



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:07 AM UTC

PDB ID : 8RP2 / pdb_00008rp2
Title : Aminodeoxychorismate synthase complex from Escherichia coli, with EDTA added
Authors : Sung, S.; Funke, F.J.; Schlee, S.; Sterner, R.; Wilmanns, M.
Deposited on : 2024-01-12
Resolution : 1.98 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

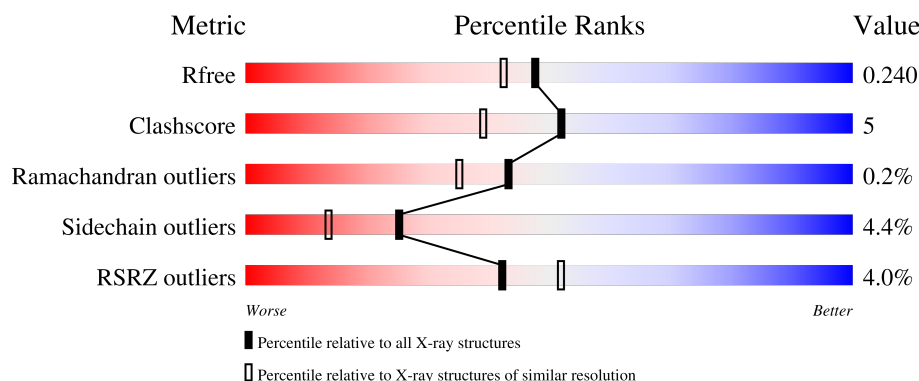
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	0% 85% 12% .
1	BBB	189	13% 86% 12% ..
2	CCC	454	2% 86% 12% .
2	DDD	454	3% 89% 11% .

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20537 atoms, of which 10045 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	76	2	0
			2967	945	1480	264	269	9			
1	BBB	187	Total	C	H	N	O	S	74	1	0
			2915	931	1454	256	265	9			

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	193	1	0
			7139	2275	3530	631	689	14			
2	DDD	454	Total	C	H	N	O	S	191	0	0
			7111	2267	3515	627	688	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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Cl	0	0
			1	1		

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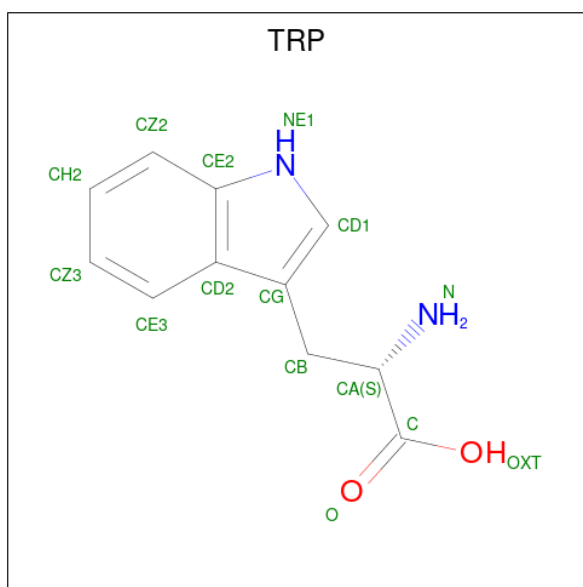
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CCC	5	Total	Cl	0	0
			5	5		
3	DDD	4	Total	Cl	0	0
			4	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂) (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	1	Total	Mg	0	0
			1	1		
6	DDD	2	Total	Mg	0	0
			2	2		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	CCC	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
7	DDD	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

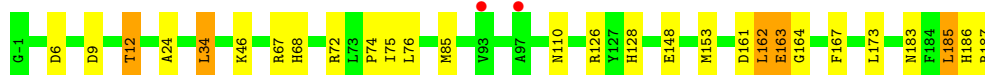
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	31	Total 31	O 31	0	0
9	BBB	8	Total 8	O 8	0	0
9	CCC	94	Total 94	O 94	0	0
9	DDD	107	Total 107	O 107	0	0

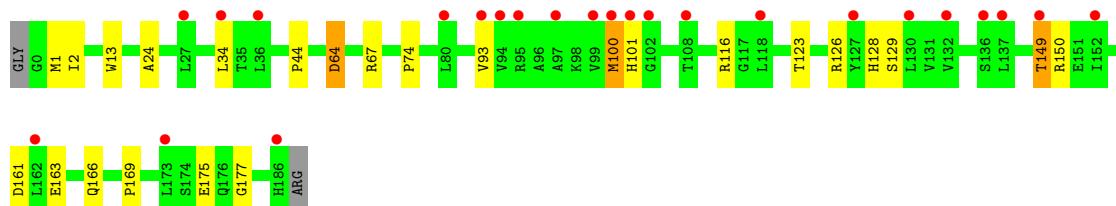
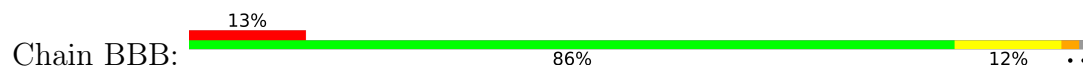
3 Residue-property plots

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.

