



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 01:29 PM JST

PDB ID : 9IVH / pdb_00009ivh
Title : Structure of TF9 mutant of aminotransferase from Mycolicibacterium neoaurum in complex with LLP and G4O
Authors : Wei, H.; Cong, L.; You, S.; Liu, W.
Deposited on : 2024-07-23
Resolution : 2.02 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

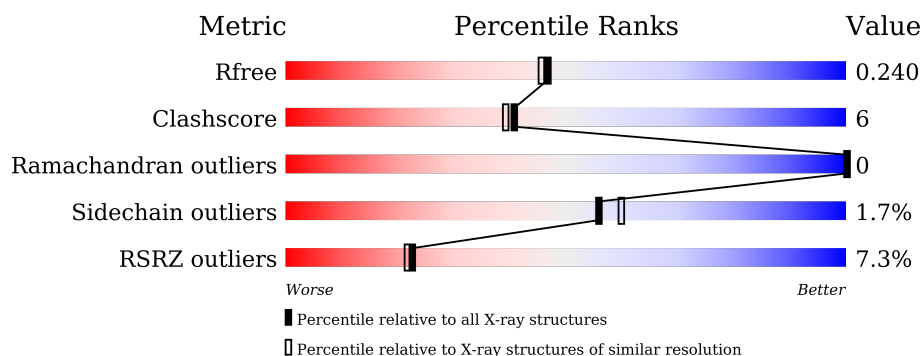
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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	323	
1	B	323	
1	C	323	
1	D	323	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10650 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 Branched-chain amino acid transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	P	S	0	0	0
			2410	1523	411	467	1	8			
1	B	311	Total	C	N	O	P	S	0	0	0
			2415	1526	412	468	1	8			
1	C	313	Total	C	N	O	P	S	0	0	0
			2426	1533	414	470	1	8			
1	D	311	Total	C	N	O	P	S	0	0	0
			2415	1526	412	468	1	8			

There are 28 discrepancies between the modelled and reference sequences:

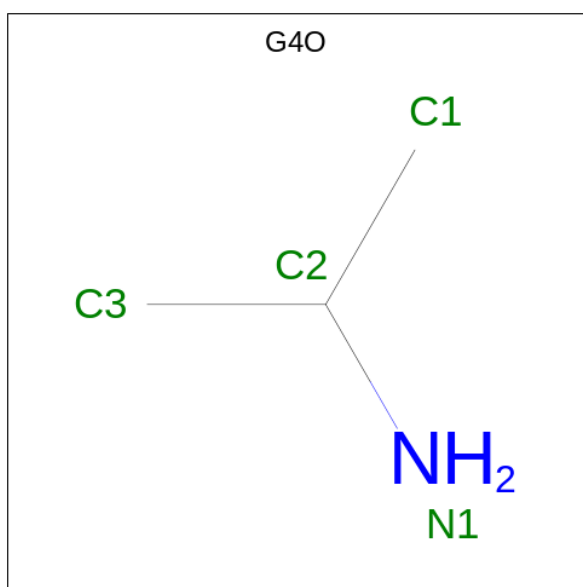
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	SER	ALA	conflict	UNP V5X927
A	259	ILE	LEU	conflict	UNP V5X927
A	261	ASP	GLU	conflict	UNP V5X927
A	279	ASP	GLU	conflict	UNP V5X927
A	302	ALA	PRO	conflict	UNP V5X927
A	307	ALA	GLU	conflict	UNP V5X927
A	310	PRO	GLU	conflict	UNP V5X927
B	119	SER	ALA	conflict	UNP V5X927
B	259	ILE	LEU	conflict	UNP V5X927
B	261	ASP	GLU	conflict	UNP V5X927
B	279	ASP	GLU	conflict	UNP V5X927
B	302	ALA	PRO	conflict	UNP V5X927
B	307	ALA	GLU	conflict	UNP V5X927
B	310	PRO	GLU	conflict	UNP V5X927
C	119	SER	ALA	conflict	UNP V5X927
C	259	ILE	LEU	conflict	UNP V5X927
C	261	ASP	GLU	conflict	UNP V5X927
C	279	ASP	GLU	conflict	UNP V5X927
C	302	ALA	PRO	conflict	UNP V5X927
C	307	ALA	GLU	conflict	UNP V5X927
C	310	PRO	GLU	conflict	UNP V5X927

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Chain	Residue	Modelled	Actual	Comment	Reference
D	119	SER	ALA	conflict	UNP V5X927
D	259	ILE	LEU	conflict	UNP V5X927
D	261	ASP	GLU	conflict	UNP V5X927
D	279	ASP	GLU	conflict	UNP V5X927
D	302	ALA	PRO	conflict	UNP V5X927
D	307	ALA	GLU	conflict	UNP V5X927
D	310	PRO	GLU	conflict	UNP V5X927

- Molecule 2 is propan-2-amine (CCD ID: G4O) (formula: C₃H₉N) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	241	Total O 241 241	0	0

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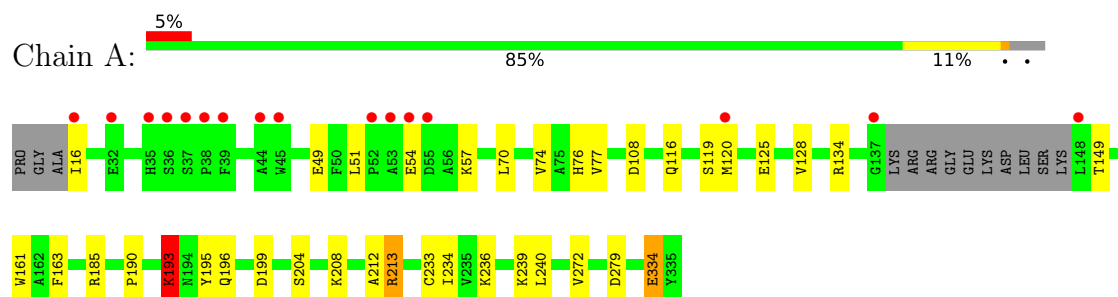
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	265	Total 265	O 265	0	0
3	C	252	Total 252	O 252	0	0
3	D	210	Total 210	O 210	0	0

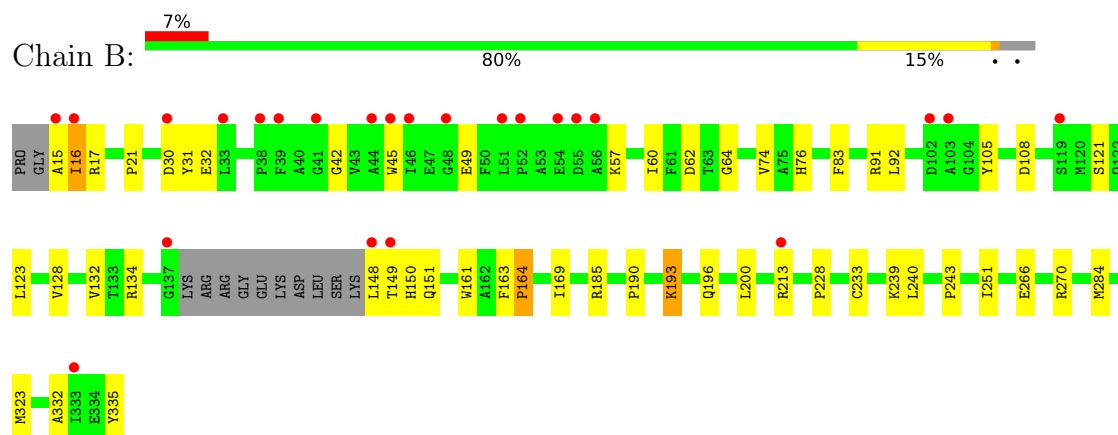
3 Residue-property plots [i](#)

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.

