



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:51 PM UTC

PDB ID : 8GOA / pdb_00008goa
Title : Crystal Structure of Glycerol Dehydrogenase in the absence of NAD⁺
Authors : Park, T.; Hoang, H.N.; Kang, J.Y.; Park, J.; Mun, S.A.; Jin, M.; Yang, J.;
Jung, C.-H.; Eom, S.H.
Deposited on : 2022-08-24
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

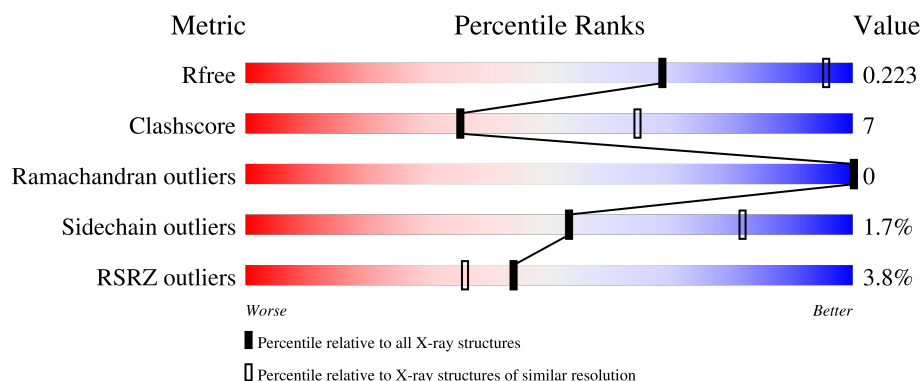
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	A	375	5% 83% 14% .
1	B	375	4% 85% 13% ..
1	C	375	% 84% 14% .
1	D	375	5% 79% 18% ..

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	TRS	A	403	-	-	X	-
3	TRS	B	403	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11323 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 Glycerol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2711	1717	460	520	14			
1	B	367	Total	C	N	O	S	0	0	0
			2715	1719	460	522	14			
1	C	367	Total	C	N	O	S	0	0	0
			2711	1716	459	522	14			
1	D	367	Total	C	N	O	S	0	0	0
			2707	1713	458	522	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	LEU	-	expression tag	UNP P0A9S5
A	369	GLU	-	expression tag	UNP P0A9S5
A	370	HIS	-	expression tag	UNP P0A9S5
A	371	HIS	-	expression tag	UNP P0A9S5
A	372	HIS	-	expression tag	UNP P0A9S5
A	373	HIS	-	expression tag	UNP P0A9S5
A	374	HIS	-	expression tag	UNP P0A9S5
A	375	HIS	-	expression tag	UNP P0A9S5
B	368	LEU	-	expression tag	UNP P0A9S5
B	369	GLU	-	expression tag	UNP P0A9S5
B	370	HIS	-	expression tag	UNP P0A9S5
B	371	HIS	-	expression tag	UNP P0A9S5
B	372	HIS	-	expression tag	UNP P0A9S5
B	373	HIS	-	expression tag	UNP P0A9S5
B	374	HIS	-	expression tag	UNP P0A9S5
B	375	HIS	-	expression tag	UNP P0A9S5
C	368	LEU	-	expression tag	UNP P0A9S5
C	369	GLU	-	expression tag	UNP P0A9S5
C	370	HIS	-	expression tag	UNP P0A9S5
C	371	HIS	-	expression tag	UNP P0A9S5
C	372	HIS	-	expression tag	UNP P0A9S5

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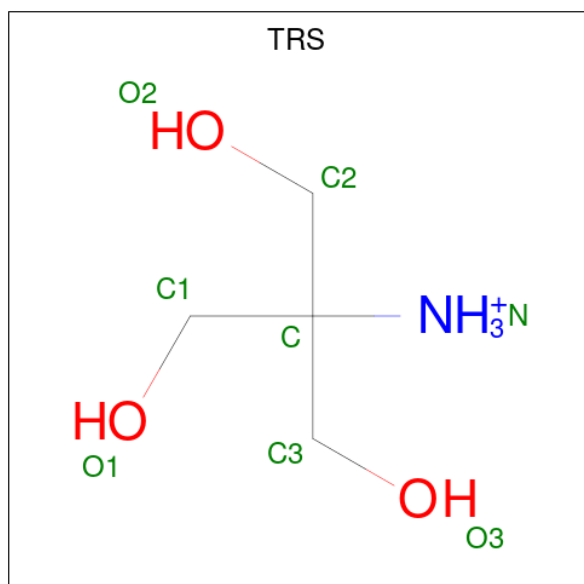
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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	HIS	-	expression tag	UNP P0A9S5
C	374	HIS	-	expression tag	UNP P0A9S5
C	375	HIS	-	expression tag	UNP P0A9S5
D	368	LEU	-	expression tag	UNP P0A9S5
D	369	GLU	-	expression tag	UNP P0A9S5
D	370	HIS	-	expression tag	UNP P0A9S5
D	371	HIS	-	expression tag	UNP P0A9S5
D	372	HIS	-	expression tag	UNP P0A9S5
D	373	HIS	-	expression tag	UNP P0A9S5
D	374	HIS	-	expression tag	UNP P0A9S5
D	375	HIS	-	expression tag	UNP P0A9S5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

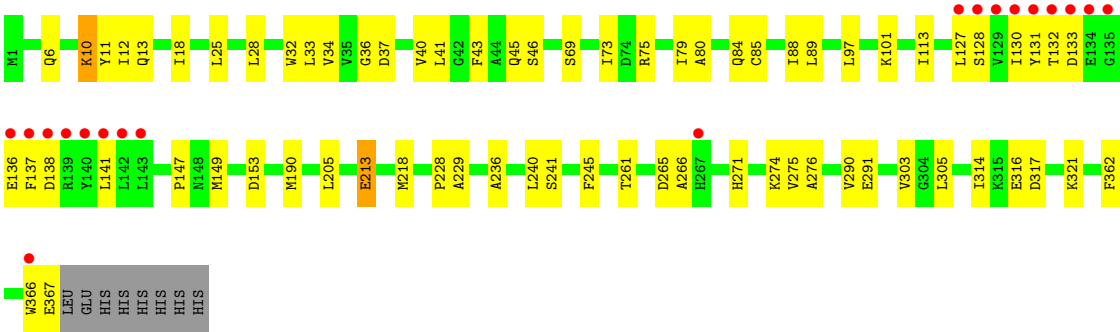
- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 8 4 1 3	0	0
3	A	1	Total C N O 8 4 1 3	0	0
3	A	1	Total C N O 8 4 1 3	0	0
3	B	1	Total C N O 8 4 1 3	0	0
3	B	1	Total C N O 8 4 1 3	0	0
3	B	1	Total C N O 8 4 1 3	0	0
3	C	1	Total C N O 8 4 1 3	0	0
3	C	1	Total C N O 8 4 1 3	0	0
3	C	1	Total C N O 8 4 1 3	0	0
3	D	1	Total C N O 8 4 1 3	0	0
3	D	1	Total C N O 8 4 1 3	0	0
3	D	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	110	Total O 110 110	0	0
4	B	92	Total O 92 92	0	0
4	C	106	Total O 106 106	0	0
4	D	71	Total O 71 71	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	161.47Å 161.47Å 291.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 2.90 49.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-2.90) 99.8 (49.24-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.220 0.196 , 0.223	Depositor DCC
R_{free} test set	4363 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11323	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: ZN, 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	A	0.41	0/2761	0.55	0/3759
1	B	0.39	0/2765	0.53	0/3764
1	C	0.39	0/2761	0.52	0/3760
1	D	0.37	0/2757	0.52	0/3756
All	All	0.39	0/11044	0.53	0/15039

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A	2711	0	2700	38	0
1	B	2715	0	2704	37	0
1	C	2711	0	2693	40	0
1	D	2707	0	2682	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	35	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	35	10	0
3	C	24	0	36	8	0
3	D	24	0	35	5	0
4	A	110	0	0	2	0
4	B	92	0	0	1	0
4	C	106	0	0	3	0
4	D	71	0	0	1	0
All	All	11323	0	10920	162	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 7.

