



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:04 PM UTC

PDB ID : 6K9Y / pdb_00006k9y
Title : Crystal structure of human VAT-1
Authors : Watanabe, Y.; Endo, T.
Deposited on : 2019-06-19
Resolution : 2.20 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

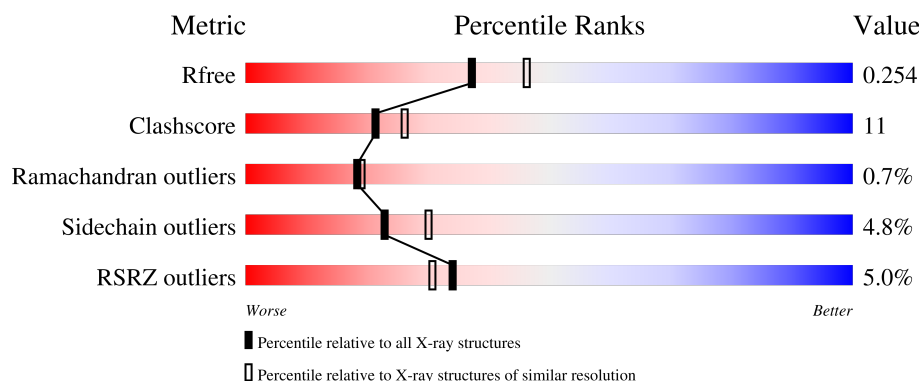
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	357	5% 68% 24% • • •
1	B	357	5% 73% 18% • 8%
1	C	357	3% 68% 22% • 9%
1	D	357	5% 66% 25% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10175 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 Synaptic vesicle membrane protein VAT-1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2584	1654	448	465	17			
1	B	328	Total	C	N	O	S	0	0	0
			2446	1564	420	446	16			
1	C	325	Total	C	N	O	S	0	0	0
			2446	1564	420	445	17			
1	D	333	Total	C	N	O	S	0	0	0
			2509	1604	432	456	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	expression tag	UNP Q99536
A	38	PRO	-	expression tag	UNP Q99536
A	39	HIS	-	expression tag	UNP Q99536
A	40	MET	-	expression tag	UNP Q99536
B	37	GLY	-	expression tag	UNP Q99536
B	38	PRO	-	expression tag	UNP Q99536
B	39	HIS	-	expression tag	UNP Q99536
B	40	MET	-	expression tag	UNP Q99536
C	37	GLY	-	expression tag	UNP Q99536
C	38	PRO	-	expression tag	UNP Q99536
C	39	HIS	-	expression tag	UNP Q99536
C	40	MET	-	expression tag	UNP Q99536
D	37	GLY	-	expression tag	UNP Q99536
D	38	PRO	-	expression tag	UNP Q99536
D	39	HIS	-	expression tag	UNP Q99536
D	40	MET	-	expression tag	UNP Q99536

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃) (labeled as "Ligand of Interest" by depositor).



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

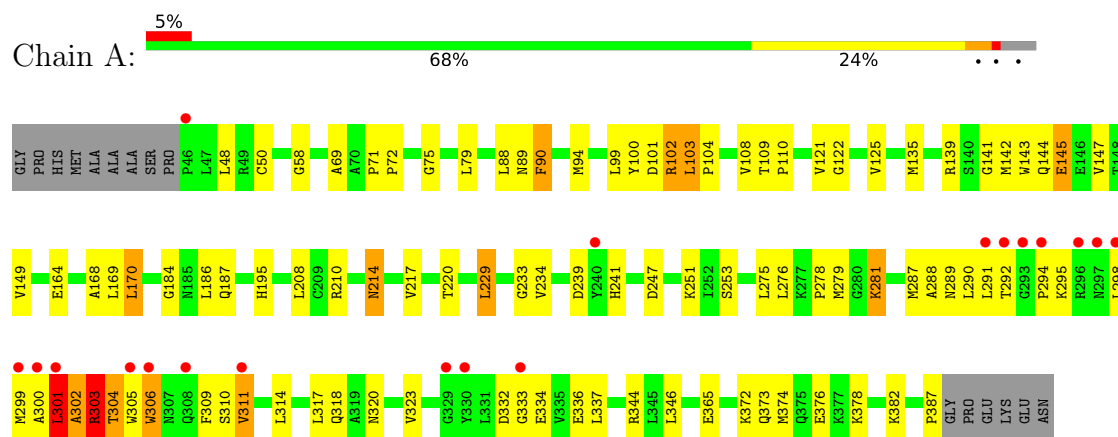
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	25	Total	O	0	0
			25	25		
3	C	52	Total	O	0	0
			52	52		
3	D	43	Total	O	0	0
			43	43		

