



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:38 PM UTC

PDB ID : 8RP1 / pdb_00008rp1
Title : Aminodeoxychorismate synthase complex from Escherichia coli, with glutamine added
Authors : Sung, S.; Franziska, J.F.; Schlee, S.; Sterner, R.; Wilmanns, M.
Deposited on : 2024-01-12
Resolution : 1.86 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

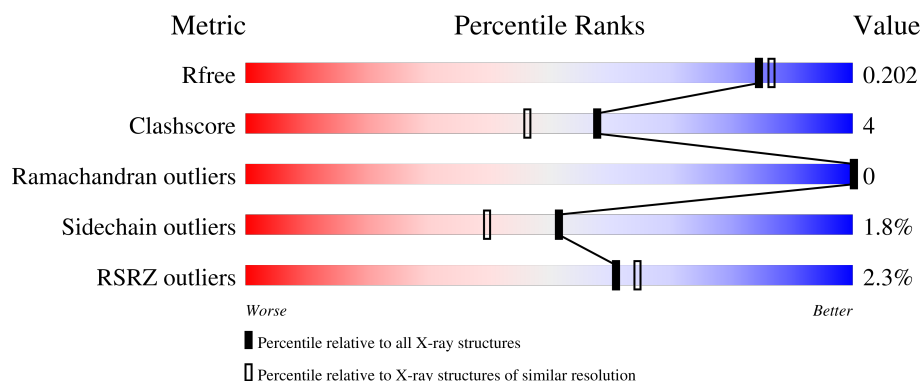
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	188	3% 91% 7%
1	BBB	188	5% 89% 10%
2	CCC	456	2% 91% 9%
2	DDD	456	% 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
3	GLU	AAA	201	-	-	X	-
5	SO4	AAA	207	-	-	X	-
6	MES	AAA	209	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21112 atoms, of which 10134 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
			2930	934	1464	259	265	8			
1	BBB	188	Total	C	H	N	O	S	73	0	0
			2930	934	1464	259	265	8			

There are 2 discrepancies between the modelled and reference sequences:

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

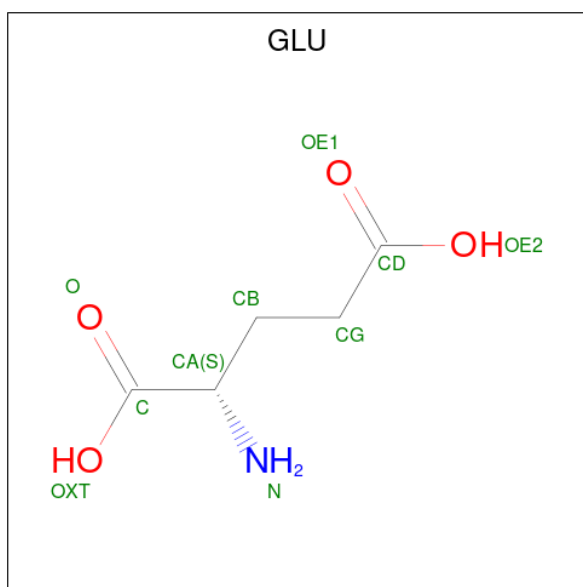
- Molecule 2 is a protein called Aminodeoxychorismate synthase component 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	CCC	456	Total	C	H	N	O	S	194	1	0
			7162	2281	3544	632	690	15			
2	DDD	455	Total	C	H	N	O	S	193	1	0
			7130	2273	3525	629	688	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-2	GLN	-	expression tag	UNP P05041
CCC	-1	GLY	-	expression tag	UNP P05041
CCC	0	HIS	-	expression tag	UNP P05041
DDD	-2	GLN	-	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).

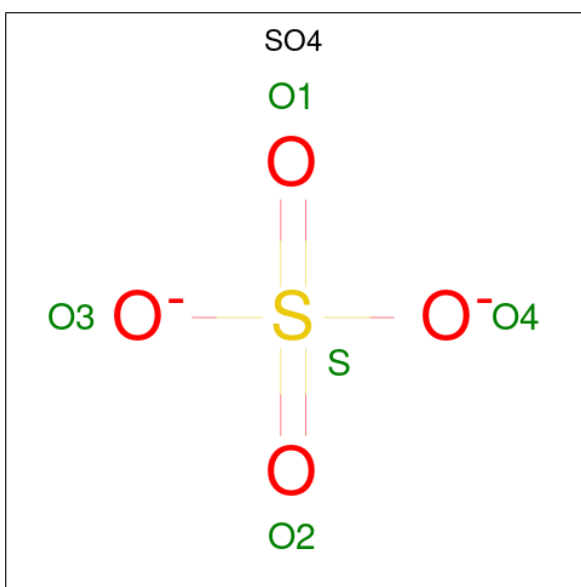


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	0	0
			17	5	8	1	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

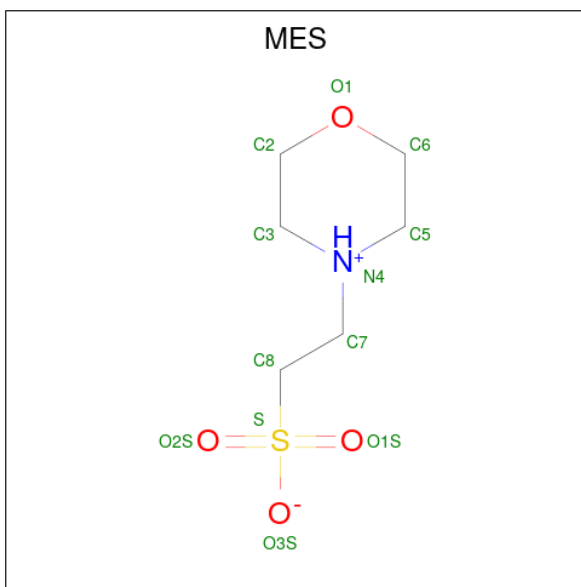
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	3	Total	Cl	0	0
			3	3		
4	CCC	8	Total	Cl	0	0
			8	8		
4	DDD	5	Total	Cl	0	0
			5	5		

