



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:59 PM UTC

PDB ID : 8RP6 / pdb_00008rp6
Title : Aminodeoxychorismate synthase complex from Escherichia coli
Authors : Sung, S.; Funke, F.J.; Schlee, S.; Sterner, R.; Wilmanns, M.
Deposited on : 2024-01-12
Resolution : 2.45 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

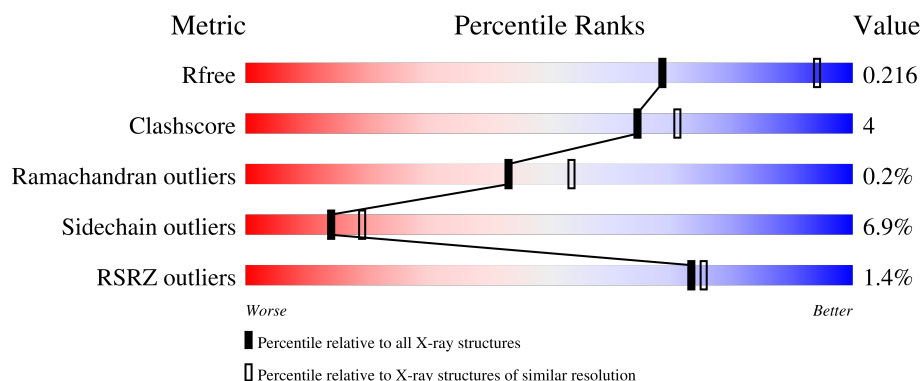
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	2% 81% 16% .
1	BBB	189	2% 83% 15% ..
2	CCC	454	% 88% 11% .
2	DDD	454	% 85% 13% .

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
6	MG	CCC	502	-	-	-	X
6	MG	DDD	502	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20274 atoms, of which 10016 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	189	Total	C	H	N	O	S	73	0	0
			2938	936	1467	260	267	8			
1	BBB	188	Total	C	H	N	O	S	73	0	0
			2929	934	1462	259	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	189	0	0
			7122	2268	3525	627	688	14			
2	DDD	454	Total	C	H	N	O	S	191	1	0
			7123	2269	3522	628	690	14			

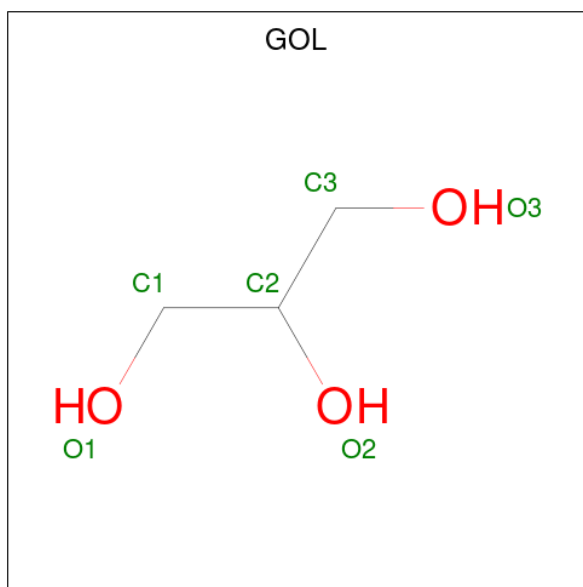
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

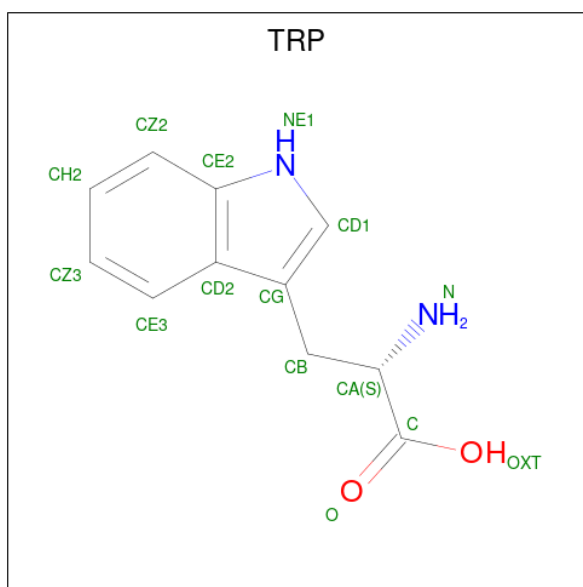
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Zn	0	0
			1	1		
3	BBB	1	Total	Zn	0	0
			1	1		

- 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	AAA	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 5 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
5	CCC	1	Total	C	H	N	O	0	0
			27	11	12	2	2		
5	DDD	1	Total	C	H	N	O	0	0
			27	11	12	2	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	4	Total	Cl	0	0
			4	4		
7	DDD	4	Total	Cl	0	0
			4	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	2	Total	O	0	0
			2	2		

