



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:22 AM UTC

PDB ID : 8OUC / pdb_00008ouc
Title : Escherichia coli DPS
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Deposited on : 2023-04-22
Resolution : 1.37 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:

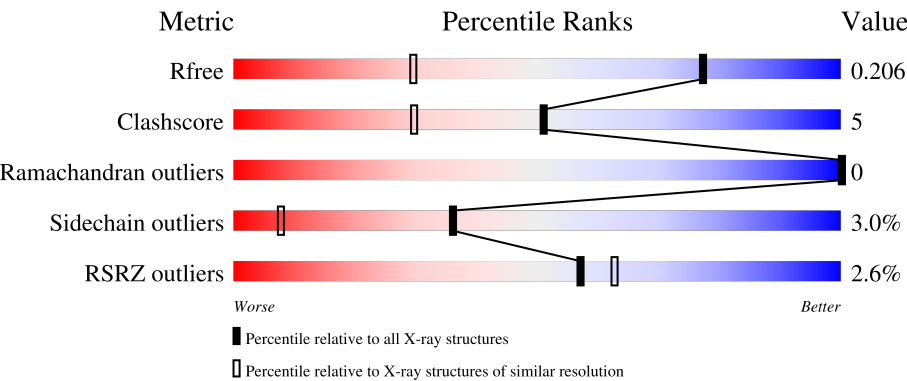
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.37 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	167	84%7%7%
1	BBB	167	80%11%7%
1	CCC	167	90%5%
1	DDD	167	88%8%
1	EEE	167	81%11%7%

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Mol	Chain	Length	Quality of chain
1	FFF	167	3% 81% 12% 7%
1	GGG	167	3% 86% 7% 7%
1	HHH	167	4% 89% 7%
1	III	167	2% 83% 13%
1	JJJ	167	% 84% 8% 7%
1	KKK	167	3% 86% 5% 7%
1	LLL	167	2% 83% 9% 7%

2 Entry composition

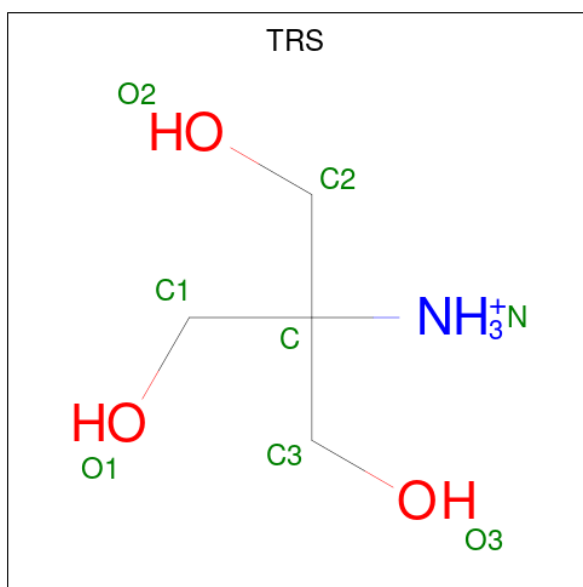
There are 3 unique types of molecules in this entry. The entry contains 17870 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA protection during starvation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	156	Total	C	N	O	S	0	0	0
			1236	776	216	241	3			
1	BBB	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	CCC	162	Total	C	N	O	S	0	0	0
			1280	805	224	248	3			
1	DDD	161	Total	C	N	O	S	0	1	0
			1281	805	225	248	3			
1	EEE	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	FFF	156	Total	C	N	O	S	0	0	0
			1236	776	216	241	3			
1	GGG	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	HHH	162	Total	C	N	O	S	0	0	0
			1280	805	224	248	3			
1	III	161	Total	C	N	O	S	0	0	0
			1272	799	223	247	3			
1	JJJ	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	KKK	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	LLL	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			8	4	1	3		
2	BBB	1	Total	C	N	O	0	0
			8	4	1	3		
2	CCC	1	Total	C	N	O	0	0
			8	4	1	3		
2	DDD	1	Total	C	N	O	0	0
			8	4	1	3		
2	EEE	1	Total	C	N	O	0	0
			8	4	1	3		
2	GGG	1	Total	C	N	O	0	0
			8	4	1	3		
2	GGG	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	246	Total	O	0	0
			246	246		
3	BBB	246	Total	O	0	0
			246	246		
3	CCC	242	Total	O	0	0
			242	242		
3	DDD	243	Total	O	0	0
			243	243		
3	EEE	227	Total	O	0	0
			227	227		

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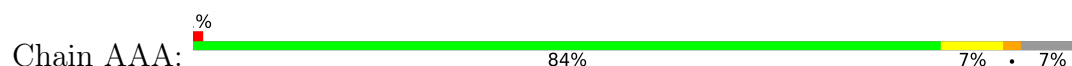
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	FFF	234	Total 234	O 234	0	0
3	GGG	250	Total 250	O 250	0	0
3	HHH	226	Total 226	O 226	0	0
3	III	245	Total 245	O 245	0	0
3	JJJ	227	Total 227	O 227	0	0
3	KKK	235	Total 235	O 235	0	0
3	LLL	234	Total 234	O 234	0	0

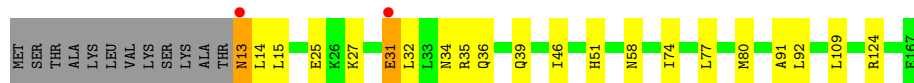
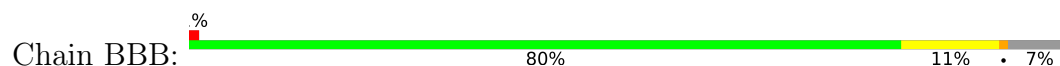
3 Residue-property plots [i](#)

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: DNA protection during starvation protein



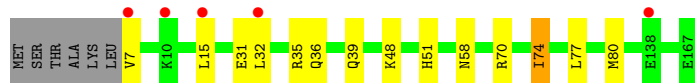
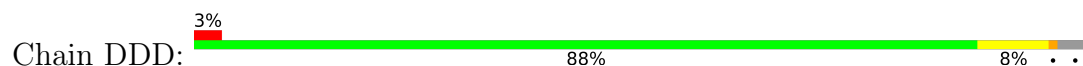
- Molecule 1: DNA protection during starvation protein



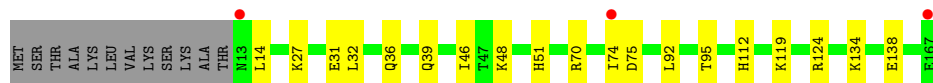
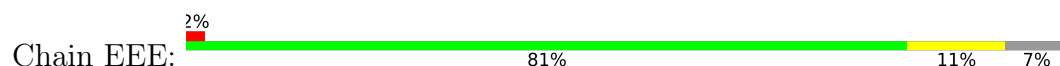
- Molecule 1: DNA protection during starvation protein



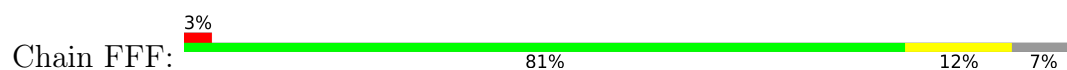
- Molecule 1: DNA protection during starvation protein



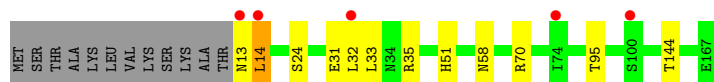
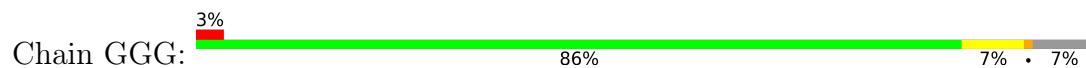
- Molecule 1: DNA protection during starvation protein



- Molecule 1: DNA protection during starvation protein



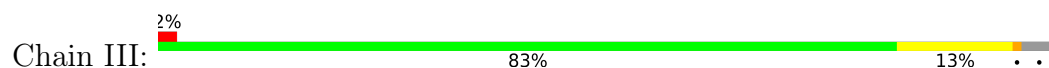
- Molecule 1: DNA protection during starvation protein



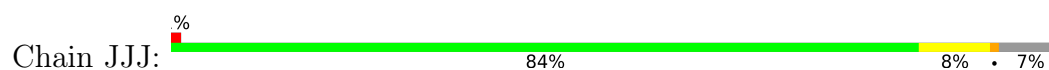
- Molecule 1: DNA protection during starvation protein



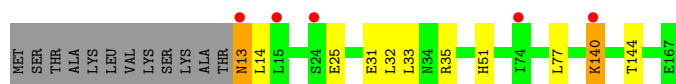
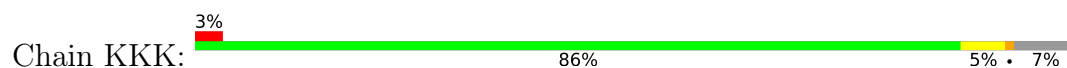
- Molecule 1: DNA protection during starvation protein



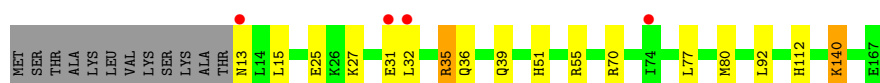
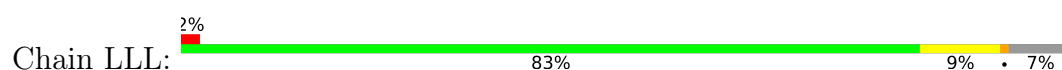
- Molecule 1: DNA protection during starvation protein



- Molecule 1: DNA protection during starvation protein



- Molecule 1: DNA protection during starvation protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.16Å 92.36Å 92.39Å 120.12° 98.91° 108.97°	Depositor
Resolution (Å)	46.12 – 1.37 46.12 – 1.37	Depositor EDS
% Data completeness (in resolution range)	90.4 (46.12-1.37) 90.4 (46.12-1.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.206 0.187 , 0.206	Depositor DCC
R_{free} test set	21618 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h-k-l,l,k 0.011 for k,h,-h-k-l 0.010 for l,-h-k-l,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17870	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS