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



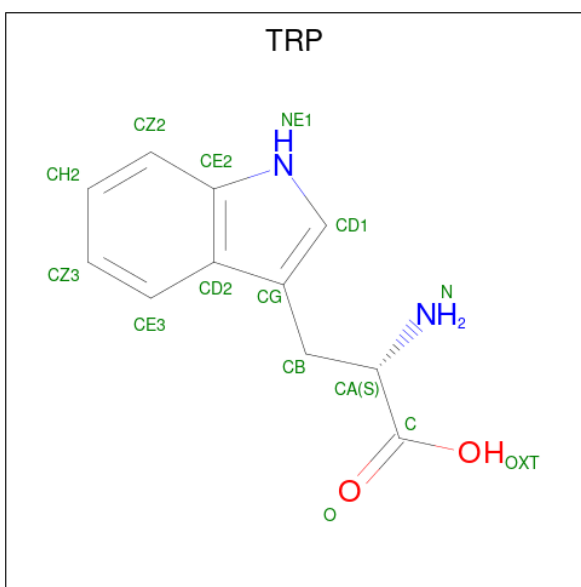
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

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

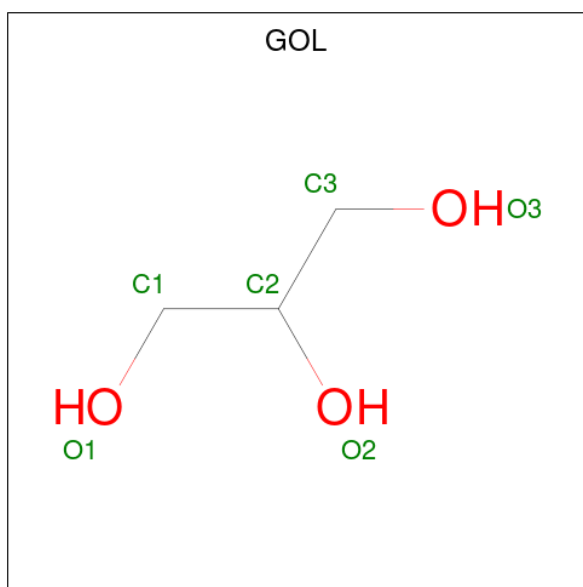


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	CCC	1	Total	C	H	N	O	0	0
			27	11	12	2	2		
7	DDD	1	Total	C	H	N	O	0	0
			27	11	12	2	2		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 10 is water.

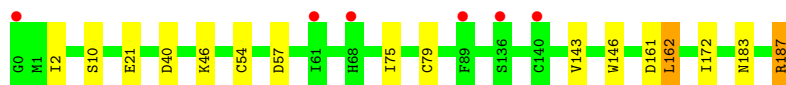
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	73	Total	O	0	0
			73	73		
10	BBB	43	Total	O	0	0
			43	43		
10	CCC	275	Total	O	0	0
			275	275		
10	DDD	234	Total	O	0	0
			234	234		

3 Residue-property plots [i](#)

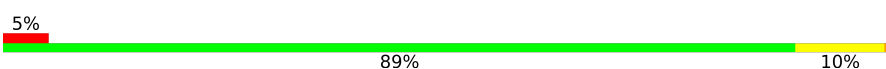
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

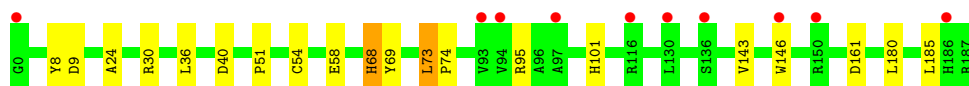
- Molecule 1: Aminodeoxychorismate synthase component 2

Chain AAA: 

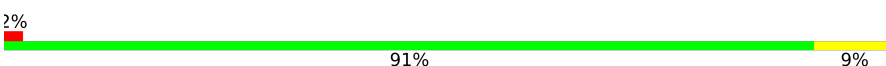


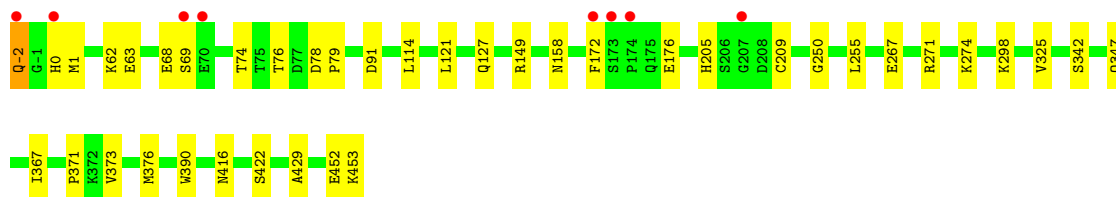
- Molecule 1: Aminodeoxychorismate synthase component 2

Chain BBB: 

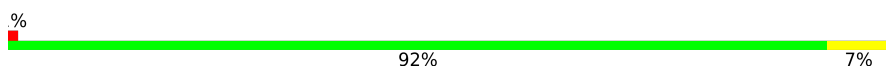


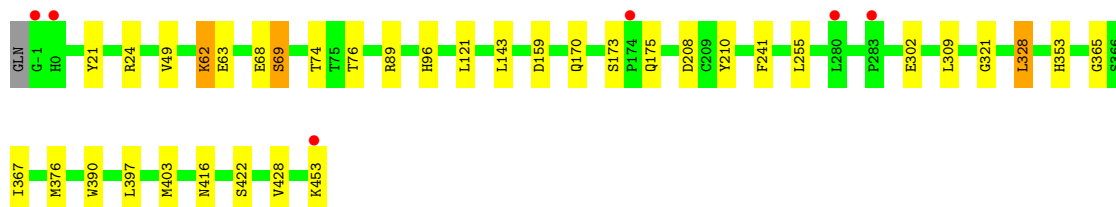
- Molecule 2: Aminodeoxychorismate synthase component 1