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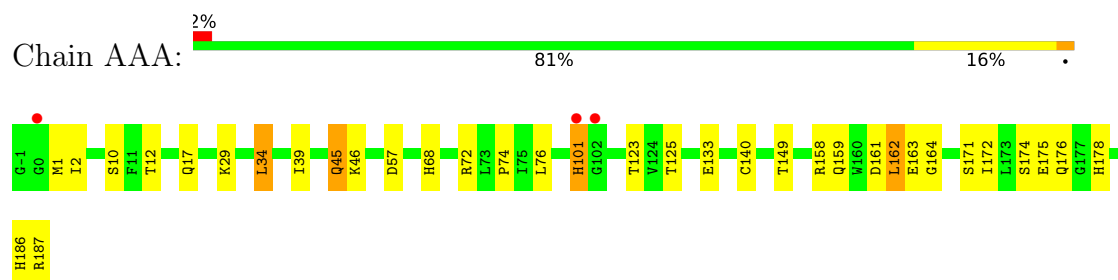
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	BBB	2	Total 2	O 2	0	0
8	CCC	35	Total 35	O 35	0	0
8	DDD	28	Total 28	O 28	0	0

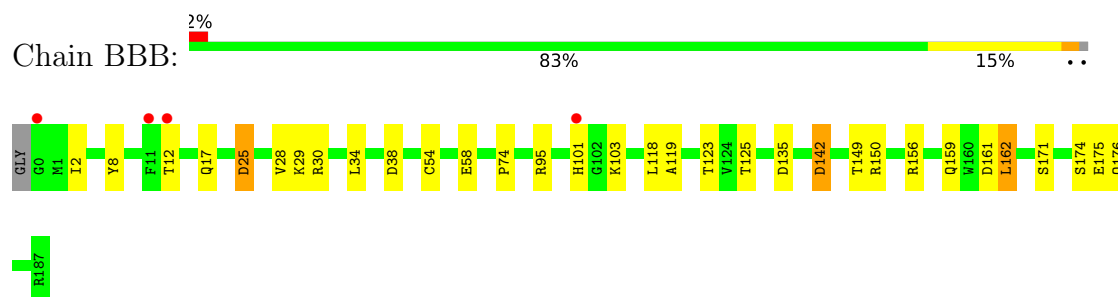
3 Residue-property plots [i](#)

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.

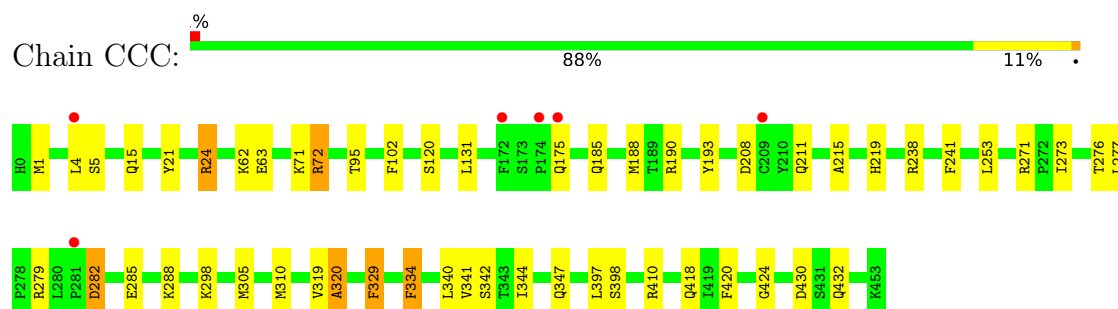
- Molecule 1: Aminodeoxychorismate synthase component 2



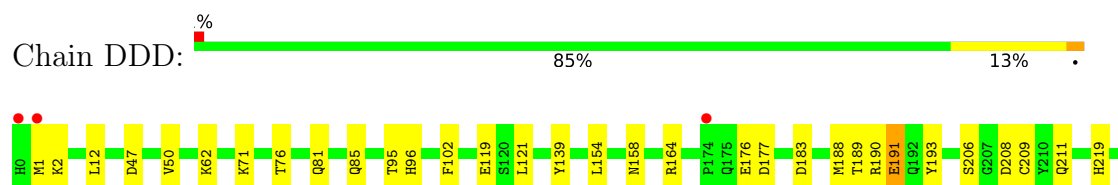
- Molecule 1: Aminodeoxychorismate synthase component 2