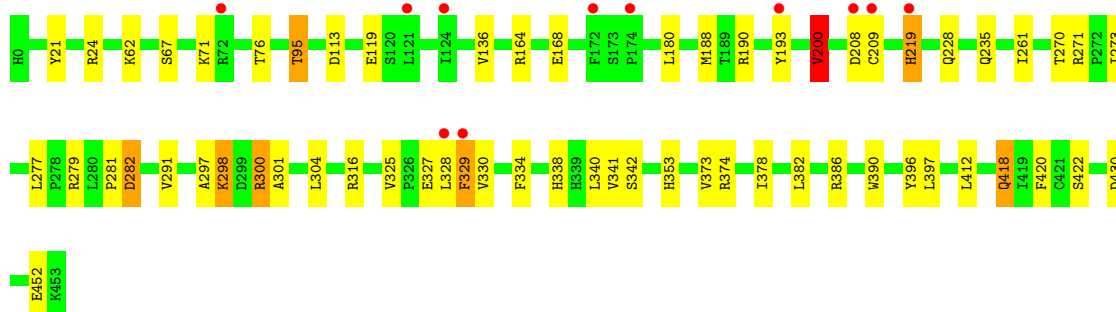
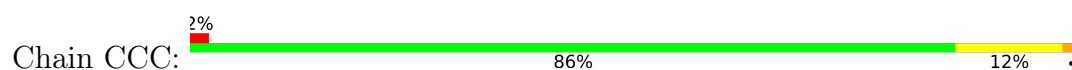
- Molecule 1: Aminodeoxychorismate synthase component 2



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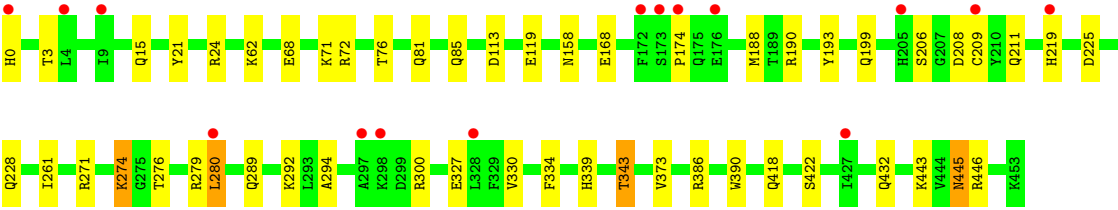


- Molecule 2: Aminodeoxychorismate synthase component 1



- 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	78.97Å 109.45Å 178.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.02 – 1.98 45.02 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.02-1.98) 100.0 (45.02-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.200 , 0.239 0.201 , 0.240	Depositor DCC
R_{free} test set	5381 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 36.8	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	20537	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: MES, MG, CL, GOL, SO4

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	1.08	0/1524	1.35	4/2070 (0.2%)
1	BBB	1.07	0/1497	1.32	2/2036 (0.1%)
2	CCC	1.02	0/3691	1.30	4/5015 (0.1%)
2	DDD	1.03	1/3677 (0.0%)	1.30	0/4997
All	All	1.04	1/10389 (0.0%)	1.31	10/14118 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	261	ILE	C-O	5.89	1.30	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	95	THR	N-CA-CB	6.07	119.04	110.36
1	AAA	163	GLU	CA-C-N	5.94	126.28	122.18
1	AAA	163	GLU	C-N-CA	5.94	126.28	122.18
1	BBB	163	GLU	CA-C-N	5.61	125.47	121.65
1	BBB	163	GLU	C-N-CA	5.61	125.47	121.65
2	CCC	95	THR	CB-CA-C	-5.60	98.20	109.68
2	CCC	208	ASP	CA-CB-CG	5.41	118.01	112.60
2	CCC	200	VAL	N-CA-CB	5.05	118.16	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	162	LEU	N-CA-CB	-5.03	103.01	110.71
1	AAA	164	GLY	CA-C-O	-5.01	116.60	121.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	DDD	208	ASP	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	1487	1480	1468	22	0
1	BBB	1461	1454	1446	11	0
2	CCC	3609	3530	3513	40	1
2	DDD	3596	3515	3498	31	0
3	AAA	1	0	0	0	0
3	CCC	5	0	0	0	0
3	DDD	4	0	0	1	0
4	AAA	10	0	0	0	0
4	CCC	5	0	0	0	0
4	DDD	5	0	0	0	0
5	CCC	15	12	9	0	0
5	DDD	15	12	9	0	0
6	CCC	1	0	0	0	0
6	DDD	2	0	0	0	1
7	CCC	12	13	13	3	0
7	DDD	12	13	13	0	0
8	CCC	6	8	8	2	0
8	DDD	6	8	8	1	0
9	AAA	31	0	0	2	0
9	BBB	8	0	0	1	0
9	CCC	94	0	0	2	0
9	DDD	107	0	0	2	0
All	All	10492	10045	9985	103	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 5.