All (162) 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:B:271:HIS:HB2	3:B:404:TRS:H12	1.51	0.89
1:D:271:HIS:HD1	3:D:403:TRS:H12	1.43	0.83
1:D:101:LYS:HD3	1:D:147:PRO:HG3	1.64	0.80
1:A:271:HIS:HA	3:A:403:TRS:H12	1.64	0.79
1:B:97:LEU:HD22	1:B:113:ILE:HG23	1.63	0.78
1:D:136:GLU:HB2	1:D:261:THR:HB	1.66	0.77
1:C:97:LEU:HD22	1:C:113:ILE:HG23	1.69	0.74
3:A:403:TRS:N	3:A:404:TRS:O1	2.21	0.74
1:D:97:LEU:HD22	1:D:113:ILE:HG23	1.70	0.72
1:C:41:LEU:HD22	1:C:45:GLN:HG3	1.72	0.71
1:C:218:MET:HG3	1:C:303:VAL:HG12	1.72	0.70
1:A:12:ILE:HG12	1:C:4:ILE:HG12	1.74	0.70
1:C:271:HIS:HB2	3:C:404:TRS:H12	1.74	0.70
1:C:211:LEU:HD23	1:C:299:LEU:HD22	1.74	0.69
1:C:77:ARG:O	1:C:81:GLU:HG3	1.92	0.69
1:C:107:MET:HG2	4:C:515:HOH:O	1.94	0.68
1:C:130:ILE:HG22	1:C:138:ASP:HB3	1.75	0.68
1:A:271:HIS:HD1	3:A:403:TRS:H32	1.59	0.67
1:B:367:GLU:N	1:B:367:GLU:OE2	2.28	0.66
3:B:403:TRS:N	3:B:404:TRS:H11	2.11	0.66
1:D:33:LEU:HD22	1:D:80:ALA:HB2	1.78	0.65
1:B:271:HIS:HA	3:B:403:TRS:H22	1.79	0.63
1:D:132:THR:HG22	1:D:133:ASP:H	1.63	0.62
1:C:270:TYR:HB2	1:C:273:GLU:HG3	1.81	0.62
1:A:270:TYR:HA	3:A:404:TRS:H12	1.82	0.62
1:D:127:LEU:HD22	1:D:190:MET:HE1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH1	1:A:83:ALA:O	2.33	0.61
1:A:123:PRO:O	1:A:124:CYS:HB2	1.99	0.61
1:D:37:ASP:O	1:D:41:LEU:HD12	2.01	0.61
1:C:271:HIS:H	3:C:404:TRS:H21	1.67	0.60
1:D:34:VAL:HG22	1:D:89:LEU:HD23	1.84	0.60
1:C:271:HIS:N	3:C:404:TRS:H21	2.17	0.60
1:A:228:PRO:HB2	1:B:287:ASN:HB2	1.83	0.59
1:B:149:MET:CE	1:B:151:ILE:HD11	2.32	0.59
1:A:252:ALA:HA	1:A:336:ILE:HD12	1.85	0.58
1:D:271:HIS:HA	3:D:403:TRS:H32	1.83	0.58
1:C:10:LYS:HB3	1:C:149:MET:HG3	1.85	0.58
1:C:252:ALA:HA	1:C:336:ILE:HD12	1.85	0.58
1:D:266:ALA:O	1:D:274:LYS:HE2	2.03	0.58
1:B:67:GLU:OE2	1:B:95:LYS:NZ	2.26	0.56
1:D:41:LEU:HB3	1:D:45:GLN:HB2	1.87	0.56
1:A:33:LEU:HD22	1:A:80:ALA:HB2	1.87	0.56
1:B:149:MET:HE3	1:B:151:ILE:HD11	1.88	0.56
1:C:287:ASN:HB2	1:D:228:PRO:HB2	1.87	0.56
1:C:41:LEU:O	1:C:45:GLN:HB2	2.06	0.55
1:D:131:TYR:OH	3:D:403:TRS:H11	2.06	0.55
1:A:250:LEU:HB2	1:A:335:THR:HG21	1.89	0.55
1:D:271:HIS:O	1:D:275:VAL:HG23	2.06	0.54
1:D:28:LEU:HD22	1:D:149:MET:HE3	1.89	0.54
1:D:131:TYR:CD1	1:D:137:PHE:HA	2.43	0.54
1:A:10:LYS:HB3	1:A:149:MET:HG2	1.88	0.54
1:A:274:LYS:NZ	3:A:403:TRS:H11	2.23	0.54
1:B:33:LEU:HD22	1:B:80:ALA:HB2	1.91	0.53
1:B:270:TYR:HD1	3:B:404:TRS:H22	1.73	0.53
1:B:131:TYR:CZ	3:B:403:TRS:H12	2.44	0.52
1:B:316:GLU:O	1:B:321:LYS:NZ	2.29	0.52
1:B:167:ALA:O	1:B:272:GLY:HA3	2.10	0.52
1:B:271:HIS:HD1	3:B:403:TRS:H32	1.75	0.52
1:B:270:TYR:HB2	1:B:273:GLU:HG3	1.90	0.52
1:A:267:HIS:HB3	4:A:588:HOH:O	2.10	0.51
1:A:257:HIS:NE2	3:A:403:TRS:O1	2.32	0.51
1:D:40:VAL:HA	1:D:43:PHE:CE1	2.46	0.51
1:D:130:ILE:HG22	1:D:138:ASP:HB3	1.91	0.51
1:C:274:LYS:NZ	3:C:403:TRS:O2	2.44	0.51
1:C:291:GLU:H	1:C:291:GLU:CD	2.18	0.51
1:D:10:LYS:HB3	1:D:149:MET:HG3	1.94	0.50
1:D:18:ILE:HG12	1:D:153:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LYS:NZ	1:B:54:ASP:OD2	2.40	0.50
3:C:403:TRS:N	3:C:404:TRS:H22	2.26	0.50
1:A:178:GLU:CD	1:A:253:ALA:HB3	2.37	0.50
1:C:334:GLU:O	1:C:337:HIS:HD2	1.94	0.50
1:C:257:HIS:NE2	3:C:403:TRS:H21	2.27	0.49
1:A:127:LEU:HD22	1:A:190:MET:HE3	1.94	0.49
1:A:37:ASP:OD1	1:A:38:LYS:N	2.45	0.49
1:A:101:LYS:HD3	1:A:147:PRO:HG3	1.95	0.49
1:B:25:LEU:HD22	1:B:32:TRP:CH2	2.48	0.49
3:B:403:TRS:HN2	3:B:404:TRS:H11	1.76	0.49
3:B:403:TRS:HN3	3:B:404:TRS:H11	1.78	0.49
1:D:75:ARG:O	1:D:79:ILE:HG13	2.13	0.49
1:D:316:GLU:O	1:D:321:LYS:NZ	2.33	0.49
3:C:403:TRS:HN1	3:C:404:TRS:H22	1.77	0.48
1:A:97:LEU:HD22	1:A:113:ILE:HG23	1.95	0.48
3:D:404:TRS:O1	3:D:404:TRS:O3	2.30	0.48
3:D:402:TRS:O2	3:D:402:TRS:O3	2.28	0.48
1:B:254:HIS:CD2	3:B:402:TRS:H11	2.48	0.47
1:D:291:GLU:HB2	4:D:530:HOH:O	2.13	0.47
1:B:93:GLY:O	1:B:97:LEU:HG	2.13	0.47
1:A:176:TRP:CE2	1:A:204:GLU:HG3	2.49	0.47
1:B:127:LEU:HD21	1:B:190:MET:SD	2.55	0.47
1:B:131:TYR:OH	3:B:403:TRS:H31	2.14	0.47
1:C:330:CYS:HA	1:C:336:ILE:HG21	1.97	0.47
1:A:107:MET:HB2	1:A:109:VAL:HG22	1.96	0.46
1:D:11:TYR:OH	1:D:13:GLN:NE2	2.48	0.46
1:A:291:GLU:HB2	4:A:525:HOH:O	2.14	0.46
1:D:362:PHE:HA	1:D:366:TRP:HB2	1.98	0.46
1:B:330:CYS:HA	1:B:336:ILE:HG21	1.97	0.46
1:D:127:LEU:HD12	1:D:141:LEU:O	2.16	0.46
1:D:236:ALA:HA	1:D:240:LEU:HB2	1.98	0.46
1:B:33:LEU:HD12	1:B:60:GLU:HB3	1.97	0.46
1:A:93:GLY:O	1:A:97:LEU:HG	2.15	0.45
1:A:270:TYR:HD1	3:A:404:TRS:H12	1.82	0.45
1:A:205:LEU:HD22	1:C:201:ALA:HB2	1.98	0.45
1:A:271:HIS:ND1	3:A:403:TRS:H32	2.29	0.45
1:B:24:TYR:HB3	1:B:149:MET:HE1	1.98	0.45
1:A:3:ARG:HB3	1:A:196:THR:HG22	1.99	0.45
1:A:330:CYS:HA	1:A:336:ILE:HG21	1.99	0.45
1:A:245:PHE:CE2	3:A:402:TRS:H11	2.52	0.45
1:C:33:LEU:HD11	1:C:62:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HD3	1:A:84:GLN:O	2.17	0.44
1:A:131:TYR:OH	3:A:403:TRS:H31	2.17	0.44
1:B:211:LEU:HD23	1:B:299:LEU:HD22	1.98	0.44
1:C:18:ILE:HD13	1:C:156:ILE:HD11	2.00	0.44
1:D:131:TYR:HD1	1:D:137:PHE:HA	1.83	0.44
1:C:33:LEU:HD22	1:C:80:ALA:HB2	2.00	0.44
1:D:127:LEU:HD22	1:D:190:MET:CE	2.47	0.44
1:A:45:GLN:O	1:A:49:GLU:HG3	2.18	0.43
1:A:17:VAL:HA	1:A:20:ARG:NH2	2.33	0.43
1:C:334:GLU:O	1:C:337:HIS:CD2	2.71	0.43
1:D:128:SER:HB2	1:D:141:LEU:HD23	1.99	0.43
1:A:321:LYS:O	1:A:325:VAL:HG23	2.18	0.43
1:D:236:ALA:O	1:D:241:SER:HB2	2.17	0.43
1:C:101:LYS:HD3	1:C:147:PRO:HG3	2.00	0.43
1:D:218:MET:HG3	1:D:303:VAL:HG12	2.00	0.43
1:D:265:ASP:HB2	1:D:314:ILE:HG12	2.00	0.43
1:C:25:LEU:HB3	1:C:32:TRP:CZ2	2.53	0.43
1:D:213:GLU:HG2	1:D:229:ALA:HA	2.01	0.43
1:A:270:TYR:HD1	3:A:404:TRS:C1	2.31	0.43
1:D:276:ALA:HB2	1:D:305:LEU:HD13	1.99	0.43
1:D:33:LEU:HB2	1:D:85:CYS:SG	2.59	0.43
1:C:173:LEU:HB3	4:C:546:HOH:O	2.17	0.43
1:D:41:LEU:HD12	1:D:41:LEU:H	1.84	0.42
1:C:267:HIS:HB3	4:C:585:HOH:O	2.18	0.42
1:C:245:PHE:HB2	1:C:250:LEU:HD21	2.01	0.42
1:D:36:GLY:C	1:D:41:LEU:HD11	2.43	0.42
1:A:274:LYS:HZ1	3:A:403:TRS:H11	1.85	0.42
1:D:127:LEU:HG	1:D:128:SER:O	2.20	0.42
1:B:267:HIS:HB3	4:B:553:HOH:O	2.20	0.42
1:C:33:LEU:HB2	1:C:85:CYS:SG	2.60	0.42
1:C:280:LEU:HA	1:C:280:LEU:HD12	1.84	0.42
1:A:77:ARG:O	1:A:81:GLU:HG3	2.19	0.41
1:C:236:ALA:HA	1:C:240:LEU:HB2	2.01	0.41
1:B:128:SER:HB3	1:B:141:LEU:HB3	2.01	0.41
1:C:206:CYS:HB2	1:C:240:LEU:HB3	2.02	0.41
1:C:257:HIS:CE1	3:C:403:TRS:H31	2.55	0.41
1:D:25:LEU:HB3	1:D:32:TRP:CZ2	2.55	0.41
1:B:31:ARG:NH1	1:B:58:VAL:HG21	2.36	0.41
1:C:117:ILE:HD12	1:C:119:SER:OG	2.21	0.41
1:B:323:ARG:HG2	1:B:349:TYR:CE1	2.55	0.41
1:D:33:LEU:HD23	1:D:88:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HB3	1:B:32:TRP:CZ2	2.55	0.41
1:B:107:MET:HE2	1:B:107:MET:HB3	1.87	0.41
1:A:167:ALA:O	1:A:272:GLY:HA3	2.21	0.41
1:B:4:ILE:HG12	1:D:12:ILE:HG12	2.02	0.41
1:B:10:LYS:HG3	1:D:6:GLN:HG2	2.01	0.41
1:D:69:SER:O	1:D:73:ILE:HG13	2.21	0.41
1:B:130:ILE:HD11	1:B:141:LEU:HD13	2.03	0.41
1:B:236:ALA:HA	1:B:240:LEU:HB2	2.03	0.41
1:B:201:ALA:HB2	1:D:205:LEU:HD22	2.02	0.40
1:C:149:MET:HE3	1:C:149:MET:HB2	1.86	0.40
1:C:323:ARG:HD3	1:C:323:ARG:HA	1.96	0.40
1:B:173:LEU:HD12	1:B:173:LEU:HA	1.94	0.40
1:C:299:LEU:O	1:C:303:VAL:HG22	2.21	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	A	365/375 (97%)	354 (97%)	11 (3%)	0	100	100
1	B	365/375 (97%)	357 (98%)	8 (2%)	0	100	100
1	C	365/375 (97%)	355 (97%)	10 (3%)	0	100	100
1	D	365/375 (97%)	356 (98%)	9 (2%)	0	100	100
All	All	1460/1500 (97%)	1422 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/283 (96%)	270 (99%)	3 (1%)	65	88
1	B	274/283 (97%)	270 (98%)	4 (2%)	57	84
1	C	273/283 (96%)	269 (98%)	4 (2%)	57	84
1	D	272/283 (96%)	264 (97%)	8 (3%)	37	71
All	All	1092/1132 (96%)	1073 (98%)	19 (2%)	53	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	37	ASP
1	A	141	LEU
1	B	10	LYS
1	B	28	LEU
1	B	58	VAL
1	B	290	VAL
1	C	47	THR
1	C	290	VAL
1	C	317	ASP
1	C	336	ILE
1	D	10	LYS
1	D	46	SER
1	D	84	GLN
1	D	213	GLU
1	D	245	PHE
1	D	290	VAL
1	D	317	ASP
1	D	367	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	237	ASN
1	A	357	GLN
1	B	84	GLN
1	B	301	HIS
1	B	364	GLN
1	C	6	GLN
1	C	337	HIS
1	D	13	GLN
1	D	105	HIS
1	D	145	ASN
1	D	237	ASN
1	D	258	ASN
1	D	337	HIS

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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
3	TRS	D	402	2	7,7,7	0.51	0	9,9,9	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRS	A	404	-	7,7,7	0.74	0	9,9,9	1.04	0
3	TRS	C	404	-	7,7,7	0.55	0	9,9,9	0.80	0
3	TRS	B	402	2	7,7,7	0.55	0	9,9,9	0.75	0
3	TRS	B	404	-	7,7,7	0.52	0	9,9,9	0.92	0
3	TRS	D	403	-	7,7,7	0.56	0	9,9,9	0.79	0
3	TRS	C	402	2	7,7,7	0.55	0	9,9,9	0.97	0
3	TRS	C	403	-	7,7,7	0.60	0	9,9,9	1.08	1 (11%)
3	TRS	A	403	-	7,7,7	0.66	0	9,9,9	1.29	1 (11%)
3	TRS	B	403	-	7,7,7	0.60	0	9,9,9	1.01	1 (11%)
3	TRS	D	404	-	7,7,7	0.61	0	9,9,9	0.74	0
3	TRS	A	402	2	7,7,7	0.60	0	9,9,9	1.07	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
3	TRS	D	402	2	-	6/9/9/9	-
3	TRS	A	404	-	-	0/9/9/9	-
3	TRS	C	404	-	-	7/9/9/9	-
3	TRS	B	402	2	-	6/9/9/9	-
3	TRS	B	404	-	-	9/9/9/9	-
3	TRS	D	403	-	-	8/9/9/9	-
3	TRS	C	402	2	-	6/9/9/9	-
3	TRS	C	403	-	-	7/9/9/9	-
3	TRS	A	403	-	-	3/9/9/9	-
3	TRS	B	403	-	-	8/9/9/9	-
3	TRS	D	404	-	-	8/9/9/9	-
3	TRS	A	402	2	-	6/9/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	TRS	C3-C-C2	-2.25	104.66	110.66
3	A	403	TRS	O3-C3-C	2.18	116.94	110.88
3	C	403	TRS	O1-C1-C	2.10	116.72	110.88

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	TRS	C3-C-C1-O1
3	A	402	TRS	N-C-C1-O1
3	A	402	TRS	N-C-C3-O3
3	A	403	TRS	C1-C-C3-O3
3	A	403	TRS	C2-C-C3-O3
3	B	402	TRS	C2-C-C1-O1
3	B	402	TRS	C3-C-C1-O1
3	B	402	TRS	N-C-C1-O1
3	B	402	TRS	C1-C-C3-O3
3	B	402	TRS	C2-C-C3-O3
3	B	402	TRS	N-C-C3-O3
3	B	404	TRS	C2-C-C1-O1
3	B	404	TRS	C3-C-C1-O1
3	B	404	TRS	N-C-C1-O1
3	B	404	TRS	C1-C-C3-O3
3	C	403	TRS	N-C-C1-O1
3	C	403	TRS	C1-C-C3-O3
3	C	403	TRS	C2-C-C3-O3
3	C	403	TRS	N-C-C3-O3
3	C	404	TRS	C1-C-C2-O2
3	C	404	TRS	C3-C-C2-O2
3	D	402	TRS	C2-C-C1-O1
3	D	402	TRS	C3-C-C1-O1
3	D	402	TRS	N-C-C1-O1
3	D	402	TRS	C1-C-C3-O3
3	D	402	TRS	C2-C-C3-O3
3	D	402	TRS	N-C-C3-O3
3	D	403	TRS	C3-C-C1-O1
3	D	403	TRS	N-C-C2-O2
3	D	403	TRS	C1-C-C3-O3
3	D	403	TRS	C2-C-C3-O3
3	D	403	TRS	N-C-C3-O3
3	D	404	TRS	C1-C-C3-O3
3	D	404	TRS	C2-C-C3-O3
3	D	404	TRS	N-C-C3-O3
3	A	402	TRS	C2-C-C1-O1
3	B	403	TRS	C1-C-C2-O2
3	B	404	TRS	C1-C-C2-O2
3	B	404	TRS	C2-C-C3-O3
3	D	403	TRS	C2-C-C1-O1

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Mol	Chain	Res	Type	Atoms
3	A	402	TRS	C2-C-C3-O3
3	B	403	TRS	C3-C-C1-O1
3	B	403	TRS	N-C-C2-O2
3	B	404	TRS	N-C-C2-O2
3	C	402	TRS	N-C-C1-O1
3	C	402	TRS	N-C-C3-O3
3	C	403	TRS	C2-C-C1-O1
3	C	404	TRS	N-C-C2-O2
3	D	403	TRS	C1-C-C2-O2
3	D	404	TRS	C1-C-C2-O2
3	D	404	TRS	N-C-C2-O2
3	B	403	TRS	C2-C-C1-O1
3	B	403	TRS	C3-C-C2-O2
3	B	403	TRS	C1-C-C3-O3
3	B	404	TRS	C3-C-C2-O2
3	C	402	TRS	C2-C-C1-O1
3	D	404	TRS	C3-C-C1-O1
3	D	404	TRS	C3-C-C2-O2
3	A	403	TRS	N-C-C3-O3
3	B	403	TRS	N-C-C1-O1
3	B	404	TRS	N-C-C3-O3
3	C	404	TRS	C1-C-C3-O3
3	D	403	TRS	N-C-C1-O1
3	A	402	TRS	C1-C-C3-O3
3	B	403	TRS	C2-C-C3-O3
3	C	402	TRS	C3-C-C2-O2
3	C	402	TRS	C1-C-C3-O3
3	C	402	TRS	C2-C-C3-O3
3	C	403	TRS	C3-C-C1-O1
3	C	403	TRS	C3-C-C2-O2
3	C	404	TRS	C3-C-C1-O1
3	C	404	TRS	C2-C-C3-O3
3	C	404	TRS	N-C-C1-O1
3	D	404	TRS	N-C-C1-O1

There are no ring outliers.