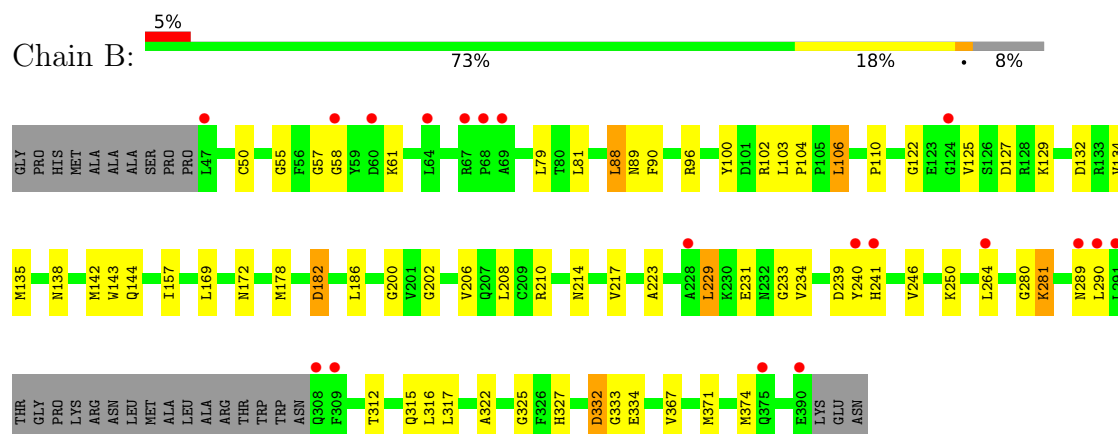
3 Residue-property plots [i](#)

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.

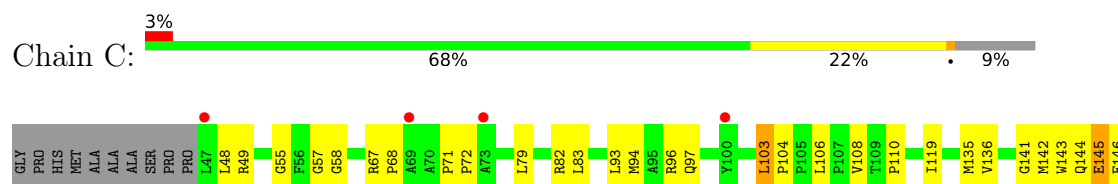
- Molecule 1: Synaptic vesicle membrane protein VAT-1 homolog

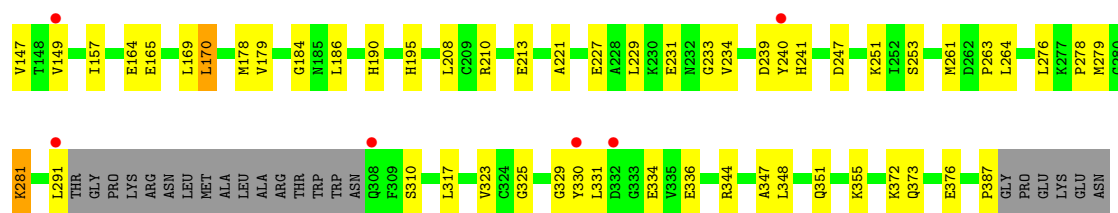


- Molecule 1: Synaptic vesicle membrane protein VAT-1 homolog

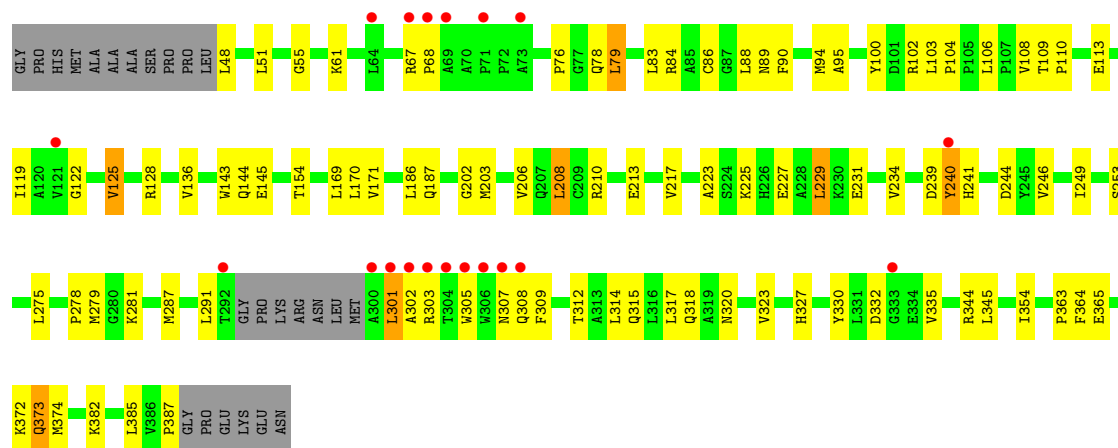


- Molecule 1: Synaptic vesicle membrane protein VAT-1 homolog





● Molecule 1: Synaptic vesicle membrane protein VAT-1 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.16Å 131.72Å 174.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.20) 99.6 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.255 0.222 , 0.254	Depositor DCC
R_{free} test set	7924 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.9	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	0.95	EDS
Total number of atoms	10175	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 3.47% 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: NO3