All (103) 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:292:LYS:CB	9:DDD:698:HOH:O	2.17	0.90
1:AAA:183:ASN:O	1:AAA:187:ARG:HB2	1.73	0.87
1:AAA:67:ARG:NH2	9:AAA:902:HOH:O	2.13	0.81
1:AAA:9:ASP:HB3	1:AAA:12:THR:HG22	1.63	0.80
2:DDD:276:THR:HG21	2:DDD:443:LYS:HE2	1.66	0.75
2:DDD:276:THR:HG22	2:DDD:339:HIS:ND1	2.02	0.74
2:DDD:276:THR:HG22	2:DDD:339:HIS:HD1	1.53	0.72
2:CCC:219:HIS:HE1	2:CCC:418:GLN:HE21	1.37	0.71
1:AAA:34:LEU:O	9:AAA:901:HOH:O	2.09	0.70
2:DDD:276:THR:HG22	2:DDD:339:HIS:CE1	2.27	0.69
2:DDD:373:VAL:HB	8:DDD:509:GOL:H2	1.75	0.69
1:AAA:163:GLU:OE2	1:AAA:187:ARG:NH2	2.19	0.67
2:CCC:329:PHE:HB2	2:CCC:340:LEU:HG	1.78	0.66
2:CCC:325:VAL:O	7:CCC:508:MES:H62	1.97	0.65
1:BBB:100:MET:HE3	1:BBB:126:ARG:CZ	2.27	0.64
2:DDD:188:MET:HE1	2:DDD:193:TYR:HD1	1.64	0.63
2:CCC:188:MET:HE1	2:CCC:193:TYR:HD1	1.64	0.63
2:DDD:81:GLN:HE21	2:DDD:85:GLN:HE22	1.47	0.63
2:CCC:338:HIS:HD2	9:CCC:684:HOH:O	1.81	0.62
2:CCC:298:LYS:H	8:CCC:509:GOL:H11	1.65	0.62
2:DDD:327:GLU:HB3	2:DDD:343:THR:HG23	1.82	0.61
1:AAA:6:ASP:OD1	1:AAA:12:THR:HG21	2.00	0.61
2:DDD:280:LEU:HD23	2:DDD:289:GLN:CG	2.30	0.61
2:DDD:168:GLU:OE2	9:DDD:601:HOH:O	2.16	0.61
2:CCC:304:LEU:HD22	2:CCC:328:LEU:HD22	1.83	0.60
1:AAA:68[B]:HIS:CE1	1:AAA:72:ARG:HH12	2.19	0.59
2:DDD:276:THR:HG23	3:DDD:507:CL:CL	2.39	0.59
2:CCC:281:PRO:O	2:CCC:282:ASP:HB3	2.02	0.59
2:CCC:300:ARG:O	2:CCC:304:LEU:HG	2.04	0.58
2:CCC:329:PHE:CB	2:CCC:340:LEU:HG	2.34	0.57
2:DDD:81:GLN:HE21	2:DDD:85:GLN:NE2	2.03	0.57
2:DDD:119:GLU:HG2	2:DDD:373:VAL:HG22	1.87	0.56
2:CCC:188:MET:HE3	2:CCC:193:TYR:HA	1.89	0.55
1:AAA:126:ARG:HD2	1:AAA:128:HIS:NE2	2.21	0.55
2:DDD:188:MET:HE3	2:DDD:193:TYR:HA	1.89	0.54
2:CCC:338:HIS:CD2	9:CCC:684:HOH:O	2.59	0.53
2:DDD:280:LEU:HD23	2:DDD:289:GLN:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:85:MET:SD	1:AAA:162:LEU:HD13	2.49	0.52
2:CCC:304:LEU:CD2	2:CCC:328:LEU:HD22	2.39	0.52
2:CCC:21:TYR:O	2:CCC:24:ARG:HG2	2.10	0.52
2:CCC:374:ARG:O	2:CCC:378:ILE:HG12	2.09	0.52
1:BBB:2:ILE:HD13	1:BBB:24:ALA:HB1	1.92	0.51
2:DDD:225:ASP:OD2	2:DDD:228:GLN:NE2	2.44	0.51
1:BBB:149:THR:O	1:BBB:149:THR:OG1	2.29	0.50
1:BBB:169:PRO:O	1:BBB:177:GLY:HA3	2.11	0.50
1:AAA:85:MET:CG	1:AAA:162:LEU:HD11	2.42	0.50
1:AAA:110:ASN:HA	7:CCC:508:MES:H52	1.93	0.50
1:BBB:74:PRO:HA	1:BBB:161:ASP:O	2.13	0.49
2:CCC:261:ILE:HD13	2:CCC:270:THR:HB	1.94	0.49
1:AAA:75:ILE:HB	1:AAA:162:LEU:HD22	1.93	0.49
2:CCC:164:ARG:O	2:CCC:168:GLU:HG2	2.12	0.49