11 monomers are involved in 35 short contacts:

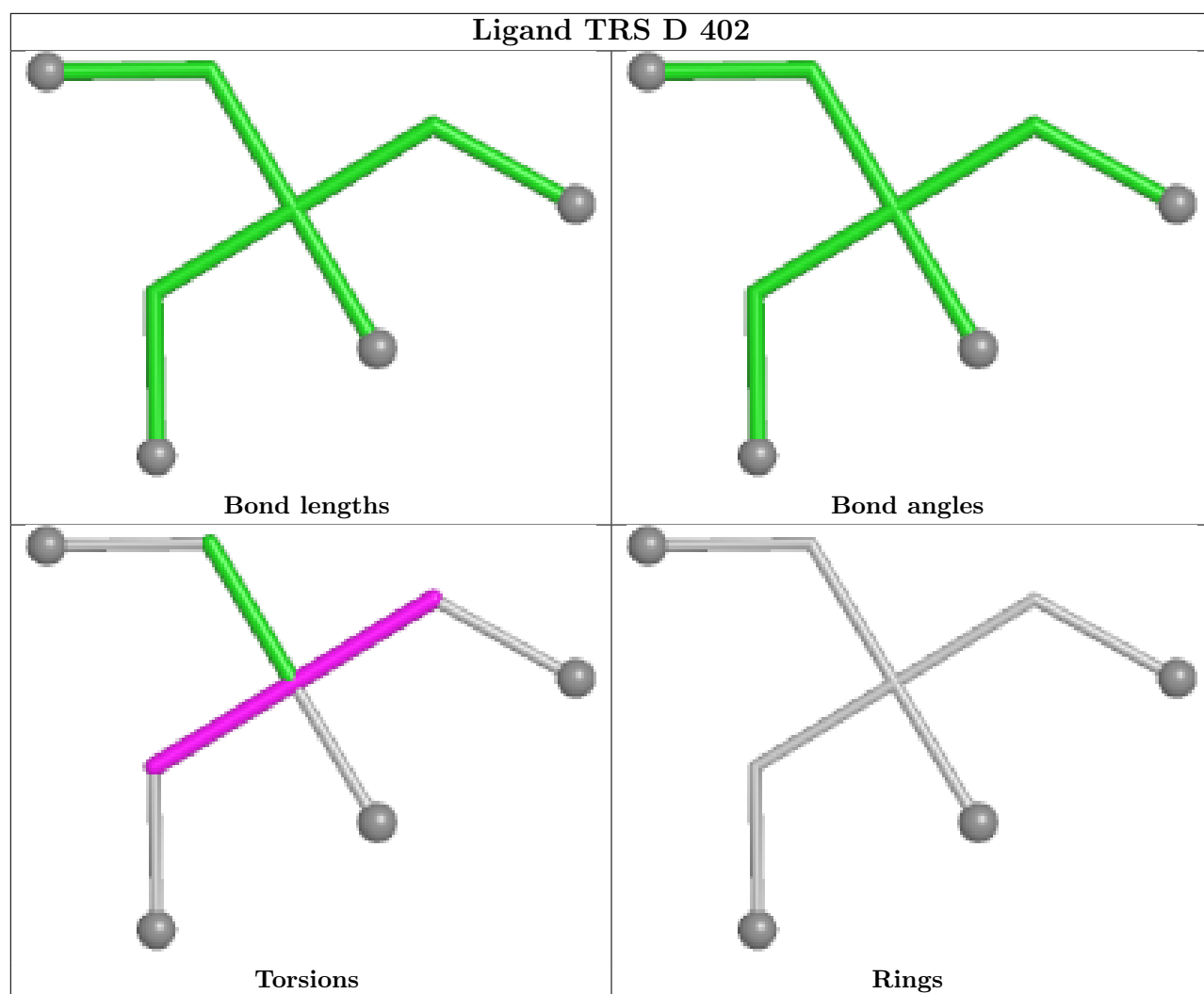
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	TRS	1	0
3	A	404	TRS	4	0
3	C	404	TRS	5	0

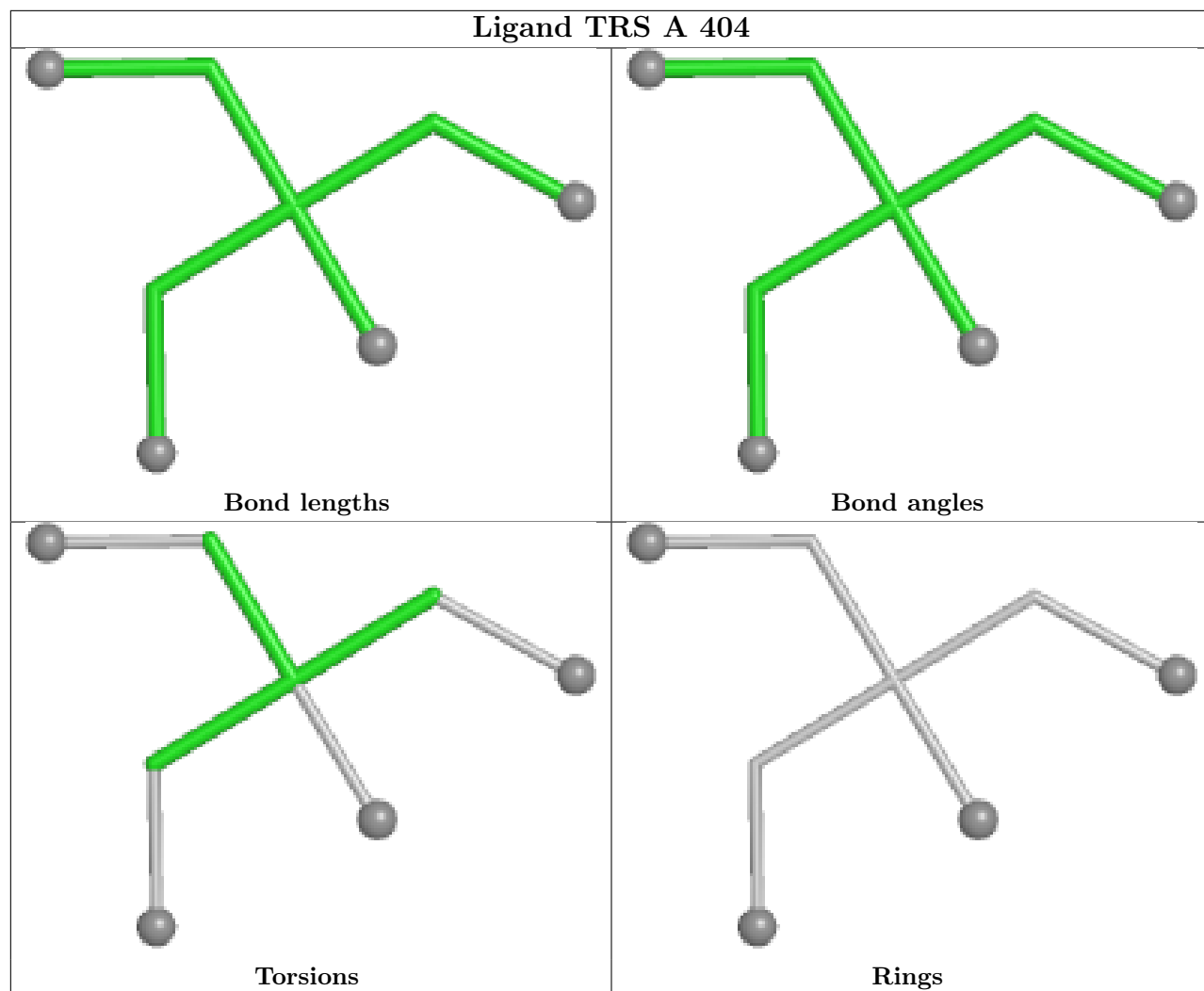
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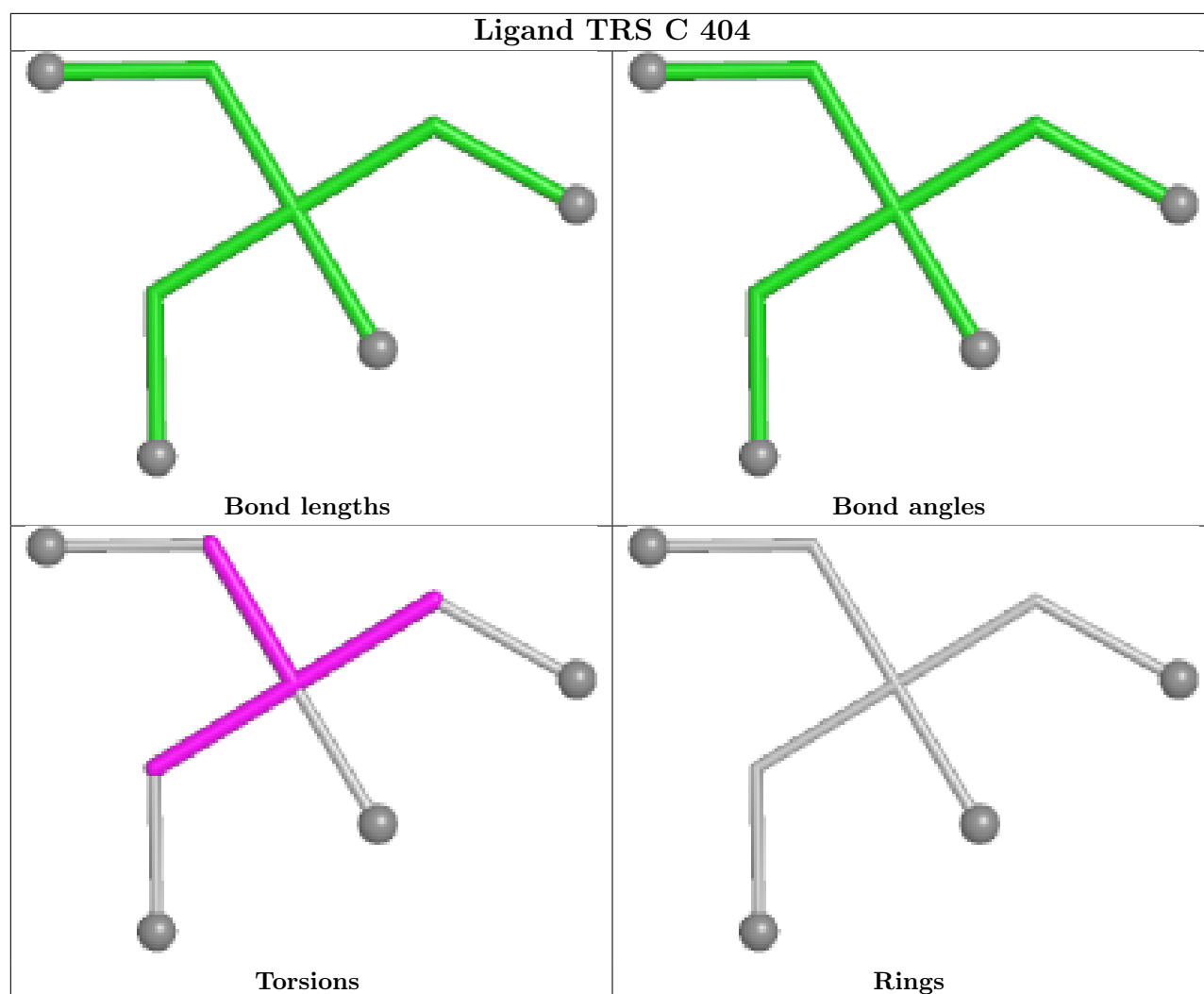
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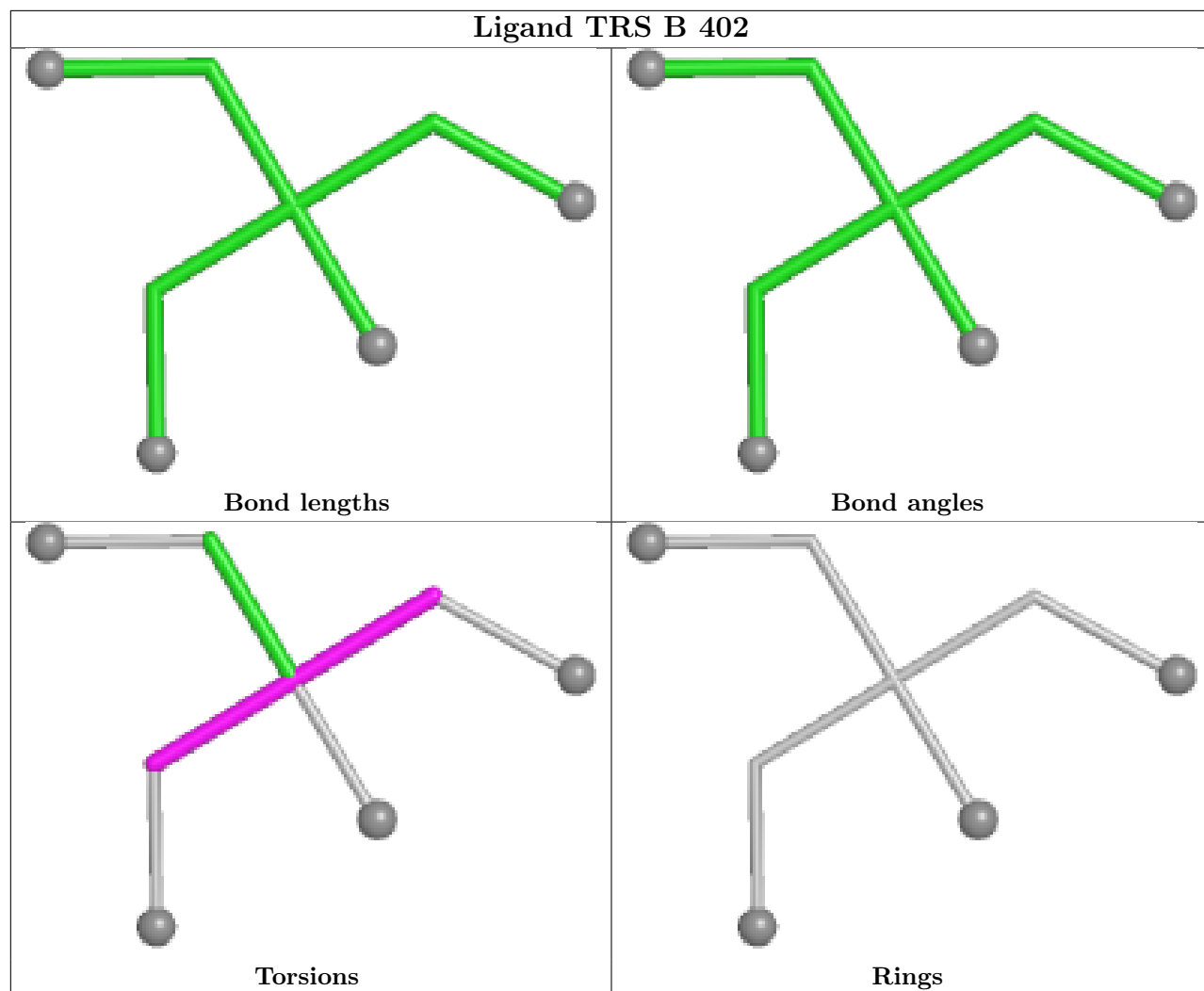
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	TRS	1	0
3	B	404	TRS	5	0
3	D	403	TRS	3	0
3	C	403	TRS	5	0
3	A	403	TRS	8	0
3	B	403	TRS	7	0
3	D	404	TRS	1	0
3	A	402	TRS	1	0

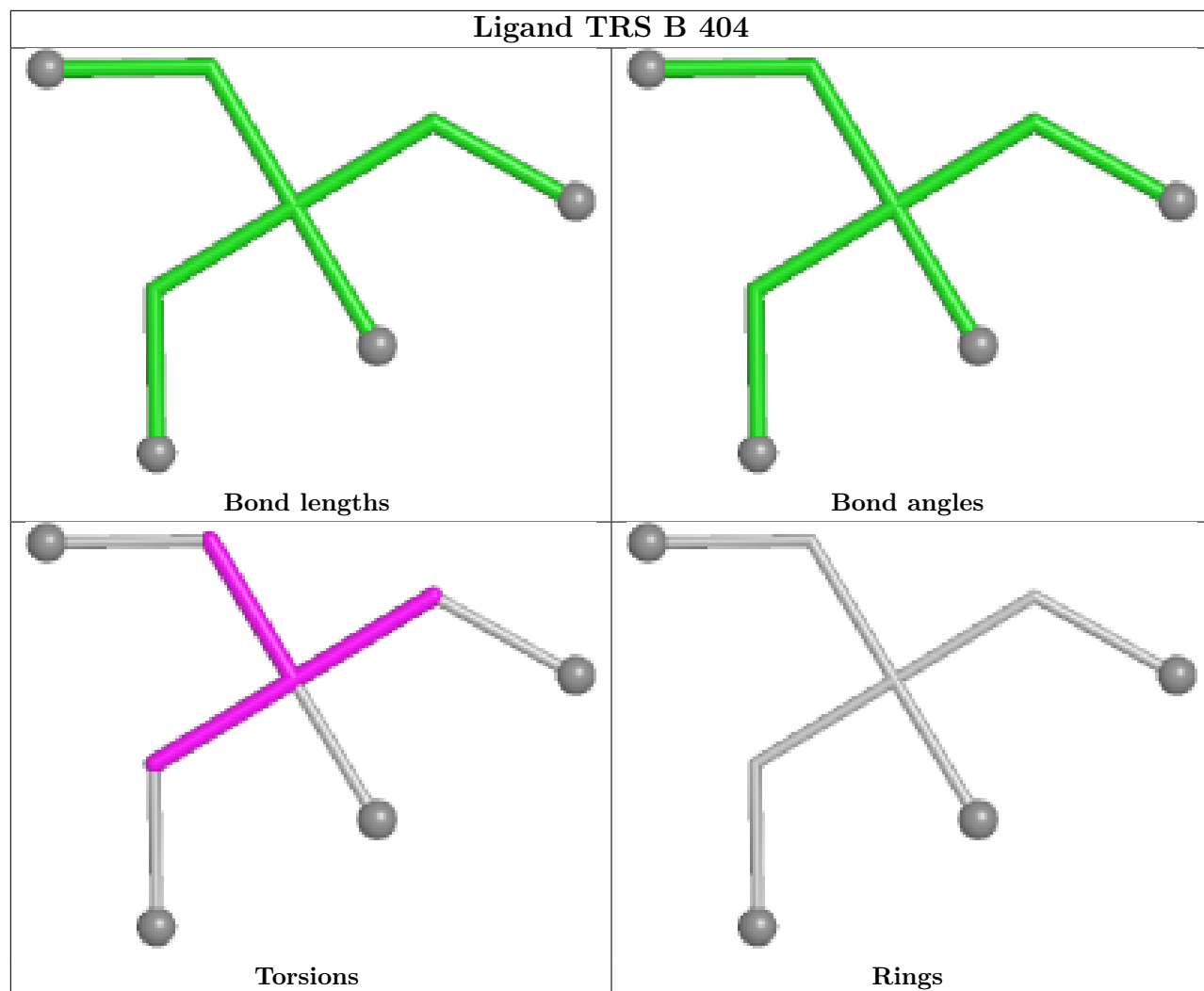
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