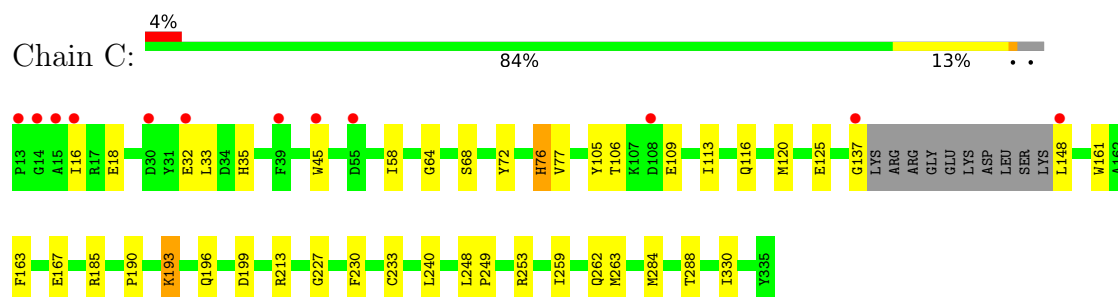
- Molecule 1: Branched-chain amino acid transferase



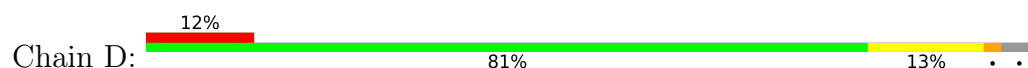
- Molecule 1: Branched-chain amino acid transferase

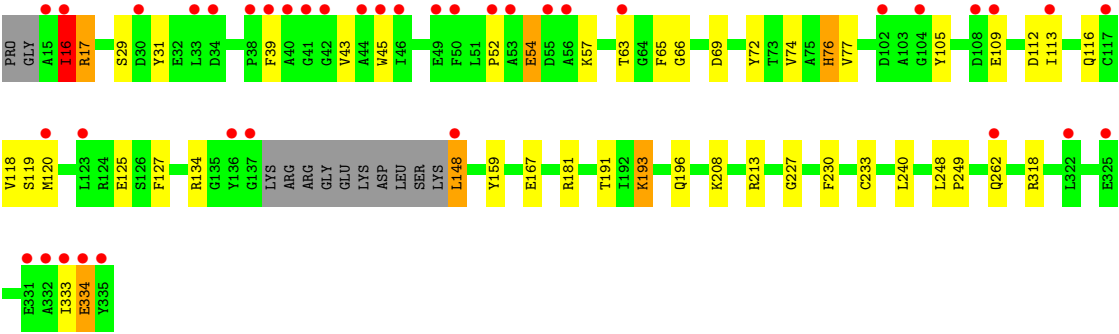


- Molecule 1: Branched-chain amino acid transferase



- Molecule 1: Branched-chain amino acid transferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.61Å 78.59Å 91.54Å 96.96° 108.42° 113.07°	Depositor
Resolution (Å)	42.55 – 2.02 42.55 – 2.02	Depositor EDS
% Data completeness (in resolution range)	92.2 (42.55-2.02) 92.2 (42.55-2.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.01Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.200 , 0.240 0.201 , 0.240	Depositor DCC
R_{free} test set	97290 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10650	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: G4O, LLP