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	0.44	0/2640	0.95	14/3588 (0.4%)
1	B	0.43	0/2496	0.91	5/3392 (0.1%)
1	C	0.46	0/2495	0.95	9/3387 (0.3%)
1	D	0.45	0/2560	0.93	9/3477 (0.3%)
All	All	0.44	0/10191	0.94	37/13844 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LEU	N-CA-C	9.08	122.96	111.24
1	B	169	LEU	N-CA-C	7.73	121.21	111.24
1	D	169	LEU	N-CA-C	7.20	120.53	111.24
1	A	302	ALA	N-CA-C	-6.73	104.54	112.89
1	D	335	VAL	N-CA-C	6.67	116.82	110.42
1	A	301	LEU	N-CA-C	-6.59	104.46	113.30
1	C	241	HIS	N-CA-C	6.30	119.12	111.82
1	A	217	VAL	N-CA-C	6.18	116.77	107.80
1	C	145	GLU	N-CA-C	5.91	117.39	111.07
1	D	253	SER	CA-C-N	5.86	126.00	119.32
1	D	253	SER	C-N-CA	5.86	126.00	119.32
1	A	332	ASP	N-CA-C	5.79	118.11	109.25
1	A	102	ARG	N-CA-C	5.75	117.80	110.61
1	B	332	ASP	N-CA-C	5.74	118.59	109.24
1	A	276	LEU	N-CA-C	5.70	119.20	110.20
1	C	213	GLU	N-CA-C	5.55	118.27	110.23
1	C	170	LEU	N-CA-C	5.45	122.41	110.80
1	D	83	LEU	N-CA-C	5.42	118.39	109.76
1	D	217	VAL	N-CA-C	5.42	115.71	108.11
1	A	103	LEU	N-CA-C	-5.41	102.95	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	213	GLU	N-CA-C	5.39	118.13	110.10
1	C	253	SER	CA-C-N	5.37	126.55	119.84
1	C	253	SER	C-N-CA	5.37	126.55	119.84
1	B	217	VAL	N-CA-C	5.37	115.58	107.80
1	C	264	LEU	N-CA-C	5.27	119.78	112.45
1	A	214	ASN	N-CA-C	5.26	118.45	111.30
1	C	169	LEU	N-CA-C	5.22	119.13	111.04
1	B	135	MET	N-CA-C	-5.21	101.67	109.95
1	D	84	ARG	N-CA-C	-5.19	107.08	113.41
1	A	145	GLU	N-CA-C	5.12	116.94	111.36
1	D	171	VAL	N-CA-C	5.09	115.52	110.23
1	A	253	SER	CA-C-N	5.08	125.11	119.32
1	A	253	SER	C-N-CA	5.08	125.11	119.32
1	A	303	ARG	N-CA-C	-5.06	105.96	111.82
1	A	170	LEU	N-CA-C	5.05	121.56	110.80
1	C	276	LEU	N-CA-C	5.01	118.12	110.20
1	B	241	HIS	N-CA-C	5.00	119.09	112.89

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	2584	0	2630	72	0
1	B	2446	0	2471	48	0
1	C	2446	0	2490	54	0
1	D	2509	0	2547	58	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	38	0	0	0	0
3	B	25	0	0	0	0
3	C	52	0	0	0	0
3	D	43	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10175	0	10138	219	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 11.

