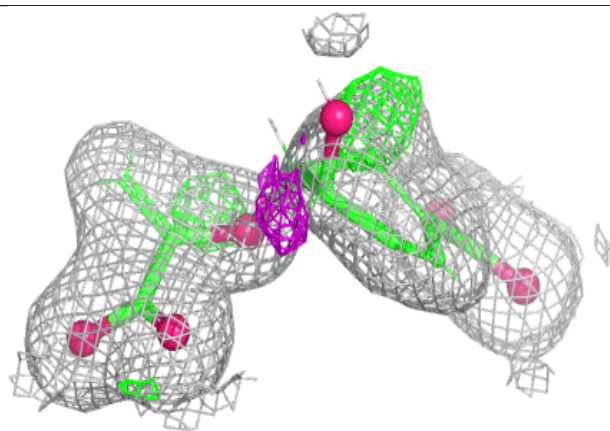
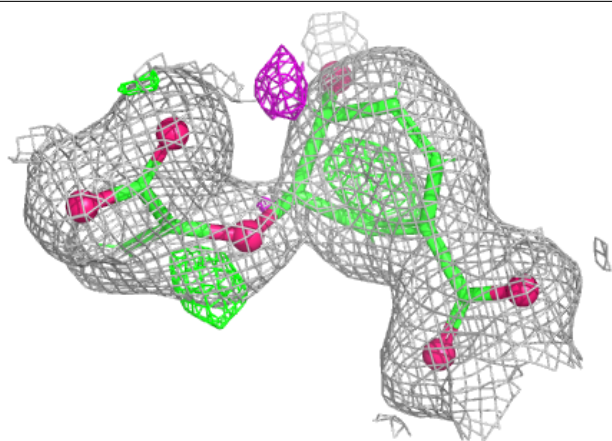
Electron density around ISJ DDD 501:

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



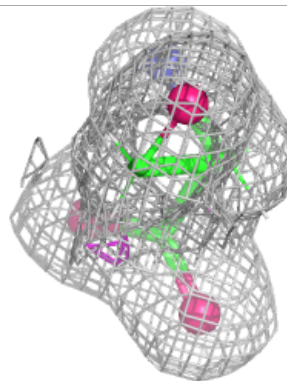
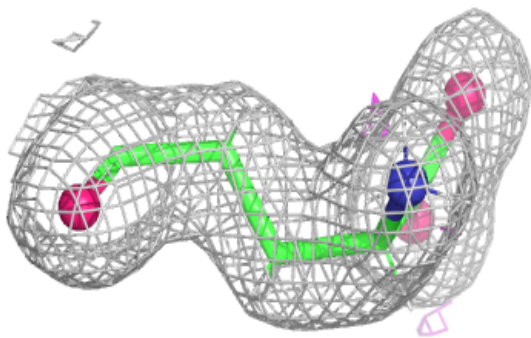
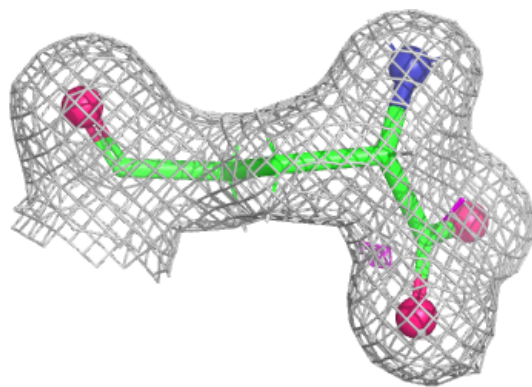
Electron density around ISJ CCC 501:

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



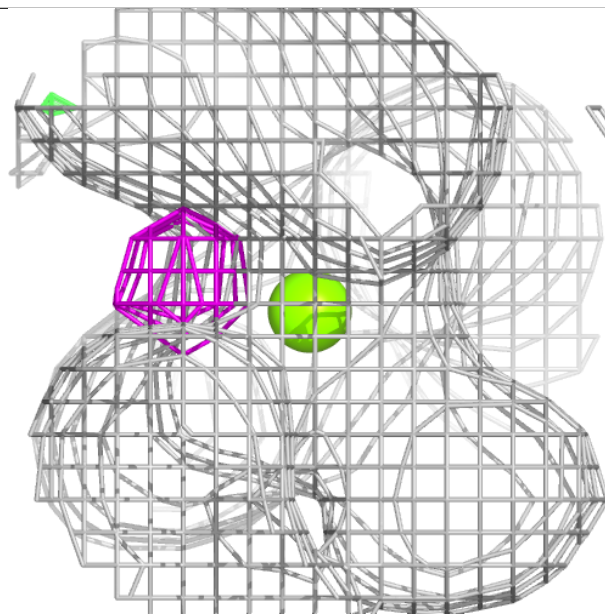
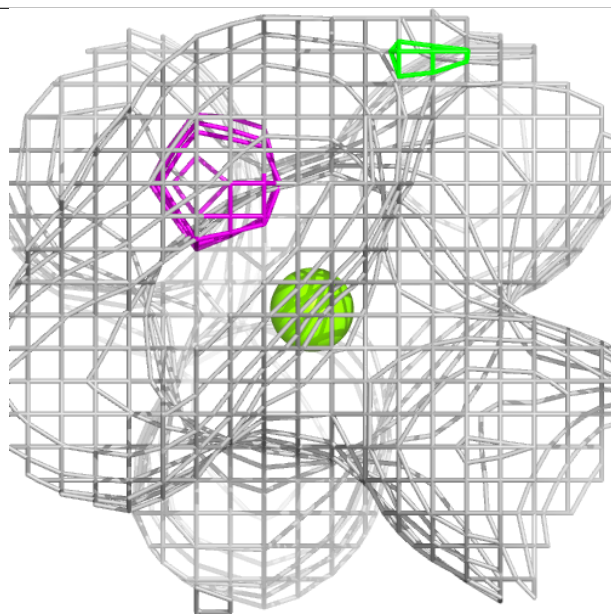
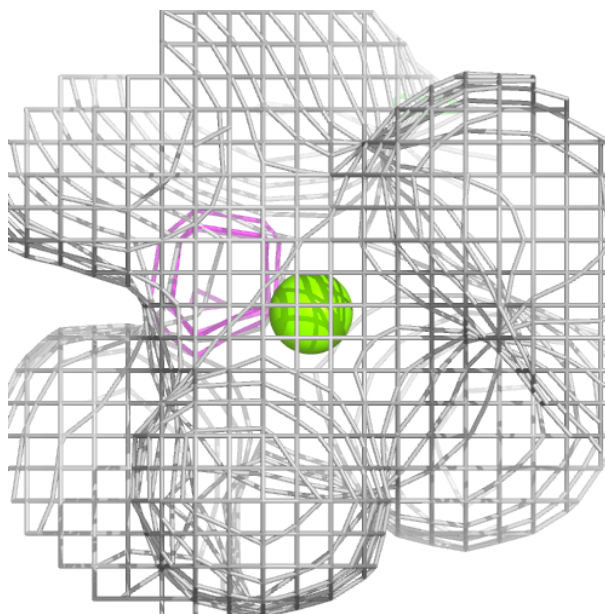
Electron density around GLU AAA 201:

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



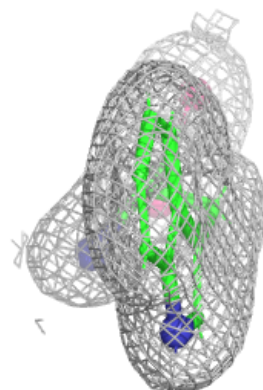
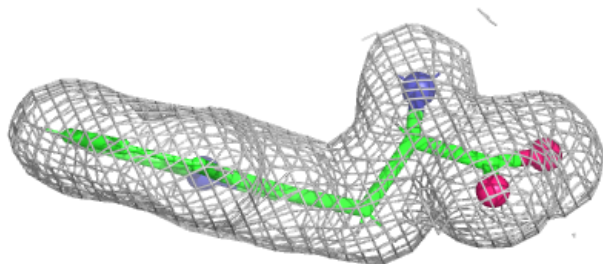
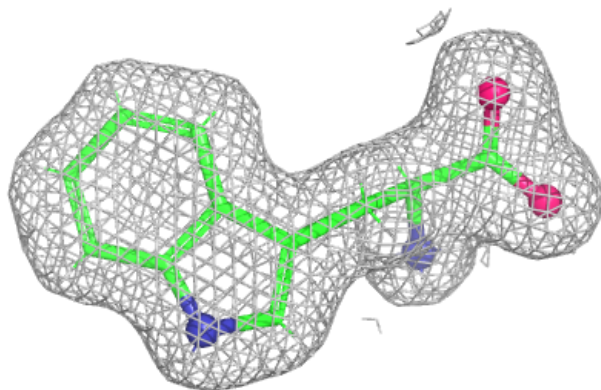
Electron density around MG DDD 503:

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



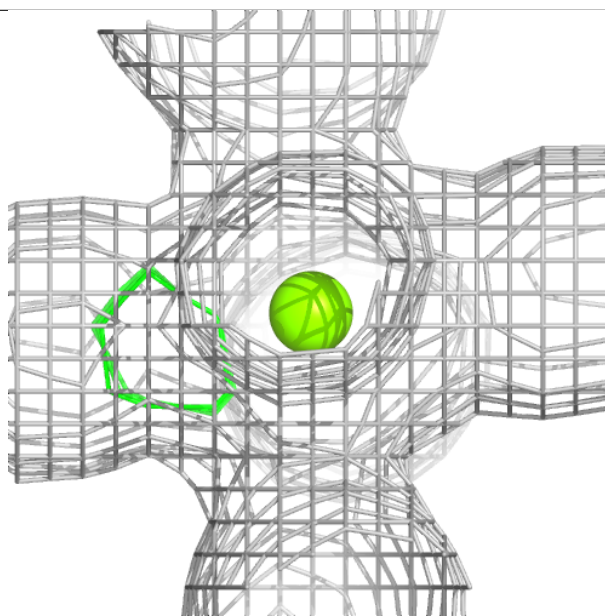
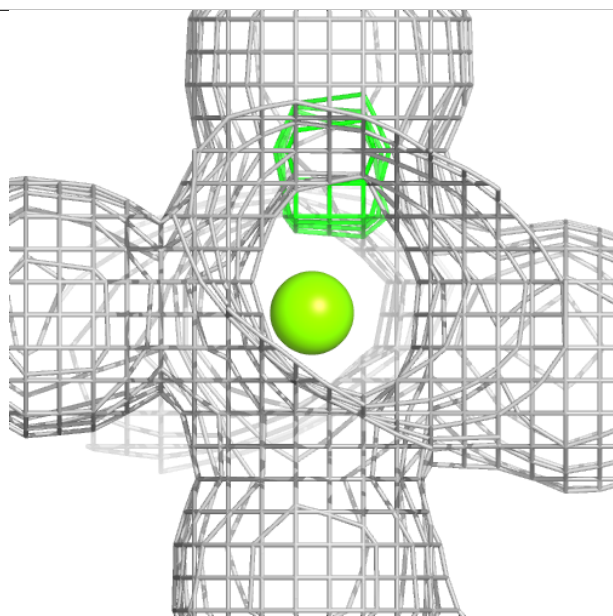
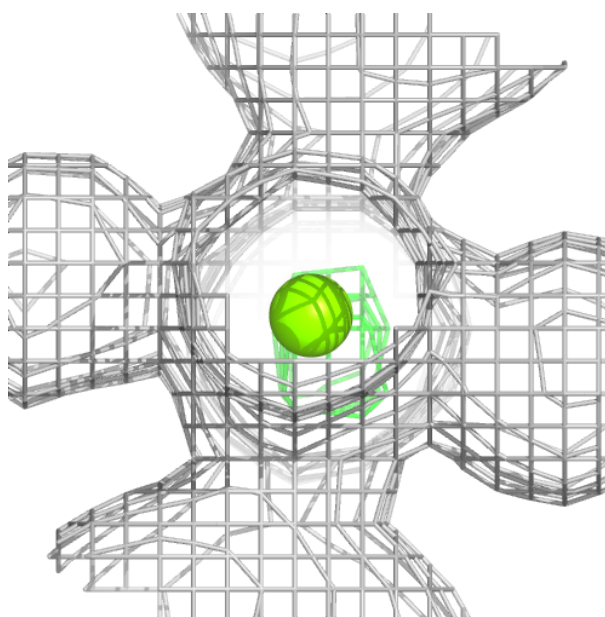
Electron density around TRP CCC 502:

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



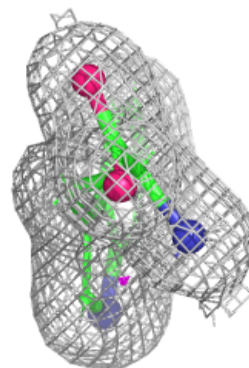
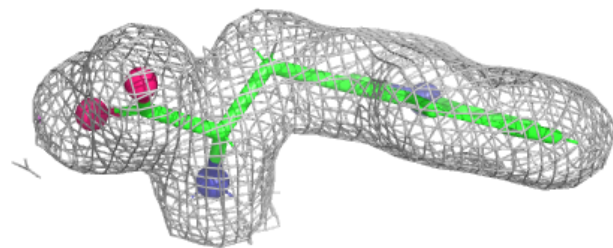
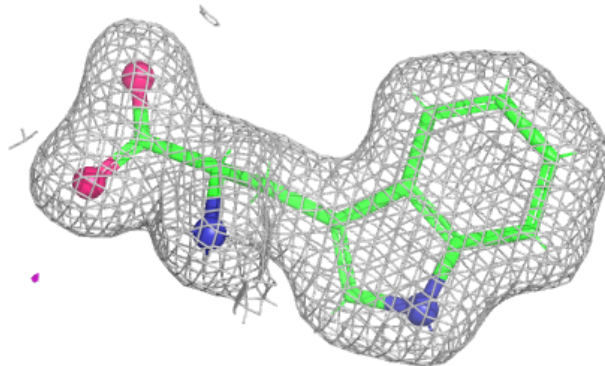
Electron density around MG DDD 504:

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



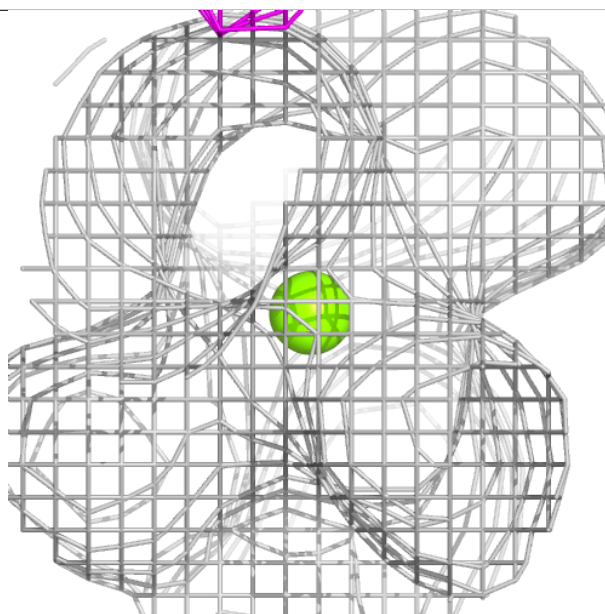
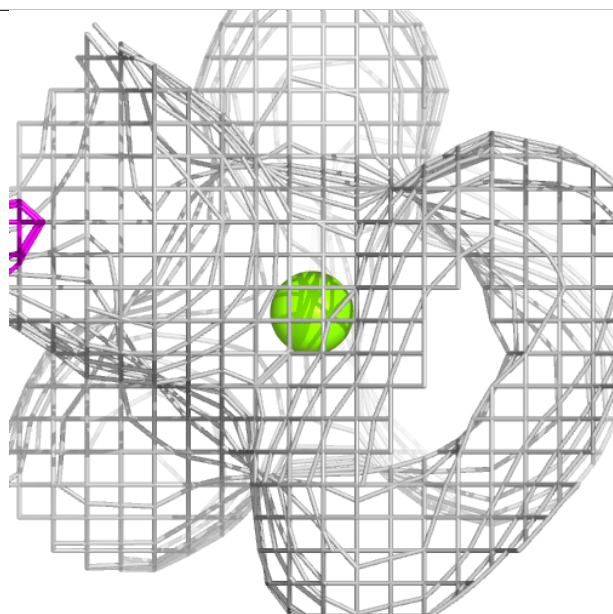
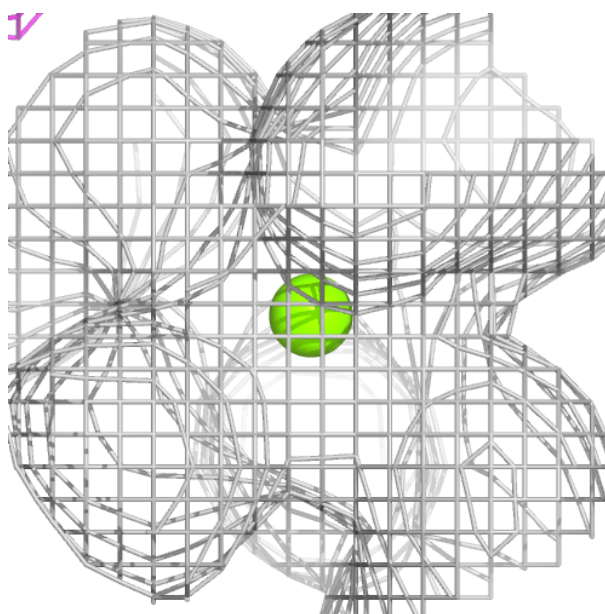
Electron density around TRP DDD 502:

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



Electron density around MG CCC 503:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.