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	0.46	1/2441 (0.0%)	0.53	0/3322
1	B	0.54	3/2446 (0.1%)	0.58	1/3329 (0.0%)
1	C	0.38	0/2458	0.51	0/3345
1	D	0.45	0/2446	0.61	4/3329 (0.1%)
All	All	0.46	4/9791 (0.0%)	0.56	5/13325 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	HIS	CG-ND1	-7.04	1.30	1.38
1	B	164	PRO	CA-C	6.77	1.55	1.51
1	A	212	ALA	C-O	-5.74	1.16	1.23
1	B	150	HIS	CD2-NE2	-5.67	1.31	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	334	GLU	N-CA-CB	-5.76	101.97	110.49
1	B	164	PRO	O-C-N	5.25	123.73	121.31
1	D	333	ILE	CA-C-N	5.21	130.68	122.34
1	D	333	ILE	C-N-CA	5.21	130.68	122.34
1	D	16	ILE	N-CA-C	5.07	118.23	111.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	LLP	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2410	0	2326	22	0
1	B	2415	0	2330	33	0
1	C	2426	0	2342	27	0
1	D	2415	0	2331	44	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	241	0	0	4	0
3	B	265	0	0	10	2
3	C	252	0	0	3	2
3	D	210	0	0	11	0
All	All	10650	0	9329	122	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (122) 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:32:GLU:O	3:B:501:HOH:O	1.56	1.23
1:D:120:MET:SD	3:D:501:HOH:O	2.15	1.04
1:D:16:ILE:HD11	1:D:31:TYR:CZ	1.98	0.98
1:D:116:GLN:OE1	3:D:501:HOH:O	1.90	0.89
1:C:106:THR:HB	1:C:109:GLU:HG3	1.59	0.84
1:B:16:ILE:HG22	3:B:533:HOH:O	1.82	0.78
1:A:54:GLU:OE1	3:A:501:HOH:O	2.05	0.74
1:D:116:GLN:O	1:D:120:MET:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLY:N	3:B:503:HOH:O	2.22	0.70
1:D:39:PHE:HB3	1:D:43:VAL:HG22	1.74	0.70
1:B:16:ILE:HG23	1:B:17:ARG:HG2	1.74	0.70
1:D:54:GLU:HG2	3:D:617:HOH:O	1.90	0.69
1:C:233:CYS:HB3	1:C:240:LEU:HD11	1.75	0.69
1:D:54:GLU:CG	3:D:617:HOH:O	2.41	0.68
1:A:16:ILE:N	3:A:502:HOH:O	2.28	0.67
1:C:262:GLN:NE2	3:C:503:HOH:O	2.26	0.64
1:D:109:GLU:O	1:D:113:ILE:HD12	1.98	0.63
1:D:17:ARG:NH2	1:D:29:SER:O	2.32	0.62
1:D:39:PHE:HE1	1:D:52:PRO:HD3	1.64	0.62
1:D:134:ARG:HG3	1:D:148:LEU:HD21	1.82	0.61
1:C:116:GLN:O	1:C:120:MET:HG3	2.01	0.61
1:B:239:LYS:HE3	1:B:266:GLU:OE1	2.02	0.60
1:B:233:CYS:HB2	1:B:284:MET:HG2	1.83	0.59
1:A:239:LYS:HE3	3:A:696:HOH:O	2.01	0.59
1:D:17:ARG:NH1	1:D:31:TYR:O	2.31	0.58
1:B:16:ILE:HD11	1:B:31:TYR:CE2	2.39	0.58
1:A:185:ARG:HA	1:A:190:PRO:HD2	1.85	0.58
1:B:15:ALA:HB1	3:B:533:HOH:O	2.04	0.58
1:B:233:CYS:HB3	1:B:240:LEU:HD11	1.86	0.58
1:D:76:HIS:HD1	1:D:159:TYR:HE2	1.51	0.57
1:B:121:SER:HB2	3:B:503:HOH:O	2.05	0.56
1:A:119:SER:OG	1:A:334:GLU:O	2.17	0.56
1:B:16:ILE:HD11	1:B:31:TYR:CZ	2.40	0.56
1:D:112:ASP:O	1:D:116:GLN:HB2	2.05	0.56
1:A:234:ILE:HD13	1:A:272:VAL:HG11	1.86	0.55
1:A:236:LYS:NZ	1:A:279:ASP:OD2	2.36	0.55
1:B:108:ASP:OD1	3:B:502:HOH:O	2.18	0.55
1:B:149:THR:HA	3:B:529:HOH:O	2.05	0.54
1:D:262:GLN:CD	3:D:512:HOH:O	2.50	0.54
1:C:16:ILE:HD11	1:C:33:LEU:HD11	1.90	0.54
1:B:161:TRP:HB3	1:B:163:PHE:O	2.09	0.53
1:B:196:GLN:HB3	1:D:196:GLN:HB3	1.89	0.53
1:C:193:LLP:HE2	1:C:193:LLP:O3	2.07	0.53
1:D:39:PHE:HB3	1:D:43:VAL:CG2	2.39	0.53
1:A:204:SER:O	1:A:208:LYS:HG2	2.10	0.52
1:D:167:GLU:OE2	1:D:213:ARG:HD2	2.10	0.52
1:D:262:GLN:NE2	3:D:512:HOH:O	2.42	0.51
1:D:227:GLY:HA3	1:D:230:PHE:CE1	2.45	0.51
1:C:77:VAL:O	1:C:125:GLU:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ILE:HD11	1:D:31:TYR:CE2	2.44	0.50
1:B:92:LEU:HD11	1:B:132:VAL:HG23	1.93	0.50
1:B:62:ASP:OD1	1:B:64:GLY:N	2.42	0.50
1:C:248:LEU:HD12	1:C:249:PRO:HD2	1.93	0.50
1:D:233:CYS:HB3	1:D:240:LEU:HD11	1.93	0.50
1:B:134:ARG:O	1:B:134:ARG:HG3	2.12	0.49
1:D:181:ARG:NH1	3:D:508:HOH:O	2.35	0.49
1:B:45:TRP:HH2	1:B:105:TYR:CZ	2.31	0.49
1:D:66:GLY:HA3	3:D:679:HOH:O	2.13	0.48
1:A:193:LLP:HE2	1:A:193:LLP:O3	2.12	0.48
1:D:227:GLY:HA3	1:D:230:PHE:CZ	2.49	0.48
1:B:332:ALA:HB1	3:B:583:HOH:O	2.13	0.47
1:C:185:ARG:HA	1:C:190:PRO:HD2	1.97	0.47
1:C:137:GLY:HA2	1:C:148:LEU:HB2	1.96	0.47
1:C:199:ASP:OD1	1:C:199:ASP:N	2.46	0.47
1:C:259:ILE:O	1:C:263:MET:HG3	2.15	0.47
1:D:77:VAL:O	1:D:125:GLU:HA	2.15	0.47
1:A:199:ASP:OD1	1:A:199:ASP:N	2.47	0.46
1:D:119:SER:OG	1:D:334:GLU:O	2.14	0.46
1:B:193:LLP:HE2	1:B:193:LLP:O3	2.14	0.46
1:C:233:CYS:HB2	1:C:284:MET:HG2	1.97	0.46
1:B:164:PRO:HD3	1:B:213:ARG:HH22	1.79	0.46
1:D:72:TYR:CE1	1:D:193:LLP:HG3	2.51	0.46
1:C:33:LEU:HB2	1:C:35:HIS:CE1	2.51	0.46
1:A:116:GLN:O	1:A:120:MET:HG3	2.15	0.46
1:A:77:VAL:O	1:A:125:GLU:HA	2.16	0.45
1:C:45:TRP:HH2	1:C:105:TYR:CZ	2.34	0.45
1:A:161:TRP:HB3	1:A:163:PHE:O	2.15	0.45
1:C:249:PRO:HA	1:C:253:ARG:NH2	2.32	0.45
1:C:330:ILE:O	3:C:501:HOH:O	2.21	0.45
1:D:167:GLU:OE2	1:D:213:ARG:NH1	2.44	0.45
1:B:123:LEU:O	1:B:335:TYR:OH	2.32	0.45
1:B:21:PRO:HG2	1:B:169:ILE:HG13	1.99	0.45
1:B:200:LEU:HD13	1:B:228:PRO:HA	1.99	0.45
1:D:74:VAL:HG11	1:D:127:PHE:CE2	2.52	0.45
1:D:113:ILE:HD12	1:D:113:ILE:H	1.82	0.45
1:B:57:LYS:HB3	1:D:57:LYS:HB3	1.99	0.44
1:D:208:LYS:NZ	3:D:523:HOH:O	2.50	0.44
1:A:49:GLU:OE2	1:A:51:LEU:HD21	2.18	0.44
1:A:233:CYS:HB3	1:A:240:LEU:HD11	1.99	0.44
1:A:70:LEU:HD21	1:A:195:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:PRO:HA	1:B:270:ARG:O	2.19	0.43
1:C:64:GLY:O	1:C:68:SER:HA	2.19	0.43
1:C:76:HIS:HB3	1:C:288:THR:HG22	2.01	0.43
1:D:45:TRP:CD2	1:D:113:ILE:HG21	2.53	0.43
1:D:76:HIS:CD2	3:D:596:HOH:O	2.71	0.43
1:A:213:ARG:HD2	1:A:213:ARG:HA	1.83	0.43
1:B:185:ARG:HA	1:B:190:PRO:HD2	2.01	0.43
1:C:167:GLU:OE1	1:C:213:ARG:HG3	2.19	0.43
1:A:108:ASP:HB2	3:A:551:HOH:O	2.18	0.42
1:D:45:TRP:HH2	1:D:105:TYR:CZ	2.38	0.42
1:A:134:ARG:O	1:A:134:ARG:HG3	2.19	0.42
1:A:196:GLN:HB3	1:C:196:GLN:HB3	2.02	0.42
1:B:16:ILE:N	3:B:533:HOH:O	2.53	0.42
1:C:18:GLU:HG2	3:C:534:HOH:O	2.20	0.42
1:D:77:VAL:HG21	1:D:118:VAL:HG11	2.00	0.42
1:D:63:THR:C	1:D:65:PHE:N	2.78	0.41
1:B:74:VAL:HA	1:B:128:VAL:O	2.21	0.41
1:C:45:TRP:CE3	1:C:113:ILE:HG21	2.54	0.41
1:A:57:LYS:HD3	1:C:58:ILE:C	2.45	0.41
1:C:72:TYR:OH	1:C:193:LLP:HE3	2.20	0.41
1:C:161:TRP:HB3	1:C:163:PHE:O	2.21	0.41
1:D:318:ARG:HA	1:D:318:ARG:HD2	1.77	0.41
1:B:83:PHE:CE1	1:B:323:MET:HE1	2.55	0.41
1:D:16:ILE:HD11	1:D:31:TYR:CE1	2.52	0.41
1:D:63:THR:HG22	1:D:69:ASP:CB	2.51	0.41
1:B:91:ARG:NH1	1:B:251:ILE:HG12	2.36	0.41
1:D:191:THR:HG21	3:D:611:HOH:O	2.21	0.41
1:A:74:VAL:HA	1:A:128:VAL:O	2.21	0.40
1:B:151:GLN:HG3	3:B:544:HOH:O	2.19	0.40
1:C:227:GLY:HA3	1:C:230:PHE:CZ	2.56	0.40
1:D:248:LEU:HD12	1:D:249:PRO:HD2	2.02	0.40
1:D:120:MET:HG3	1:D:120:MET:H	1.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:674:HOH:O	3:C:501:HOH:O[1_665]	1.99	0.21
3:B:674:HOH:O	3:C:710:HOH:O[1_665]	2.14	0.06