1:BBB:13:TRP:CE2	2:CCC:316:ARG:HD2	2.48	0.48
2:CCC:180:LEU:HD12	2:CCC:452:GLU:HA	1.95	0.48
2:CCC:279:ARG:HD2	2:CCC:334:PHE:O	2.13	0.48
1:BBB:128:HIS:CE1	1:BBB:166:GLN:HG3	2.48	0.48
2:CCC:119:GLU:HG2	2:CCC:373:VAL:HG22	1.96	0.48
1:AAA:68[B]:HIS:CE1	1:AAA:72:ARG:NH1	2.82	0.47
2:DDD:21:TYR:O	2:DDD:24:ARG:HG2	2.15	0.47
2:CCC:390:TRP:CD2	2:CCC:422:SER:HB2	2.49	0.47
1:AAA:186:HIS:HB2	2:CCC:291:VAL:HG21	1.96	0.47
2:CCC:271:ARG:HA	2:CCC:342:SER:O	2.15	0.46
1:BBB:67:ARG:HD3	9:BBB:204:HOH:O	2.14	0.46
2:DDD:445:ASN:HD22	2:DDD:445:ASN:HA	1.60	0.46
1:BBB:1:MET:HE2	1:BBB:44:PRO:HB3	1.98	0.46
1:AAA:46:LYS:HE3	1:AAA:185:LEU:O	2.16	0.46
1:BBB:64:ASP:OD2	1:BBB:64:ASP:N	2.48	0.46
1:AAA:153:MET:CE	1:AAA:167:PHE:HD1	2.29	0.46
2:CCC:297:ALA:HA	2:CCC:300:ARG:HG2	1.97	0.46
1:AAA:74:PRO:HA	1:AAA:161:ASP:O	2.17	0.45
7:CCC:508:MES:H31	7:CCC:508:MES:H81	1.78	0.45
2:DDD:271:ARG:HE	2:DDD:343:THR:CG2	2.29	0.45
2:CCC:396:TYR:C	2:CCC:397:LEU:HD22	2.42	0.45
1:BBB:123:THR:HB	1:BBB:175:GLU:OE2	2.17	0.44
2:CCC:298:LYS:N	8:CCC:509:GOL:H11	2.31	0.44
2:DDD:158:ASN:HD22	2:DDD:158:ASN:HA	1.63	0.44
2:CCC:200:VAL:HG12	2:CCC:382:LEU:CD1	2.47	0.44
2:DDD:279:ARG:HD2	2:DDD:334:PHE:O	2.17	0.44
2:CCC:219:HIS:CE1	2:CCC:418:GLN:HE21	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:9:ASP:HB3	1:AAA:12:THR:CG2	2.40	0.44
1:AAA:24:ALA:HB2	1:AAA:185:LEU:HD11	2.00	0.44
2:DDD:390:TRP:CD2	2:DDD:422:SER:HB2	2.52	0.44
2:DDD:327:GLU:CD	2:DDD:330:VAL:HG21	2.43	0.44
2:CCC:113:ASP:OD2	2:CCC:386:ARG:HB3	2.18	0.43
2:CCC:273:ILE:HG12	2:CCC:341:VAL:HG22	2.01	0.43
2:DDD:113:ASP:OD2	2:DDD:386:ARG:HB3	2.18	0.43
2:CCC:328:LEU:O	2:CCC:329:PHE:O	2.35	0.43
2:DDD:294:ALA:O	2:DDD:300:ARG:NH1	2.51	0.43
2:CCC:374:ARG:CZ	2:CCC:378:ILE:HD11	2.49	0.42
2:CCC:281:PRO:O	2:CCC:282:ASP:CB	2.66	0.42
2:CCC:327:GLU:OE2	2:CCC:330:VAL:HG21	2.19	0.42
2:CCC:300:ARG:HG3	2:CCC:301:ALA:N	2.35	0.42
2:DDD:327:GLU:CG	2:DDD:330:VAL:HG21	2.50	0.42
2:DDD:62:LYS:O	2:DDD:76:THR:HA	2.20	0.42
2:DDD:276:THR:CG2	2:DDD:339:HIS:CE1	3.00	0.42
1:AAA:161:ASP:OD1	1:AAA:187:ARG:NH1	2.53	0.41
2:CCC:329:PHE:HB2	2:CCC:340:LEU:CG	2.49	0.41
2:CCC:412:LEU:HA	2:CCC:420:PHE:O	2.21	0.41
2:DDD:211:GLN:HE22	2:DDD:274:LYS:HE3	1.86	0.41
1:AAA:85:MET:HG3	1:AAA:162:LEU:HD11	2.01	0.41
2:DDD:188:MET:HE3	2:DDD:193:TYR:CA	2.51	0.41
2:CCC:261:ILE:CD1	2:CCC:270:THR:HB	2.51	0.40
2:CCC:62:LYS:O	2:CCC:76:THR:HA	2.22	0.40
1:AAA:85:MET:CG	1:AAA:162:LEU:CD1	2.99	0.40