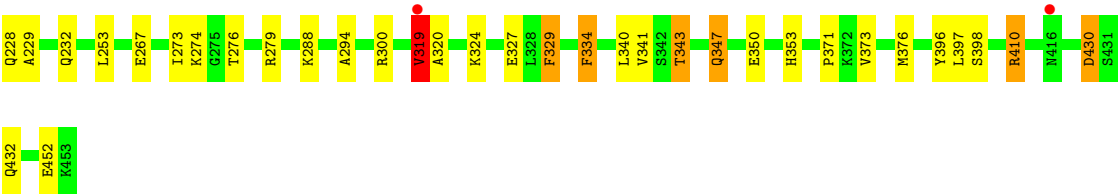


- Molecule 2: Aminodeoxychorismate synthase component 1



- Molecule 2: Aminodeoxychorismate synthase component 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.50Å 108.33Å 179.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.43 – 2.45 46.43 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.43-2.45) 100.0 (46.43-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.204 , 0.254 0.207 , 0.216	Depositor DCC
R_{free} test set	2872 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20274	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AAA	0.99	0/1507	1.39	1/2047 (0.0%)
1	BBB	1.01	0/1503	1.44	3/2042 (0.1%)
2	CCC	0.95	0/3677	1.35	6/4995 (0.1%)
2	DDD	0.95	0/3681	1.37	7/5002 (0.1%)
All	All	0.97	0/10368	1.37	17/14086 (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
2	DDD	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	208	ASP	CA-CB-CG	6.39	118.99	112.60
2	CCC	329	PHE	CB-CA-C	-6.04	102.17	111.66
1	BBB	25	ASP	CA-CB-CG	6.04	118.64	112.60
2	DDD	430	ASP	CA-CB-CG	5.75	118.35	112.60
2	CCC	432	GLN	CA-C-N	5.72	128.74	120.79
2	CCC	432	GLN	C-N-CA	5.72	128.74	120.79
2	DDD	432	GLN	CA-C-N	5.47	128.40	120.79
2	DDD	432	GLN	C-N-CA	5.47	128.40	120.79
2	CCC	208	ASP	CA-CB-CG	5.42	118.02	112.60
1	AAA	162	LEU	CB-CA-C	5.38	118.95	109.80
2	DDD	47	ASP	CA-CB-CG	5.31	117.91	112.60
1	BBB	142	ASP	CA-CB-CG	5.23	117.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	329	PHE	CB-CA-C	-5.22	103.47	111.66
2	DDD	334	PHE	CB-CA-C	5.19	117.11	109.22
2	CCC	241	PHE	CA-CB-CG	-5.11	108.69	113.80
1	BBB	162	LEU	CA-C-O	-5.05	114.89	120.24
2	CCC	334	PHE	CB-CA-C	5.04	116.87	109.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	DDD	319	VAL	Mainchain

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	1471	1467	1457	18	1
1	BBB	1467	1462	1454	12	0
2	CCC	3597	3525	3511	23	0
2	DDD	3601	3522	3505	28	2
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
4	AAA	12	16	16	2	0
5	CCC	15	12	9	0	0
5	DDD	15	12	9	0	0
6	CCC	2	0	0	0	1
6	DDD	1	0	0	0	0
7	CCC	4	0	0	2	0
7	DDD	4	0	0	1	0
8	AAA	2	0	0	0	0
8	BBB	2	0	0	0	0
8	CCC	35	0	0	0	0
8	DDD	28	0	0	1	0
All	All	10258	10016	9961	79	2

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 4.