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	305/323 (94%)	297 (97%)	8 (3%)	0	100	100
1	B	306/323 (95%)	297 (97%)	9 (3%)	0	100	100
1	C	308/323 (95%)	301 (98%)	7 (2%)	0	100	100
1	D	306/323 (95%)	298 (97%)	8 (3%)	0	100	100
All	All	1225/1292 (95%)	1193 (97%)	32 (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	250/260 (96%)	246 (98%)	4 (2%)	58	62
1	B	250/260 (96%)	244 (98%)	6 (2%)	44	46
1	C	251/260 (96%)	249 (99%)	2 (1%)	79	83
1	D	250/260 (96%)	245 (98%)	5 (2%)	50	53
All	All	1001/1040 (96%)	984 (98%)	17 (2%)	56	60

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	149	THR

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Mol	Chain	Res	Type
1	A	213	ARG
1	A	334	GLU
1	B	16	ILE
1	B	30	ASP
1	B	49	GLU
1	B	60	ILE
1	B	76	HIS
1	B	148	LEU
1	C	32	GLU
1	C	76	HIS
1	D	16	ILE
1	D	17	ARG
1	D	54	GLU
1	D	76	HIS
1	D	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	B	231	ASN
1	C	35	HIS
1	C	231	ASN
1	D	81	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	D	193	1	23,24,25	1.11	1 (4%)	25,32,34	1.69	9 (36%)
1	LLP	B	193	1	23,24,25	1.35	2 (8%)	25,32,34	1.95	10 (40%)
1	LLP	A	193	1	23,24,25	1.27	2 (8%)	25,32,34	1.87	7 (28%)
1	LLP	C	193	1	23,24,25	1.23	1 (4%)	25,32,34	1.91	7 (28%)

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
1	LLP	D	193	1	-	4/16/17/19	0/1/1/1
1	LLP	B	193	1	-	4/16/17/19	0/1/1/1
1	LLP	A	193	1	-	3/16/17/19	0/1/1/1
1	LLP	C	193	1	-	4/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	LLP	P-OP4	4.26	1.73	1.60
1	B	193	LLP	P-OP4	4.18	1.73	1.60
1	A	193	LLP	P-OP4	3.98	1.73	1.60
1	D	193	LLP	P-OP4	3.63	1.71	1.60
1	B	193	LLP	O3-C3	-2.37	1.31	1.37
1	A	193	LLP	CE-NZ	-2.05	1.42	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	LLP	CE-NZ-C4'	3.97	131.11	118.90
1	A	193	LLP	C5-C4-C4'	-3.93	115.09	121.56
1	C	193	LLP	OP3-P-OP2	3.70	121.77	107.64
1	B	193	LLP	OP3-P-OP4	-3.68	96.94	106.73
1	C	193	LLP	CD-CE-NZ	3.46	119.41	110.93
1	A	193	LLP	C3-C4-C4'	3.34	126.64	120.41
1	D	193	LLP	CE-NZ-C4'	3.34	129.14	118.90
1	B	193	LLP	CE-NZ-C4'	3.31	129.07	118.90
1	A	193	LLP	CE-NZ-C4'	3.02	128.19	118.90
1	B	193	LLP	CG-CD-CE	-2.98	103.18	113.57
1	C	193	LLP	OP3-P-OP4	-2.95	98.87	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	LLP	CD-CG-CB	2.93	123.99	113.62
1	B	193	LLP	OP3-P-OP2	2.89	118.69	107.64
1	B	193	LLP	CD-CE-NZ	2.82	117.83	110.93
1	B	193	LLP	C5-C4-C4'	-2.82	116.92	121.56
1	B	193	LLP	C3-C4-C4'	2.75	125.54	120.41
1	A	193	LLP	OP3-P-OP2	2.75	118.15	107.64
1	D	193	LLP	C5-C4-C4'	-2.65	117.20	121.56
1	A	193	LLP	OP2-P-OP4	-2.64	99.70	106.73
1	D	193	LLP	C3-C4-C4'	2.63	125.31	120.41
1	D	193	LLP	OP2-P-OP4	-2.63	99.74	106.73
1	A	193	LLP	CG-CD-CE	-2.56	104.64	113.57
1	C	193	LLP	CG-CD-CE	-2.47	104.98	113.57
1	D	193	LLP	CG-CD-CE	-2.32	105.50	113.57
1	C	193	LLP	C5-C4-C4'	-2.29	117.79	121.56
1	B	193	LLP	OP3-P-OP1	2.29	119.63	110.68
1	D	193	LLP	CD-CE-NZ	2.28	116.53	110.93
1	D	193	LLP	OP3-P-OP1	2.20	119.29	110.68
1	B	193	LLP	O3-C3-C4	2.20	125.50	119.60
1	B	193	LLP	CD-CG-CB	2.19	121.38	113.62
1	D	193	LLP	OP3-P-OP2	2.17	115.93	107.64
1	A	193	LLP	C4-C4'-NZ	2.12	134.01	124.31
1	D	193	LLP	C4-C4'-NZ	2.10	133.94	124.31

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	193	LLP	C4-C4'-NZ-CE
1	B	193	LLP	C4-C4'-NZ-CE
1	C	193	LLP	C4-C4'-NZ-CE
1	D	193	LLP	C4-C4'-NZ-CE
1	D	193	LLP	CG-CD-CE-NZ
1	A	193	LLP	CG-CD-CE-NZ
1	B	193	LLP	CG-CD-CE-NZ
1	C	193	LLP	CG-CD-CE-NZ
1	D	193	LLP	C5'-OP4-P-OP3
1	B	193	LLP	N-CA-CB-CG
1	A	193	LLP	C3-C4-C4'-NZ
1	B	193	LLP	C3-C4-C4'-NZ
1	C	193	LLP	C3-C4-C4'-NZ
1	D	193	LLP	C3-C4-C4'-NZ
1	C	193	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	193	LLP	1	0
1	B	193	LLP	1	0
1	A	193	LLP	1	0
1	C	193	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	G4O	C	401	-	2,3,3	0.18	0	1,3,3	0.28	0
2	G4O	B	401	-	2,3,3	0.16	0	1,3,3	0.05	0
2	G4O	D	401	-	2,3,3	0.09	0	1,3,3	0.03	0
2	G4O	A	401	-	2,3,3	0.11	0	1,3,3	0.03	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