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	6:DDD:503:MG:MG[3_555]	1.29	0.31

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	189/189 (100%)	182 (96%)	7 (4%)	0	100	100
1	BBB	186/189 (98%)	180 (97%)	6 (3%)	0	100	100
2	CCC	453/454 (100%)	439 (97%)	12 (3%)	2 (0%)	30	20
2	DDD	452/454 (100%)	437 (97%)	14 (3%)	1 (0%)	43	35
All	All	1280/1286 (100%)	1238 (97%)	39 (3%)	3 (0%)	43	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CCC	282	ASP
2	CCC	329	PHE
2	DDD	174	PRO

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	159/157 (101%)	153 (96%)	6 (4%)	29	19
1	BBB	157/157 (100%)	148 (94%)	9 (6%)	18	8
2	CCC	391/391 (100%)	376 (96%)	15 (4%)	29	19
2	DDD	389/391 (100%)	371 (95%)	18 (5%)	24	12
All	All	1096/1096 (100%)	1048 (96%)	48 (4%)	25	14

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	12	THR
1	AAA	34	LEU
1	AAA	76	LEU
1	AAA	148	GLU
1	AAA	173	LEU

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Mol	Chain	Res	Type
1	AAA	185	LEU
1	BBB	34	LEU
1	BBB	64	ASP
1	BBB	93	VAL
1	BBB	100	MET
1	BBB	101	HIS
1	BBB	116	ARG
1	BBB	129	SER
1	BBB	149	THR
1	BBB	150	ARG
2	CCC	67	SER
2	CCC	71	LYS
2	CCC	95	THR
2	CCC	136	VAL
2	CCC	190	ARG
2	CCC	200	VAL
2	CCC	209	CYS
2	CCC	219	HIS
2	CCC	228	GLN
2	CCC	235	GLN
2	CCC	277	LEU
2	CCC	298	LYS
2	CCC	300	ARG
2	CCC	418	GLN
2	CCC	430	ASP
2	DDD	0	HIS
2	DDD	3	THR
2	DDD	15	GLN
2	DDD	68	GLU
2	DDD	71	LYS
2	DDD	72	ARG
2	DDD	190	ARG
2	DDD	199	GLN
2	DDD	206	SER
2	DDD	209	CYS
2	DDD	219	HIS
2	DDD	274	LYS
2	DDD	280	LEU
2	DDD	343	THR
2	DDD	418	GLN
2	DDD	432	GLN
2	DDD	445	ASN

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Mol	Chain	Res	Type
2	DDD	446	ARG

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 23 ligands modelled in this entry, 13 are monoatomic - leaving 10 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	$\# Z > 2$
7	MES	DDD	508	-	12,12,12	0.86	0	15,16,16	0.44	0
5	TRP	DDD	501	-	15,16,16	0.57	0	18,22,22	0.60	0
5	TRP	CCC	501	-	15,16,16	0.60	0	18,22,22	0.53	0
4	SO4	CCC	510	-	4,4,4	0.30	0	6,6,6	0.13	0
4	SO4	DDD	510	-	4,4,4	0.29	0	6,6,6	0.05	0
7	MES	CCC	508	-	12,12,12	0.83	0	15,16,16	0.82	0
8	GOL	DDD	509	-	5,5,5	0.07	0	5,5,5	0.32	0
8	GOL	CCC	509	-	5,5,5	0.15	0	5,5,5	0.46	0
4	SO4	AAA	803	-	4,4,4	0.29	0	6,6,6	0.08	0
4	SO4	AAA	802	-	4,4,4	0.29	0	6,6,6	0.25	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
7	MES	DDD	508	-	-	4/6/14/14	0/1/1/1
5	TRP	DDD	501	-	-	0/8/8/8	0/2/2/2
5	TRP	CCC	501	-	-	0/8/8/8	0/2/2/2
7	MES	CCC	508	-	-	2/6/14/14	0/1/1/1
8	GOL	DDD	509	-	-	4/4/4/4	-
8	GOL	CCC	509	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	CCC	508	MES	C8-C7-N4-C3
7	DDD	508	MES	C8-C7-N4-C3
8	CCC	509	GOL	C1-C2-C3-O3
8	DDD	509	GOL	O1-C1-C2-O2
8	DDD	509	GOL	O1-C1-C2-C3
8	DDD	509	GOL	C1-C2-C3-O3
8	CCC	509	GOL	O2-C2-C3-O3
8	DDD	509	GOL	O2-C2-C3-O3
7	DDD	508	MES	C7-C8-S-O3S
7	DDD	508	MES	C7-C8-S-O1S
7	DDD	508	MES	C7-C8-S-O2S
7	CCC	508	MES	N4-C7-C8-S