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	0.68	0/1254	0.98	1/1698 (0.1%)
1	BBB	0.68	0/1247	0.98	0/1688
1	CCC	0.71	0/1298	0.98	2/1756 (0.1%)
1	DDD	0.67	0/1299	0.95	0/1756
1	EEE	0.72	0/1247	0.97	0/1688
1	FFF	0.73	0/1254	0.97	0/1698
1	GGG	0.69	0/1247	0.95	0/1688
1	HHH	0.70	0/1298	1.01	1/1756 (0.1%)
1	III	0.72	0/1290	1.01	0/1745
1	JJJ	0.69	0/1247	0.95	0/1688
1	KKK	0.70	0/1247	0.95	0/1688
1	LLL	0.68	1/1247 (0.1%)	0.95	0/1688
All	All	0.70	1/15175 (0.0%)	0.97	4/20537 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	LLL	112	HIS	CE1-NE2	5.93	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HHH	31	GLU	CB-CG-CD	7.12	124.71	112.60
1	CCC	31	GLU	CB-CG-CD	6.71	124.01	112.60
1	AAA	51	HIS	CA-CB-CG	5.36	119.16	113.80
1	CCC	71	THR	CA-CB-OG1	-5.21	101.78	109.60

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	1236	0	1232	12	0
1	BBB	1229	0	1225	16	0
1	CCC	1280	0	1288	7	0
1	DDD	1281	0	1289	17	0
1	EEE	1229	0	1225	14	0
1	FFF	1236	0	1232	17	0
1	GGG	1229	0	1225	12	0
1	HHH	1280	0	1288	14	0
1	III	1272	0	1277	12	0
1	JJJ	1229	0	1225	12	0
1	KKK	1229	0	1225	11	0
1	LLL	1229	0	1225	13	0
2	AAA	8	0	12	0	0
2	BBB	8	0	12	0	0
2	CCC	8	0	12	0	0
2	DDD	8	0	12	0	0
2	EEE	8	0	12	0	0
2	GGG	16	0	24	0	0
3	AAA	246	0	0	6	0
3	BBB	246	0	0	7	0
3	CCC	242	0	0	5	0
3	DDD	243	0	0	7	0
3	EEE	227	0	0	4	0
3	FFF	234	0	0	8	0
3	GGG	250	0	0	11	0
3	HHH	226	0	0	5	0
3	III	245	0	0	9	0
3	JJJ	227	0	0	4	0
3	KKK	235	0	0	4	0
3	LLL	234	0	0	8	0
All	All	17870	0	15040	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (156) 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:III:32:LEU:HD12	3:III:201:HOH:O	1.71	0.89
1:GGG:31:GLU:HG3	3:GGG:455:HOH:O	1.78	0.84
1:EEE:32:LEU:HD12	3:EEE:312:HOH:O	1.77	0.83
1:BBB:32:LEU:HD12	3:BBB:302:HOH:O	1.83	0.78
3:GGG:504:HOH:O	1:HHH:74:ILE:CG1	2.32	0.77
1:GGG:32:LEU:HD22	3:GGG:367:HOH:O	1.86	0.73
1:DDD:32:LEU:HD12	3:DDD:302:HOH:O	1.88	0.73
1:BBB:31:GLU:HG2	3:BBB:476:HOH:O	1.88	0.73
1:DDD:31:GLU:HG3	3:DDD:301:HOH:O	1.90	0.72
3:CCC:489:HOH:O	1:DDD:74:ILE:CG1	2.37	0.71
1:LLL:32:LEU:HD12	3:LLL:207:HOH:O	1.93	0.68
1:JJJ:32:LEU:HD21	1:JJJ:148:LEU:HD11	1.78	0.64
1:FFF:31:GLU:HG2	3:FFF:361:HOH:O	1.97	0.64
1:LLL:27:LYS:O	1:LLL:31:GLU:HG2	1.98	0.64
1:FFF:35:ARG:NH1	3:FFF:201:HOH:O	2.32	0.62
1:KKK:140:LYS:HD3	1:KKK:140:LYS:H	1.64	0.62
1:KKK:25:GLU:HG3	1:KKK:140:LYS:HE3	1.80	0.61
1:JJJ:75:ASP:HB2	3:JJJ:352:HOH:O	1.98	0.61
1:AAA:25:GLU:HG3	3:AAA:328:HOH:O	1.99	0.61
1:GGG:95:THR:HG23	3:GGG:463:HOH:O	2.00	0.60
3:III:399:HOH:O	1:JJJ:74:ILE:CG1	2.49	0.60
1:HHH:32:LEU:HD21	1:HHH:148:LEU:HD11	1.83	0.59
3:GGG:504:HOH:O	1:HHH:74:ILE:CB	2.49	0.59
1:GGG:13:ASN:ND2	1:GGG:14:LEU:H	2.01	0.59
1:III:35:ARG:NH1	3:III:201:HOH:O	2.37	0.58
1:BBB:35:ARG:NH1	3:BBB:302:HOH:O	2.37	0.57
1:KKK:31:GLU:CD	3:KKK:209:HOH:O	2.46	0.57
3:GGG:504:HOH:O	1:HHH:74:ILE:HG21	2.05	0.57
1:JJJ:35:ARG:NH1	3:JJJ:201:HOH:O	2.38	0.57
1:DDD:35:ARG:NH1	3:DDD:302:HOH:O	2.38	0.56
1:DDD:15:LEU:HD12	3:DDD:313:HOH:O	2.04	0.56
1:KKK:140:LYS:H	1:KKK:140:LYS:CD	2.19	0.56
1:BBB:92:LEU:HB2	3:BBB:404:HOH:O	2.06	0.56
1:DDD:36:GLN:NE2	1:DDD:39:GLN:HE21	2.04	0.55
1:HHH:134:LYS:CE	3:HHH:220:HOH:O	2.55	0.55
1:III:36:GLN:NE2	1:III:39:GLN:HE21	2.05	0.54
1:LLL:36:GLN:NE2	1:LLL:39:GLN:HE21	2.06	0.54
1:EEE:112:HIS:CE1	1:FFF:15:LEU:HD11	2.42	0.54
3:III:399:HOH:O	1:JJJ:74:ILE:HG21	2.07	0.54
1:DDD:58:ASN:HB2	3:III:361:HOH:O	2.07	0.54
1:AAA:92:LEU:HB2	3:AAA:433:HOH:O	2.08	0.53
1:BBB:34:ASN:HD21	1:BBB:91:ALA:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AAA:307:HOH:O	1:EEE:134:LYS:CE	2.55	0.53
1:FFF:58:ASN:HB2	3:FFF:358:HOH:O	2.08	0.53
1:III:77:LEU:HA	1:III:80:MET:HE2	1.89	0.53
1:EEE:36:GLN:NE2	1:EEE:39:GLN:HE21	2.06	0.53
1:AAA:94:THR:O	1:AAA:98:ILE:HG12	2.09	0.53
1:JJJ:77:LEU:HA	1:JJJ:80:MET:HE3	1.91	0.53
1:GGG:32:LEU:C	1:GGG:32:LEU:HD13	2.34	0.53
1:AAA:32:LEU:C	1:AAA:32:LEU:HD23	2.34	0.52
1:AAA:25:GLU:CG	3:AAA:328:HOH:O	2.57	0.52
1:BBB:77:LEU:HA	1:BBB:80:MET:HE3	1.92	0.52
3:GGG:504:HOH:O	1:HHH:74:ILE:HG12	2.03	0.52
1:HHH:35:ARG:NH1	3:HHH:201:HOH:O	2.41	0.52
1:CCC:7:VAL:HG13	1:CCC:16:TYR:HB3	1.92	0.51
1:BBB:77:LEU:HA	1:BBB:80:MET:CE	2.40	0.51
1:III:31:GLU:HG2	3:III:219:HOH:O	2.10	0.51
1:DDD:48:LYS:HE3	1:DDD:70:ARG:NH1	2.26	0.51
1:LLL:25:GLU:HG3	3:LLL:354:HOH:O	2.10	0.51
1:AAA:58:ASN:HB2	3:JJJ:358:HOH:O	2.10	0.51
1:LLL:15:LEU:CD2	3:LLL:296:HOH:O	2.58	0.51
1:DDD:77:LEU:HA	1:DDD:80:MET:CE	2.42	0.50
1:EEE:92:LEU:HB2	3:EEE:410:HOH:O	2.11	0.50
1:FFF:31:GLU:CG	3:FFF:361:HOH:O	2.58	0.50
1:AAA:35:ARG:NH1	3:AAA:302:HOH:O	2.45	0.49
1:HHH:134:LYS:HE3	3:HHH:220:HOH:O	2.12	0.49
1:BBB:13:ASN:N	3:BBB:303:HOH:O	2.43	0.49
1:LLL:36:GLN:HE22	1:LLL:39:GLN:HE21	1.60	0.49
1:HHH:77:LEU:HA	1:HHH:80:MET:HE2	1.95	0.49
1:CCC:74:ILE:CG1	3:DDD:505:HOH:O	2.61	0.49
1:DDD:36:GLN:HE22	1:DDD:39:GLN:HE21	1.61	0.49
1:EEE:48:LYS:HE3	1:EEE:70:ARG:NH2	2.27	0.48
1:FFF:36:GLN:NE2	1:FFF:39:GLN:HE21	2.10	0.48
1:EEE:14:LEU:HD11	1:EEE:27:LYS:HG3	1.94	0.48
1:EEE:138:GLU:OE1	3:EEE:301:HOH:O	2.20	0.48
1:HHH:12:THR:HA	3:HHH:246:HOH:O	2.14	0.48
1:FFF:32:LEU:HD21	1:FFF:148:LEU:HD11	1.96	0.48
1:LLL:92:LEU:HB2	3:LLL:303:HOH:O	2.13	0.48
1:CCC:74:ILE:HG21	3:DDD:505:HOH:O	2.13	0.48
1:EEE:48:LYS:HE3	1:EEE:70:ARG:CZ	2.44	0.48
1:BBB:36:GLN:NE2	1:BBB:39:GLN:HE21	2.11	0.47
1:DDD:74:ILE:HD12	1:DDD:77:LEU:HD21	1.96	0.47
1:EEE:95:THR:HG23	3:FFF:347:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LLL:77:LEU:HA	1:LLL:80:MET:HE2	1.96	0.47
3:AAA:307:HOH:O	1:EEE:134:LYS:HE3	2.15	0.46
1:FFF:13:ASN:ND2	3:FFF:203:HOH:O	2.47	0.46
1:HHH:15:LEU:CD1	3:HHH:270:HOH:O	2.62	0.46
1:III:8:LYS:HD3	1:III:15:LEU:HD22	1.96	0.46
1:III:130:ASN:O	1:III:134:LYS:HG3	2.16	0.46
1:LLL:35:ARG:NH1	3:LLL:207:HOH:O	2.48	0.46
1:CCC:94:THR:O	1:CCC:98:ILE:HG12	2.14	0.46
3:CCC:489:HOH:O	1:DDD:74:ILE:HG13	2.09	0.46
1:EEE:36:GLN:HE22	1:EEE:39:GLN:HE21	1.63	0.46
1:HHH:77:LEU:HA	1:HHH:80:MET:CE	2.45	0.46
1:BBB:13:ASN:HD22	1:BBB:14:LEU:N	2.15	0.46
1:FFF:95:THR:HG23	3:FFF:347:HOH:O	2.16	0.45
3:III:399:HOH:O	1:JJJ:74:ILE:CB	2.64	0.45
1:AAA:12:THR:HG1	1:AAA:31:GLU:CD	2.24	0.45
1:JJJ:135:ALA:HA	1:JJJ:138:GLU:HG3	1.96	0.45
1:III:36:GLN:HE22	1:III:39:GLN:HE21	1.63	0.45
1:KKK:140:LYS:CE	3:KKK:206:HOH:O	2.65	0.45
1:DDD:48:LYS:CE	1:DDD:70:ARG:NH1	2.79	0.45
1:EEE:75:ASP:OD1	3:EEE:302:HOH:O	2.21	0.45
1:FFF:77:LEU:HA	1:FFF:80:MET:HE3	1.97	0.45
1:GGG:31:GLU:HG2	3:GGG:311:HOH:O	2.17	0.45
1:LLL:13:ASN:HB3	3:LLL:287:HOH:O	2.17	0.45
1:KKK:33:LEU:HD21	1:KKK:144:THR:HG23	1.98	0.45
1:KKK:140:LYS:NZ	3:KKK:206:HOH:O	2.50	0.44
1:KKK:32:LEU:C	1:KKK:32:LEU:HD23	2.42	0.44
1:AAA:70:ARG:HD2	1:AAA:70:ARG:C	2.43	0.44
1:JJJ:77:LEU:HA	1:JJJ:80:MET:CE	2.48	0.44
1:JJJ:36:GLN:NE2	1:JJJ:39:GLN:HE21	2.16	0.43
1:BBB:27:LYS:CE	3:BBB:303:HOH:O	2.66	0.43
1:AAA:48:LYS:HE3	1:AAA:70:ARG:NH1	2.33	0.43
1:FFF:94:THR:O	1:FFF:98:ILE:HG12	2.18	0.43
1:LLL:70:ARG:HD2	1:LLL:70:ARG:C	2.43	0.43
1:FFF:92:LEU:HB2	3:FFF:294:HOH:O	2.17	0.43
1:GGG:35:ARG:NH2	3:GGG:313:HOH:O	2.51	0.43
1:GGG:35:ARG:NH2	3:GGG:312:HOH:O	2.51	0.43
1:III:48:LYS:HE3	1:III:70:ARG:CZ	2.49	0.43
1:EEE:46:ILE:HD13	1:EEE:124:ARG:HD3	2.01	0.42
1:FFF:32:LEU:C	1:FFF:32:LEU:HD23	2.44	0.42
1:FFF:70:ARG:O	1:FFF:74:ILE:HD13	2.19	0.42
1:KKK:35:ARG:CZ	3:KKK:277:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:46:ILE:HD13	1:BBB:124:ARG:HD3	2.00	0.42
1:CCC:74:ILE:HG13	3:DDD:505:HOH:O	2.19	0.42
3:GGG:504:HOH:O	1:HHH:74:ILE:CG2	2.65	0.42
1:III:112:HIS:HE1	3:III:374:HOH:O	2.01	0.42
1:FFF:36:GLN:HE22	1:FFF:39:GLN:HE21	1.67	0.42
3:CCC:462:HOH:O	1:GGG:58:ASN:HB2	2.19	0.42
1:CCC:74:ILE:HD12	1:CCC:77:LEU:HD21	2.02	0.42
1:GGG:13:ASN:HD22	1:GGG:14:LEU:H	1.68	0.42
1:BBB:58:ASN:HB2	3:LLL:365:HOH:O	2.19	0.42
1:LLL:140:LYS:CE	3:LLL:224:HOH:O	2.68	0.42
3:CCC:489:HOH:O	1:DDD:74:ILE:HG21	2.20	0.41
1:BBB:34:ASN:ND2	1:BBB:92:LEU:H	2.18	0.41
1:LLL:77:LEU:HA	1:LLL:80:MET:CE	2.50	0.41
1:KKK:13:ASN:ND2	1:KKK:14:LEU:H	2.17	0.41
1:CCC:6:LEU:HD23	1:CCC:6:LEU:HA	1.85	0.41
1:BBB:36:GLN:HE22	1:BBB:39:GLN:HE21	1.69	0.41
1:JJJ:31:GLU:HB3	3:JJJ:251:HOH:O	2.20	0.41
1:FFF:46:ILE:HD13	1:FFF:124:ARG:HD3	2.04	0.40
1:GGG:70:ARG:HD2	1:GGG:70:ARG:C	2.46	0.40
1:III:33:LEU:HD21	1:III:144:THR:HG23	2.03	0.40
1:KKK:77:LEU:HD12	1:KKK:77:LEU:C	2.46	0.40
1:BBB:27:LYS:HE3	3:BBB:303:HOH:O	2.21	0.40
1:DDD:77:LEU:HA	1:DDD:80:MET:HE2	2.03	0.40
1:III:94:THR:O	1:III:98:ILE:HG12	2.21	0.40
1:AAA:13:ASN:HD22	1:AAA:13:ASN:HA	1.59	0.40
1:AAA:32:LEU:HD21	1:AAA:148:LEU:HD11	2.03	0.40
1:FFF:70:ARG:C	1:FFF:70:ARG:HD2	2.46	0.40
1:GGG:33:LEU:HD21	1:GGG:144:THR:HG23	2.02	0.40
1:HHH:8:LYS:HE2	1:HHH:15:LEU:HD11	2.04	0.40
3:III:399:HOH:O	1:JJJ:74:ILE:HG12	2.17	0.40
3:CCC:489:HOH:O	1:DDD:74:ILE:CB	2.69	0.40
1:DDD:77:LEU:HA	1:DDD:80:MET:HE3	2.02	0.40