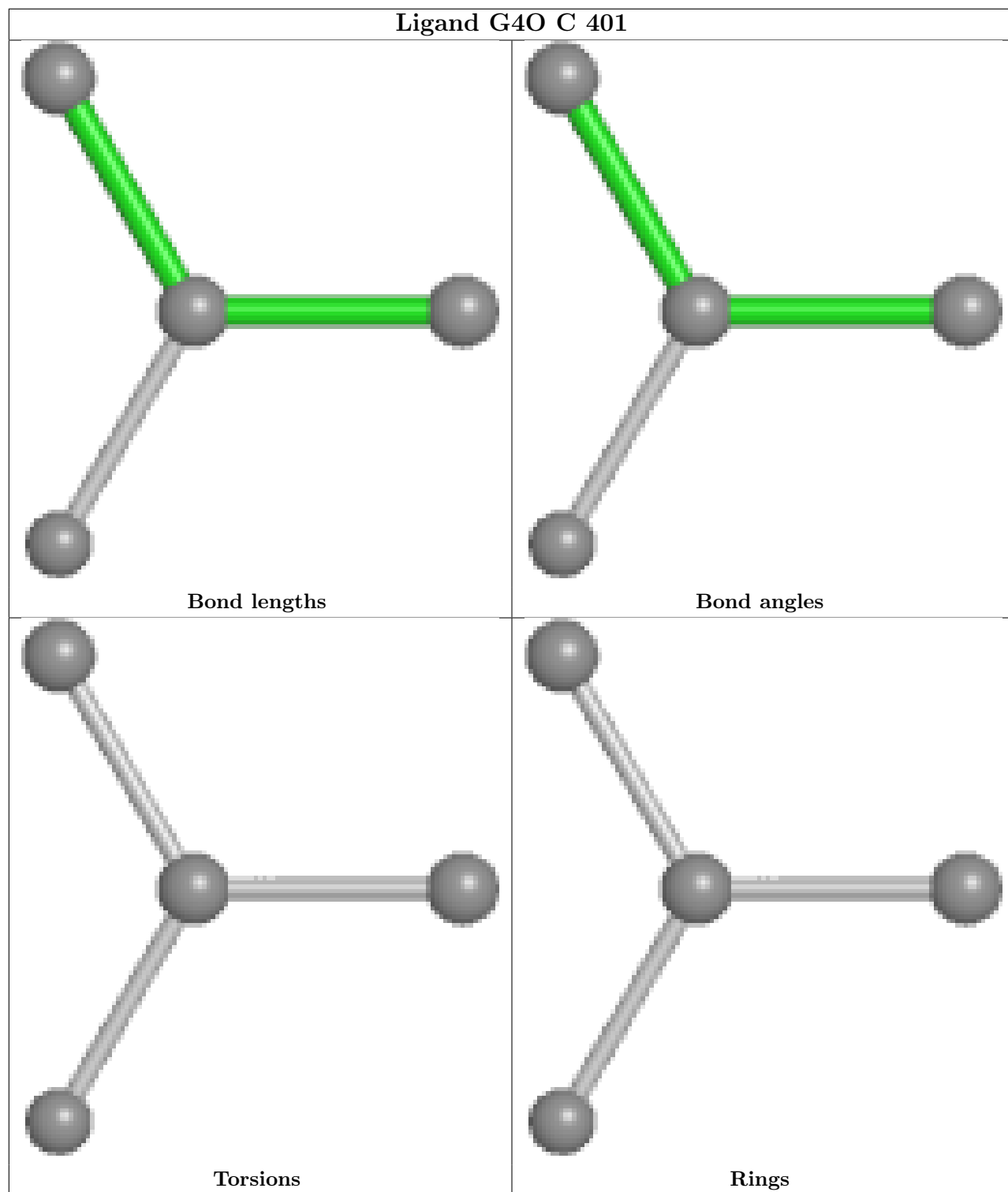
There are no torsion outliers.

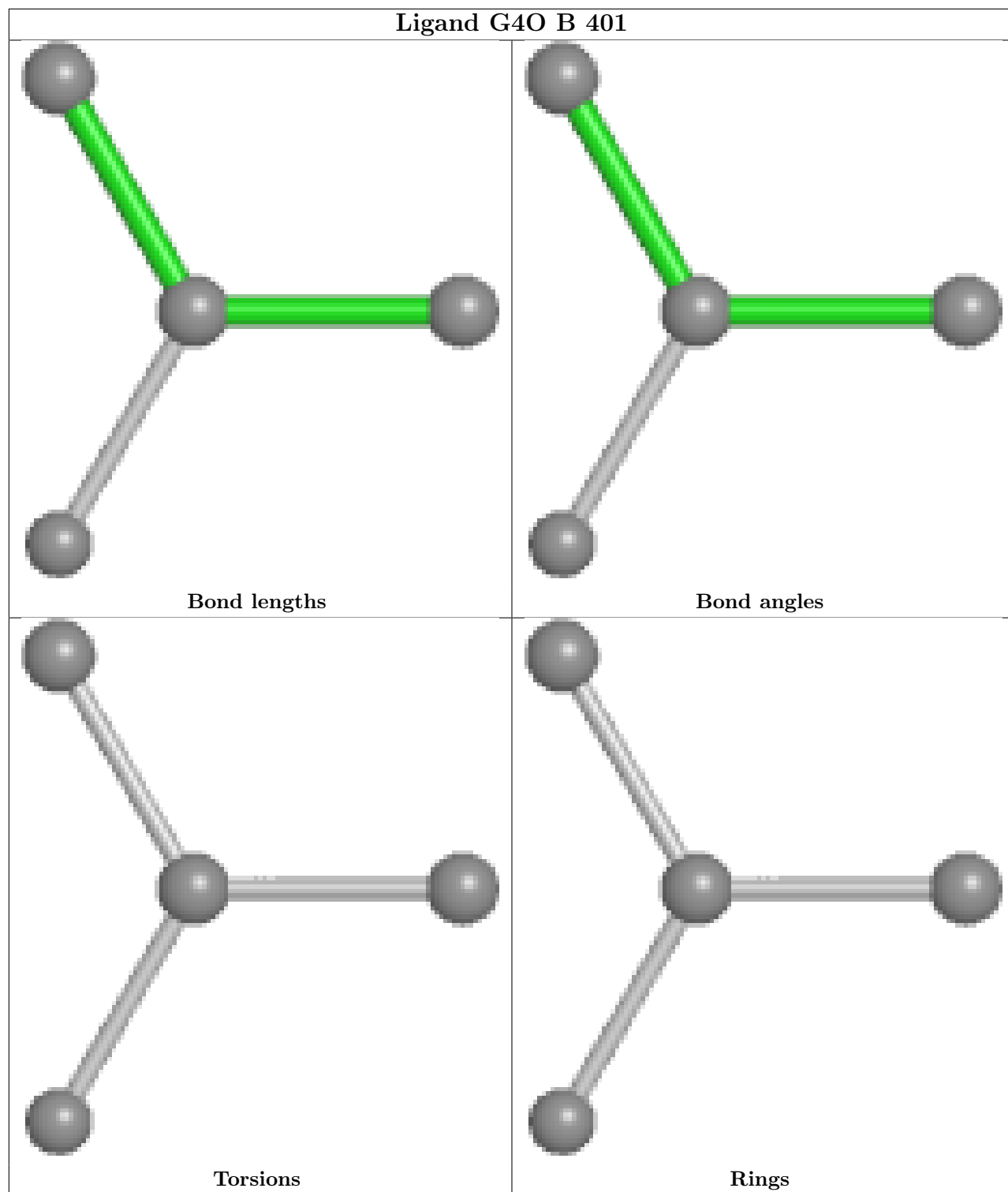
There are no ring outliers.