All (79) 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:410:ARG:NH2	7:DDD:505:CL:CL	2.28	1.03
1:AAA:176:GLN:HA	4:AAA:303:GOL:H2	1.42	1.01
2:DDD:319:VAL:HG12	2:DDD:319:VAL:O	1.61	0.97
2:CCC:410:ARG:NH2	7:CCC:505:CL:CL	2.40	0.92
2:DDD:319:VAL:O	2:DDD:319:VAL:CG1	2.23	0.86
2:CCC:219:HIS:ND1	2:CCC:418:GLN:NE2	2.26	0.84
1:AAA:178:HIS:HB2	4:AAA:303:GOL:H11	1.60	0.80
2:DDD:189:THR:HG22	2:DDD:191:GLU:H	1.54	0.72
2:CCC:279:ARG:HD3	2:CCC:334:PHE:O	1.90	0.71
2:CCC:279:ARG:CD	2:CCC:334:PHE:O	2.40	0.70
2:CCC:282:ASP:HB3	2:CCC:285:GLU:HB3	1.77	0.67
2:DDD:294:ALA:O	2:DDD:300:ARG:NH1	2.28	0.65
1:BBB:118:LEU:HD22	1:BBB:176:GLN:HE21	1.64	0.63
1:AAA:161:ASP:OD1	1:AAA:187:ARG:NH1	2.36	0.58
2:DDD:267:GLU:CD	2:DDD:347:GLN:NE2	2.61	0.58
1:BBB:125:THR:HG22	1:BBB:174:SER:OG	2.04	0.57
2:DDD:267:GLU:CD	2:DDD:347:GLN:HE22	2.13	0.56
2:DDD:96:HIS:HB3	8:DDD:617:HOH:O	2.05	0.56
1:AAA:186:HIS:O	1:AAA:187:ARG:C	2.49	0.56
1:AAA:125:THR:HG22	1:AAA:174:SER:OG	2.06	0.55
2:DDD:279:ARG:HD2	2:DDD:334:PHE:O	2.06	0.55
1:BBB:17:GLN:OE1	2:CCC:320:ALA:O	2.23	0.55
2:CCC:188:MET:HE1	2:CCC:193:TYR:HD1	1.72	0.55
2:DDD:327:GLU:OE1	2:DDD:343:THR:CG2	2.54	0.54
1:AAA:46:LYS:HG2	1:AAA:74:PRO:HB2	1.90	0.53
2:DDD:188:MET:HE1	2:DDD:193:TYR:HD1	1.73	0.53
1:AAA:101:HIS:H	1:AAA:101:HIS:CD2	2.27	0.51
2:DDD:267:GLU:OE2	2:DDD:347:GLN:NE2	2.44	0.51
1:AAA:123:THR:HB	1:AAA:175:GLU:OE1	2.12	0.50
2:DDD:121:LEU:HD11	2:DDD:376:MET:HE2	1.93	0.49
2:CCC:21:TYR:O	2:CCC:24:ARG:HG3	2.12	0.49
2:DDD:189:THR:HG22	2:DDD:191:GLU:N	2.25	0.48
2:DDD:327:GLU:OE1	2:DDD:343:THR:HG23	2.13	0.48
2:DDD:119:GLU:HG2	2:DDD:373:VAL:HG22	1.94	0.48
2:DDD:81:GLN:HE21	2:DDD:85:GLN:HE21	1.62	0.47
2:DDD:279:ARG:CD	2:DDD:334:PHE:O	2.62	0.47
1:AAA:163:GLU:HG3	1:AAA:164:GLY:N	2.29	0.47
1:AAA:34:LEU:HD13	1:AAA:39:ILE:HG12	1.97	0.47
1:BBB:119:ALA:H	1:BBB:176:GLN:HE22	1.62	0.46
1:BBB:125:THR:HG21	1:BBB:171:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:62:LYS:HE3	7:CCC:506:CL:CL	2.53	0.46
1:BBB:54:CYS:HB2	1:BBB:58:GLU:HB2	1.98	0.45
2:CCC:329:PHE:HB3	2:CCC:340:LEU:HD11	1.99	0.45
1:BBB:8:TYR:CE1	1:BBB:30:ARG:HD2	2.52	0.45
2:CCC:71:LYS:HB2	2:CCC:71:LYS:HE2	1.80	0.43
1:AAA:45:GLN:HE21	1:AAA:45:GLN:HB3	1.52	0.43
2:DDD:329:PHE:HB3	2:DDD:340:LEU:HD11	2.01	0.43
2:CCC:215:ALA:HA	2:CCC:424:GLY:HA2	2.00	0.43
2:CCC:253:LEU:HD12	2:CCC:253:LEU:N	2.34	0.43
2:DDD:102:PHE:HA	2:DDD:398:SER:HB2	2.01	0.43
1:AAA:140:CYS:O	1:AAA:158:ARG:HG3	2.19	0.43
2:CCC:271:ARG:HA	2:CCC:342:SER:O	2.18	0.43
2:CCC:319:VAL:HG12	2:CCC:320:ALA:HB3	2.01	0.43
1:AAA:125:THR:HG21	1:AAA:171:SER:OG	2.18	0.42
2:CCC:185:GLN:CD	2:CCC:219:HIS:HE2	2.26	0.42
1:AAA:74:PRO:HA	1:AAA:161:ASP:O	2.19	0.42
1:BBB:74:PRO:HA	1:BBB:161:ASP:O	2.20	0.42
2:CCC:273:ILE:HG12	2:CCC:341:VAL:HG22	2.02	0.42
2:CCC:310:MET:HB2	2:CCC:344:ILE:HD13	2.02	0.42
1:AAA:2:ILE:HD12	1:AAA:46:LYS:HB2	2.00	0.42
2:CCC:72:ARG:HE	2:CCC:72:ARG:HB3	1.55	0.42
1:AAA:158:ARG:HH22	1:BBB:175:GLU:CD	2.28	0.42
2:DDD:253:LEU:HD12	2:DDD:253:LEU:N	2.34	0.42
1:BBB:118:LEU:HA	1:BBB:176:GLN:HE22	1.85	0.41
1:BBB:28:VAL:O	1:BBB:29:LYS:HD2	2.20	0.41
2:DDD:273:ILE:HG12	2:DDD:341:VAL:HG22	2.01	0.41
2:CCC:279:ARG:HD2	2:CCC:334:PHE:O	2.20	0.41
2:DDD:62:LYS:O	2:DDD:76:THR:HA	2.21	0.41
2:DDD:209:CYS:HA	2:DDD:371:PRO:HD2	2.03	0.41
2:DDD:229:ALA:O	2:DDD:232:GLN:HG2	2.20	0.41
2:CCC:418:GLN:HG2	2:CCC:420:PHE:CZ	2.56	0.41
1:AAA:68:HIS:O	1:AAA:72:ARG:HD3	2.20	0.41
1:AAA:34:LEU:HD23	1:AAA:34:LEU:HA	1.77	0.41
2:CCC:1:MET:HE2	2:CCC:1:MET:HB2	1.83	0.41
2:CCC:102:PHE:HA	2:CCC:398:SER:HB2	2.02	0.40
2:DDD:396:TYR:C	2:DDD:397:LEU:HD12	2.46	0.40
1:BBB:34:LEU:HD22	1:BBB:38:ASP:HB2	2.02	0.40
2:DDD:12:LEU:HD12	2:DDD:12:LEU:HA	1.85	0.40
2:DDD:50:VAL:HB	2:DDD:139:TYR:CD1	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:17:GLN:OE1	2:DDD:320:ALA:O[1_455]	1.98	0.22
2:DDD:353:HIS:HE2	6:CCC:503:MG:MG[3_545]	1.47	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	187/189 (99%)	183 (98%)	4 (2%)	0	100	100
1	BBB	186/189 (98%)	179 (96%)	7 (4%)	0	100	100
2	CCC	452/454 (100%)	434 (96%)	16 (4%)	2 (0%)	30	37
2	DDD	453/454 (100%)	436 (96%)	17 (4%)	0	100	100
All	All	1278/1286 (99%)	1232 (96%)	44 (3%)	2 (0%)	43	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CCC	282	ASP
2	CCC	320	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	157/157 (100%)	143 (91%)	14 (9%)	9	10
1	BBB	157/157 (100%)	143 (91%)	14 (9%)	9	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CCC	390/391 (100%)	369 (95%)	21 (5%)	20	29
2	DDD	390/391 (100%)	363 (93%)	27 (7%)	14	19
All	All	1094/1096 (100%)	1018 (93%)	76 (7%)	14	19