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	79.40Å 109.91Å 174.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 1.86 46.93 – 1.86	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.93-1.86) 100.0 (46.93-1.86)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.167 , 0.201 0.167 , 0.202	Depositor DCC
R_{free} test set	6391 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21112	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, GOL, SO4, CL

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	1.06	0/1502	1.25	1/2042 (0.0%)
1	BBB	1.06	0/1502	1.24	0/2042
2	CCC	1.02	0/3699	1.20	2/5024 (0.0%)
2	DDD	1.01	1/3686 (0.0%)	1.19	1/5008 (0.0%)
All	All	1.03	1/10389 (0.0%)	1.21	4/14116 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	96	HIS	CE1-NE2	5.82	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	187	ARG	CA-C-O	-6.70	109.42	120.80
2	DDD	241	PHE	CA-CB-CG	-5.89	107.91	113.80
2	CCC	78	ASP	CA-CB-CG	5.30	117.90	112.60
2	CCC	158	ASN	O-C-N	5.00	125.80	121.65

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	AAA	1466	1464	1454	19	0
1	BBB	1466	1464	1455	12	0
2	CCC	3618	3544	3526	28	0
2	DDD	3605	3525	3507	26	1
3	AAA	9	8	5	5	0
4	AAA	3	0	0	0	0
4	CCC	8	0	0	2	0
4	DDD	5	0	0	0	0
5	AAA	20	0	0	2	0
5	CCC	20	0	0	0	0
5	DDD	10	0	0	0	0
6	AAA	12	13	13	8	0
6	CCC	36	39	39	7	0
6	DDD	12	13	13	4	0
7	CCC	15	12	9	0	0
7	DDD	15	12	9	0	0
8	CCC	2	0	0	0	1
8	DDD	1	0	0	0	0
9	CCC	18	24	24	3	0
9	DDD	12	16	16	0	0
10	AAA	73	0	0	4	0
10	BBB	43	0	0	0	1
10	CCC	275	0	0	5	1
10	DDD	234	0	0	7	2
All	All	10978	10134	10070	91	3