All (219) 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:D:301:LEU:HD11	1:D:303:ARG:HD2	1.50	0.92
1:C:67:ARG:HG2	1:C:68:PRO:HD2	1.56	0.87
1:D:145:GLU:HG2	1:D:387:PRO:HB3	1.57	0.86
1:A:292:THR:O	1:A:294:PRO:HD2	1.79	0.83
1:A:301:LEU:O	1:A:304:THR:HB	1.80	0.81
1:A:306:TRP:HZ3	1:C:310:SER:O	1.62	0.81
1:C:142:MET:HE1	1:C:147:VAL:HG21	1.62	0.81
1:D:95:ALA:HB1	1:D:103:LEU:HD12	1.63	0.80
1:D:136:VAL:HG22	1:D:154:THR:HG22	1.65	0.79
1:D:301:LEU:HD11	1:D:303:ARG:CD	2.12	0.78
1:A:145:GLU:HG2	1:A:387:PRO:HB3	1.67	0.77
1:A:103:LEU:HD22	1:A:104:PRO:HD2	1.68	0.75
1:A:102:ARG:HH11	1:A:139:ARG:HH22	1.33	0.74
1:A:373:GLN:OE1	1:A:378:LYS:HE3	1.87	0.74
1:D:229:LEU:HG	1:D:234:VAL:HG21	1.69	0.73
1:A:300:ALA:HB1	1:A:303:ARG:HD2	1.71	0.73
1:D:67:ARG:HB2	1:D:68:PRO:HD2	1.72	0.71
1:A:229:LEU:HG	1:A:234:VAL:HG21	1.72	0.71
1:C:97:GLN:HG3	1:C:291:LEU:HD11	1.74	0.70
1:C:58:GLY:O	1:C:96:ARG:HD3	1.92	0.69
1:C:96:ARG:NH1	1:C:97:GLN:HE21	1.90	0.69
1:A:279:MET:HE2	1:B:178:MET:HE2	1.74	0.69
1:B:367:VAL:HG22	1:B:371:MET:HE2	1.75	0.69
1:B:89:ASN:C	1:B:374:MET:HE1	2.19	0.68
1:D:301:LEU:CD1	1:D:303:ARG:H	2.07	0.68
1:C:97:GLN:HG3	1:C:291:LEU:CD1	2.24	0.67
1:D:301:LEU:HD12	1:D:302:ALA:N	2.10	0.67
1:B:246:VAL:HG12	1:B:250:LYS:HE2	1.78	0.66
1:C:247:ASP:O	1:C:251:LYS:HG3	1.95	0.66
1:B:58:GLY:O	1:B:96:ARG:HD3	1.96	0.64
1:B:210:ARG:HD2	1:B:233:GLY:HA3	1.77	0.64
1:A:142:MET:HE1	1:A:147:VAL:HG11	1.80	0.64
1:D:86:CYS:HB2	1:D:385:LEU:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ARG:HH11	1:C:97:GLN:HE21	1.45	0.63
1:C:94:MET:HE1	1:C:291:LEU:HB2	1.80	0.62
1:B:290:LEU:HD23	1:B:290:LEU:O	1.99	0.62
1:C:110:PRO:HG2	1:C:143:TRP:CE3	2.35	0.62
1:C:135:MET:HE2	1:C:157:ILE:HG12	1.81	0.62
1:B:281:LYS:HB3	1:B:322:ALA:HB3	1.80	0.61
1:A:102:ARG:NH1	1:A:139:ARG:HH22	1.99	0.61
1:B:50:CYS:HB2	1:B:144:GLN:HB3	1.83	0.60
1:D:372:LYS:HD3	3:D:540:HOH:O	2.00	0.60
1:D:100:TYR:CZ	1:D:102:ARG:HB2	2.37	0.60
1:A:89:ASN:C	1:A:374:MET:HE1	2.28	0.58
1:A:48:LEU:HG	1:A:69:ALA:HB2	1.84	0.58
1:A:110:PRO:HG2	1:A:143:TRP:CE3	2.39	0.58
1:D:303:ARG:HA	1:D:307:ASN:CB	2.33	0.58
1:A:94:MET:CB	1:A:291:LEU:HD13	2.34	0.57
1:A:314:LEU:O	1:A:318:GLN:HG3	2.05	0.57
1:C:347:ALA:O	1:C:351:GLN:HG3	2.03	0.57
1:A:135:MET:HE1	1:A:346:LEU:HD21	1.87	0.57
1:A:50:CYS:HB3	1:A:144:GLN:HB2	1.86	0.57
1:A:102:ARG:NH1	1:A:139:ARG:NH2	2.51	0.57
1:C:104:PRO:HG2	1:C:108:VAL:HG21	1.88	0.56
1:A:301:LEU:O	1:A:301:LEU:HD22	2.06	0.56
1:D:301:LEU:HD12	1:D:302:ALA:H	1.70	0.55
1:A:301:LEU:C	1:A:301:LEU:HD13	2.31	0.55
1:D:48:LEU:HB3	1:D:67:ARG:HG3	1.89	0.55
1:A:317:LEU:CD2	1:B:327:HIS:HB2	2.36	0.55
1:B:210:ARG:HG2	1:B:210:ARG:HH11	1.71	0.55
1:B:129:LYS:HE2	1:B:132:ASP:OD1	2.07	0.55
1:C:57:GLY:O	1:C:96:ARG:HD2	2.06	0.55
1:C:142:MET:CE	1:C:147:VAL:HG21	2.34	0.55
1:C:94:MET:CE	1:C:291:LEU:HD22	2.37	0.55
1:D:203:MET:HE3	3:D:541:HOH:O	2.07	0.55
1:A:75:GLY:O	1:A:122:GLY:HA3	2.07	0.54
1:A:90:PHE:CD1	1:A:374:MET:HE3	2.42	0.54
1:C:82:ARG:HG2	1:C:119:ILE:HD13	1.89	0.54
1:B:229:LEU:HG	1:B:234:VAL:HG21	1.90	0.54
1:B:312:THR:OG1	1:B:315:GLN:HG3	2.08	0.53
1:A:147:VAL:HG12	1:A:149:VAL:HG13	1.91	0.53
1:A:99:LEU:HD13	1:A:291:LEU:CD2	2.38	0.53
1:C:141:GLY:C	1:C:142:MET:HE2	2.34	0.53
1:A:147:VAL:CG1	1:A:149:VAL:HG13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HD2	1:A:233:GLY:HA3	1.91	0.53
1:B:79:LEU:HD11	1:B:81:LEU:HD23	1.90	0.53
1:D:48:LEU:O	1:D:67:ARG:HG2	2.08	0.53