There are no symmetry-related clashes.

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	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	BBB	153/167 (92%)	152 (99%)	1 (1%)	0	100	100
1	CCC	160/167 (96%)	159 (99%)	1 (1%)	0	100	100
1	DDD	160/167 (96%)	159 (99%)	1 (1%)	0	100	100
1	EEE	153/167 (92%)	151 (99%)	2 (1%)	0	100	100
1	FFF	154/167 (92%)	153 (99%)	1 (1%)	0	100	100
1	GGG	153/167 (92%)	152 (99%)	1 (1%)	0	100	100
1	HHH	160/167 (96%)	158 (99%)	2 (1%)	0	100	100
1	III	159/167 (95%)	157 (99%)	2 (1%)	0	100	100
1	JJJ	153/167 (92%)	152 (99%)	1 (1%)	0	100	100
1	KKK	153/167 (92%)	152 (99%)	1 (1%)	0	100	100
1	LLL	153/167 (92%)	152 (99%)	1 (1%)	0	100	100
All	All	1865/2004 (93%)	1849 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	134/143 (94%)	129 (96%)	5 (4%)	30	5
1	BBB	133/143 (93%)	126 (95%)	7 (5%)	20	2
1	CCC	139/143 (97%)	133 (96%)	6 (4%)	26	3
1	DDD	139/143 (97%)	136 (98%)	3 (2%)	45	14
1	EEE	133/143 (93%)	129 (97%)	4 (3%)	36	8
1	FFF	134/143 (94%)	133 (99%)	1 (1%)	76	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GGG	133/143 (93%)	130 (98%)	3 (2%)	44	13
1	HHH	139/143 (97%)	136 (98%)	3 (2%)	45	14
1	III	138/143 (96%)	133 (96%)	5 (4%)	31	5
1	JJJ	133/143 (93%)	128 (96%)	5 (4%)	29	5
1	KKK	133/143 (93%)	130 (98%)	3 (2%)	44	13
1	LLL	133/143 (93%)	129 (97%)	4 (3%)	36	8
All	All	1621/1716 (94%)	1572 (97%)	49 (3%)	36	8

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	12	THR
1	AAA	13	ASN
1	AAA	31	GLU
1	AAA	51	HIS
1	AAA	74	ILE
1	BBB	13	ASN
1	BBB	15	LEU
1	BBB	25	GLU
1	BBB	31	GLU
1	BBB	51	HIS
1	BBB	74	ILE
1	BBB	109	LEU
1	CCC	7	VAL
1	CCC	10	LYS
1	CCC	31	GLU
1	CCC	51	HIS
1	CCC	74	ILE
1	CCC	138	GLU
1	DDD	7	VAL
1	DDD	51	HIS
1	DDD	74	ILE
1	EEE	31	GLU
1	EEE	51	HIS
1	EEE	74	ILE
1	EEE	119	LYS
1	FFF	51	HIS
1	GGG	14	LEU
1	GGG	24	SER
1	GGG	51	HIS

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Mol	Chain	Res	Type
1	HHH	6	LEU
1	HHH	51	HIS
1	HHH	74	ILE
1	III	7	VAL
1	III	10	LYS
1	III	35	ARG
1	III	51	HIS
1	III	109	LEU
1	JJJ	15	LEU
1	JJJ	51	HIS
1	JJJ	74	ILE
1	JJJ	138	GLU
1	JJJ	140	LYS
1	KKK	13	ASN
1	KKK	51	HIS
1	KKK	140	LYS
1	LLL	35	ARG
1	LLL	51	HIS
1	LLL	55	ARG
1	LLL	140	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRS	GGG	202	-	7,7,7	0.18	0	9,9,9	0.29	0
2	TRS	GGG	201	-	7,7,7	0.14	0	9,9,9	0.29	0
2	TRS	EEE	201	-	7,7,7	0.18	0	9,9,9	0.29	0
2	TRS	AAA	201	-	7,7,7	0.08	0	9,9,9	0.34	0
2	TRS	CCC	201	-	7,7,7	0.19	0	9,9,9	0.26	0
2	TRS	BBB	201	-	7,7,7	0.10	0	9,9,9	0.25	0
2	TRS	DDD	201	-	7,7,7	0.15	0	9,9,9	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
2	TRS	GGG	202	-	-	0/9/9/9	-
2	TRS	GGG	201	-	-	3/9/9/9	-
2	TRS	EEE	201	-	-	2/9/9/9	-
2	TRS	AAA	201	-	-	0/9/9/9	-
2	TRS	CCC	201	-	-	0/9/9/9	-
2	TRS	BBB	201	-	-	0/9/9/9	-
2	TRS	DDD	201	-	-	1/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	GGG	201	TRS	N-C-C1-O1
2	GGG	201	TRS	C2-C-C1-O1
2	GGG	201	TRS	C3-C-C1-O1
2	DDD	201	TRS	C1-C-C3-O3
2	EEE	201	TRS	C3-C-C1-O1