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 (91) 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)
1:AAA:79:CYS:SG	3:AAA:201:GLU:CD	2.05	1.39
2:CCC:452:GLU:OE1	10:CCC:601:HOH:O	1.62	1.13
1:AAA:172:ILE:HD11	6:AAA:209:MES:O3S	1.62	1.00
6:DDD:508:MES:O3S	10:DDD:601:HOH:O	1.80	0.98
2:DDD:159:ASP:OD2	10:DDD:602:HOH:O	1.95	0.85
6:DDD:508:MES:O3S	10:DDD:603:HOH:O	1.95	0.84
2:DDD:89:ARG:NH1	10:DDD:604:HOH:O	2.14	0.79
2:CCC:205:HIS:HE1	10:CCC:602:HOH:O	1.66	0.78
1:AAA:57:ASP:OD1	10:AAA:301:HOH:O	2.01	0.77
2:CCC:-2:GLN:HB2	2:CCC:91:ASP:OD2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AAA:209:MES:O1S	10:AAA:302:HOH:O	2.03	0.76
1:AAA:172:ILE:CD1	6:AAA:209:MES:O3S	2.34	0.74
2:CCC:298:LYS:HE3	10:CCC:849:HOH:O	1.92	0.69
2:CCC:416:ASN:HD22	6:CCC:512:MES:H22	1.58	0.69
1:AAA:79:CYS:SG	3:AAA:201:GLU:CG	2.83	0.66
6:AAA:209:MES:H62	2:DDD:328:LEU:HD12	1.77	0.66
2:DDD:416:ASN:OD1	10:DDD:605:HOH:O	2.14	0.66
1:BBB:101:HIS:HD2	10:CCC:755:HOH:O	1.80	0.64
2:DDD:302:GLU:HG2	2:DDD:428:VAL:HG11	1.79	0.63
2:CCC:373:VAL:HB	9:CCC:516:GOL:H2	1.81	0.62
2:CCC:149:ARG:HD2	4:CCC:505:CL:CL	2.37	0.61
1:AAA:161:ASP:OD2	10:AAA:303:HOH:O	2.16	0.61
1:BBB:8:TYR:CE1	1:BBB:30:ARG:HD2	2.35	0.61
1:AAA:183:ASN:O	1:AAA:187:ARG:HG2	2.01	0.60
2:CCC:429:ALA:O	10:CCC:602:HOH:O	2.16	0.59
2:CCC:127:GLN:HE22	6:CCC:514:MES:H72	1.68	0.57
5:AAA:207:SO4:S	6:DDD:508:MES:H72	2.45	0.56
1:AAA:183:ASN:O	1:AAA:187:ARG:CG	2.54	0.56
2:DDD:397:LEU:HD21	2:DDD:403:MET:SD	2.47	0.55
2:CCC:267:GLU:OE2	2:CCC:347:GLN:OE1	2.24	0.54
1:AAA:75:ILE:HB	1:AAA:162:LEU:HD23	1.88	0.54
1:BBB:69:TYR:HB3	1:BBB:73:LEU:HD11	1.89	0.54
2:DDD:24:ARG:HD3	2:DDD:170:GLN:HB2	1.92	0.52
2:CCC:371:PRO:CB	9:CCC:516:GOL:H12	2.41	0.51
2:CCC:250:GLY:HA2	6:CCC:512:MES:H61	1.94	0.50
2:DDD:309:LEU:C	2:DDD:309:LEU:HD23	2.37	0.50
1:AAA:143:VAL:HG11	1:AAA:146:TRP:CE2	2.46	0.50
1:AAA:172:ILE:HD11	6:AAA:209:MES:S	2.51	0.50
2:DDD:63:GLU:HG3	2:DDD:74:THR:HG23	1.94	0.50
2:DDD:255:LEU:HD22	2:DDD:255:LEU:N	2.27	0.50
2:CCC:371:PRO:HB3	9:CCC:516:GOL:H12	1.95	0.49
1:AAA:172:ILE:HD11	6:AAA:209:MES:H81	1.93	0.49
1:BBB:143:VAL:HG11	1:BBB:146:TRP:CE2	2.49	0.48
6:AAA:209:MES:C6	2:DDD:328:LEU:HD12	2.43	0.48
2:CCC:390:TRP:CD2	2:CCC:422:SER:HB2	2.49	0.47
1:AAA:10:SER:HB3	2:DDD:309:LEU:HG	1.96	0.47
2:DDD:68:GLU:O	2:DDD:69:SER:C	2.57	0.47
2:DDD:309:LEU:HD22	2:DDD:365:GLY:HA3	1.96	0.47
1:BBB:8:TYR:CZ	1:BBB:30:ARG:HD2	2.50	0.47
2:CCC:267:GLU:CD	2:CCC:347:GLN:OE1	2.58	0.47
2:CCC:255:LEU:HD22	2:CCC:255:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:416:ASN:ND2	6:CCC:512:MES:H22	2.28	0.46
1:BBB:9:ASP:HB2	1:BBB:51:PRO:O	2.16	0.46
6:CCC:512:MES:H82	6:CCC:512:MES:H51	1.83	0.45
2:DDD:376[A]:MET:CE	10:DDD:725:HOH:O	2.64	0.45
2:CCC:68:GLU:O	2:CCC:69:SER:C	2.59	0.45
1:AAA:2:ILE:HD12	1:AAA:46:LYS:HB2	1.99	0.44
1:BBB:69:TYR:HB3	1:BBB:73:LEU:CD1	2.47	0.44
1:BBB:74:PRO:HA	1:BBB:161:ASP:O	2.17	0.44
2:CCC:325:VAL:O	6:CCC:513:MES:H22	2.18	0.44
2:DDD:21:TYR:O	2:DDD:24:ARG:HG2	2.18	0.44
3:AAA:201:GLU:HG2	2:DDD:210:TYR:OH	2.17	0.44
2:DDD:390:TRP:CD2	2:DDD:422:SER:HB2	2.53	0.43
1:AAA:79:CYS:SG	3:AAA:201:GLU:OE1	2.66	0.43
1:BBB:54:CYS:HB2	1:BBB:58:GLU:HB2	2.00	0.43
1:AAA:54:CYS:HA	10:DDD:619:HOH:O	2.17	0.43
2:DDD:49:VAL:HB	2:DDD:143:LEU:HB3	2.01	0.43
5:AAA:207:SO4:O3	6:DDD:508:MES:H51	2.18	0.43
2:CCC:63:GLU:HG3	2:CCC:74:THR:HG23	2.00	0.43
2:CCC:79:PRO:HG2	2:CCC:114:LEU:HD11	2.01	0.42
1:AAA:172:ILE:HD11	6:AAA:209:MES:C8	2.48	0.42
2:CCC:-2:GLN:H2	2:CCC:1:MET:HE1	1.85	0.42
1:AAA:21:GLU:CG	2:DDD:321:GLY:HA2	2.50	0.42
2:CCC:390:TRP:CE2	2:CCC:422:SER:HB2	2.55	0.42
4:CCC:511:CL:CL	6:CCC:512:MES:H72	2.57	0.41
1:BBB:24:ALA:HB2	1:BBB:185:LEU:HD11	2.02	0.41
2:CCC:121:LEU:HD11	2:CCC:376[A]:MET:HE2	2.02	0.41
1:BBB:36:LEU:HD13	1:BBB:68:HIS:CE1	2.56	0.41
2:DDD:121:LEU:CD1	2:DDD:376[A]:MET:HE2	2.50	0.41
2:CCC:271:ARG:HA	2:CCC:342:SER:O	2.21	0.41
1:AAA:183:ASN:O	1:AAA:187:ARG:HG3	2.21	0.41
2:DDD:367:ILE:HD12	2:DDD:367:ILE:C	2.46	0.41
3:AAA:201:GLU:CD	10:AAA:337:HOH:O	2.63	0.41
2:CCC:62:LYS:O	2:CCC:76:THR:HA	2.21	0.41
2:CCC:63:GLU:HG3	2:CCC:74:THR:CG2	2.50	0.41
2:CCC:367:ILE:HD12	2:CCC:367:ILE:C	2.46	0.41
2:DDD:24:ARG:CD	2:DDD:170:GLN:HB2	2.50	0.41
2:DDD:63:GLU:CG	2:DDD:74:THR:HG23	2.51	0.41
2:DDD:397:LEU:CD2	2:DDD:403:MET:SD	3.09	0.40
2:DDD:62:LYS:O	2:DDD:76:THR:HA	2.20	0.40
1:BBB:180:LEU:C	1:BBB:180:LEU:HD23	2.47	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CCC:793:HOH:O	10:DDD:604:HOH:O[3_454]	1.81	0.39
2:DDD:353:HIS:HE2	8:CCC:503:MG:MG[3_444]	1.33	0.27
10:BBB:208:HOH:O	10:DDD:602:HOH:O[3_454]	2.12	0.08

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	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
1	BBB	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
2	CCC	455/456 (100%)	442 (97%)	13 (3%)	0	100	100
2	DDD	454/456 (100%)	442 (97%)	12 (3%)	0	100	100
All	All	1281/1288 (100%)	1248 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	155 (99%)	2 (1%)	61	51
1	BBB	157/157 (100%)	153 (98%)	4 (2%)	42	27
2	CCC	391/392 (100%)	384 (98%)	7 (2%)	51	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DDD	389/392 (99%)	382 (98%)	7 (2%)	51	40
All	All	1094/1098 (100%)	1074 (98%)	20 (2%)	51	40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	40	ASP
1	AAA	162	LEU
1	BBB	40	ASP
1	BBB	68	HIS
1	BBB	73	LEU
1	BBB	95	ARG
2	CCC	-2	GLN
2	CCC	0	HIS
2	CCC	172	PHE
2	CCC	176	GLU
2	CCC	209	CYS
2	CCC	274	LYS
2	CCC	453	LYS
2	DDD	62	LYS
2	DDD	69	SER
2	DDD	173	SER
2	DDD	175	GLN
2	DDD	208	ASP
2	DDD	328	LEU
2	DDD	453	LYS