1:A:101:ASP:C	1:A:102:ARG:HG3	2.33	0.53
1:A:336:GLU:OE2	1:A:336:GLU:HA	2.09	0.53
1:B:264:LEU:HB3	1:B:289:ASN:ND2	2.24	0.52
1:C:344:ARG:NH2	1:C:348:LEU:HD21	2.25	0.52
1:C:184:GLY:HA2	1:C:281:LYS:HG3	1.92	0.52
1:C:323:VAL:HG22	1:D:323:VAL:HG23	1.92	0.52
1:D:314:LEU:O	1:D:318:GLN:HG3	2.10	0.51
1:A:300:ALA:O	1:A:303:ARG:HD2	2.10	0.51
1:D:110:PRO:HG2	1:D:143:TRP:CE3	2.46	0.51
1:A:104:PRO:HG2	1:A:108:VAL:HG21	1.92	0.51
1:A:164:GLU:H	1:A:164:GLU:CD	2.18	0.51
1:A:90:PHE:HA	1:A:374:MET:CE	2.40	0.51
1:A:99:LEU:HD13	1:A:291:LEU:HD23	1.92	0.51
1:C:83:LEU:HD12	1:C:144:GLN:O	2.11	0.50
1:D:227:GLU:HG2	1:D:231:GLU:OE2	2.11	0.50
1:A:214:ASN:HD22	1:A:214:ASN:N	2.08	0.50
1:B:100:TYR:CD2	1:B:103:LEU:HB2	2.47	0.50
1:D:79:LEU:HD12	1:D:79:LEU:C	2.36	0.50
1:D:125:VAL:HG22	1:D:125:VAL:O	2.11	0.50
1:C:79:LEU:C	1:C:79:LEU:HD12	2.37	0.50
1:D:89:ASN:C	1:D:374:MET:HE1	2.37	0.50
1:B:79:LEU:HD12	1:B:79:LEU:C	2.36	0.50
1:B:110:PRO:HG2	1:B:143:TRP:CE3	2.47	0.49
1:A:317:LEU:HD23	1:B:327:HIS:HB2	1.94	0.49
1:A:323:VAL:HG23	1:B:316:LEU:HD11	1.94	0.49
1:A:299:MET:C	1:A:301:LEU:H	2.20	0.49
1:B:122:GLY:O	1:B:125:VAL:HG12	2.12	0.49
1:C:103:LEU:HD22	1:C:104:PRO:HD2	1.94	0.49
1:C:164:GLU:H	1:C:164:GLU:CD	2.21	0.49
1:B:88:LEU:HD13	1:B:143:TRP:HZ2	1.78	0.48
1:C:49:ARG:HG3	1:C:145:GLU:OE1	2.13	0.48
1:A:135:MET:HG3	1:A:170:LEU:HD11	1.94	0.48
1:C:210:ARG:HD2	1:C:233:GLY:HA3	1.95	0.48
1:B:172:ASN:OD1	1:B:200:GLY:HA3	2.13	0.48
1:B:264:LEU:HB3	1:B:289:ASN:HD21	1.77	0.48
1:B:88:LEU:HD12	1:B:89:ASN:N	2.29	0.48
1:B:317:LEU:C	1:B:317:LEU:HD23	2.39	0.48
1:C:178:MET:HE2	1:D:279:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:CYS:HB2	1:B:144:GLN:CB	2.44	0.48
1:C:336:GLU:H	1:C:336:GLU:CD	2.22	0.48
1:A:288:ALA:C	1:A:290:LEU:H	2.22	0.48
1:C:136:VAL:HG21	1:C:149:VAL:HG21	1.96	0.48
1:D:363:PRO:HB2	1:D:365:GLU:OE1	2.14	0.47
1:D:67:ARG:NH2	1:D:144:GLN:OE1	2.47	0.47
1:D:202:GLY:O	1:D:206:VAL:HG23	2.14	0.47
1:A:214:ASN:HD22	1:A:214:ASN:H	1.61	0.47
1:B:138:ASN:CB	1:B:142:MET:HE3	2.44	0.47
1:C:48:LEU:HD11	1:C:82:ARG:NH2	2.29	0.47
1:C:71:PRO:HA	1:C:72:PRO:HD3	1.80	0.47
1:D:301:LEU:CD1	1:D:303:ARG:HD2	2.34	0.47
1:A:100:TYR:HD2	1:A:103:LEU:HB2	1.80	0.47
1:A:195:HIS:HA	1:A:220:THR:OG1	2.15	0.47
1:D:94:MET:HE1	1:D:291:LEU:HG	1.95	0.47
1:D:106:LEU:HD12	1:D:106:LEU:N	2.30	0.47
1:D:240:TYR:HD1	1:D:240:TYR:H	1.63	0.47
1:A:287:MET:HE3	1:B:317:LEU:HD13	1.97	0.46
1:C:49:ARG:NH2	1:C:387:PRO:O	2.49	0.46
1:D:125:VAL:HG21	1:D:128:ARG:HB2	1.98	0.46
1:A:122:GLY:O	1:A:125:VAL:HG12	2.15	0.46
1:B:100:TYR:CZ	1:B:102:ARG:HB2	2.51	0.46
1:A:323:VAL:HG23	1:B:316:LEU:CD1	2.45	0.46
1:B:231:GLU:C	1:B:231:GLU:CD	2.83	0.46
1:C:229:LEU:HG	1:C:234:VAL:HG21	1.98	0.45
1:A:88:LEU:HD13	1:A:143:TRP:CZ2	2.52	0.45
1:B:88:LEU:HD13	1:B:143:TRP:CZ2	2.52	0.45
1:A:239:ASP:OD1	1:A:241:HIS:HB2	2.17	0.45
1:C:49:ARG:HH21	1:C:387:PRO:C	2.25	0.45
1:A:247:ASP:O	1:A:251:LYS:HG3	2.17	0.45
1:A:306:TRP:CZ3	1:C:310:SER:O	2.53	0.45
1:D:76:PRO:O	1:D:78:GLN:HG2	2.17	0.45
1:A:141:GLY:C	1:A:142:MET:HE2	2.42	0.45
1:B:57:GLY:N	1:B:61:LYS:HG3	2.32	0.45
1:C:227:GLU:O	1:C:231:GLU:HG3	2.17	0.44
1:C:278:PRO:O	1:C:279:MET:HB2	2.17	0.44
1:B:178:MET:O	1:B:182:ASP:HB2	2.17	0.44
1:B:280:GLY:C	1:B:281:LYS:HD3	2.43	0.44
1:D:55:GLY:O	1:D:61:LYS:HB3	2.18	0.44
1:D:317:LEU:C	1:D:317:LEU:HD23	2.42	0.44
1:D:373:GLN:OE1	1:D:373:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:HB2	1:B:239:ASP:OD2	2.17	0.44