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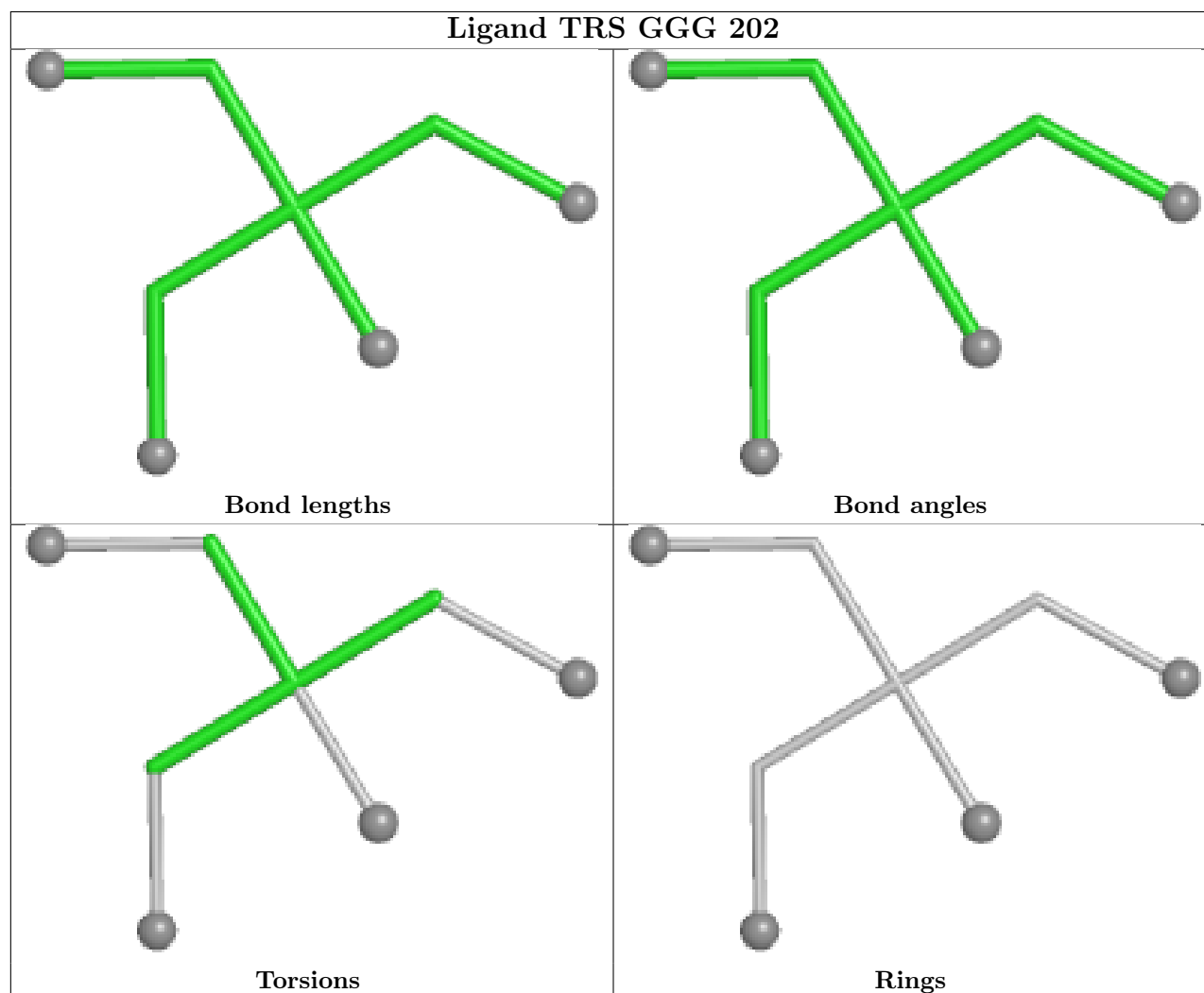
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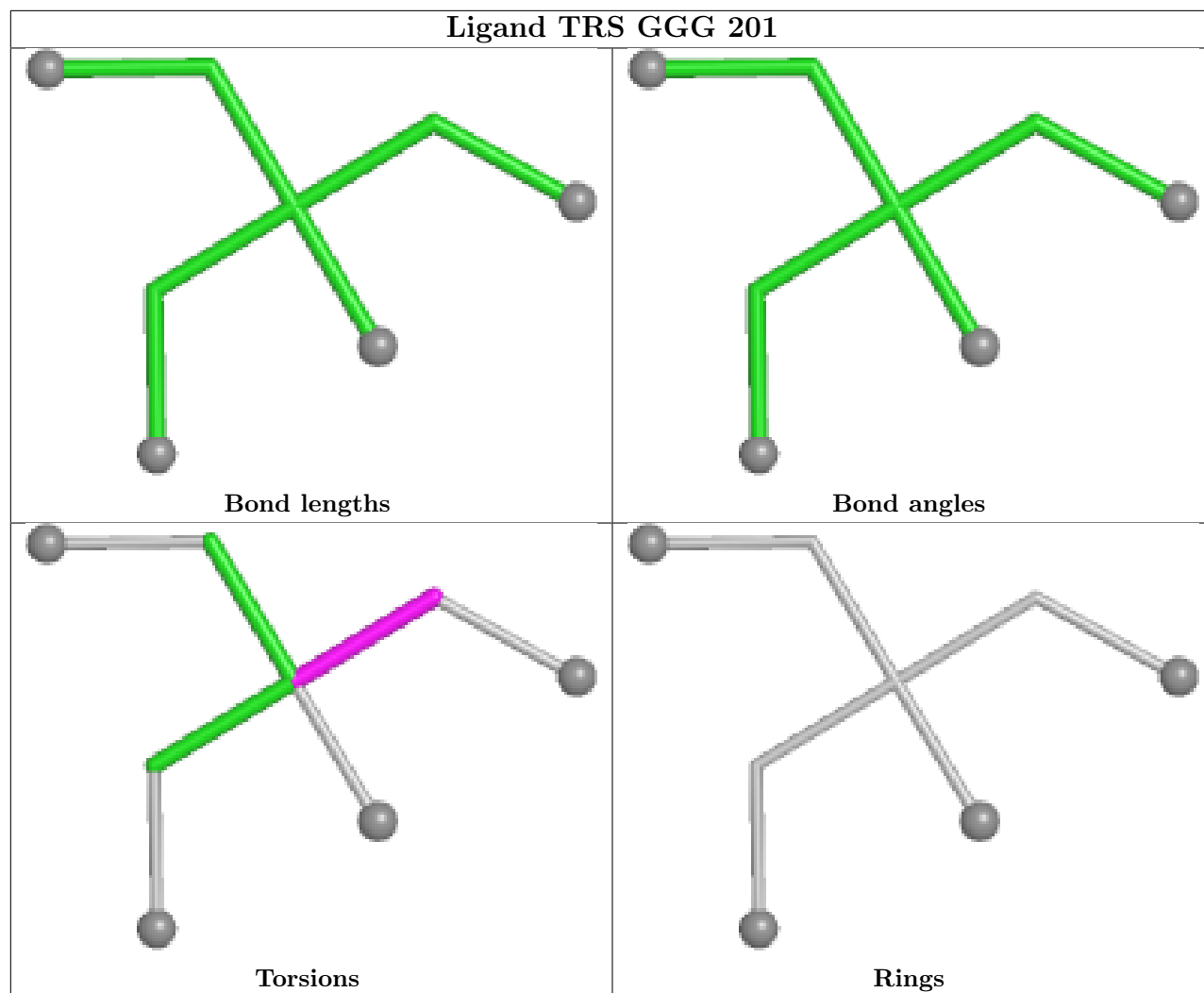
Mol	Chain	Res	Type	Atoms
2	EEE	201	TRS	C1-C-C2-O2

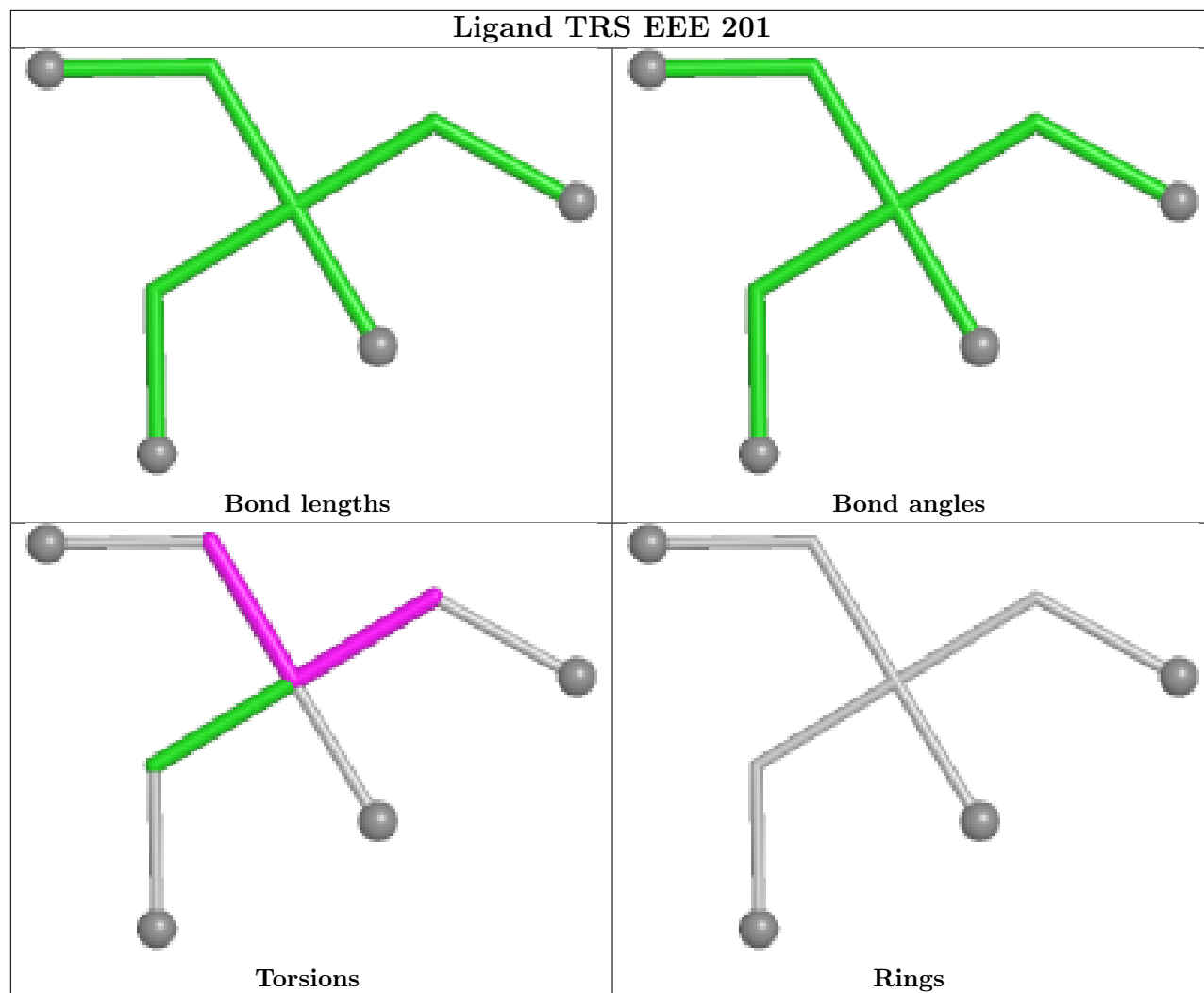
There are no ring outliers.