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1	MET
1	AAA	10	SER
1	AAA	12	THR
1	AAA	29	LYS
1	AAA	34	LEU
1	AAA	45	GLN
1	AAA	57	ASP
1	AAA	76	LEU
1	AAA	101	HIS
1	AAA	133	GLU
1	AAA	149	THR
1	AAA	159	GLN
1	AAA	162	LEU
1	AAA	172	ILE
1	BBB	2	ILE
1	BBB	12	THR
1	BBB	25	ASP
1	BBB	95	ARG
1	BBB	101	HIS
1	BBB	103	LYS
1	BBB	123	THR
1	BBB	135	ASP
1	BBB	142	ASP
1	BBB	149	THR
1	BBB	150	ARG
1	BBB	156	ARG
1	BBB	159	GLN
1	BBB	162	LEU
2	CCC	4	LEU
2	CCC	5	SER
2	CCC	15	GLN
2	CCC	24	ARG
2	CCC	63	GLU
2	CCC	72	ARG

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Mol	Chain	Res	Type
2	CCC	95	THR
2	CCC	120	SER
2	CCC	131	LEU
2	CCC	175	GLN
2	CCC	190	ARG
2	CCC	211	GLN
2	CCC	238	ARG
2	CCC	276	THR
2	CCC	277	LEU
2	CCC	288	LYS
2	CCC	298	LYS
2	CCC	305	MET
2	CCC	347	GLN
2	CCC	397	LEU
2	CCC	430	ASP
2	DDD	1	MET
2	DDD	2	LYS
2	DDD	71	LYS
2	DDD	95	THR
2	DDD	154	LEU
2	DDD	158	ASN
2	DDD	164	ARG
2	DDD	176	GLU
2	DDD	177	ASP
2	DDD	183	ASP
2	DDD	190	ARG
2	DDD	191	GLU
2	DDD	206	SER
2	DDD	211	GLN
2	DDD	219	HIS
2	DDD	228	GLN
2	DDD	274	LYS
2	DDD	276	THR
2	DDD	288	LYS
2	DDD	319	VAL
2	DDD	324	LYS
2	DDD	343	THR
2	DDD	347	GLN
2	DDD	350	GLU
2	DDD	410	ARG
2	DDD	430	ASP
2	DDD	452	GLU

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 17 ligands modelled in this entry, 13 are monoatomic - leaving 4 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	AAA	303	-	5,5,5	0.12	0	5,5,5	0.30	0
4	GOL	AAA	302	-	5,5,5	0.16	0	5,5,5	0.36	0
5	TRP	CCC	501	-	15,16,16	0.64	1 (6%)	18,22,22	0.57	0
5	TRP	DDD	501	-	15,16,16	0.89	1 (6%)	18,22,22	0.63	1 (5%)

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	AAA	303	-	-	2/4/4/4	-
4	GOL	AAA	302	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRP	CCC	501	-	-	0/8/8/8	0/2/2/2
5	TRP	DDD	501	-	-	0/8/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	DDD	501	TRP	OXT-C	-3.07	1.20	1.30
5	CCC	501	TRP	OXT-C	-2.13	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	DDD	501	TRP	OXT-C-O	-2.15	119.21	124.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	302	GOL	C1-C2-C3-O3
4	AAA	302	GOL	O1-C1-C2-C3
4	AAA	303	GOL	O1-C1-C2-C3
4	AAA	302	GOL	O2-C2-C3-O3
4	AAA	302	GOL	O1-C1-C2-O2
4	AAA	303	GOL	O1-C1-C2-O2