1:B:55:GLY:HA2	1:B:106:LEU:HD23	2.00	0.44
1:D:327:HIS:HB3	1:D:330:TYR:HD2	1.82	0.44
1:A:94:MET:HA	1:A:291:LEU:HD22	2.00	0.44
1:A:108:VAL:HG22	1:A:109:THR:N	2.33	0.44
1:D:51:LEU:O	1:D:109:THR:HG23	2.17	0.44
1:C:372:LYS:HG3	1:C:376:GLU:OE2	2.18	0.43
1:B:332:ASP:O	1:B:334:GLU:HG2	2.17	0.43
1:C:55:GLY:HA2	1:C:106:LEU:HD23	2.00	0.43
1:D:208:LEU:HD12	1:D:208:LEU:HA	1.85	0.43
1:C:195:HIS:HB2	1:C:263:PRO:HD2	2.00	0.43
1:D:103:LEU:HD21	1:D:108:VAL:HG11	2.00	0.43
1:D:278:PRO:O	1:D:279:MET:HB2	2.18	0.43
1:A:372:LYS:HG2	1:A:376:GLU:OE1	2.18	0.43
1:B:125:VAL:O	1:B:125:VAL:HG13	2.18	0.43
1:B:134:VAL:HA	1:B:157:ILE:HG13	2.01	0.43
1:C:94:MET:HE3	1:C:291:LEU:HD22	1.99	0.43
1:A:168:ALA:CB	1:A:382:LYS:HG2	2.48	0.43
1:D:244:ASP:OD1	1:D:246:VAL:HB	2.18	0.43
1:A:320:ASN:HA	1:B:325:GLY:O	2.18	0.43
1:A:334:GLU:HB3	1:A:337:LEU:HB3	2.01	0.43
1:C:82:ARG:NE	1:C:146:GLU:HB2	2.33	0.43
1:A:309:PHE:CZ	1:A:311:VAL:HG13	2.54	0.42
1:D:113:GLU:OE1	1:D:382:LYS:NZ	2.43	0.42
1:A:279:MET:CE	1:B:178:MET:HE2	2.46	0.42
1:C:329:GLY:C	1:C:331:LEU:H	2.27	0.42
1:B:210:ARG:HG2	1:B:210:ARG:NH1	2.34	0.42
1:B:240:TYR:CD1	1:B:240:TYR:C	2.98	0.42
1:A:298:LEU:O	1:A:301:LEU:HB3	2.19	0.42
1:C:221:ALA:O	1:C:239:ASP:HA	2.19	0.42
1:A:50:CYS:HB3	1:A:144:GLN:CB	2.50	0.42
1:D:210:ARG:HG2	1:D:210:ARG:HH11	1.85	0.42
1:D:301:LEU:HD11	1:D:303:ARG:H	1.83	0.42
1:A:300:ALA:HB1	1:A:303:ARG:CD	2.47	0.42
1:A:301:LEU:HD13	1:A:302:ALA:N	2.35	0.42
1:C:179:VAL:HG11	1:C:261:MET:HE3	2.01	0.42
1:D:223:ALA:C	1:D:225:LYS:H	2.27	0.41
1:D:122:GLY:O	1:D:125:VAL:HG13	2.20	0.41
1:C:103:LEU:HD13	1:C:104:PRO:O	2.20	0.41
1:D:239:ASP:OD1	1:D:241:HIS:HB2	2.21	0.41
1:A:278:PRO:O	1:A:279:MET:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLY:O	1:B:206:VAL:HG23	2.20	0.41
1:B:317:LEU:HD23	1:B:317:LEU:O	2.21	0.41
1:D:100:TYR:OH	1:D:102:ARG:HB2	2.20	0.41
1:A:71:PRO:HA	1:A:72:PRO:HD3	1.80	0.41
1:A:164:GLU:CD	1:A:164:GLU:N	2.79	0.41
1:D:104:PRO:HG2	1:D:108:VAL:HG21	2.02	0.41
1:A:103:LEU:HD13	1:A:104:PRO:O	2.21	0.41
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.91	0.41
1:C:79:LEU:HD12	1:C:79:LEU:O	2.20	0.41
1:C:82:ARG:HD3	1:C:82:ARG:HA	1.88	0.41
1:C:240:TYR:CD1	1:C:240:TYR:C	2.99	0.41
1:C:165:GLU:OE2	1:C:355:LYS:HE3	2.21	0.41
1:C:317:LEU:HD23	1:C:317:LEU:C	2.46	0.41
1:C:325:GLY:O	1:D:320:ASN:HA	2.21	0.41
1:D:345:LEU:O	1:D:354:ILE:HD12	2.20	0.40
1:A:184:GLY:O	1:A:281:LYS:HE3	2.21	0.40
1:D:312:THR:OG1	1:D:315:GLN:HG3	2.21	0.40
1:A:58:GLY:HA2	1:A:295:LYS:O	2.21	0.40
1:D:88:LEU:HD13	1:D:143:TRP:CZ2	2.56	0.40
1:D:125:VAL:CG2	1:D:128:ARG:HB2	2.52	0.40
1:D:249:ILE:HD12	1:D:275:LEU:HD21	2.04	0.40
1:D:363:PRO:O	1:D:364:PHE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/357 (95%)	324 (95%)	14 (4%)	2 (1%)	21	23
1	B	324/357 (91%)	310 (96%)	12 (4%)	2 (1%)	21	23
1	C	321/357 (90%)	307 (96%)	12 (4%)	2 (1%)	21	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	329/357 (92%)	305 (93%)	21 (6%)	3 (1%)	14	14
All	All	1314/1428 (92%)	1246 (95%)	59 (4%)	9 (1%)	18	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	170	LEU
1	D	308	GLN
1	C	330	TYR
1	A	289	ASN
1	D	170	LEU
1	D	305	TRP
1	B	333	GLY
1	A	333	GLY
1	B	104	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/286 (96%)	256 (94%)	17 (6%)	16	20
1	B	257/286 (90%)	247 (96%)	10 (4%)	28	39
1	C	260/286 (91%)	252 (97%)	8 (3%)	35	48
1	D	265/286 (93%)	249 (94%)	16 (6%)	17	21
All	All	1055/1144 (92%)	1004 (95%)	51 (5%)	23	30