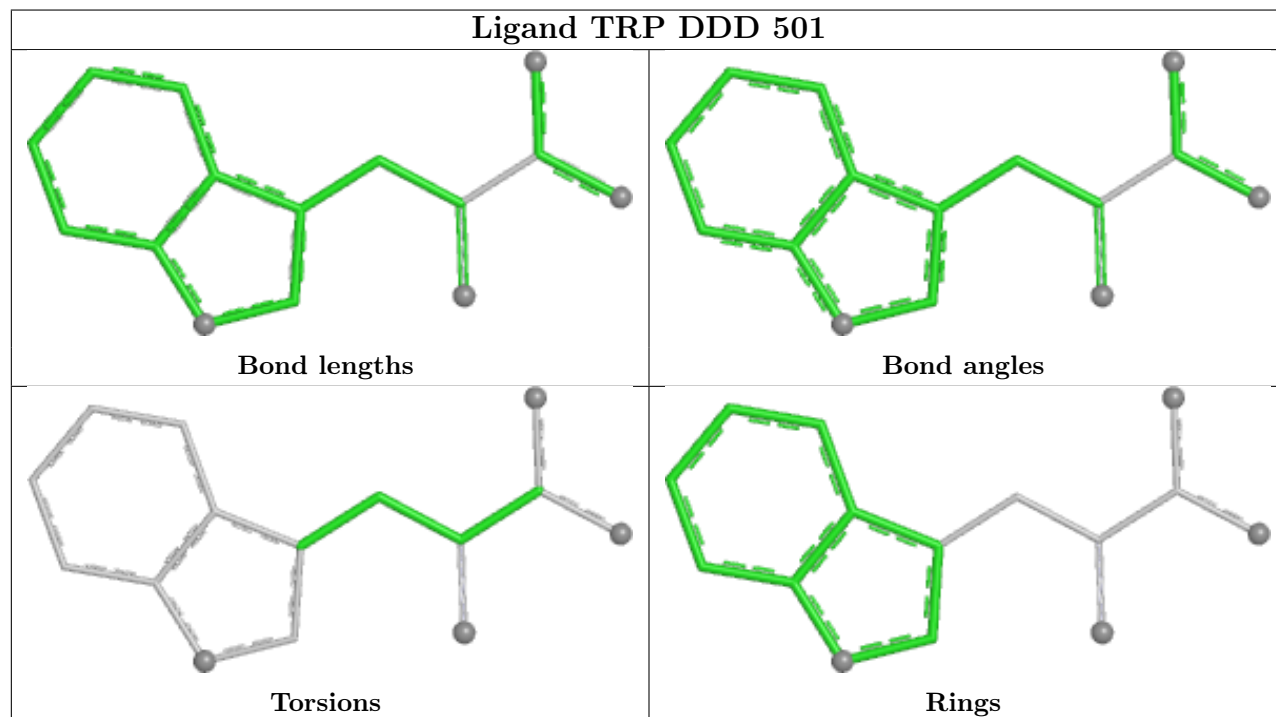
There are no ring outliers.