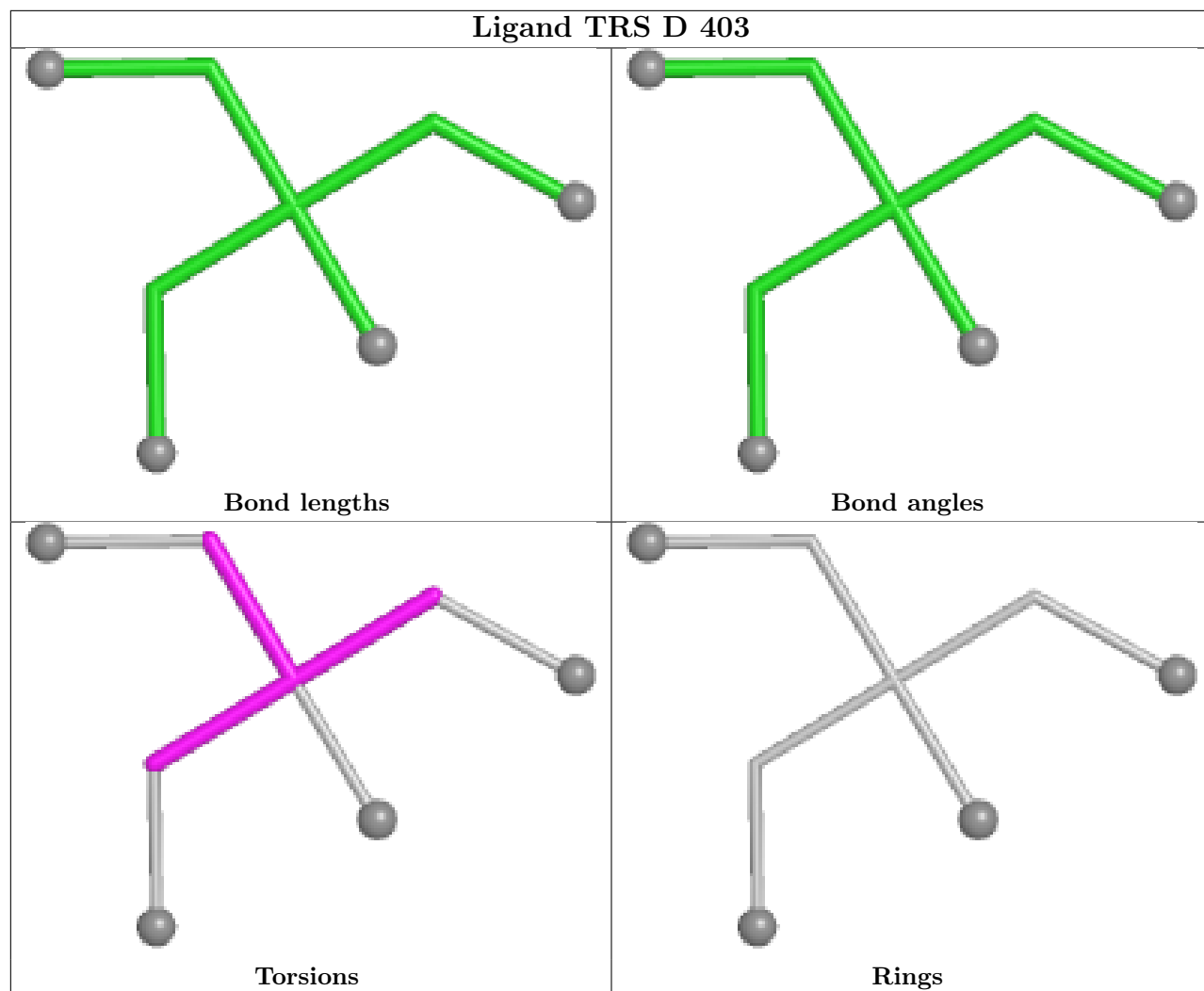


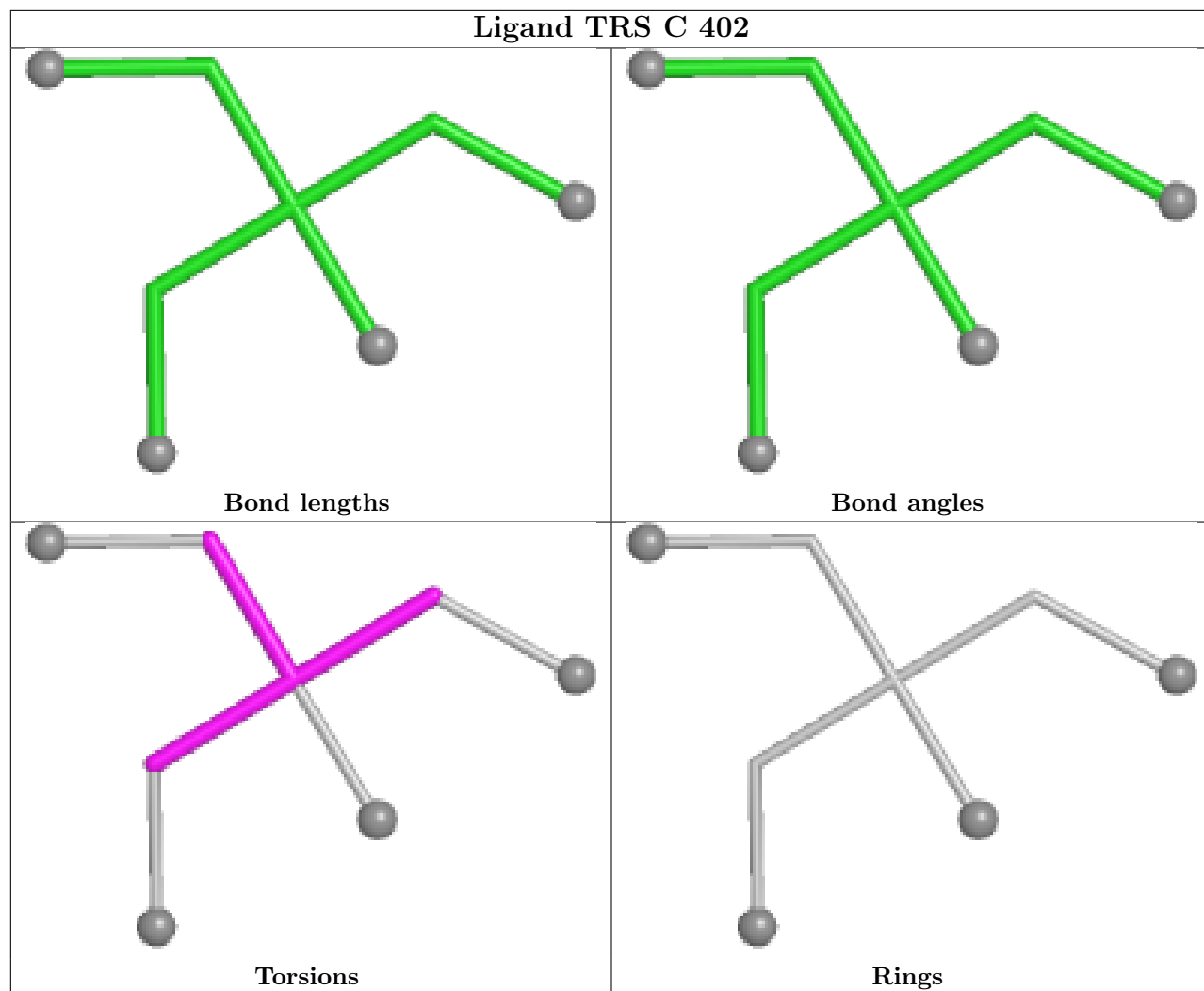


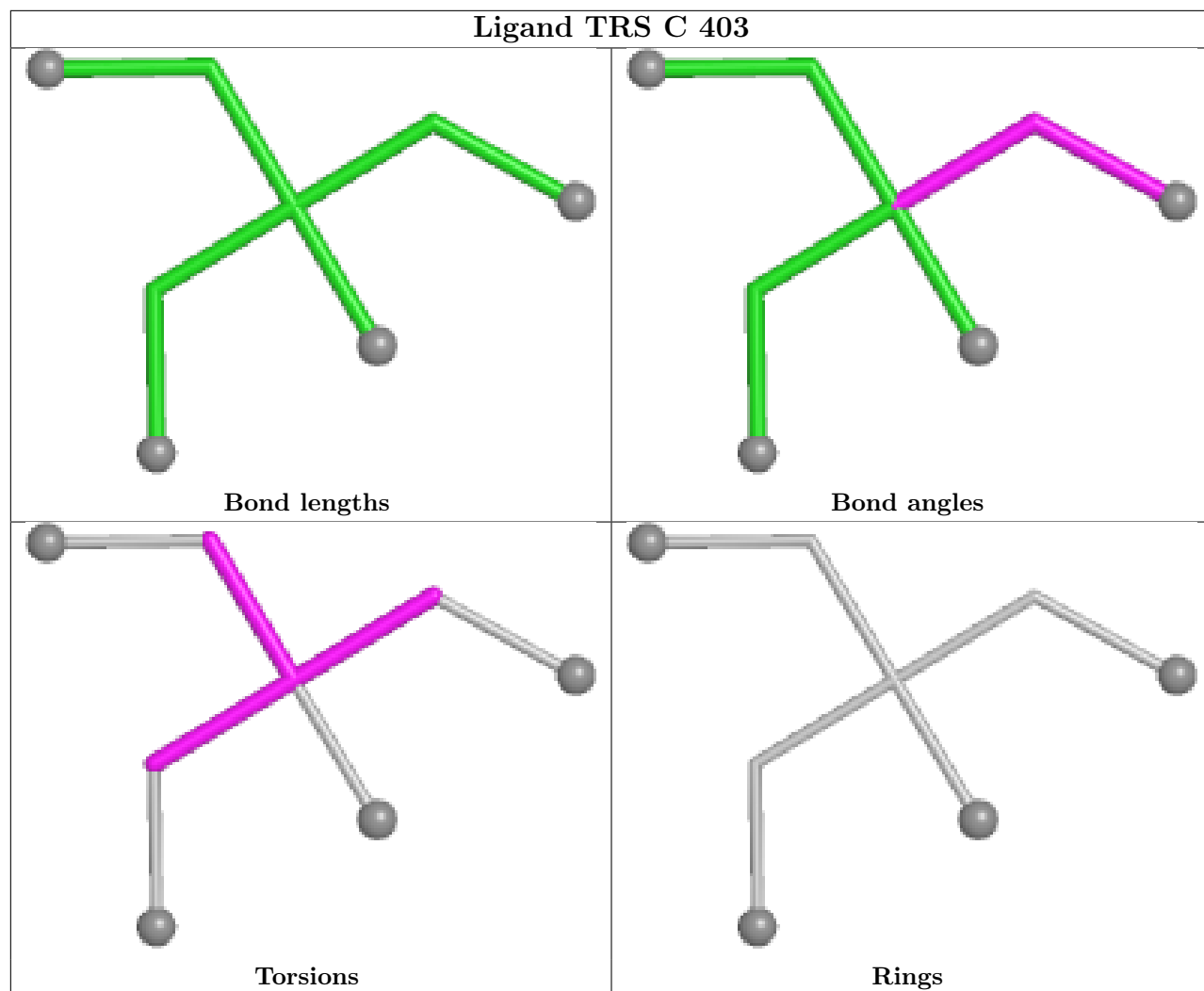


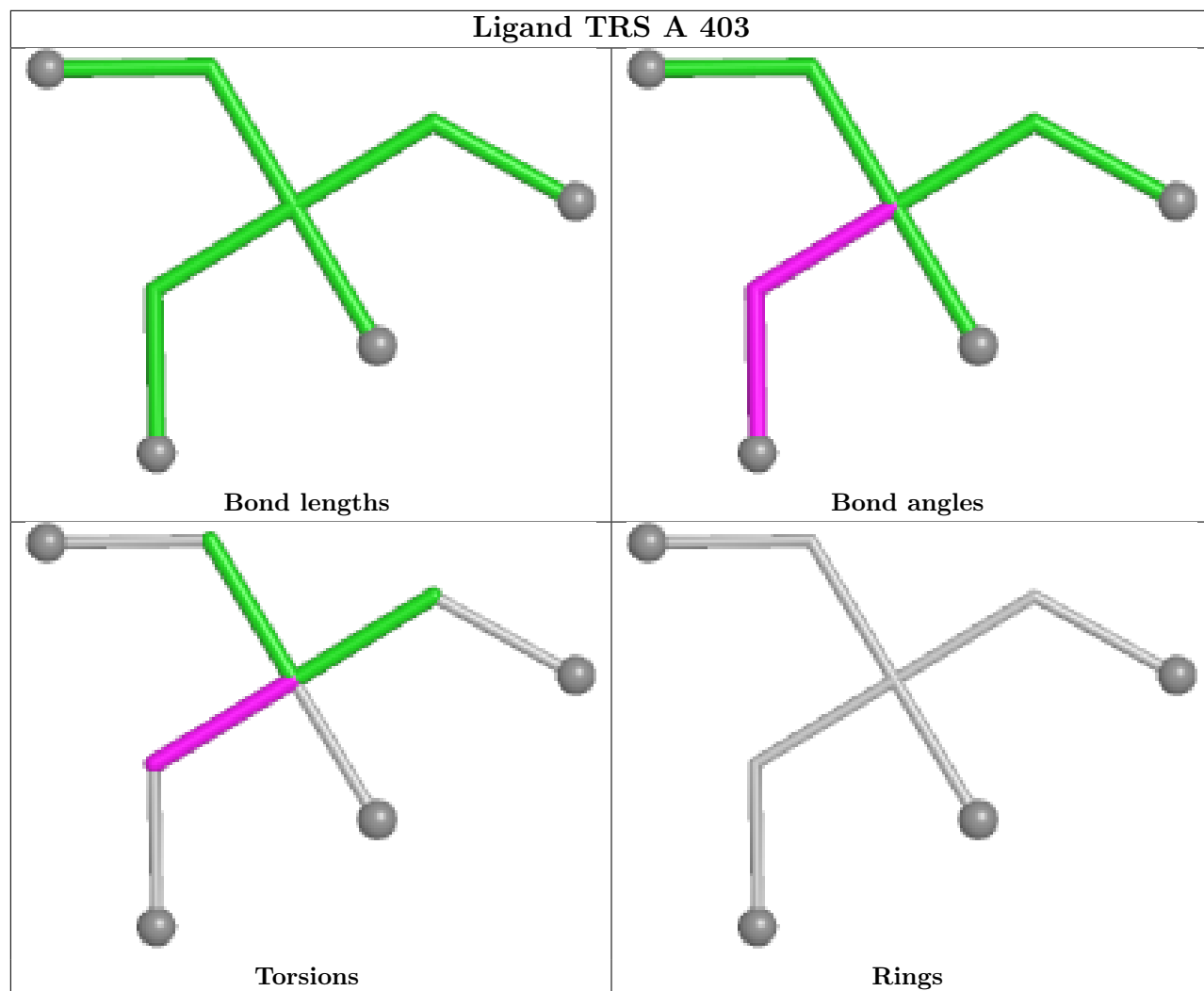


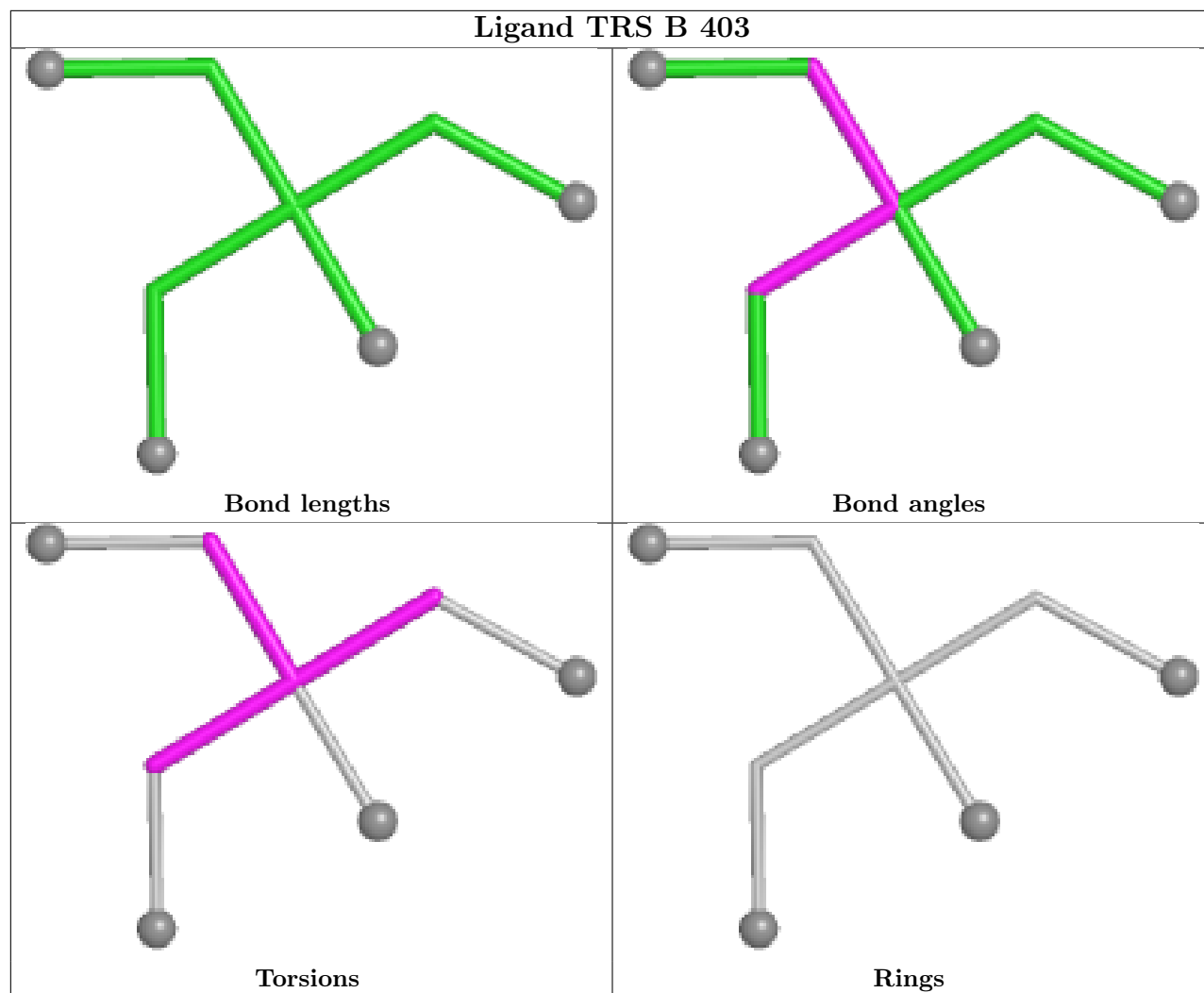


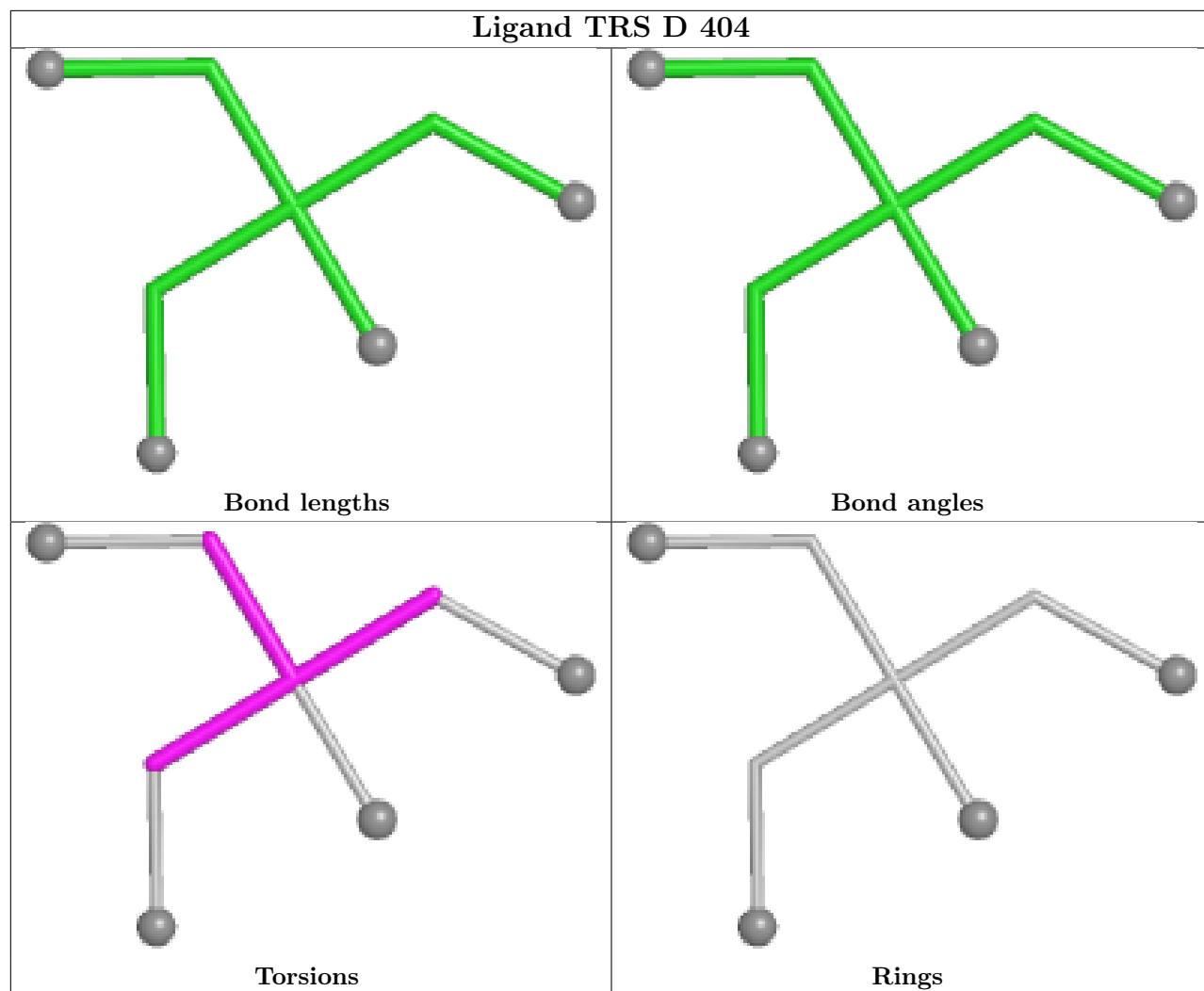


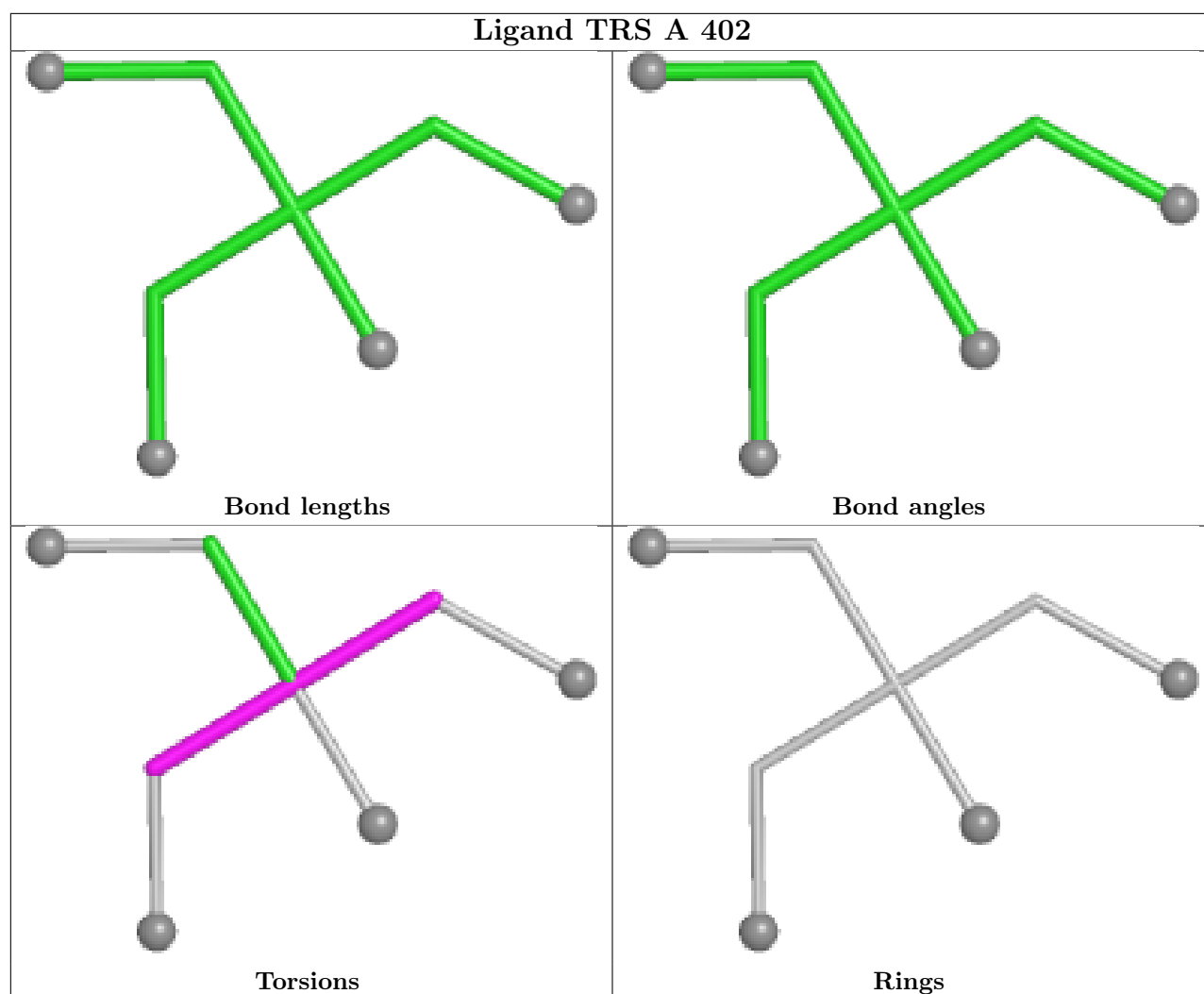












5.7 Other polymers [i](#)

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	A	367/375 (97%)	-0.25	19 (5%) 33 26	37, 52, 84, 139	0
1	B	367/375 (97%)	-0.38	16 (4%) 39 30	39, 51, 81, 131	0
1	C	367/375 (97%)	-0.43	2 (0%) 87 83	38, 52, 72, 95	0
1	D	367/375 (97%)	0.02	19 (5%) 33 26	43, 60, 100, 163	0
All	All	1468/1500 (97%)	-0.26	56 (3%) 44 36	37, 54, 88, 163	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	129	VAL	9.1
1	D	130	ILE	5.5
1	A	130	ILE	5.5
1	D	128	SER	5.3
1	D	131	TYR	5.3
1	D	137	PHE	5.1
1	C	367	GLU	5.1
1	D	135	GLY	4.7