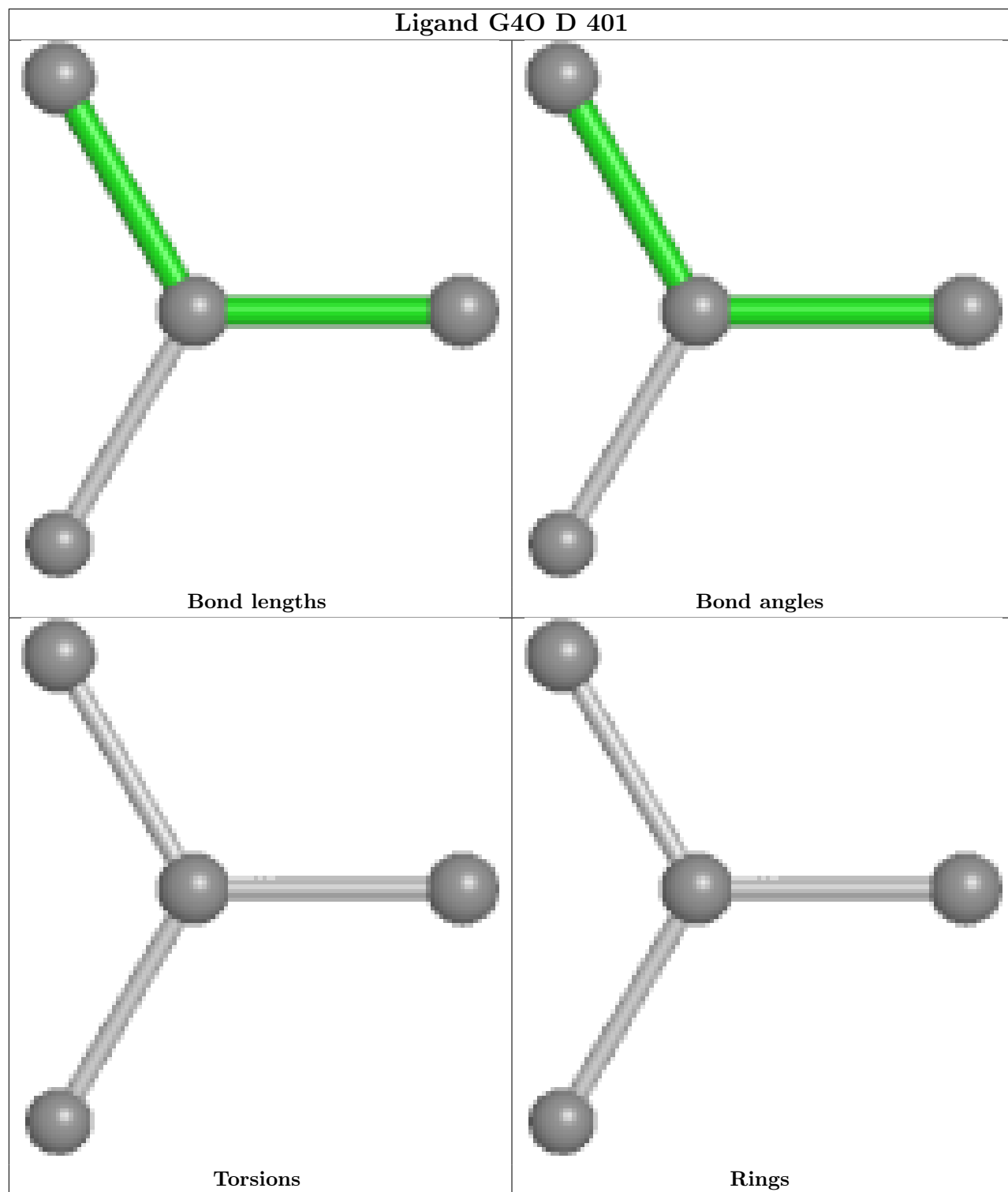
No monomer is involved in short contacts.

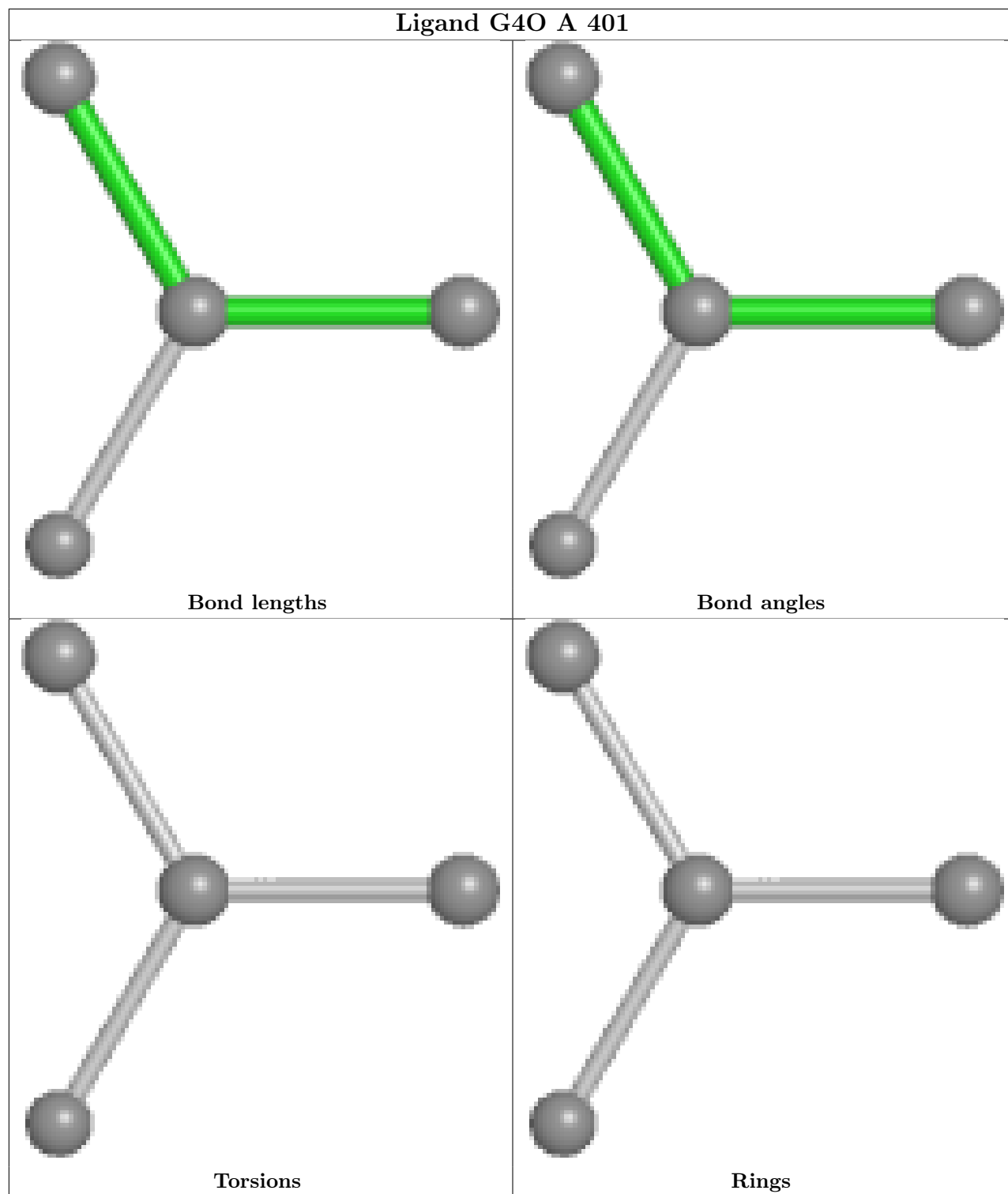
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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 ⓘ