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

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 19 are monoatomic - leaving 23 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	$\# Z > 2$
6	MES	DDD	508	-	12,12,12	0.88	0	15,16,16	0.62	0
5	SO4	CCC	520	-	4,4,4	0.39	0	6,6,6	0.14	0
5	SO4	CCC	521	-	4,4,4	0.27	0	6,6,6	0.17	0
5	SO4	AAA	208	-	4,4,4	0.38	0	6,6,6	0.13	0
5	SO4	DDD	511	-	4,4,4	0.30	0	6,6,6	0.12	0
7	TRP	CCC	501	-	15,16,16	0.53	0	18,22,22	0.61	0
9	GOL	DDD	510	-	5,5,5	0.16	0	5,5,5	0.41	0
5	SO4	AAA	206	-	4,4,4	0.28	0	6,6,6	0.17	0
9	GOL	CCC	517	-	5,5,5	0.08	0	5,5,5	0.31	0
5	SO4	CCC	518	-	4,4,4	0.31	0	6,6,6	0.31	0
5	SO4	AAA	205	-	4,4,4	0.30	0	6,6,6	0.22	0
9	GOL	CCC	515	-	5,5,5	0.14	0	5,5,5	0.41	0
7	TRP	DDD	501	-	15,16,16	0.76	1 (6%)	18,22,22	0.74	0
5	SO4	AAA	207	-	4,4,4	0.25	0	6,6,6	0.15	0
6	MES	CCC	514	-	12,12,12	0.69	0	15,16,16	0.50	0
3	GLU	AAA	201	-	6,8,9	0.78	0	6,9,11	0.77	0
6	MES	CCC	513	-	12,12,12	0.79	0	15,16,16	0.64	0
9	GOL	CCC	516	-	5,5,5	0.27	0	5,5,5	0.33	0
5	SO4	DDD	512	-	4,4,4	0.29	0	6,6,6	0.19	0
6	MES	CCC	512	-	12,12,12	1.17	1 (8%)	15,16,16	0.95	0
9	GOL	DDD	509	-	5,5,5	0.23	0	5,5,5	0.52	0
6	MES	AAA	209	-	12,12,12	0.93	0	15,16,16	0.71	0
5	SO4	CCC	519	-	4,4,4	0.33	0	6,6,6	0.28	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
6	MES	DDD	508	-	-	3/6/14/14	0/1/1/1
6	MES	CCC	514	-	-	3/6/14/14	0/1/1/1
9	GOL	CCC	515	-	-	4/4/4/4	-
9	GOL	DDD	509	-	-	4/4/4/4	-
6	MES	CCC	513	-	-	5/6/14/14	0/1/1/1
3	GLU	AAA	201	-	-	0/8/8/9	-
7	TRP	CCC	501	-	-	0/8/8/8	0/2/2/2
9	GOL	DDD	510	-	-	2/4/4/4	-
9	GOL	CCC	516	-	-	4/4/4/4	-
6	MES	AAA	209	-	-	5/6/14/14	0/1/1/1
6	MES	CCC	512	-	-	5/6/14/14	0/1/1/1
7	TRP	DDD	501	-	-	0/8/8/8	0/2/2/2
9	GOL	CCC	517	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CCC	512	MES	C8-S	2.68	1.81	1.77
7	DDD	501	TRP	OXT-C	-2.28	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	209	MES	C7-C8-S-O1S
6	AAA	209	MES	C7-C8-S-O2S
6	CCC	512	MES	C8-C7-N4-C5
6	CCC	513	MES	C8-C7-N4-C3
6	CCC	513	MES	C7-C8-S-O2S
6	CCC	513	MES	C7-C8-S-O3S
6	CCC	514	MES	N4-C7-C8-S
9	CCC	515	GOL	O1-C1-C2-C3
9	CCC	515	GOL	C1-C2-C3-O3
9	CCC	516	GOL	O1-C1-C2-C3
9	CCC	516	GOL	C1-C2-C3-O3
9	CCC	516	GOL	O2-C2-C3-O3
9	CCC	517	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	CCC	517	GOL	C1-C2-C3-O3
9	DDD	509	GOL	C1-C2-C3-O3
9	DDD	509	GOL	O2-C2-C3-O3
9	CCC	515	GOL	O2-C2-C3-O3
6	DDD	508	MES	C7-C8-S-O3S
9	DDD	509	GOL	O1-C1-C2-C3
9	DDD	510	GOL	O1-C1-C2-C3
9	CCC	515	GOL	O1-C1-C2-O2
9	CCC	516	GOL	O1-C1-C2-O2
9	CCC	517	GOL	O1-C1-C2-O2
9	DDD	509	GOL	O1-C1-C2-O2
6	AAA	209	MES	C7-C8-S-O3S
6	CCC	514	MES	C8-C7-N4-C5
9	CCC	517	GOL	O2-C2-C3-O3
9	DDD	510	GOL	O1-C1-C2-O2
6	CCC	512	MES	C7-C8-S-O1S
6	CCC	513	MES	C7-C8-S-O1S
6	DDD	508	MES	C7-C8-S-O1S
6	DDD	508	MES	C7-C8-S-O2S
6	AAA	209	MES	N4-C7-C8-S
6	CCC	512	MES	N4-C7-C8-S
6	CCC	513	MES	N4-C7-C8-S
6	CCC	514	MES	C8-C7-N4-C3
6	CCC	512	MES	C7-C8-S-O3S
6	CCC	512	MES	C7-C8-S-O2S
6	AAA	209	MES	C8-C7-N4-C3