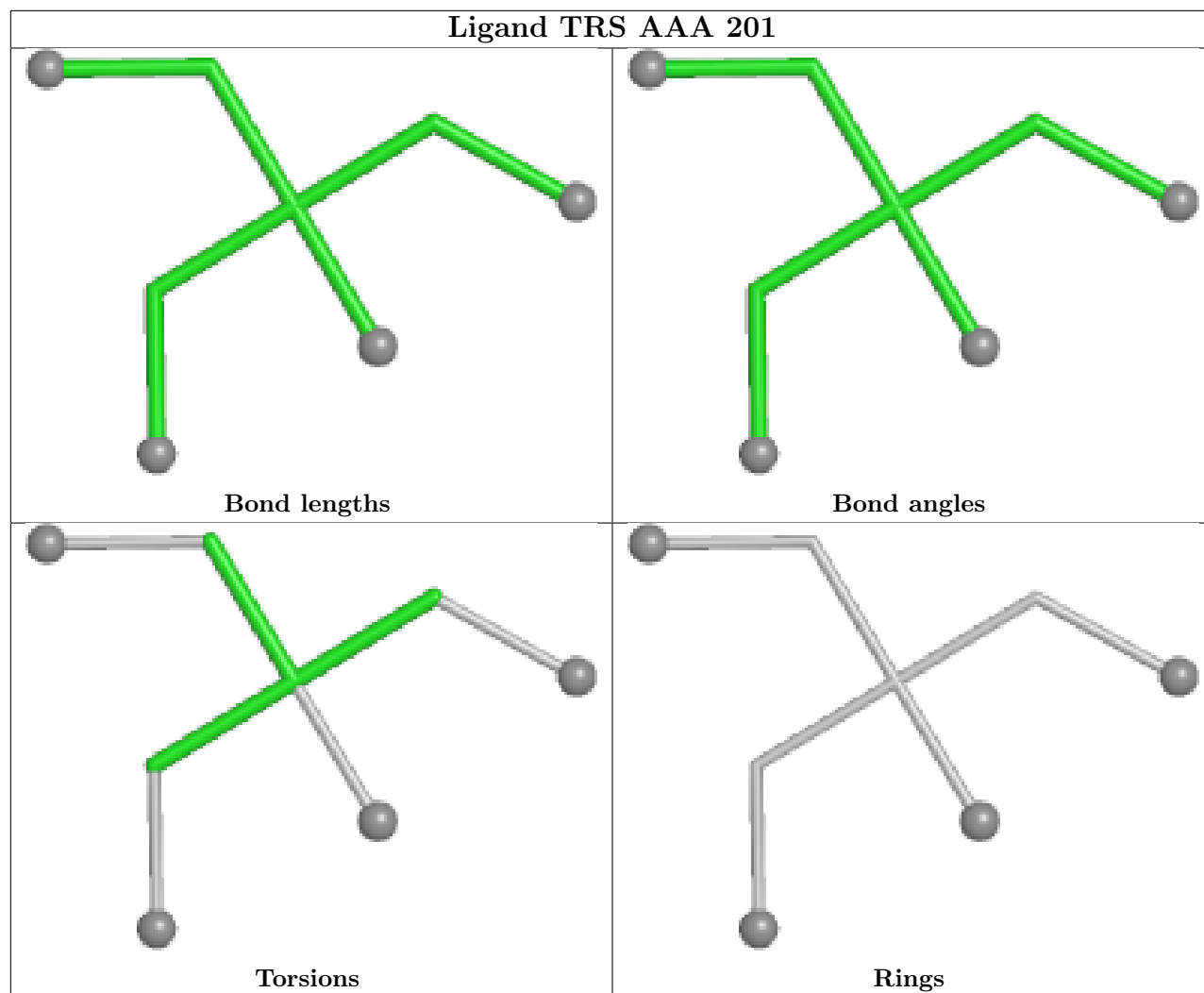
No monomer is involved in short contacts.

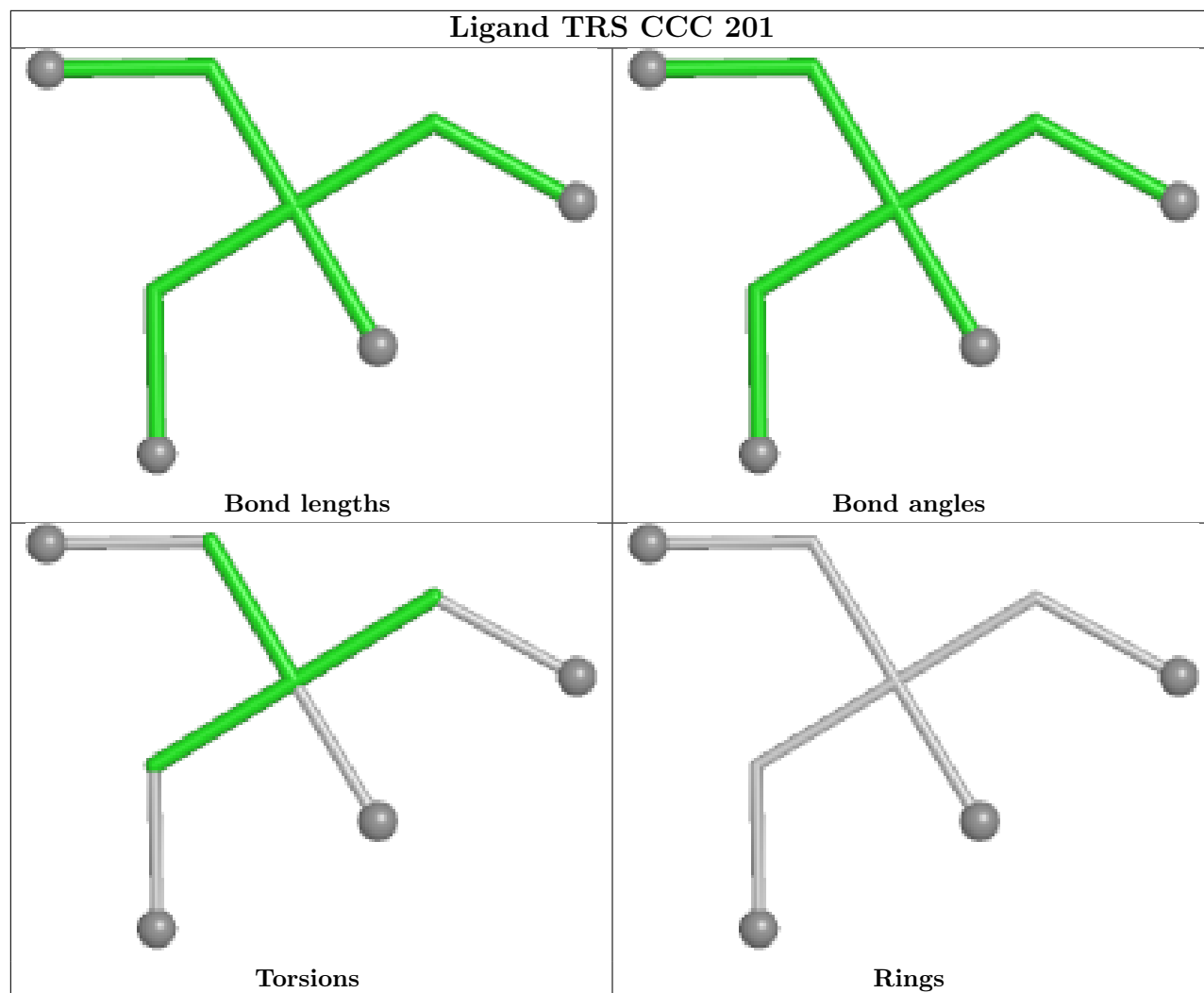
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