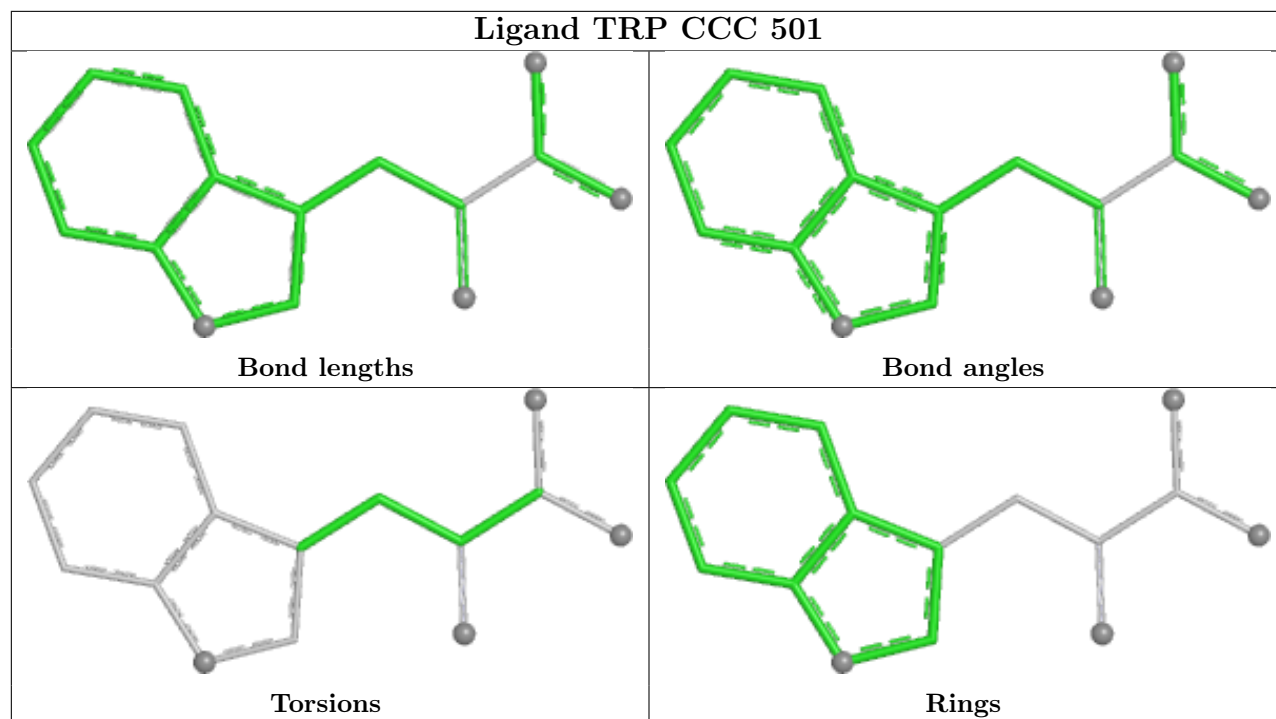
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	CCC	508	MES	3	0
8	DDD	509	GOL	1	0
8	CCC	509	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.21	2 (1%) 78 84	18, 44, 72, 100	2 (1%)
1	BBB	187/189 (98%)	1.00	24 (12%) 7 11	23, 58, 96, 128	1 (0%)
2	CCC	454/454 (100%)	0.22	11 (2%) 59 69	15, 43, 73, 114	1 (0%)
2	DDD	454/454 (100%)	0.27	15 (3%) 49 59	28, 44, 74, 115	0
All	All	1284/1286 (99%)	0.35	52 (4%) 42 52	15, 46, 78, 128	4 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	101	HIS	4.7
2	DDD	4	LEU	3.9
1	BBB	173	LEU	3.9
2	CCC	329	PHE	3.7
1	BBB	99	VAL	3.6
1	BBB	130	LEU	3.5
1	BBB	93	VAL	3.3
2	DDD	297	ALA	3.3
1	BBB	127	TYR	3.2
1	BBB	80	LEU	3.1
1	BBB	94	VAL	2.9
2	CCC	209	CYS	2.9
1	BBB	162	LEU	2.9
1	BBB	97	ALA	2.7
2	CCC	121	LEU	2.7
2	CCC	208	ASP	2.6
2	CCC	174	PRO	2.6
1	BBB	27	LEU	2.6
2	DDD	427	ILE	2.6
2	DDD	172	PHE	2.6
1	BBB	36	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	97	ALA	2.6
2	DDD	9	ILE	2.5
1	BBB	132	VAL	2.5
1	BBB	108	THR	2.5
2	CCC	172	PHE	2.5
1	BBB	136	SER	2.5
2	CCC	219	HIS	2.4
2	DDD	174	PRO	2.4
2	DDD	205	HIS	2.4
1	BBB	95	ARG	2.3
1	BBB	100	MET	2.3
2	DDD	280	LEU	2.3
2	CCC	193	TYR	2.2
2	DDD	0	HIS	2.2
1	BBB	152	ILE	2.2
2	DDD	298	LYS	2.2
2	DDD	209	CYS	2.2
1	BBB	186	HIS	2.1
2	DDD	219	HIS	2.1
1	BBB	102	GLY	2.1
2	DDD	328	LEU	2.1
2	CCC	124	ILE	2.1
1	AAA	93	VAL	2.1
1	BBB	34	LEU	2.1
1	BBB	118	LEU	2.1
2	DDD	176	GLU	2.1
2	DDD	173	SER	2.0
1	BBB	149	THR	2.0
1	BBB	137	LEU	2.0
2	CCC	328	LEU	2.0
2	CCC	72	ARG	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 ⓘ