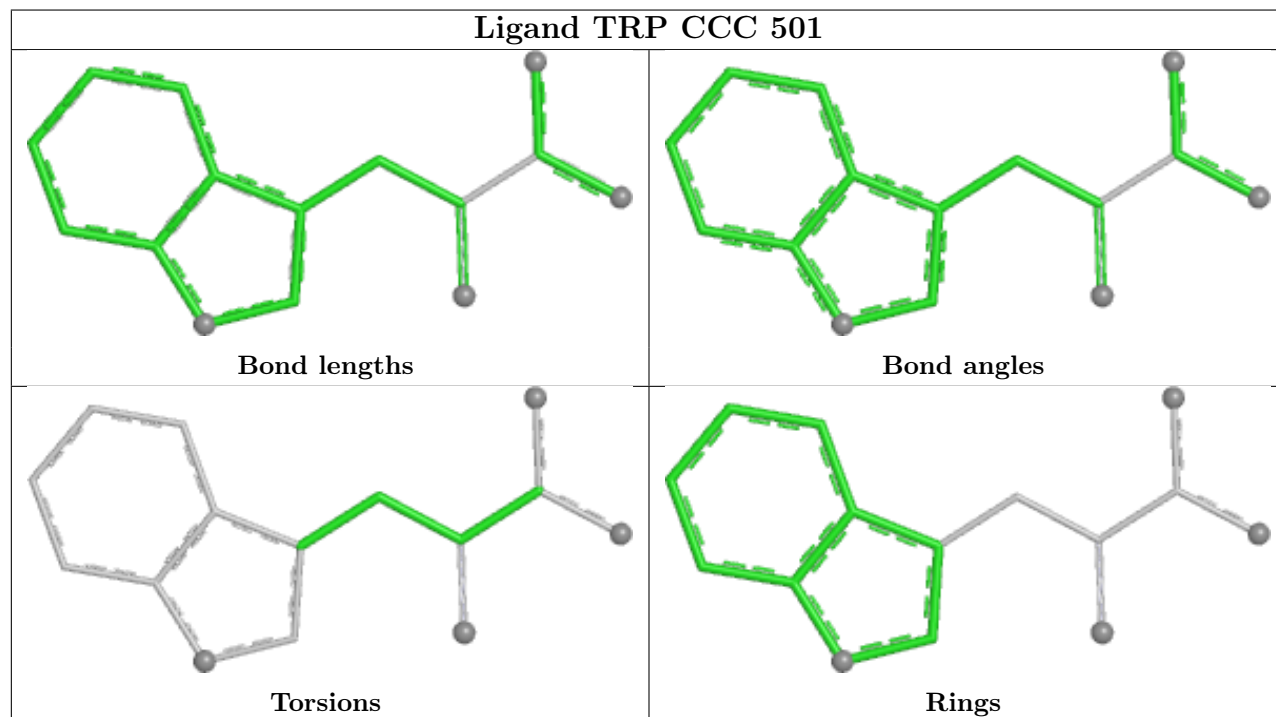
There are no ring outliers.