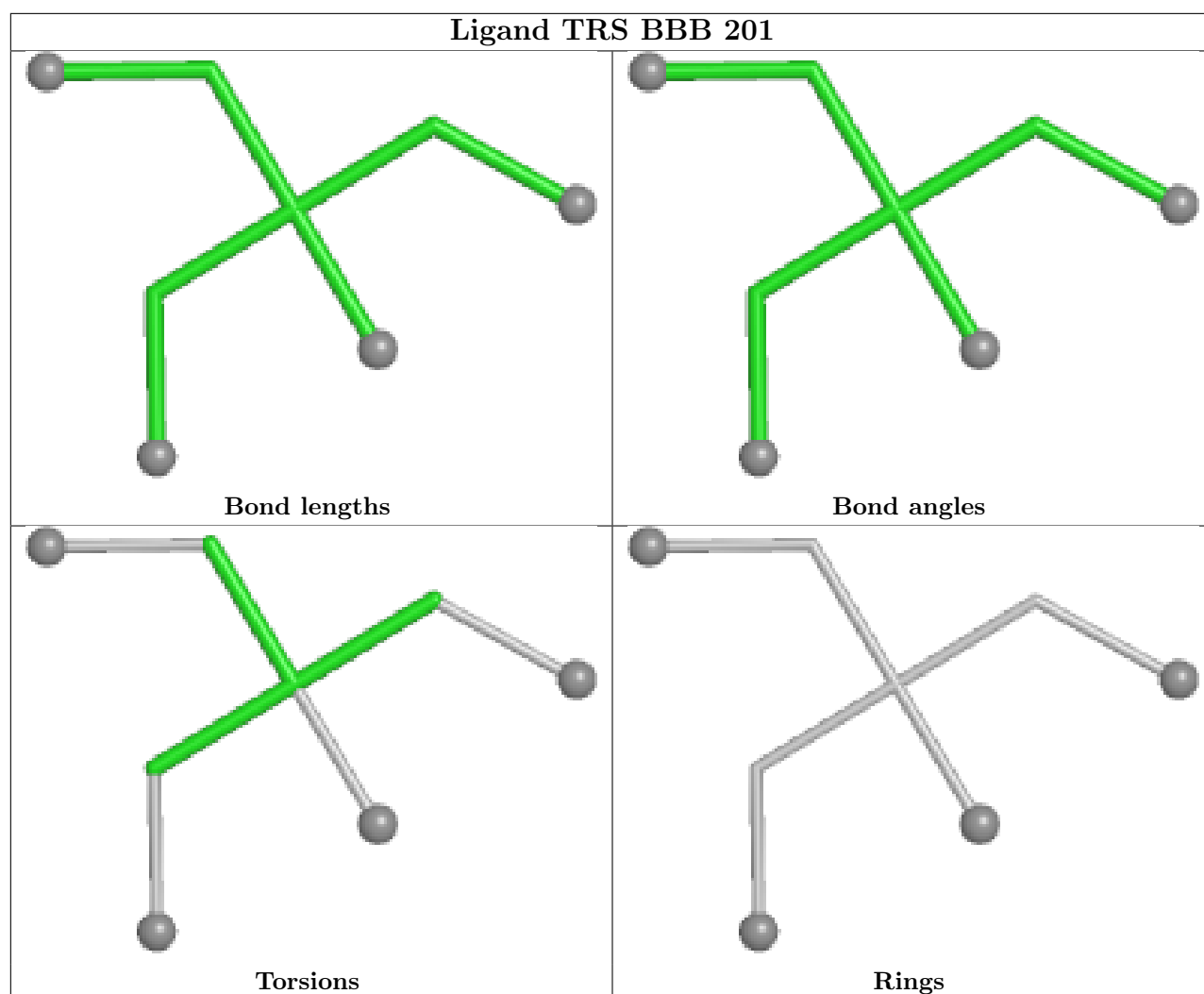


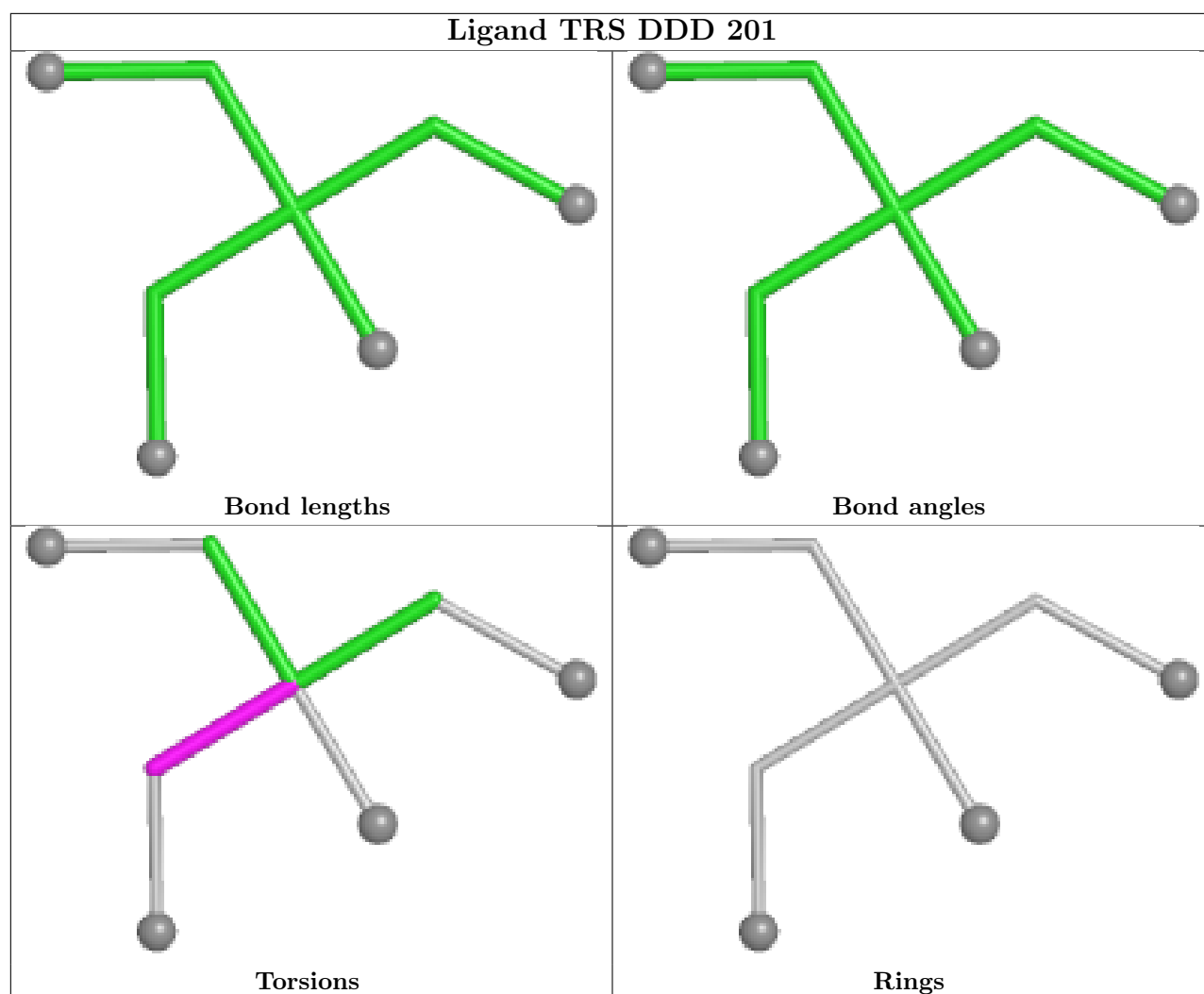












5.7 Other polymers [i](#)

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	156/167 (93%)	0.19	2 (1%) 75 81	11, 14, 27, 60	0
1	BBB	155/167 (92%)	0.19	2 (1%) 75 81	12, 15, 25, 35	0
1	CCC	162/167 (97%)	0.24	6 (3%) 45 51	11, 14, 28, 68	0
1	DDD	161/167 (96%)	0.18	5 (3%) 51 57	11, 15, 28, 47	1 (0%)
1	EEE	155/167 (92%)	0.20	3 (1%) 66 72	12, 15, 27, 37	0
1	FFF	156/167 (93%)	0.21	5 (3%) 50 55	11, 15, 26, 72	0
1	GGG	155/167 (92%)	0.18	5 (3%) 50 55	11, 15, 27, 54	0
1	HHH	162/167 (97%)	0.25	7 (4%) 40 45	12, 14, 29, 59	0
1	III	161/167 (96%)	0.18	4 (2%) 58 64	11, 14, 26, 50	0
1	JJJ	155/167 (92%)	0.16	2 (1%) 75 81	11, 16, 28, 53	0
1	KKK	155/167 (92%)	0.18	5 (3%) 50 55	11, 16, 27, 60	0
1	LLL	155/167 (92%)	0.17	4 (2%) 57 63	12, 16, 26, 39	0
All	All	1888/2004 (94%)	0.19	50 (2%) 57 63	11, 15, 27, 72	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	III	7	VAL	8.4
1	CCC	7	VAL	7.0
1	CCC	6	LEU	6.7
1	AAA	12	THR	5.1
1	JJJ	13	ASN	4.9
1	DDD	7	VAL	4.7
1	HHH	6	LEU	4.7
1	BBB	13	ASN	4.5
1	FFF	12	THR	4.2
1	EEE	13	ASN	4.1
1	GGG	13	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	GGG	14	LEU	4.0
1	LLL	13	ASN	4.0
1	AAA	13	ASN	3.9
1	CCC	10	LYS	3.6
1	HHH	11	ALA	3.5
1	HHH	10	LYS	3.5
1	KKK	13	ASN	3.5
1	GGG	32	LEU	3.4
1	KKK	140	LYS	3.3
1	HHH	7	VAL	3.3
1	CCC	32	LEU	3.2
1	LLL	31	GLU	3.0
1	III	11	ALA	2.9
1	DDD	10	LYS	2.8
1	CCC	11	ALA	2.8
1	FFF	13	ASN	2.8
1	DDD	32	LEU	2.6
1	FFF	74	ILE	2.5
1	FFF	100	SER	2.5
1	HHH	50	ALA	2.4
1	KKK	24	SER	2.4
1	III	10	LYS	2.4
1	HHH	9	SER	2.4
1	EEE	167	GLU	2.4
1	CCC	167	GLU	2.3
1	DDD	15	LEU	2.3
1	JJJ	15	LEU	2.3
1	GGG	100	SER	2.3
1	EEE	74	ILE	2.3
1	KKK	15	LEU	2.3
1	III	100	SER	2.2
1	BBB	31	GLU	2.2
1	DDD	138	GLU	2.2
1	FFF	24	SER	2.2
1	LLL	32	LEU	2.1
1	LLL	74	ILE	2.1
1	HHH	12	THR	2.0
1	GGG	74	ILE	2.0
1	KKK	74	ILE	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](#)