1	D	140	TYR	4.7
1	A	140	TYR	4.6
1	D	132	THR	4.5
1	D	136	GLU	4.5
1	D	366	TRP	4.3
1	D	139	ARG	4.3
1	A	128	SER	4.3
1	A	134	GLU	4.2
1	D	141	LEU	4.1
1	B	130	ILE	3.8
1	A	129	VAL	3.8
1	A	367	GLU	3.5
1	B	131	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	128	SER	3.4
1	A	141	LEU	3.3
1	C	268	HIS	3.2
1	B	366	TRP	3.2
1	B	132	THR	3.1
1	A	135	GLY	3.0
1	A	139	ARG	3.0
1	B	134	GLU	3.0
1	B	138	ASP	2.9
1	A	366	TRP	2.9
1	B	135	GLY	2.8
1	A	137	PHE	2.8
1	A	138	ASP	2.8
1	B	133	ASP	2.8
1	A	142	LEU	2.7
1	B	139	ARG	2.7
1	B	367	GLU	2.7
1	B	129	VAL	2.7
1	B	127	LEU	2.7
1	D	127	LEU	2.6
1	D	134	GLU	2.6
1	B	361	ARG	2.5
1	D	138	ASP	2.5
1	A	132	THR	2.4
1	D	133	ASP	2.4
1	A	136	GLU	2.3
1	D	142	LEU	2.3
1	B	142	LEU	2.3
1	A	337	HIS	2.3
1	D	143	LEU	2.2
1	D	267	HIS	2.1
1	A	267	HIS	2.1
1	A	131	TYR	2.1
1	A	332	GLU	2.1
1	B	365	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