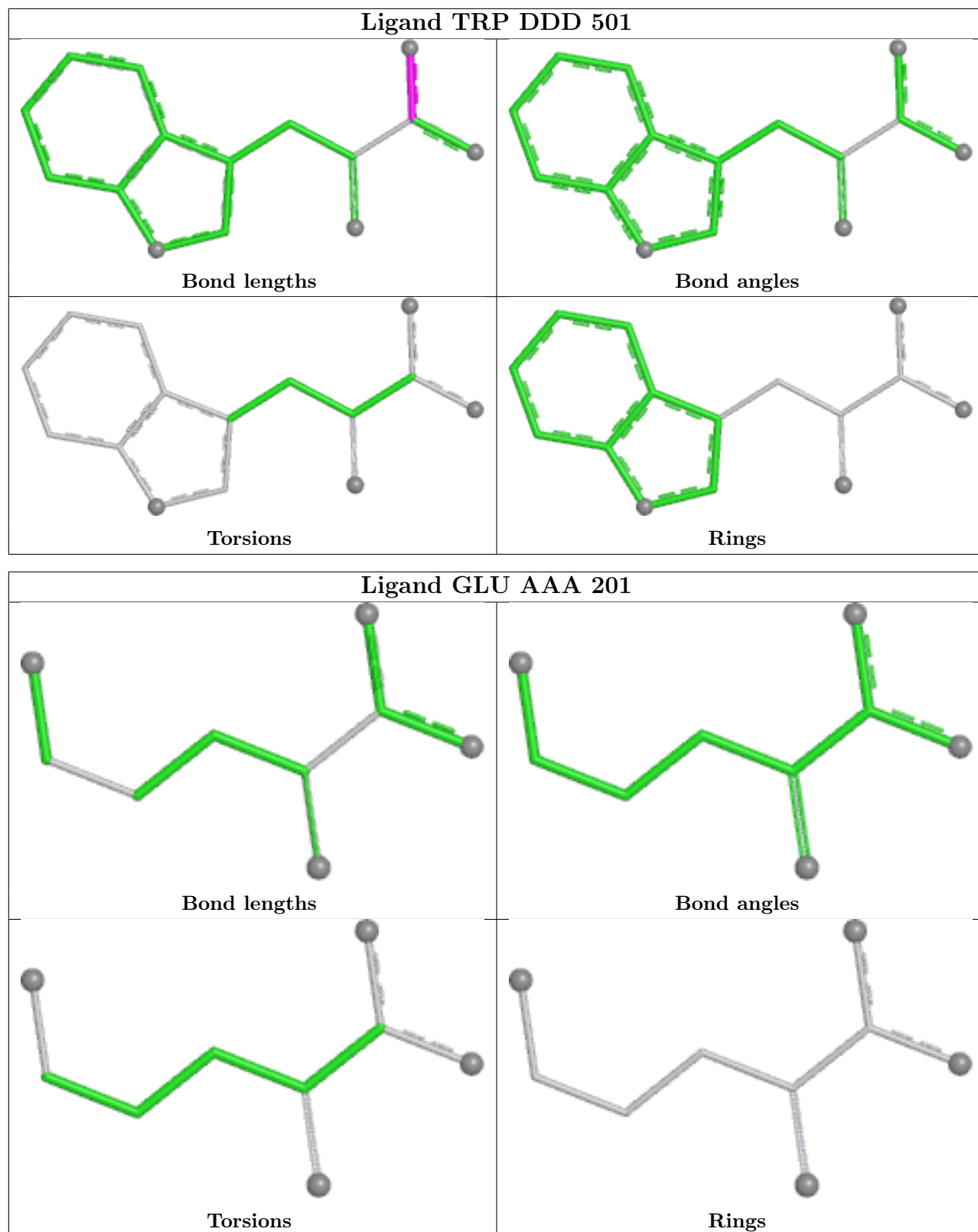
8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	DDD	508	MES	4	0
5	AAA	207	SO4	2	0
6	CCC	514	MES	1	0
3	AAA	201	GLU	5	0
6	CCC	513	MES	1	0
9	CCC	516	GOL	3	0
6	CCC	512	MES	5	0
6	AAA	209	MES	8	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	188/188 (100%)	0.12	6 (3%)	50	54	22, 36, 58, 80	0
1	BBB	188/188 (100%)	0.38	10 (5%)	32	35	23, 40, 68, 94	0
2	CCC	456/456 (100%)	-0.31	8 (1%)	67	71	14, 30, 50, 95	2 (0%)
2	DDD	455/456 (99%)	-0.18	6 (1%)	75	79	14, 32, 55, 100	2 (0%)
All	All	1287/1288 (99%)	-0.10	30 (2%)	61	64	14, 32, 57, 100	4 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	CCC	173	SER	4.9
2	CCC	172	PHE	4.8
1	BBB	0	GLY	4.4
2	DDD	-1	GLY	3.8
2	CCC	174	PRO	3.6
1	BBB	97	ALA	3.6
2	DDD	0	HIS	3.5
2	CCC	-2	GLN	3.5
2	CCC	70	GLU	2.9
1	BBB	94	VAL	2.8
1	BBB	136	SER	2.7
2	DDD	453	LYS	2.6
1	BBB	130	LEU	2.5
1	BBB	146	TRP	2.5
2	DDD	280	LEU	2.5
1	AAA	61	ILE	2.5
2	CCC	0	HIS	2.4
1	BBB	93	VAL	2.4
1	AAA	136	SER	2.3
1	BBB	116	ARG	2.2
1	BBB	150	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	0	GLY	2.2
1	AAA	89	PHE	2.2
2	CCC	207	GLY	2.2
1	AAA	140	CYS	2.2
2	DDD	174	PRO	2.1
1	AAA	68	HIS	2.1
1	BBB	186	HIS	2.1
2	DDD	283	PRO	2.1
2	CCC	69	SER	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(Å ²)	Q<0.9
6	MES	CCC	512	12/12	0.66	0.21	40,69,76,79	3
5	SO4	AAA	208	5/5	0.69	0.16	47,52,77,78	3
6	MES	CCC	514	12/12	0.70	0.19	65,83,90,98	1
9	GOL	CCC	517	6/6	0.70	0.16	6,64,67,68	2
9	GOL	DDD	510	6/6	0.73	0.16	6,52,57,66	2
6	MES	DDD	508	12/12	0.78	0.18	39,89,95,95	3
4	CL	DDD	506	1/1	0.80	0.15	81,81,81,81	0
9	GOL	DDD	509	6/6	0.82	0.14	6,56,60,71	2
5	SO4	AAA	207	5/5	0.82	0.13	74,82,92,93	0
5	SO4	DDD	512	5/5	0.84	0.12	70,75,75,84	0
4	CL	CCC	508	1/1	0.85	0.19	78,78,78,78	0
5	SO4	CCC	520	5/5	0.86	0.12	67,72,86,97	0
4	CL	CCC	505	1/1	0.87	0.13	74,74,74,74	0
9	GOL	CCC	515	6/6	0.89	0.12	41,55,72,75	2