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	90	PHE
1	A	121	VAL
1	A	186	LEU
1	A	187	GLN

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Mol	Chain	Res	Type
1	A	208	LEU
1	A	229	LEU
1	A	281	LYS
1	A	301	LEU
1	A	303	ARG
1	A	304	THR
1	A	305	TRP
1	A	306	TRP
1	A	310	SER
1	A	311	VAL
1	A	344	ARG
1	A	365	GLU
1	B	88	LEU
1	B	90	PHE
1	B	106	LEU
1	B	127	ASP
1	B	182	ASP
1	B	186	LEU
1	B	208	LEU
1	B	214	ASN
1	B	229	LEU
1	B	281	LYS
1	C	93	LEU
1	C	103	LEU
1	C	186	LEU
1	C	190	HIS
1	C	208	LEU
1	C	281	LYS
1	C	334	GLU
1	C	373	GLN
1	D	79	LEU
1	D	90	PHE
1	D	119	ILE
1	D	125	VAL
1	D	186	LEU
1	D	187	GLN
1	D	208	LEU
1	D	229	LEU
1	D	240	TYR
1	D	281	LYS
1	D	287	MET
1	D	301	LEU

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Mol	Chain	Res	Type
1	D	309	PHE
1	D	332	ASP
1	D	344	ARG
1	D	373	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	97	GLN
1	A	187	GLN
1	A	214	ASN
1	A	308	GLN
1	A	350	ASN
1	B	78	GLN
1	B	144	GLN
1	B	153	GLN
1	B	236	HIS
1	B	289	ASN
1	B	351	GLN
1	B	375	GLN
1	C	65	GLN
1	C	78	GLN
1	C	97	GLN
1	C	153	GLN
1	C	187	GLN
1	C	190	HIS
1	C	236	HIS
1	C	241	HIS
1	C	373	GLN
1	D	78	GLN
1	D	153	GLN
1	D	187	GLN
1	D	308	GLN

5.3.3 RNA ⓘ

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](#)

8 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	NO3	D	401	-	1,3,3	0.32	0	0,3,3	-	-
2	NO3	B	401	-	1,3,3	0.35	0	0,3,3	-	-
2	NO3	C	401	-	1,3,3	0.24	0	0,3,3	-	-
2	NO3	D	402	-	1,3,3	0.34	0	0,3,3	-	-
2	NO3	A	401	-	1,3,3	0.33	0	0,3,3	-	-
2	NO3	B	402	-	1,3,3	0.34	0	0,3,3	-	-
2	NO3	A	402	-	1,3,3	0.36	0	0,3,3	-	-
2	NO3	C	402	-	1,3,3	0.42	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

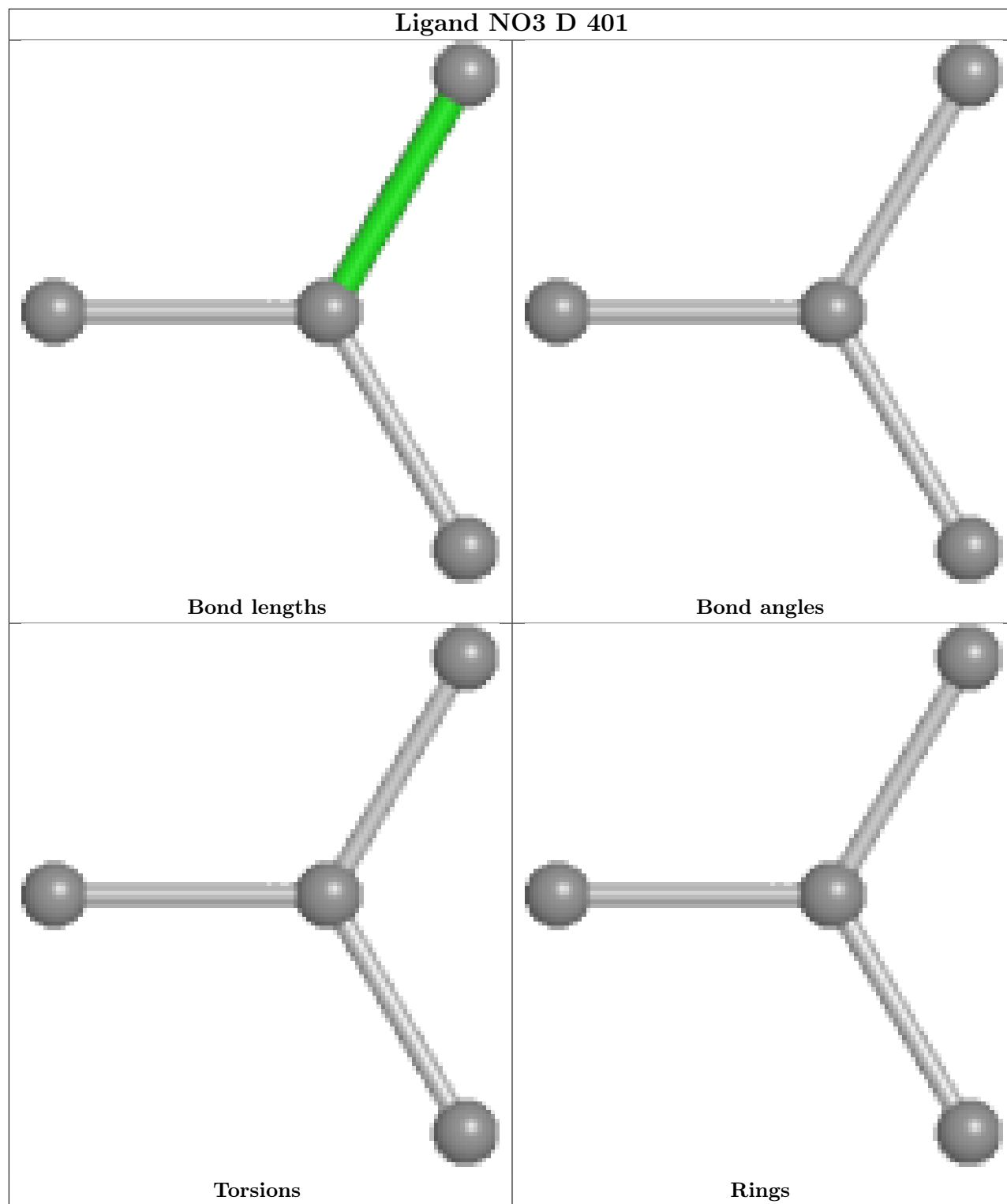
There are no torsion outliers.