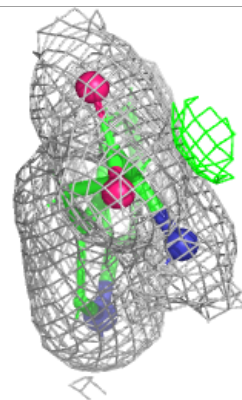
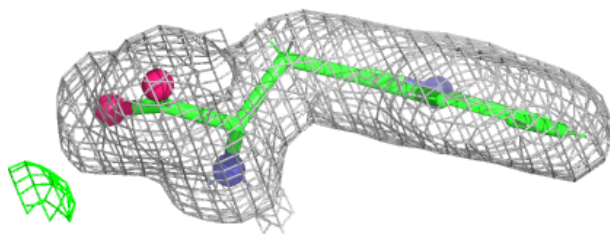
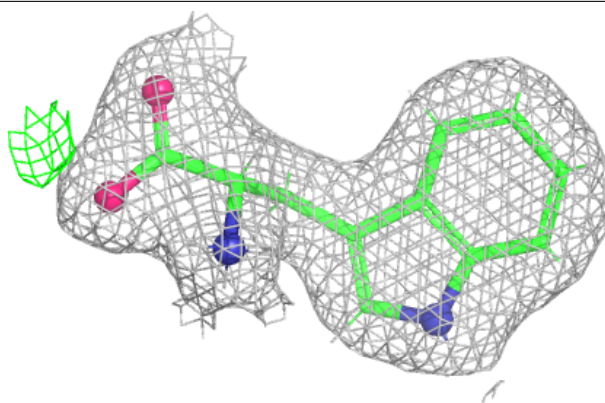
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	DDD	502	1/1	0.40	0.22	82,82,82,82	0
4	SO4	DDD	510	5/5	0.70	0.10	93,96,112,113	0
8	GOL	CCC	509	6/6	0.73	0.12	69,77,80,85	2
6	MG	CCC	502	1/1	0.75	0.24	70,70,70,70	0
4	SO4	AAA	803	5/5	0.79	0.10	87,90,92,98	0
7	MES	CCC	508	12/12	0.79	0.17	55,90,98,102	0
4	SO4	CCC	510	5/5	0.79	0.15	114,116,124,124	0
4	SO4	AAA	802	5/5	0.83	0.09	58,67,84,84	0
3	CL	AAA	801	1/1	0.85	0.20	82,82,82,82	0
7	MES	DDD	508	12/12	0.86	0.14	50,69,73,74	0
3	CL	CCC	504	1/1	0.86	0.19	78,78,78,78	0
8	GOL	DDD	509	6/6	0.87	0.10	50,60,69,71	2
3	CL	DDD	507	1/1	0.90	0.15	59,59,59,59	0
3	CL	DDD	506	1/1	0.91	0.19	79,79,79,79	0
3	CL	CCC	507	1/1	0.92	0.21	77,77,77,77	0
3	CL	CCC	506	1/1	0.94	0.17	55,55,55,55	0
3	CL	DDD	505	1/1	0.94	0.13	58,58,58,58	0
3	CL	DDD	504	1/1	0.95	0.09	53,53,53,53	0
3	CL	CCC	503	1/1	0.95	0.16	66,66,66,66	0
3	CL	CCC	505	1/1	0.96	0.08	52,52,52,52	0
5	TRP	CCC	501	15/15	0.97	0.05	27,30,33,35	0
5	TRP	DDD	501	15/15	0.97	0.05	30,31,35,37	0
6	MG	DDD	503	1/1	0.99	0.03	37,37,37,37	0

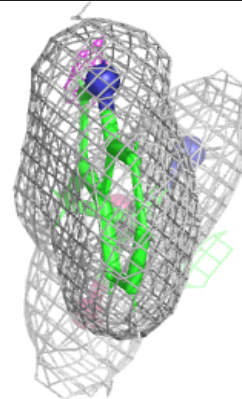
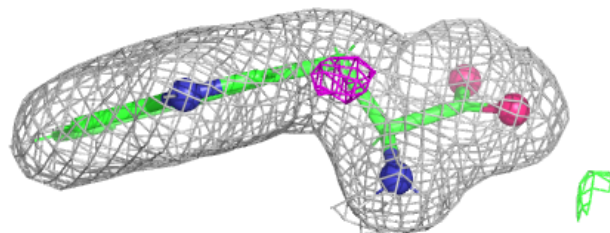
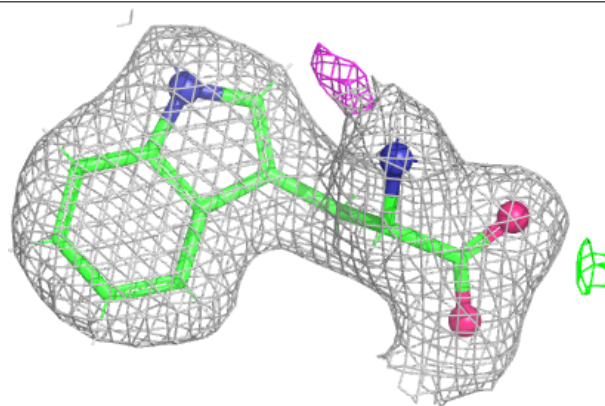
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TRP 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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.