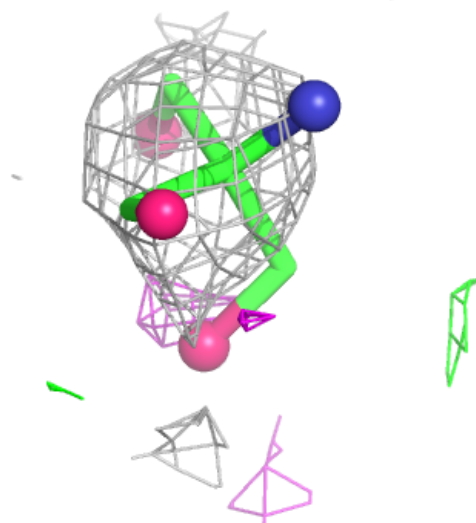
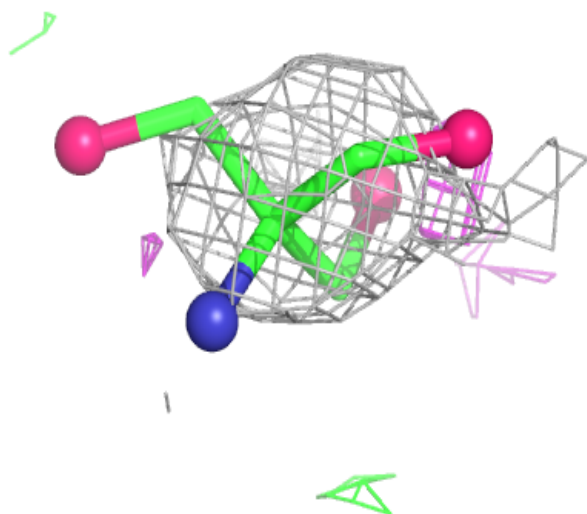
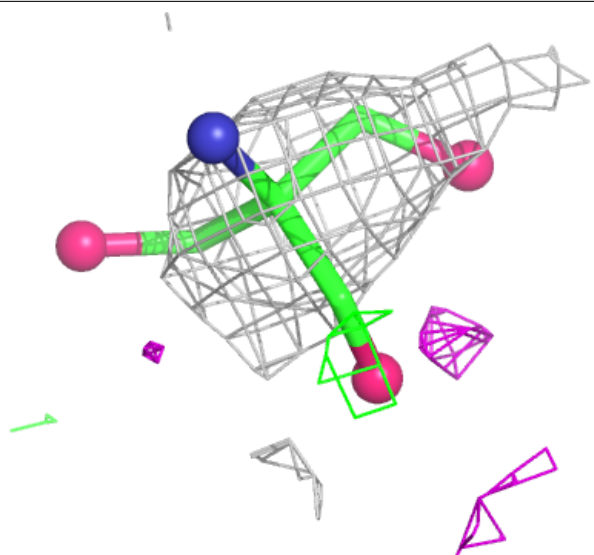
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TRS	D	403	8/8	0.78	0.23	87,97,110,110	0
3	TRS	C	404	8/8	0.79	0.19	79,85,94,113	0
3	TRS	C	403	8/8	0.79	0.21	79,90,101,105	0
3	TRS	B	403	8/8	0.83	0.22	66,75,93,95	8
3	TRS	A	404	8/8	0.85	0.21	60,74,85,91	0
3	TRS	D	404	8/8	0.85	0.20	73,79,89,97	0
3	TRS	A	403	8/8	0.90	0.14	70,83,101,107	0
3	TRS	B	404	8/8	0.91	0.20	64,75,81,89	0
3	TRS	D	402	8/8	0.93	0.19	86,91,98,130	0
3	TRS	C	402	8/8	0.95	0.19	52,73,79,83	8
3	TRS	A	402	8/8	0.95	0.21	74,75,88,95	8
3	TRS	B	402	8/8	0.95	0.17	87,89,119,133	0
2	ZN	A	401	1/1	1.00	0.06	49,49,49,49	0
2	ZN	B	401	1/1	1.00	0.01	44,44,44,44	0
2	ZN	C	401	1/1	1.00	0.05	53,53,53,53	0
2	ZN	D	401	1/1	1.00	0.04	57,57,57,57	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.

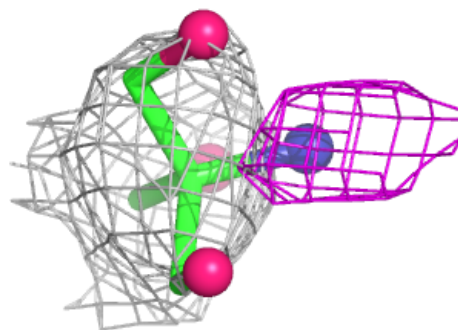
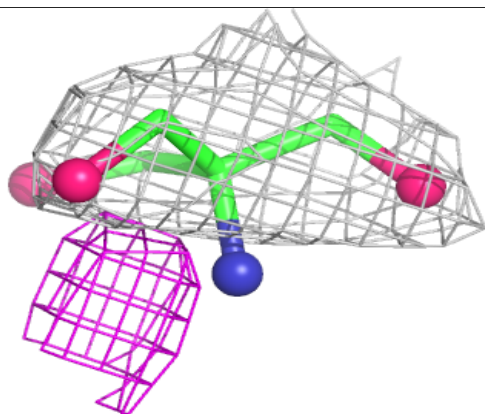
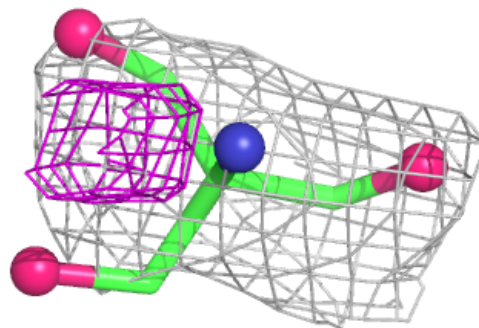
Electron density around TRS D 403:

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



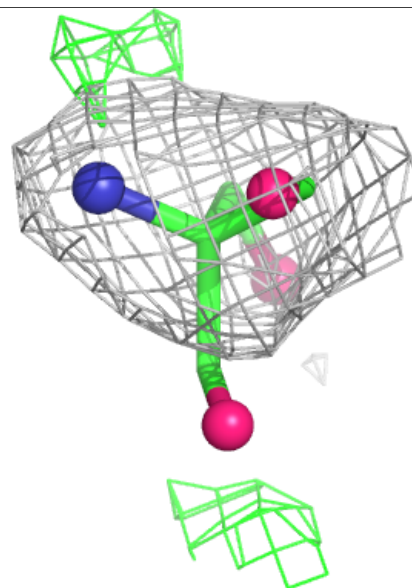
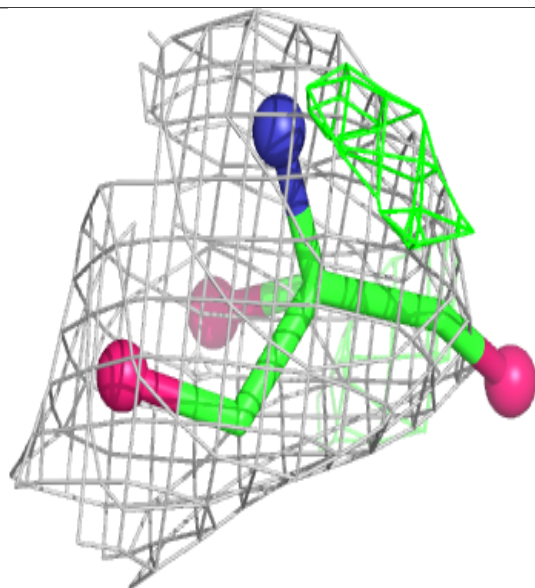
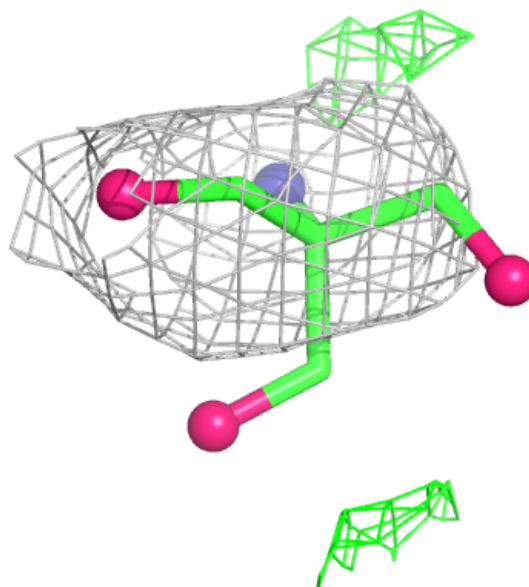
Electron density around TRS C 404:

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



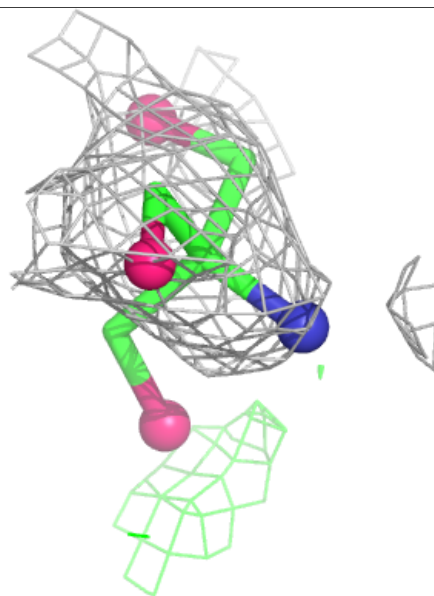
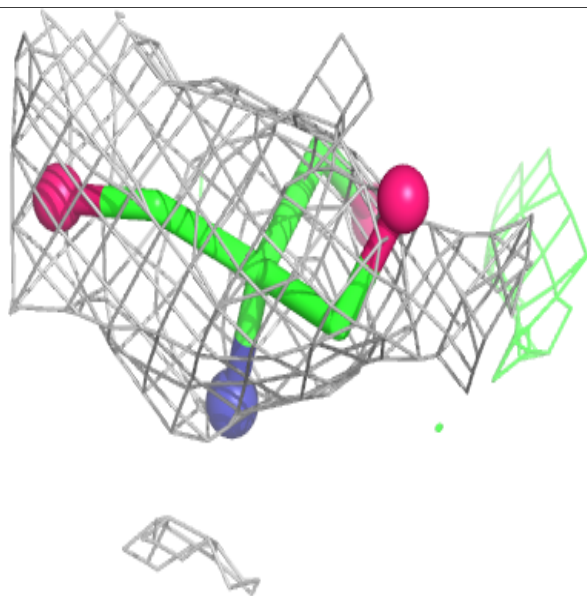
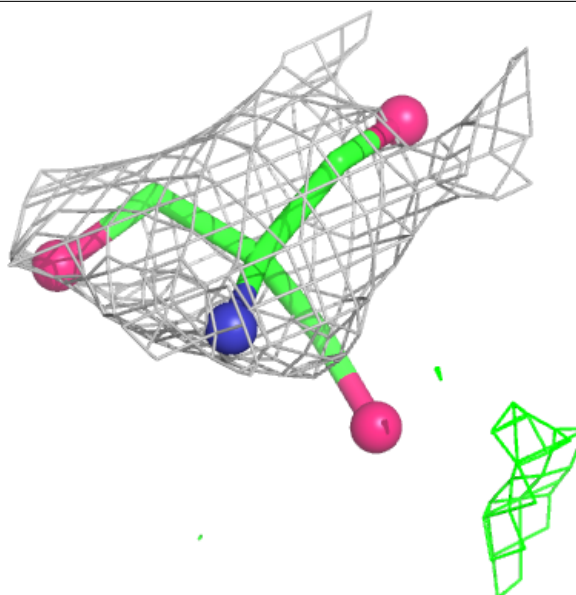
Electron density around TRS C 403:

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



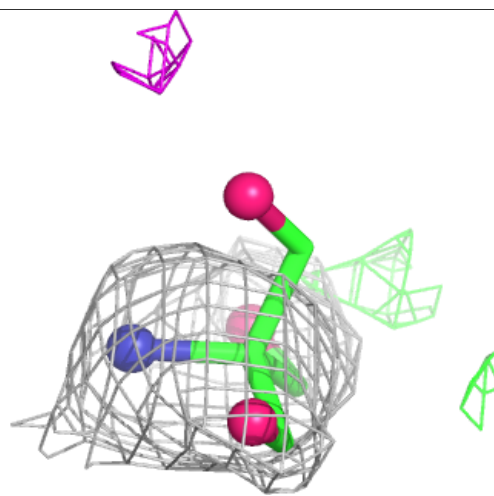
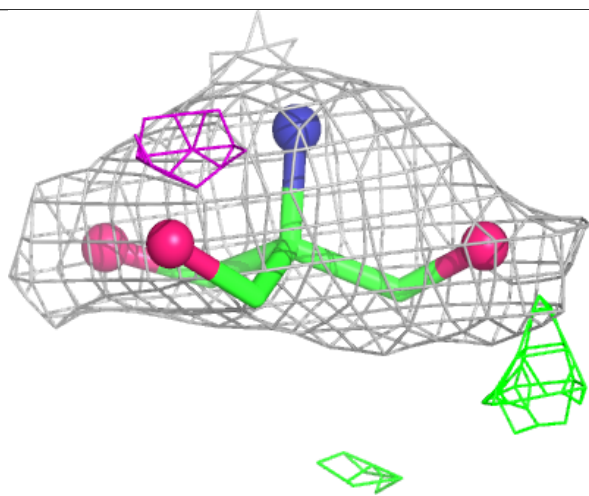
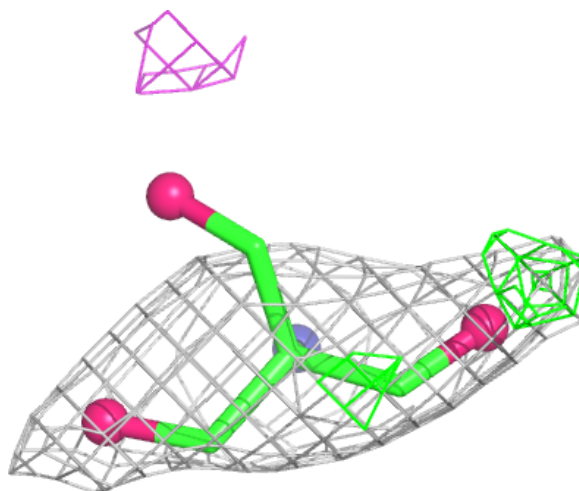
Electron density around TRS B 403:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



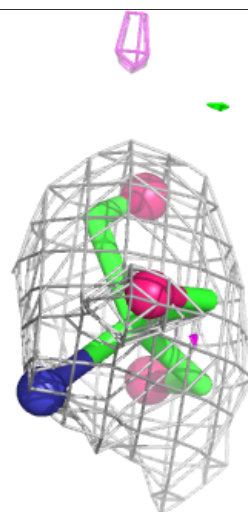
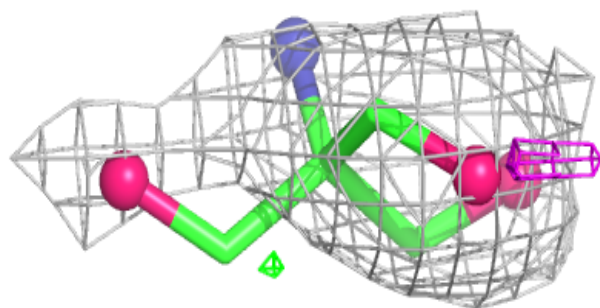
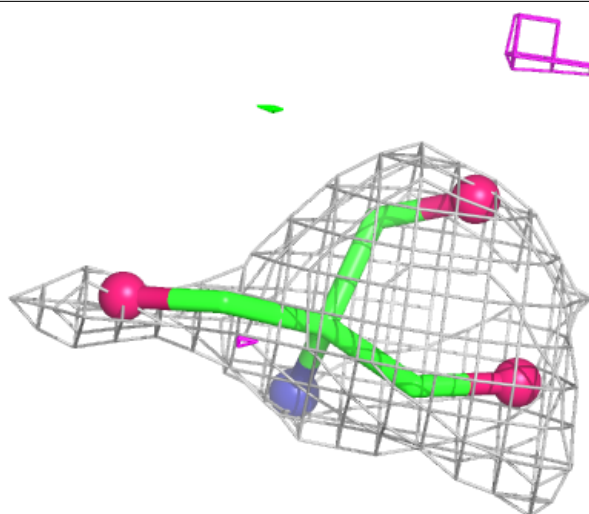
Electron density around TRS A 404:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