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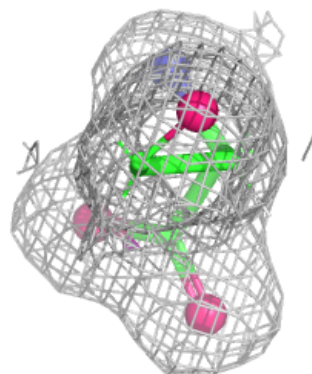
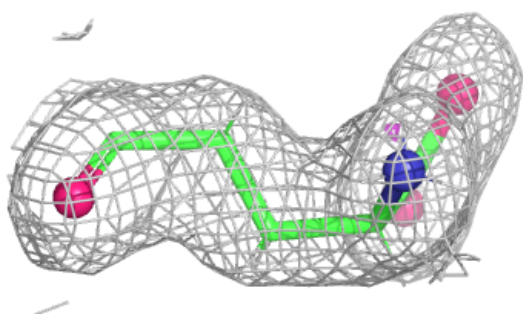
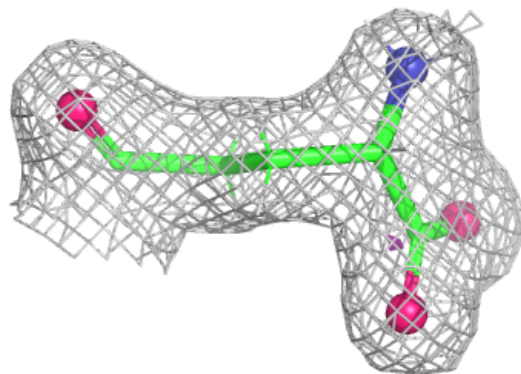
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GOL	CCC	516	6/6	0.89	0.09	6,44,47,54	2
6	MES	CCC	513	12/12	0.89	0.14	45,65,69,79	0
5	SO4	CCC	519	5/5	0.89	0.08	49,58,61,68	0
5	SO4	CCC	521	5/5	0.89	0.08	72,76,82,87	0
8	MG	DDD	502	1/1	0.90	0.14	60,60,60,60	0
4	CL	CCC	510	1/1	0.90	0.14	70,70,70,70	0
5	SO4	AAA	206	5/5	0.90	0.09	70,76,78,79	0
5	SO4	DDD	511	5/5	0.91	0.08	54,55,61,67	0
4	CL	AAA	204	1/1	0.91	0.19	76,76,76,76	0
5	SO4	CCC	518	5/5	0.92	0.08	56,58,60,62	0
6	MES	AAA	209	12/12	0.92	0.10	44,56,58,60	0
4	CL	CCC	511	1/1	0.93	0.09	57,57,57,57	0
4	CL	CCC	504	1/1	0.93	0.10	51,51,51,51	0
4	CL	DDD	503	1/1	0.94	0.20	68,68,68,68	0
4	CL	DDD	504	1/1	0.94	0.14	70,70,70,70	0
4	CL	AAA	202	1/1	0.94	0.13	61,61,61,61	0
5	SO4	AAA	205	5/5	0.94	0.07	30,44,48,55	5
4	CL	DDD	507	1/1	0.95	0.23	47,47,47,47	0
4	CL	CCC	506	1/1	0.95	0.15	56,56,56,56	0
3	GLU	AAA	201	9/10	0.96	0.06	31,33,35,36	0
7	TRP	DDD	501	15/15	0.97	0.05	22,25,27,29	0
4	CL	AAA	203	1/1	0.98	0.13	50,50,50,50	0
4	CL	CCC	509	1/1	0.98	0.05	35,35,35,35	0
4	CL	DDD	505	1/1	0.98	0.05	37,37,37,37	0
8	MG	CCC	502	1/1	0.99	0.04	40,40,40,40	0
8	MG	CCC	503	1/1	0.99	0.04	27,27,27,27	0
7	TRP	CCC	501	15/15	0.99	0.03	21,22,24,25	0
4	CL	CCC	507	1/1	0.99	0.04	34,34,34,34	0

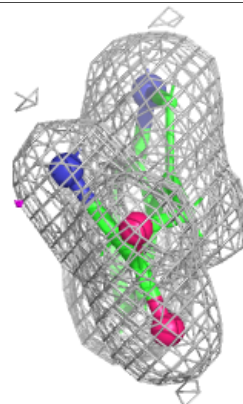
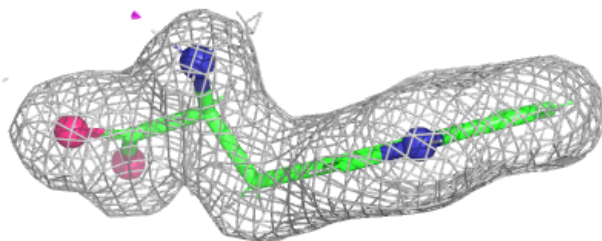
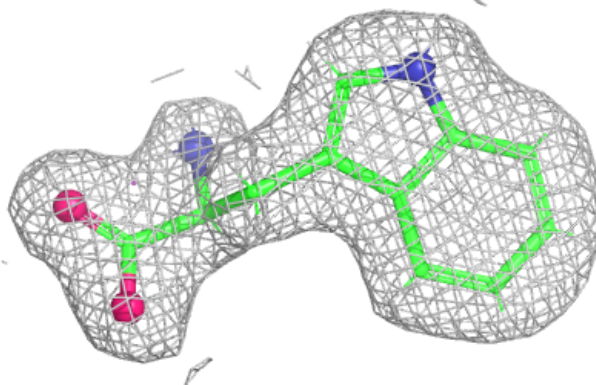
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

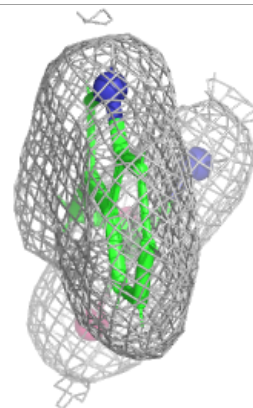
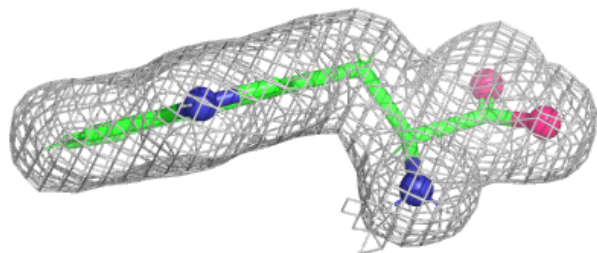
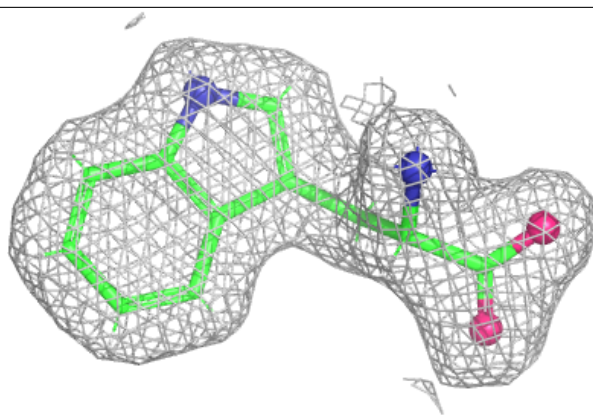
**Electron density around TRP DDD 501:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.