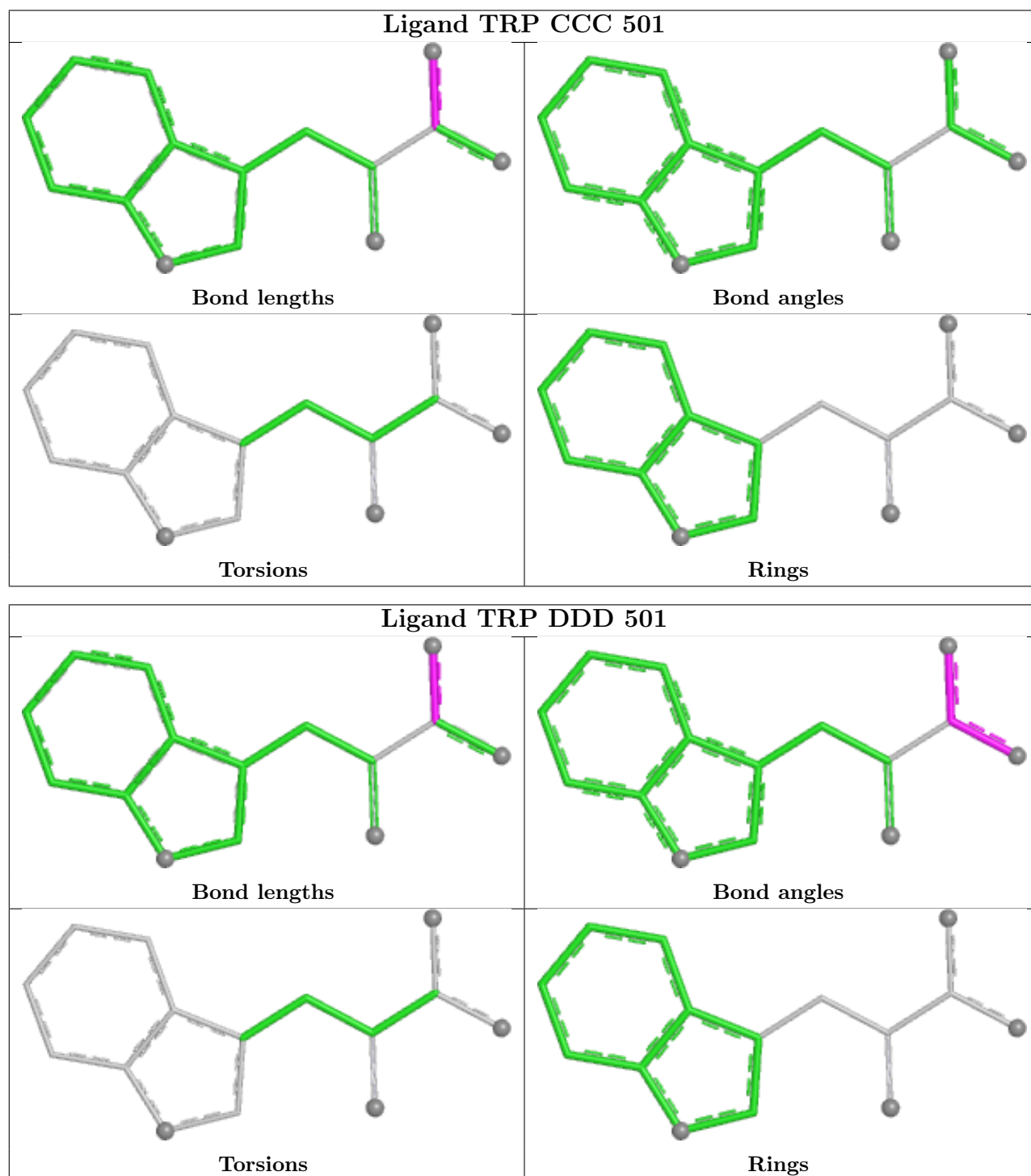
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	303	GOL	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	AAA	189/189 (100%)	0.23	3 (1%) 70 73	39, 60, 95, 130	0
1	BBB	188/189 (99%)	0.28	4 (2%) 63 65	42, 67, 95, 126	0
2	CCC	454/454 (100%)	-0.07	6 (1%) 75 77	32, 54, 90, 130	0
2	DDD	454/454 (100%)	-0.00	5 (1%) 78 79	27, 55, 95, 128	1 (0%)
All	All	1285/1286 (99%)	0.05	18 (1%) 73 75	27, 58, 95, 130	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	DDD	0	HIS	4.2
1	BBB	0	GLY	3.9
2	DDD	416[A]	ASN	3.9
1	BBB	101	HIS	3.0
1	AAA	101	HIS	2.9
2	CCC	209	CYS	2.8
2	CCC	174	PRO	2.7
2	CCC	4	LEU	2.7
1	BBB	11	PHE	2.6
1	AAA	102	GLY	2.6
2	CCC	172	PHE	2.5
2	CCC	175	GLN	2.4
2	CCC	281	PRO	2.4
2	DDD	319	VAL	2.3
1	AAA	0	GLY	2.2
1	BBB	12	THR	2.1
2	DDD	1	MET	2.1
2	DDD	174	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

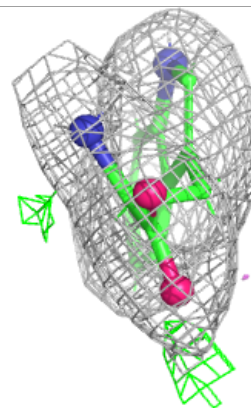
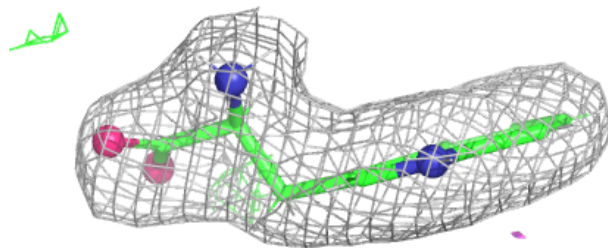
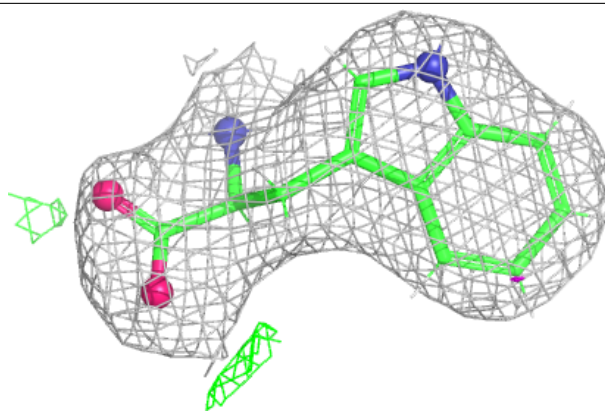
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	MG	DDD	502	1/1	0.61	0.41	79,79,79,79	0
6	MG	CCC	502	1/1	0.73	0.45	72,72,72,72	0
4	GOL	AAA	303	6/6	0.73	0.13	68,80,88,88	2
7	CL	DDD	503	1/1	0.78	0.21	90,90,90,90	0
4	GOL	AAA	302	6/6	0.82	0.13	71,78,80,81	2
7	CL	CCC	504	1/1	0.86	0.13	86,86,86,86	0
7	CL	DDD	505	1/1	0.91	0.13	65,65,65,65	0
7	CL	DDD	504	1/1	0.93	0.16	84,84,84,84	0
7	CL	CCC	505	1/1	0.93	0.10	63,63,63,63	0
7	CL	CCC	506	1/1	0.94	0.11	78,78,78,78	0
7	CL	CCC	507	1/1	0.95	0.27	54,54,54,54	0
5	TRP	DDD	501	15/15	0.97	0.07	33,37,42,54	0
5	TRP	CCC	501	15/15	0.97	0.06	34,36,45,53	0
7	CL	DDD	506	1/1	0.97	0.25	57,57,57,57	0
3	ZN	BBB	301	1/1	0.99	0.02	76,76,76,76	0
3	ZN	AAA	301	1/1	0.99	0.04	79,79,79,79	0
6	MG	CCC	503	1/1	0.99	0.01	48,48,48,48	0