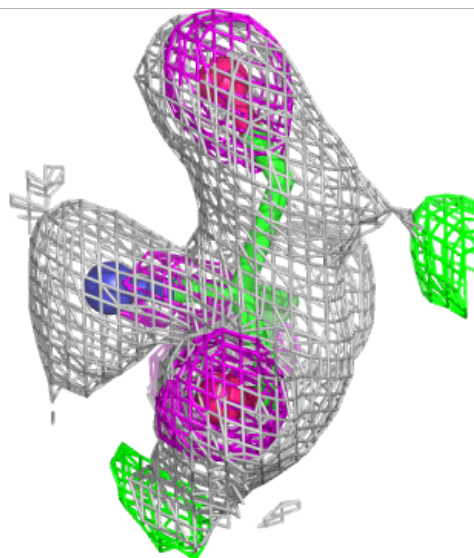
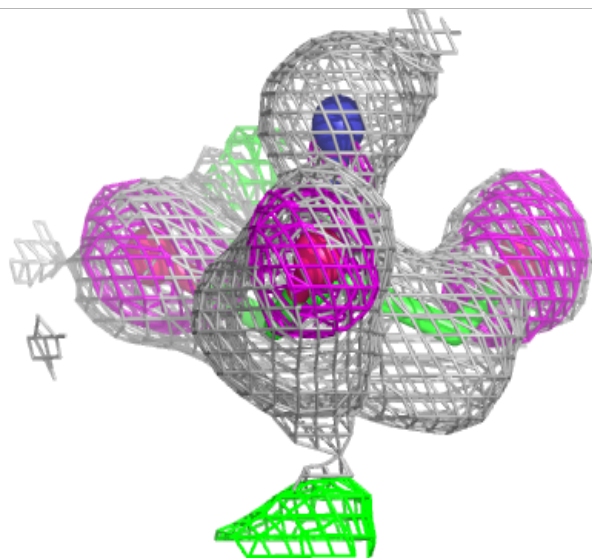
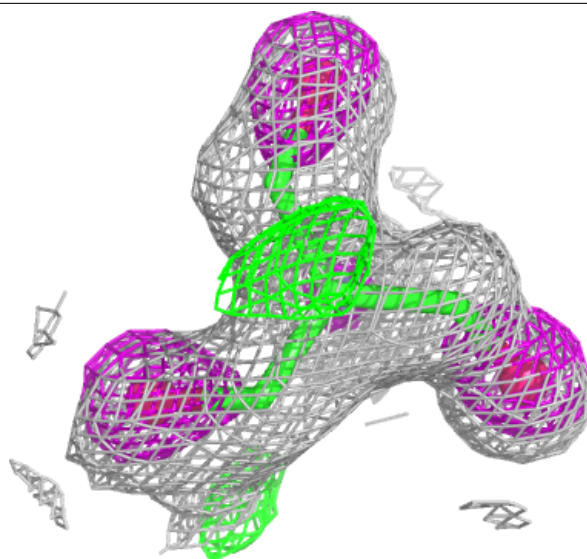
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	TRS	EEE	201	8/8	0.87	0.12	20,20,20,20	0
2	TRS	GGG	201	8/8	0.87	0.12	20,20,20,20	0
2	TRS	DDD	201	8/8	0.92	0.09	20,20,20,20	0
2	TRS	AAA	201	8/8	0.95	0.08	20,20,20,20	0
2	TRS	CCC	201	8/8	0.96	0.07	20,20,20,20	0
2	TRS	GGG	202	8/8	0.96	0.08	20,20,20,20	0
2	TRS	BBB	201	8/8	0.97	0.07	20,20,20,20	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.

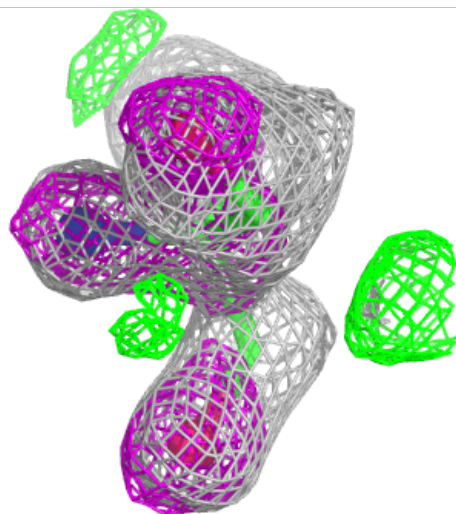
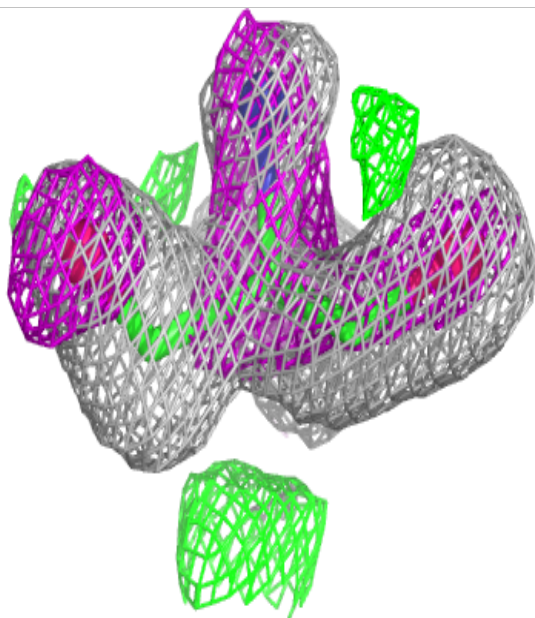
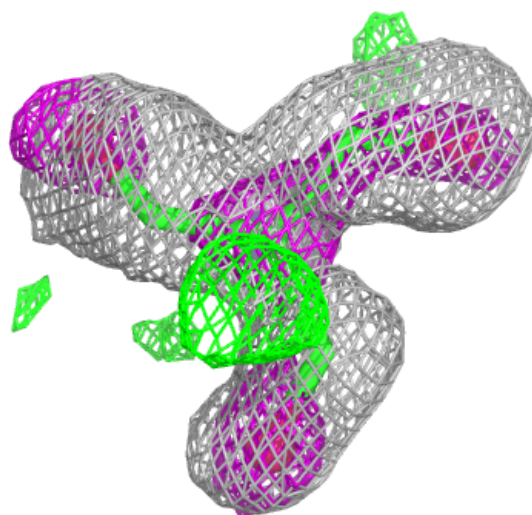
Electron density around TRS EEE 201:

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



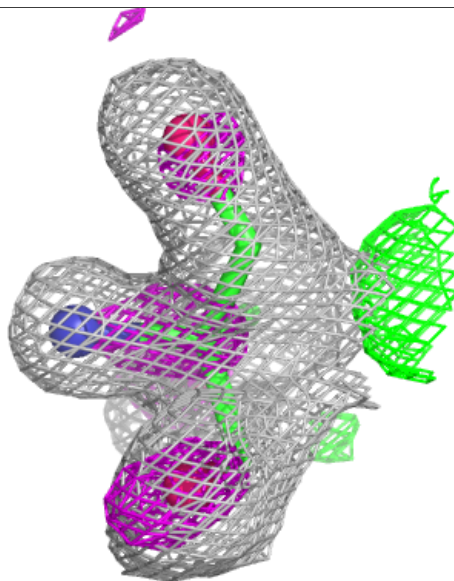
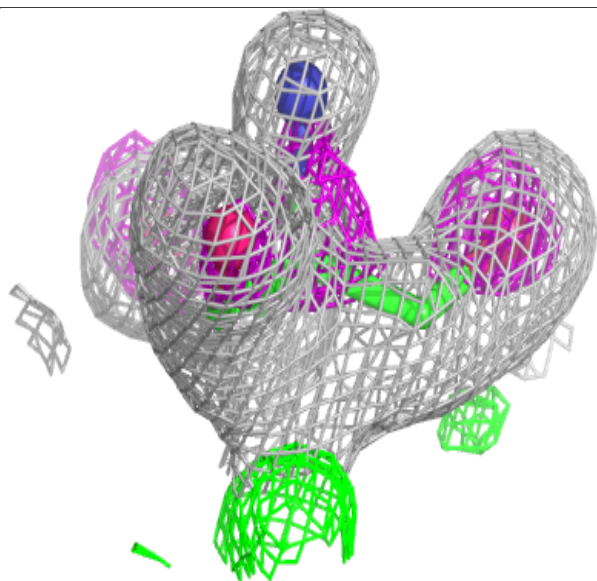
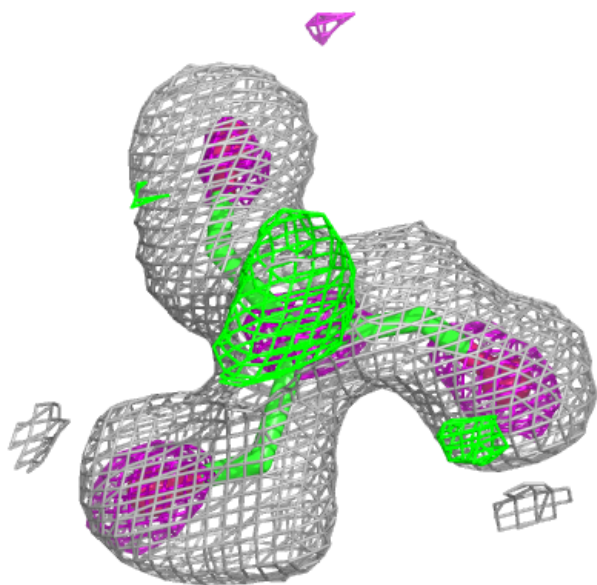
Electron density around TRS GGG 201:

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



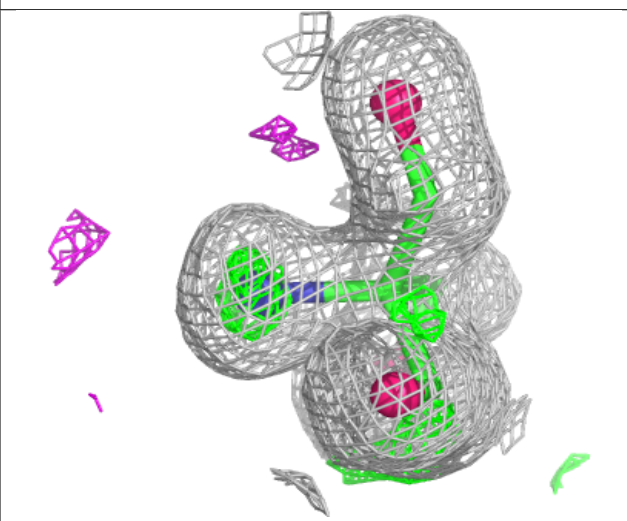
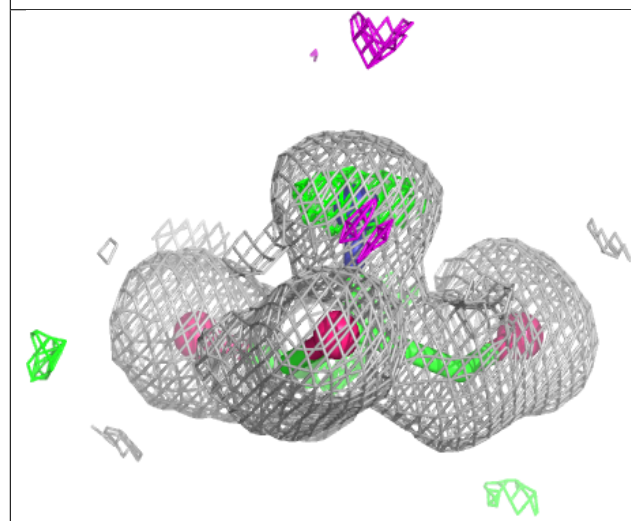
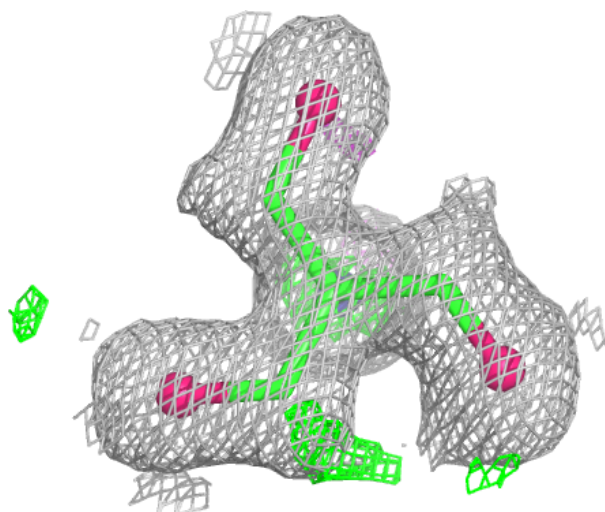
Electron density around TRS DDD 201:

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



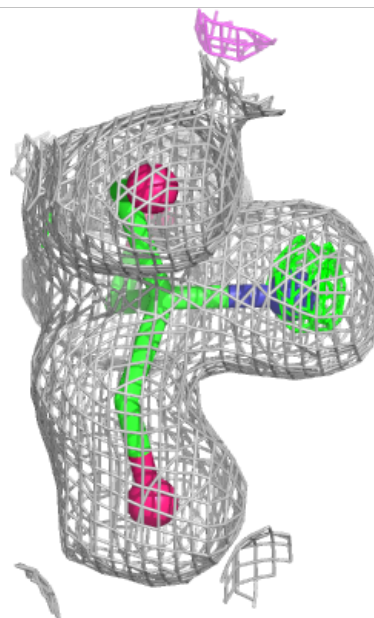
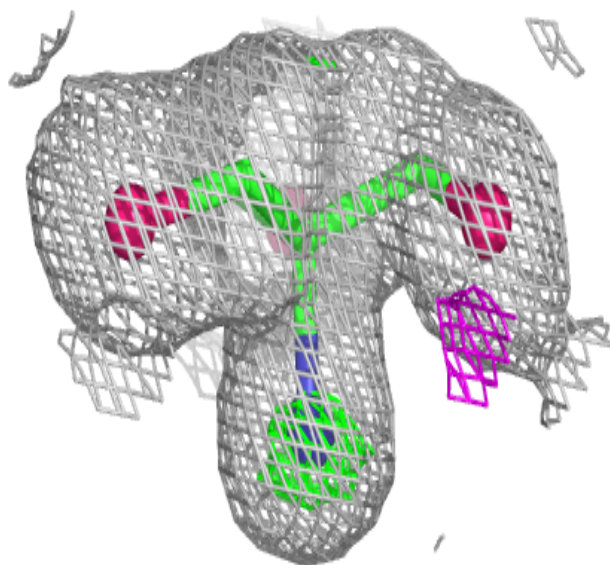
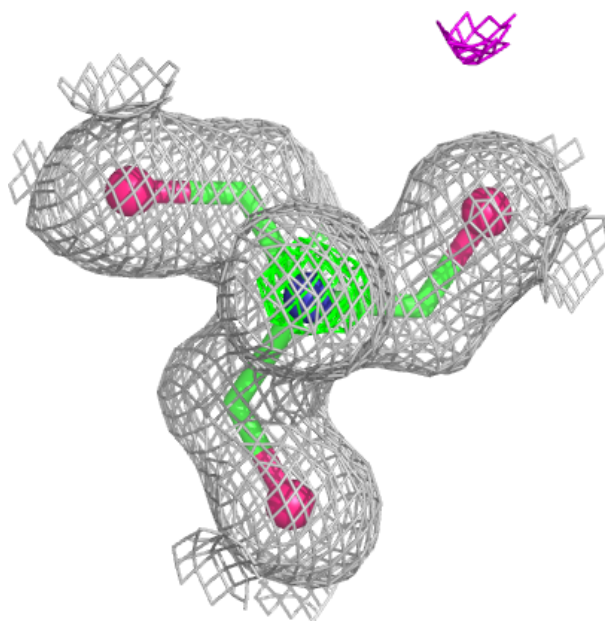
Electron density around TRS AAA 201:

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



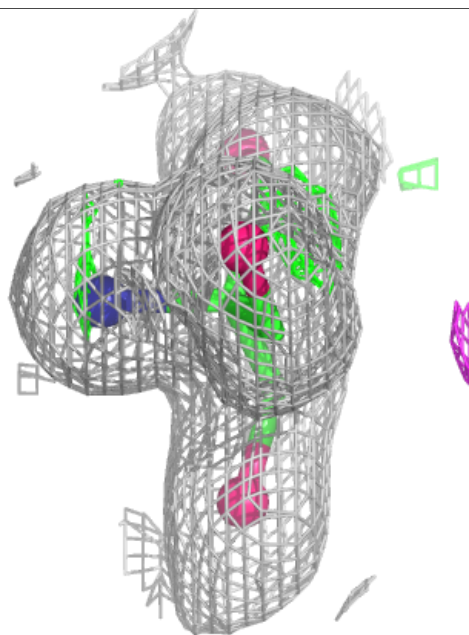
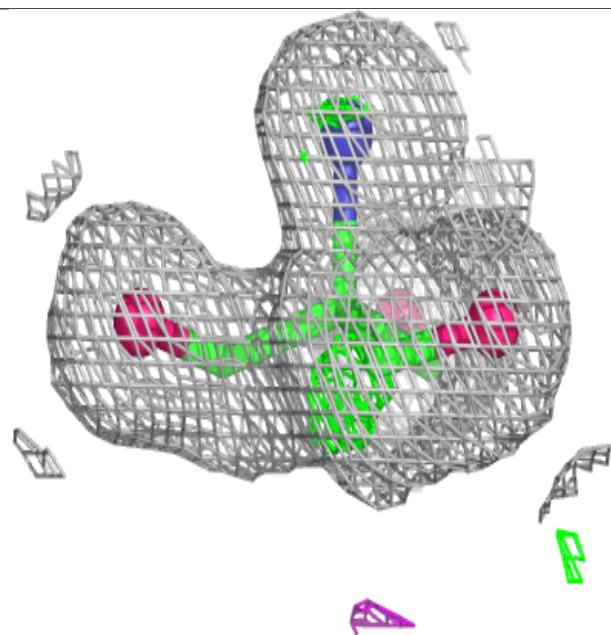
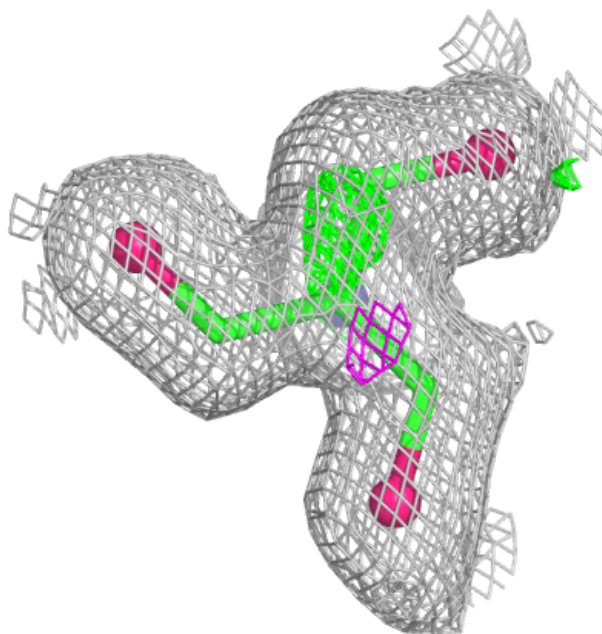
Electron density around TRS CCC 201:

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



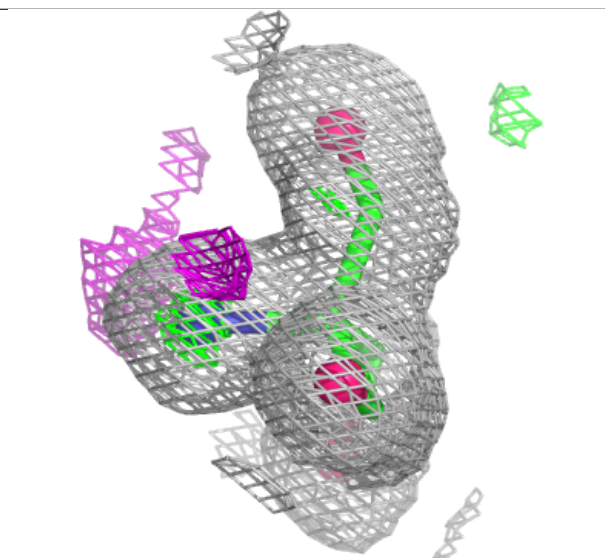
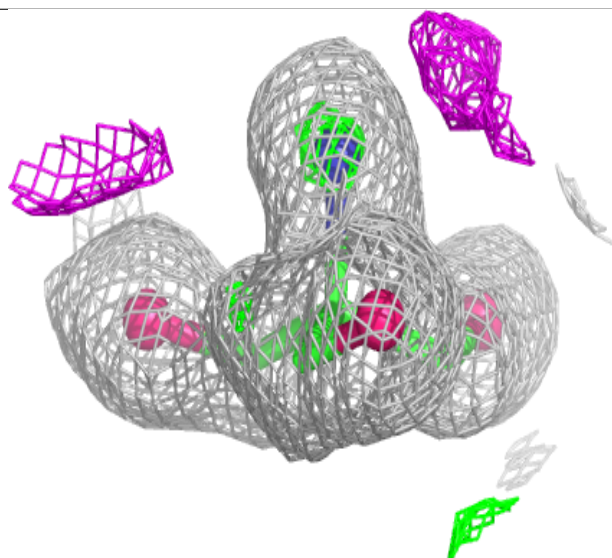
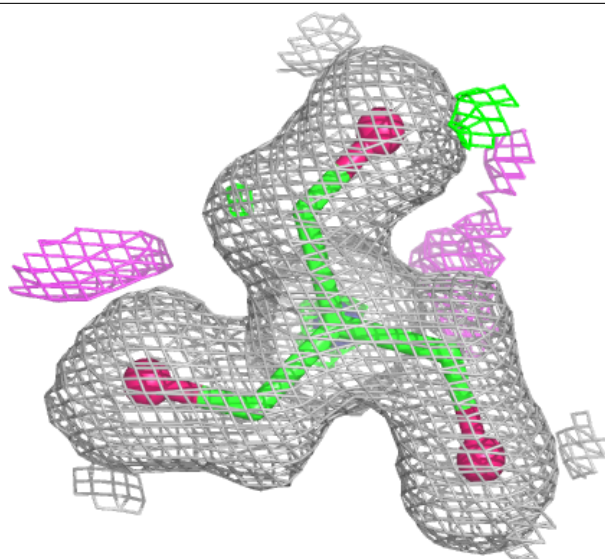
Electron density around TRS GGG 202:

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



Electron density around TRS BBB 201:

$2mF_o-DF_c$ (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.