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	309/323 (95%)	0.30	16 (5%) 34 33	18, 29, 52, 72	0
1	B	310/323 (95%)	0.36	24 (7%) 21 20	17, 29, 52, 81	0
1	C	312/323 (96%)	0.37	12 (3%) 44 43	19, 31, 52, 76	0
1	D	310/323 (95%)	0.64	39 (12%) 9 8	18, 34, 63, 79	0
All	All	1241/1292 (96%)	0.42	91 (7%) 22 22	17, 31, 57, 81	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	ALA	5.5
1	C	148	LEU	5.0
1	A	55	ASP	4.9
1	C	13	PRO	4.6
1	B	55	ASP	4.2
1	D	40	ALA	3.9
1	B	16	ILE	3.8
1	B	51	LEU	3.8
1	B	39	PHE	3.7
1	D	39	PHE	3.7
1	D	334	GLU	3.6
1	C	14	GLY	3.5
1	B	38	PRO	3.3
1	C	137	GLY	3.3
1	A	54	GLU	3.2
1	B	41	GLY	3.2
1	D	50	PHE	3.1
1	D	333	ILE	2.9
1	D	148	LEU	2.9
1	B	333	ILE	2.9
1	B	30	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	16	ILE	2.9
1	D	325	GLU	2.9
1	D	30	ASP	2.8
1	A	148	LEU	2.8
1	D	63	THR	2.8
1	D	137	GLY	2.7
1	D	49	GLU	2.7
1	B	46	ILE	2.7
1	B	15	ALA	2.7
1	B	54	GLU	2.7
1	A	137	GLY	2.7
1	B	56	ALA	2.6
1	B	52	PRO	2.6
1	D	33	LEU	2.6
1	D	15	ALA	2.6
1	D	41	GLY	2.6
1	D	120	MET	2.6
1	D	46	ILE	2.6
1	D	53	ALA	2.5
1	B	119	SER	2.5
1	D	45	TRP	2.5
1	D	55	ASP	2.5
1	D	108	ASP	2.5
1	A	38	PRO	2.5
1	A	52	PRO	2.5
1	C	45	TRP	2.4
1	B	213	ARG	2.4
1	D	52	PRO	2.4
1	D	113	ILE	2.4
1	B	33	LEU	2.4
1	B	44	ALA	2.4
1	B	149	THR	2.4
1	A	39	PHE	2.4
1	B	137	GLY	2.4
1	A	120	MET	2.3
1	A	36	SER	2.3
1	D	38	PRO	2.3
1	C	30	ASP	2.3
1	D	136	TYR	2.3
1	D	104	GLY	2.2
1	A	45	TRP	2.2
1	D	16	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	32	GLU	2.2
1	B	103	ALA	2.2
1	D	332	ALA	2.2
1	B	48	GLY	2.2
1	D	331	GLU	2.2
1	D	322	LEU	2.2
1	B	45	TRP	2.2
1	A	37	SER	2.2
1	D	44	ALA	2.2
1	B	102	ASP	2.2
1	C	55	ASP	2.2
1	A	35	HIS	2.2
1	C	16	ILE	2.1
1	C	108	ASP	2.1
1	D	56	ALA	2.1
1	D	102	ASP	2.1
1	B	148	LEU	2.1
1	C	39	PHE	2.1
1	D	34	ASP	2.1
1	D	123	LEU	2.1
1	A	53	ALA	2.1
1	D	42	GLY	2.1
1	A	32	GLU	2.1
1	A	44	ALA	2.0
1	D	262	GLN	2.0
1	D	109	GLU	2.0
1	D	335	TYR	2.0
1	D	117	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	B	193	24/25	0.94	0.09	18,24,29,38	0
1	LLP	A	193	24/25	0.95	0.08	19,23,31,37	0
1	LLP	C	193	24/25	0.95	0.09	20,24,34,35	0
1	LLP	D	193	24/25	0.95	0.10	22,26,39,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

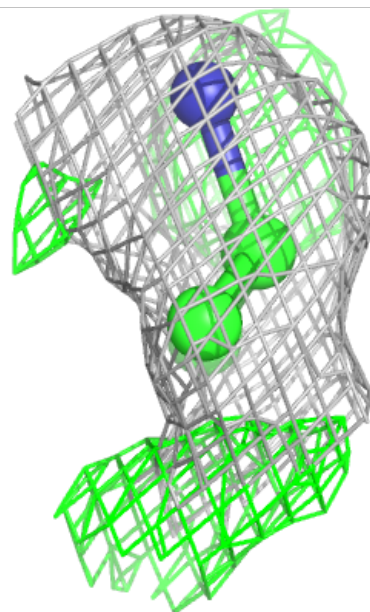
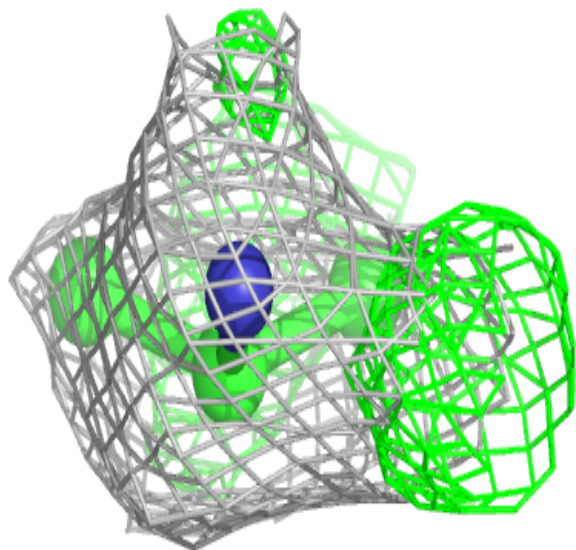
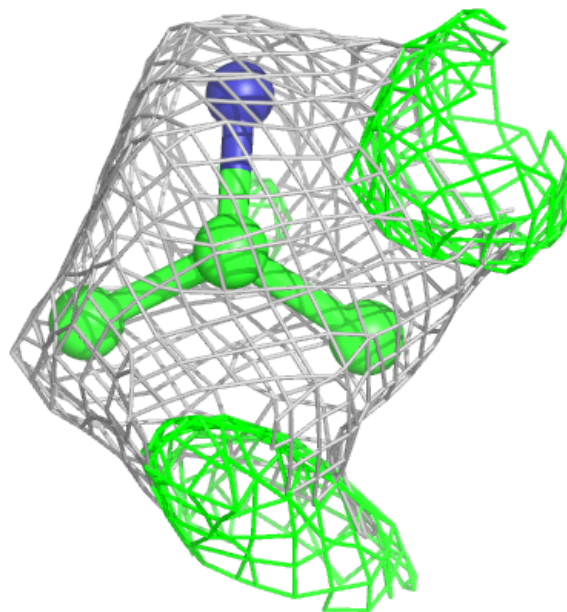
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	G4O	A	401	4/4	0.74	0.21	34,40,41,44	0
2	G4O	C	401	4/4	0.74	0.28	38,41,41,46	0
2	G4O	B	401	4/4	0.81	0.19	30,39,44,45	0
2	G4O	D	401	4/4	0.83	0.18	40,40,43,50	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.

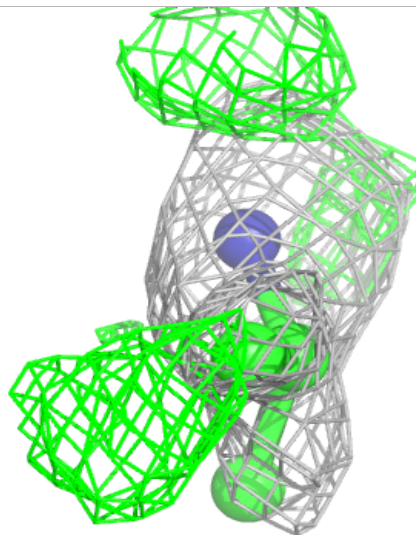
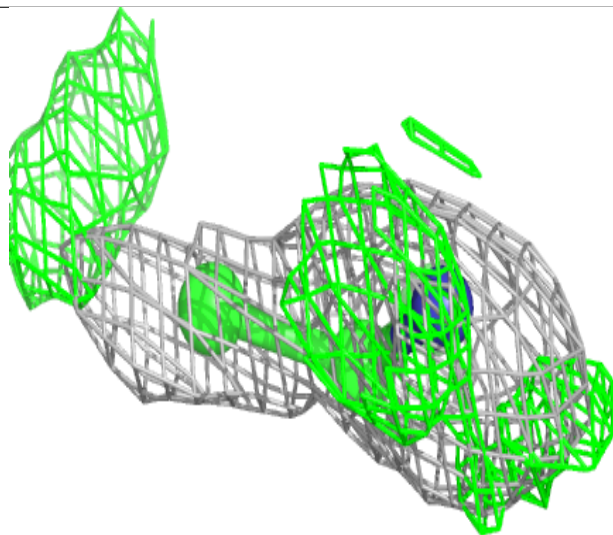
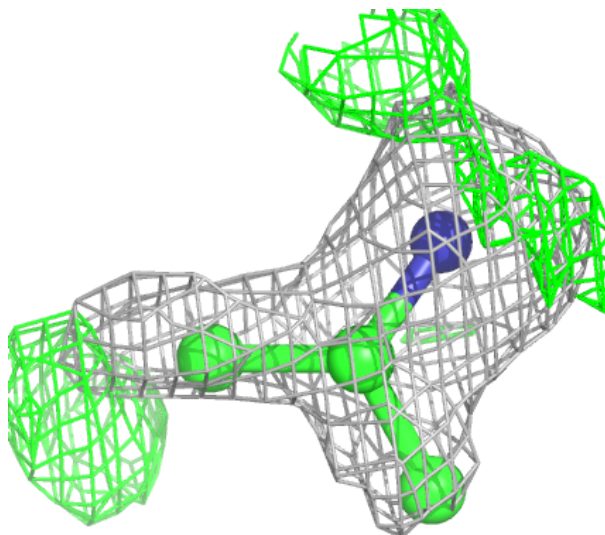
Electron density around G4O A 401:

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



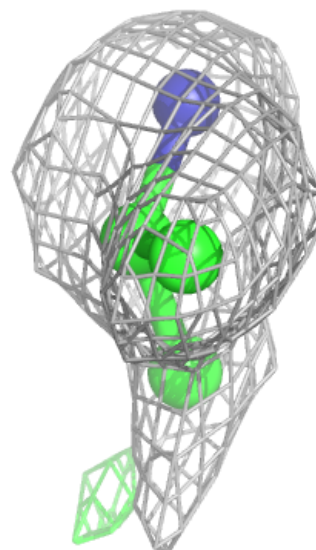
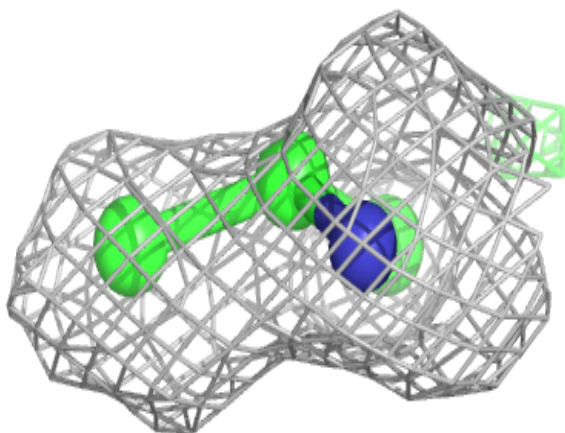
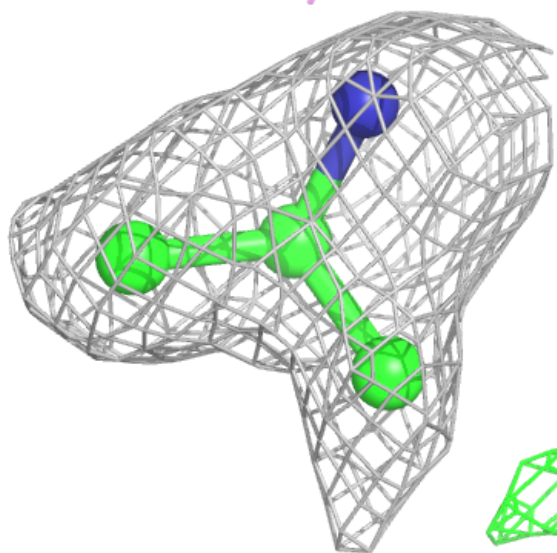
Electron density around G4O C 401:

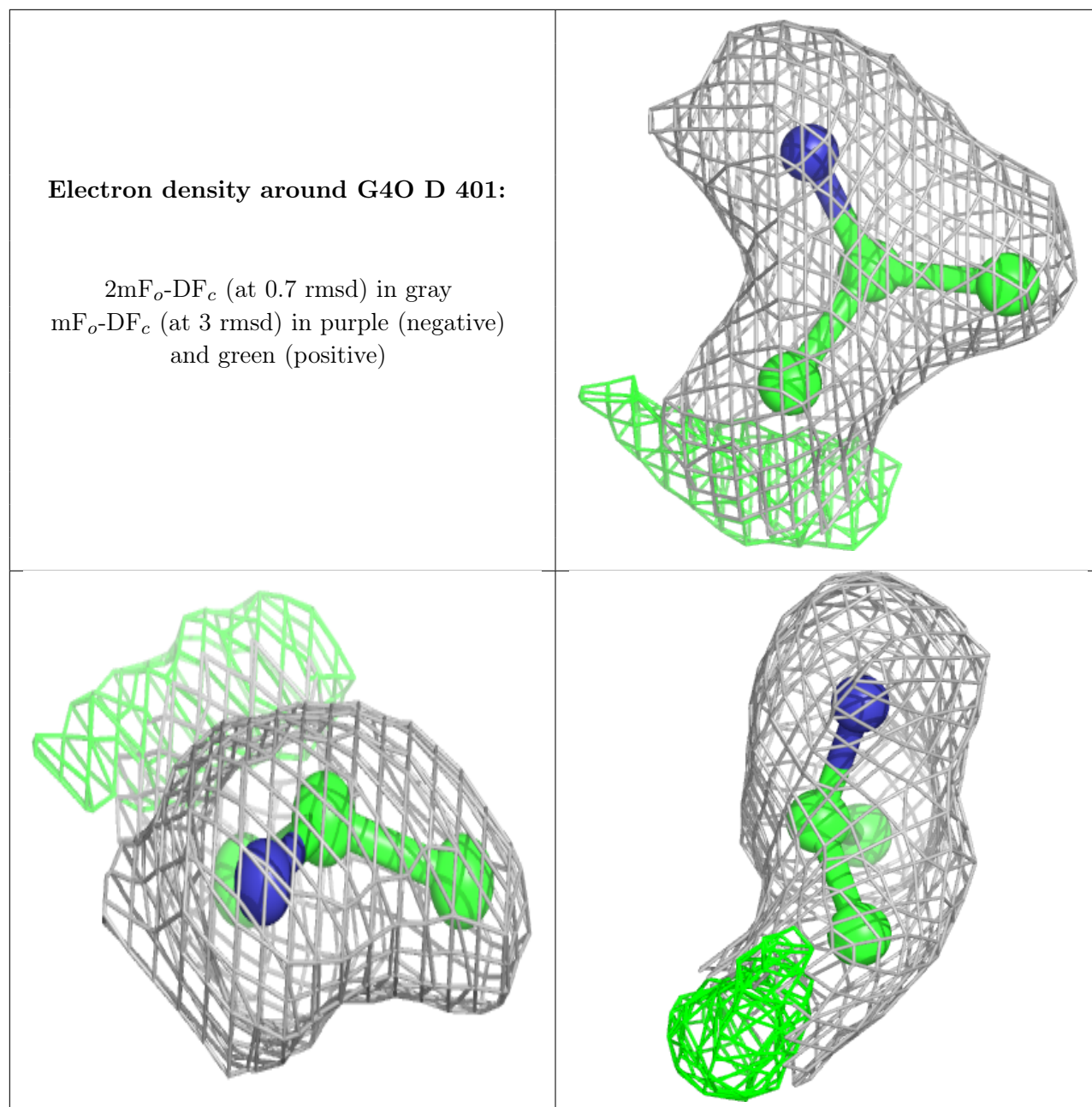
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G4O 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.