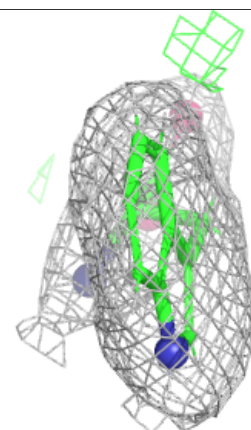
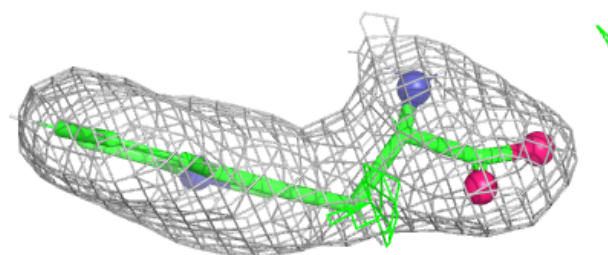
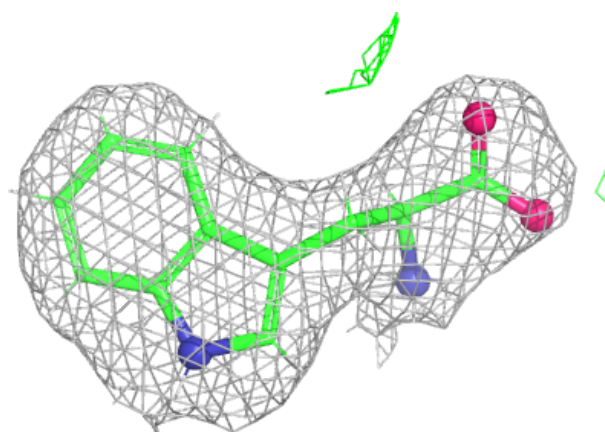
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TRP 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)

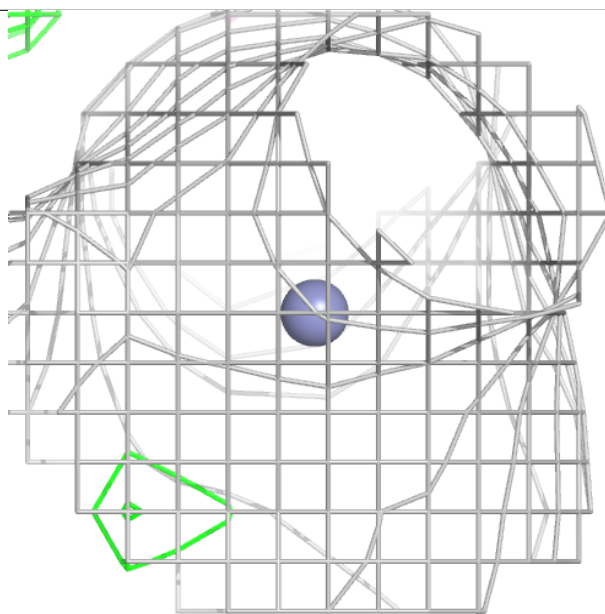
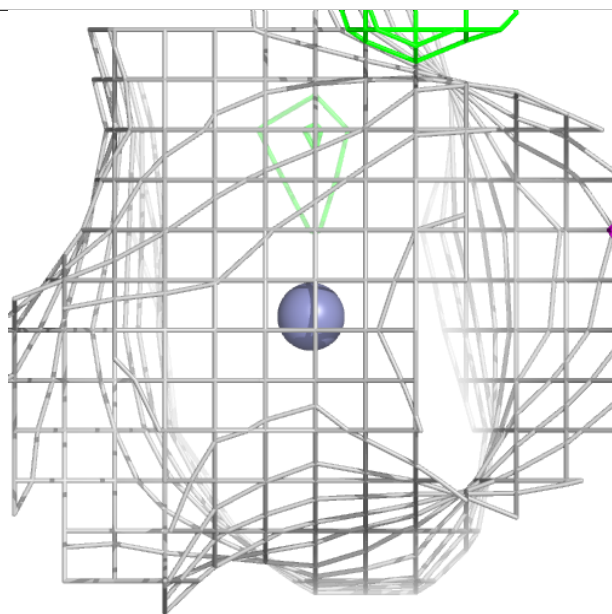
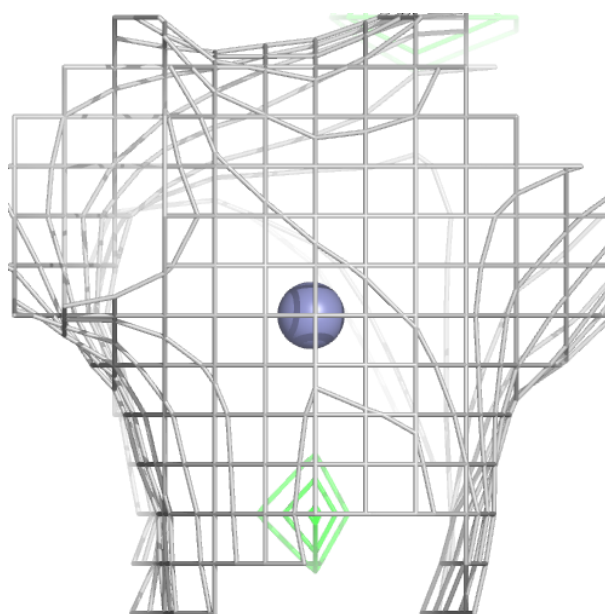
**Electron density around TRP CCC 501:**