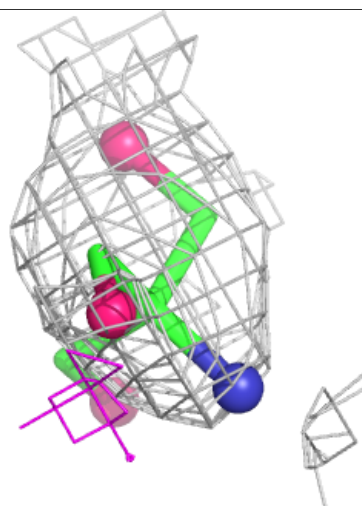
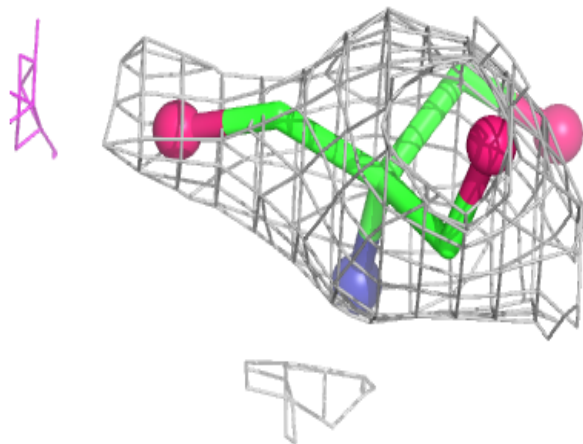
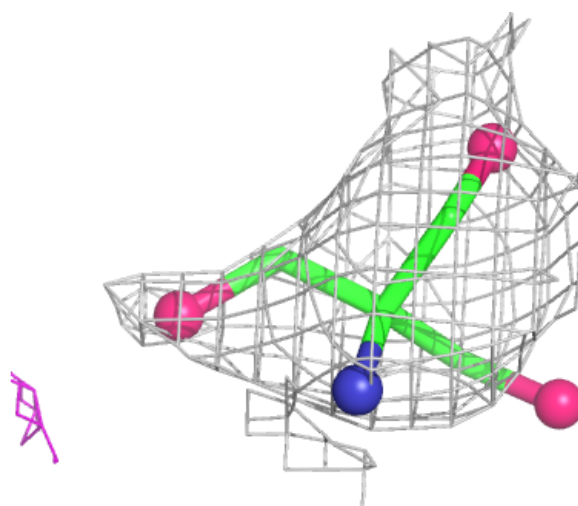
Electron density around TRS D 404:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



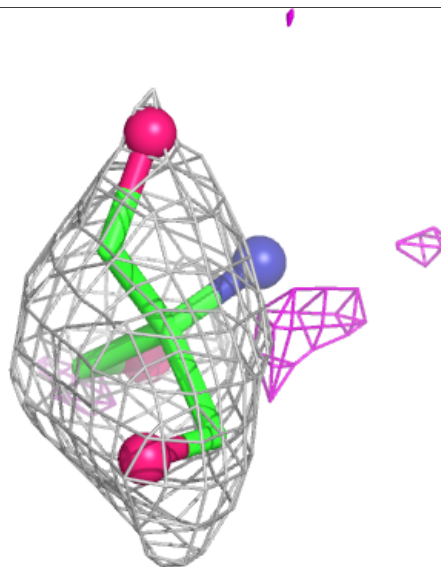
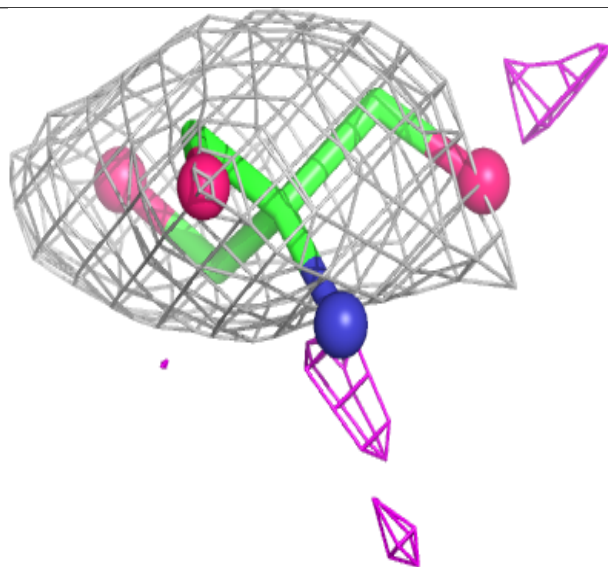
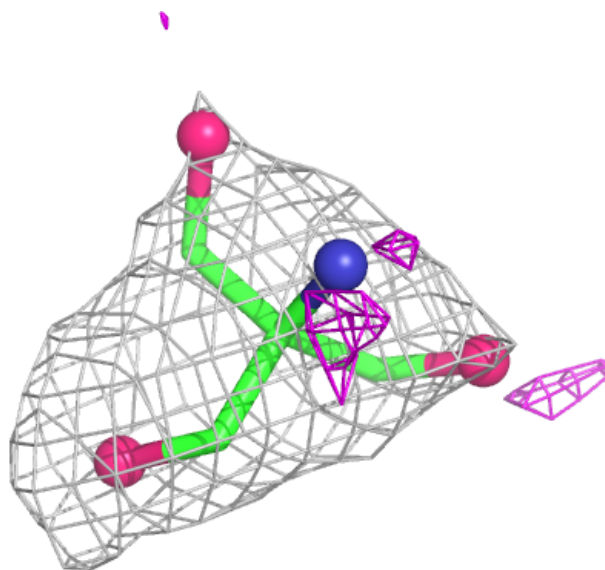
Electron density around TRS A 403:

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



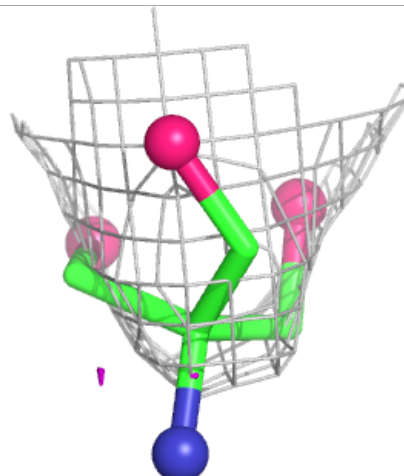
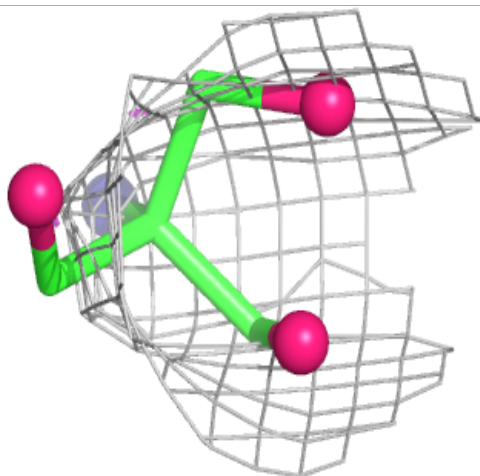
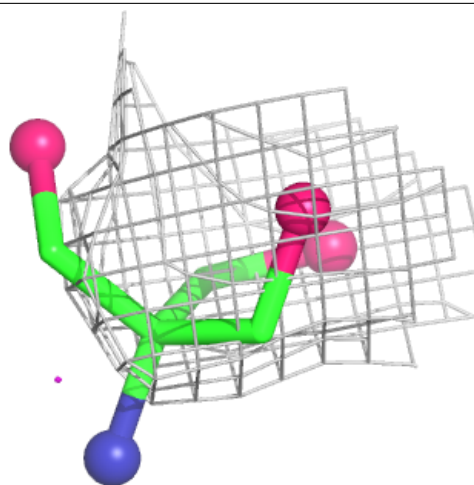
Electron density around TRS B 404:

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



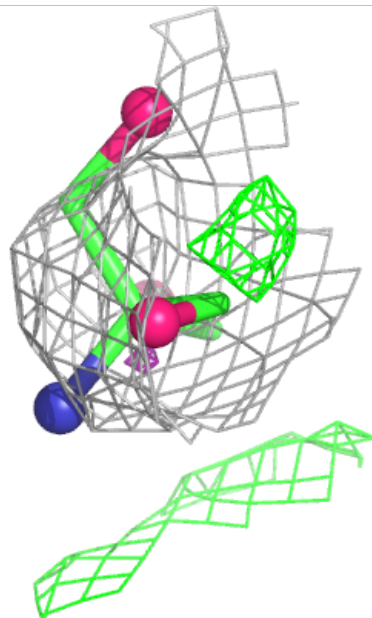
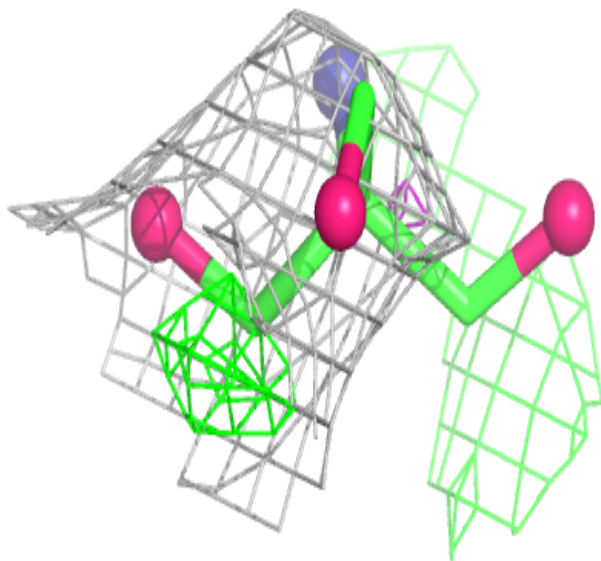
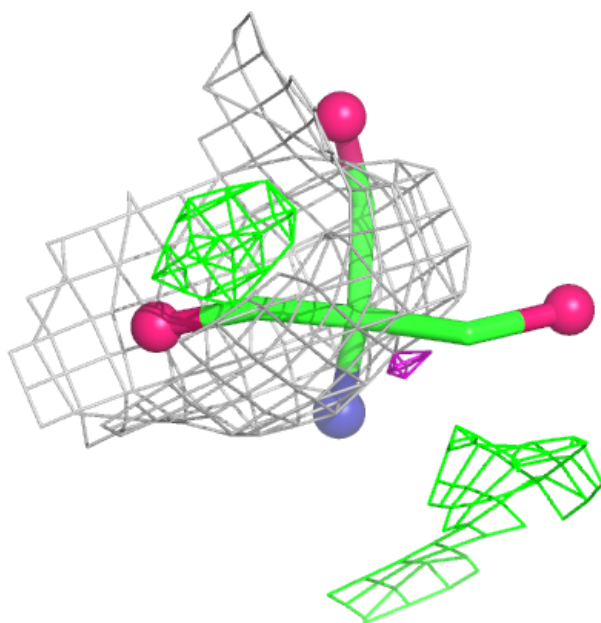
Electron density around TRS D 402:

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



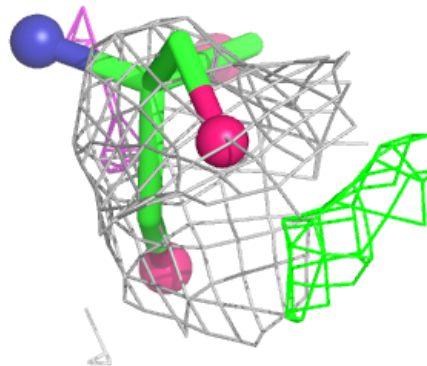
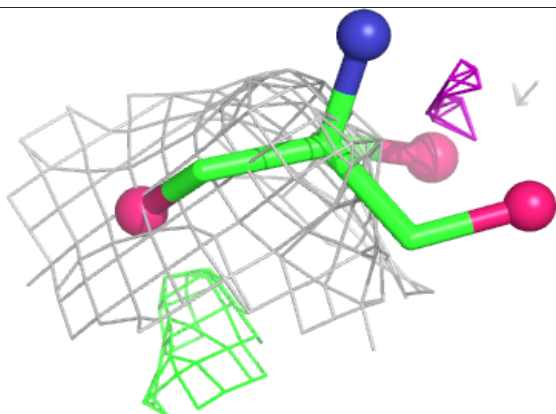
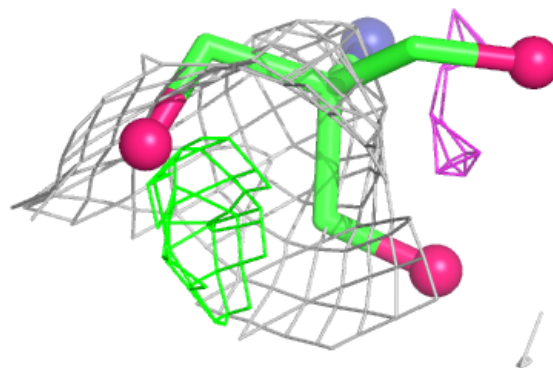
Electron density around TRS C 402:

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



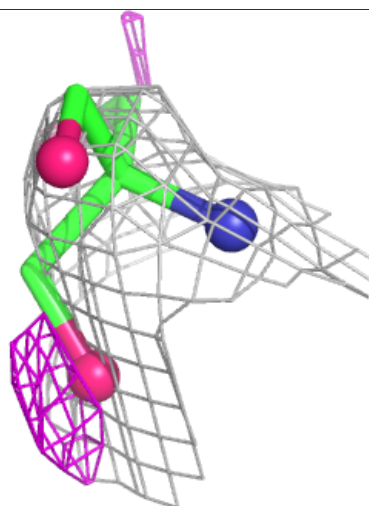
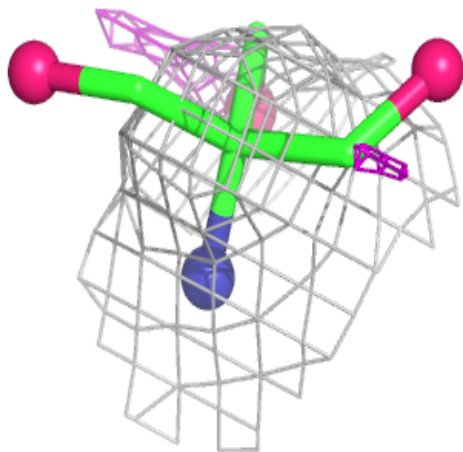
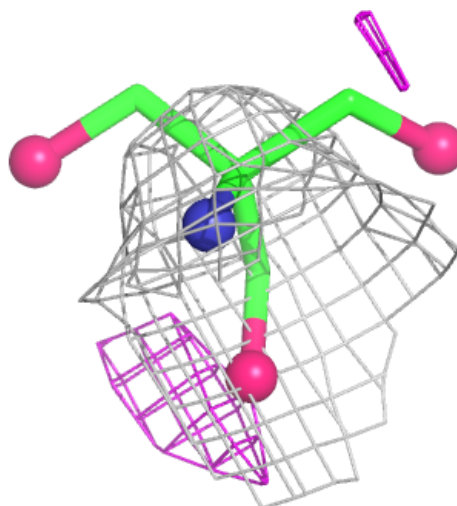
Electron density around TRS A 402:

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



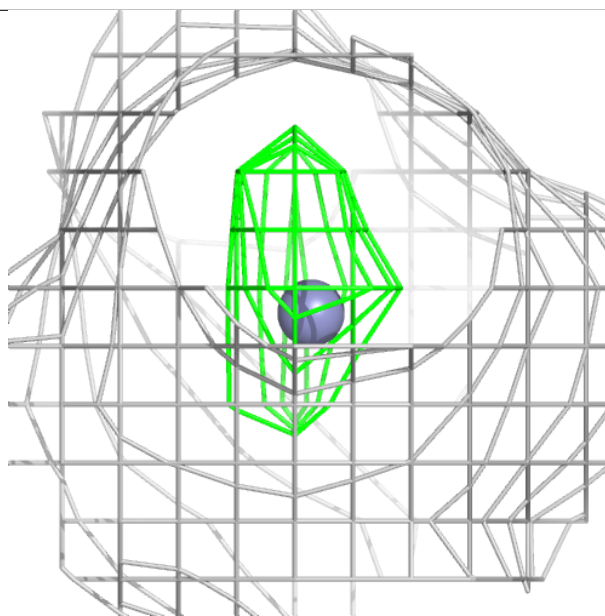
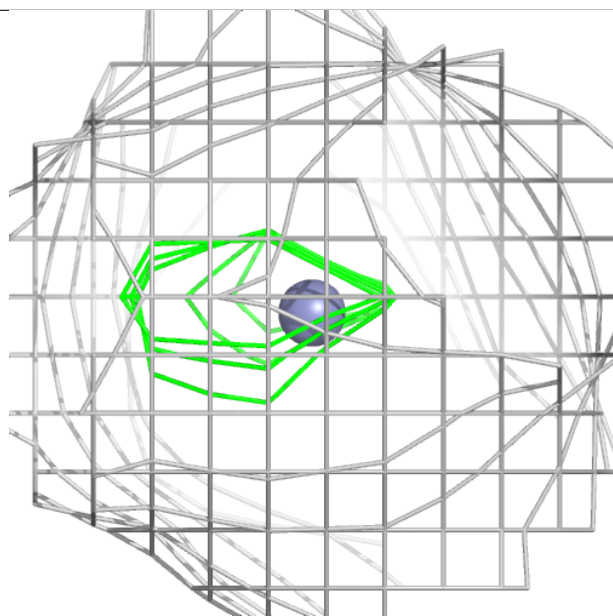
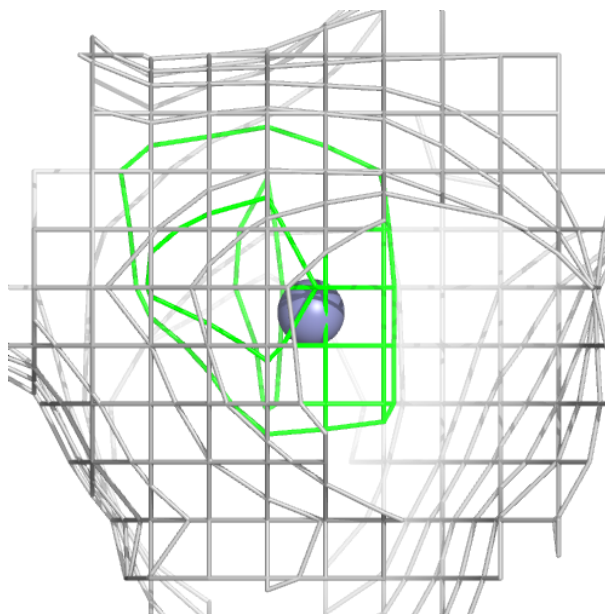
Electron density around TRS B 402:

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



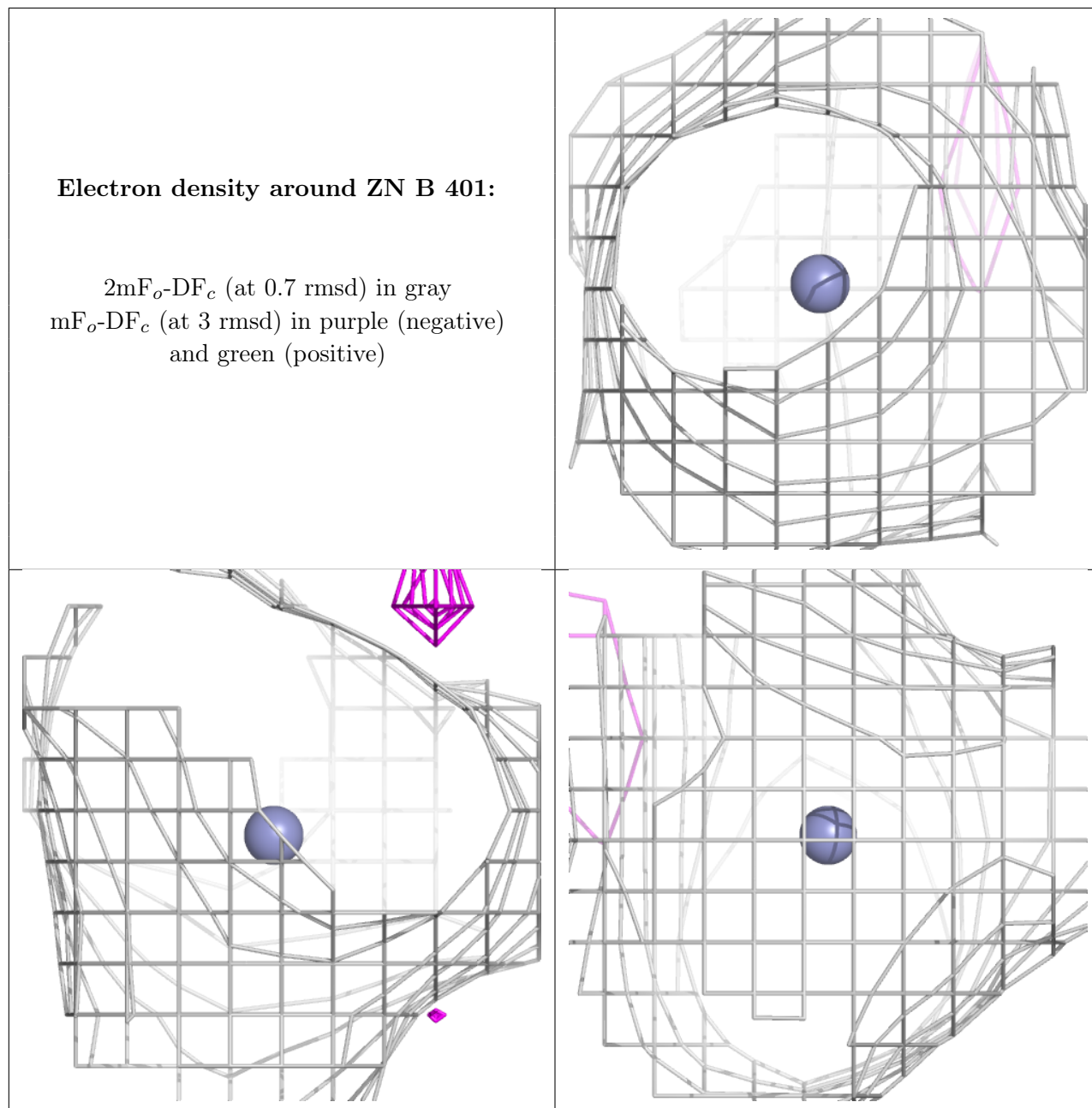
Electron density around ZN A 401:

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



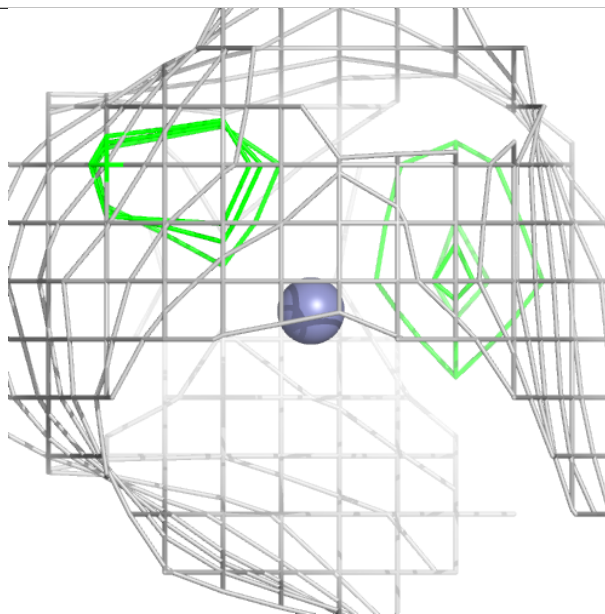
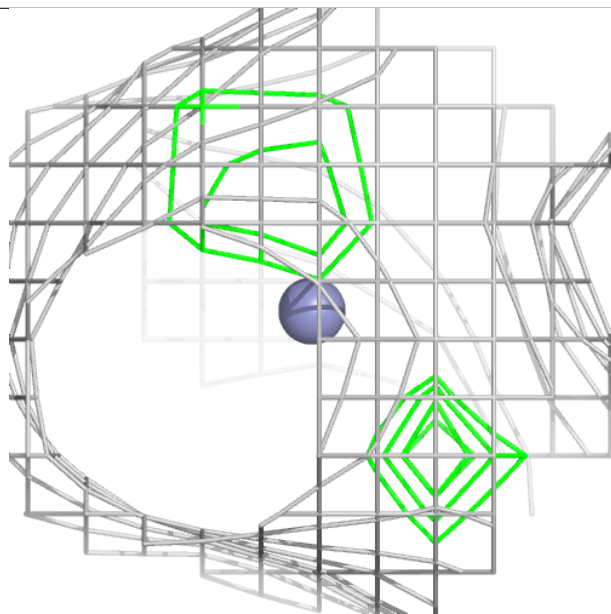
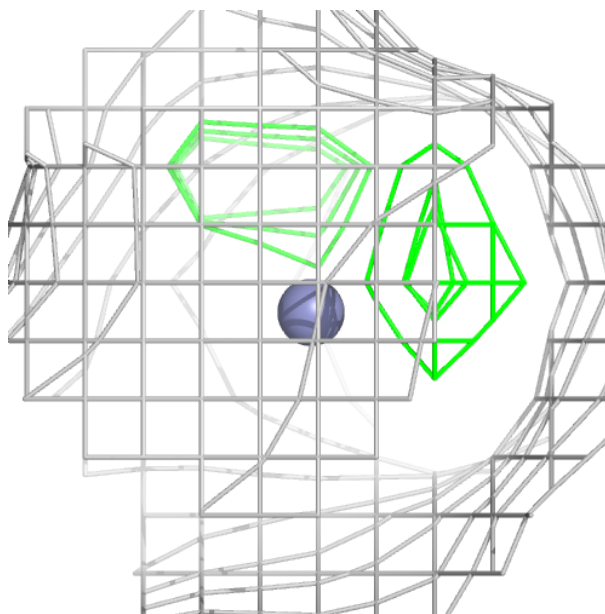
Electron density around ZN B 401:

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



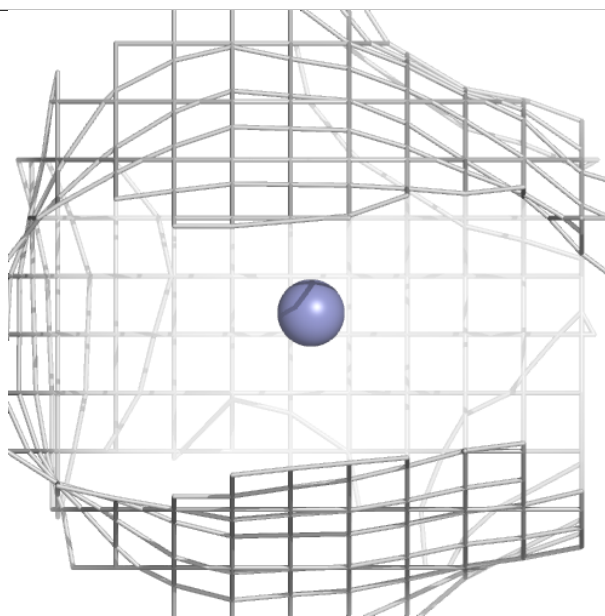
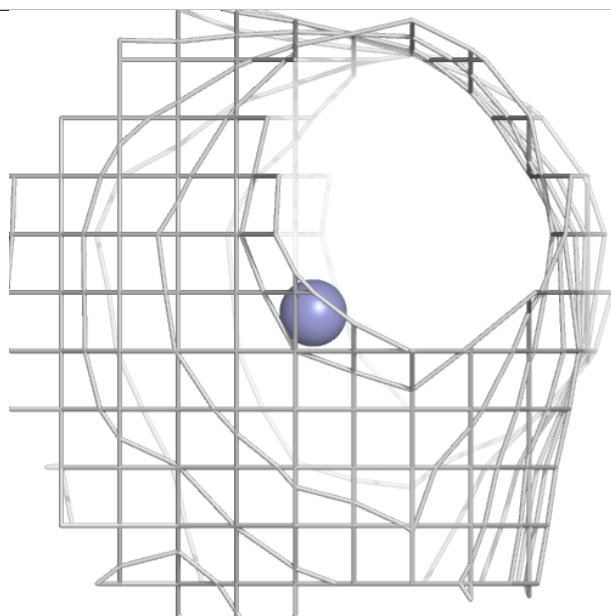
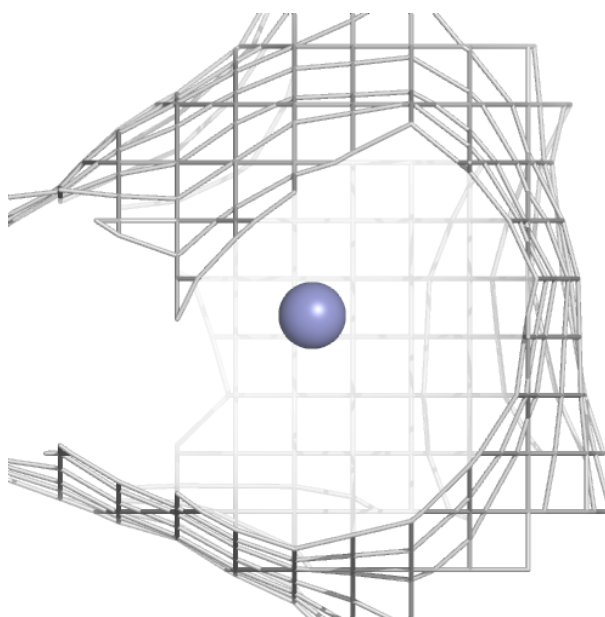
Electron density around ZN C 401:

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



Electron density around ZN D 401:

$2mF_o-DF_c$ (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.