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



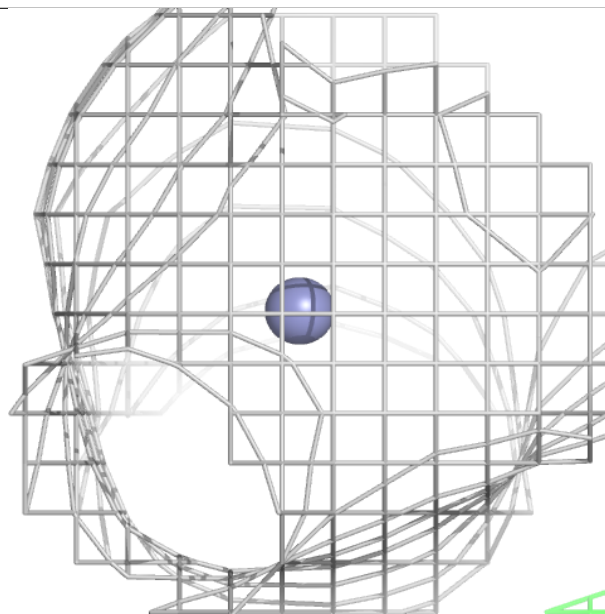
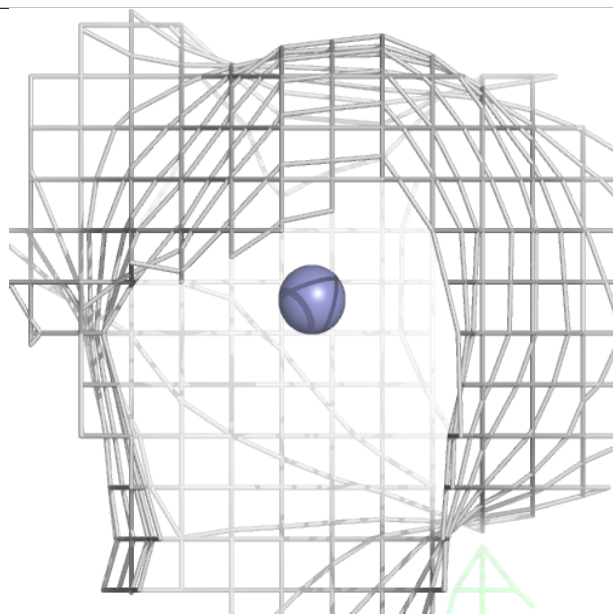
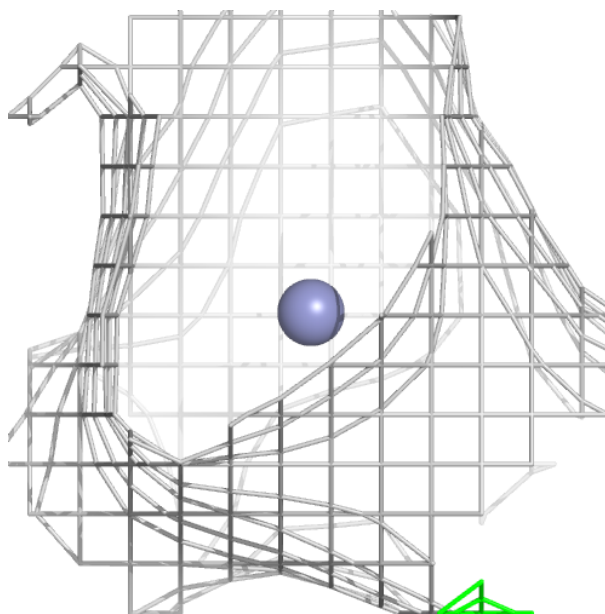
Electron density around ZN BBB 301:

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



Electron density around ZN AAA 301:

$2mF_o-DF_c$ (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.