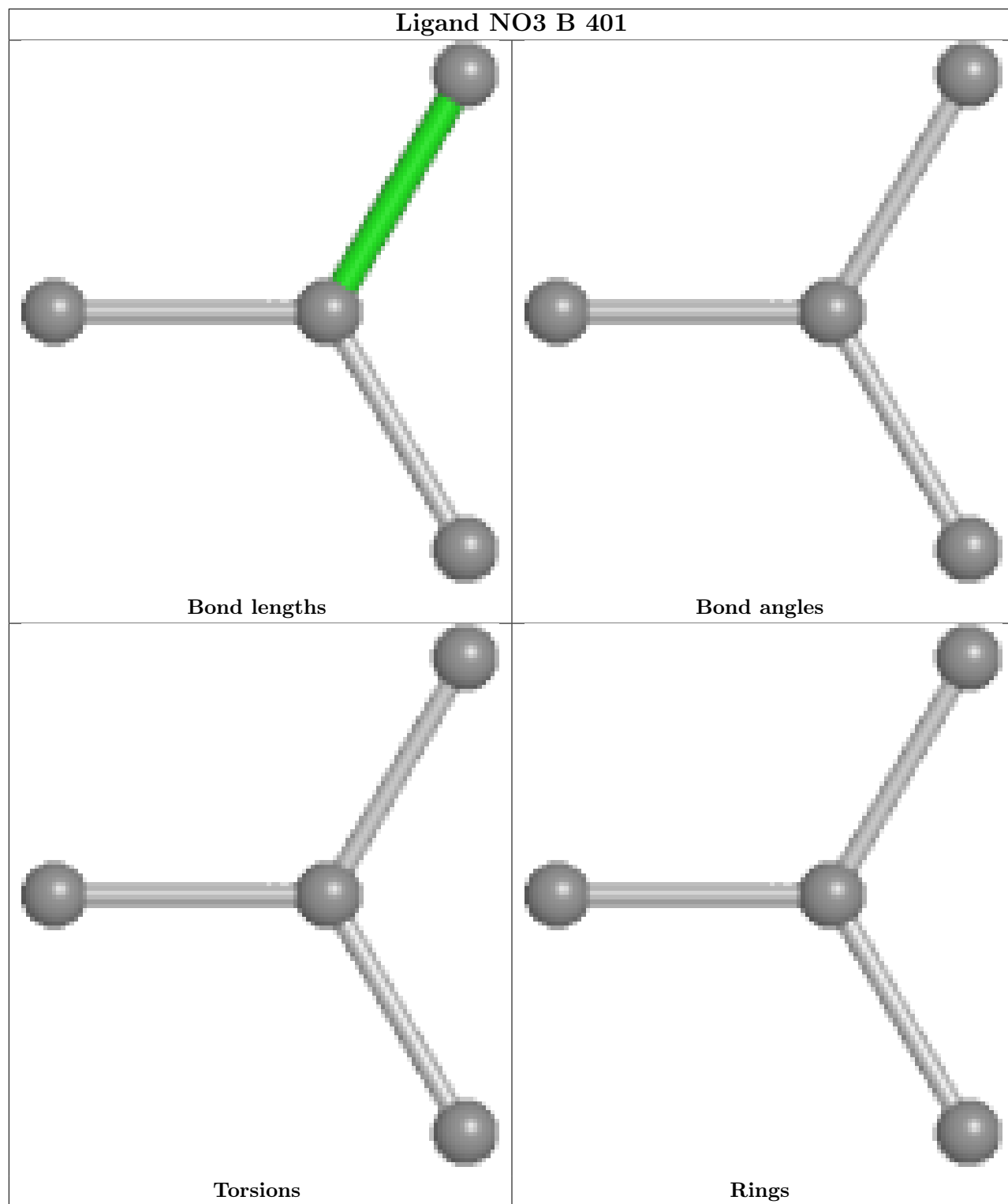
There are no ring outliers.

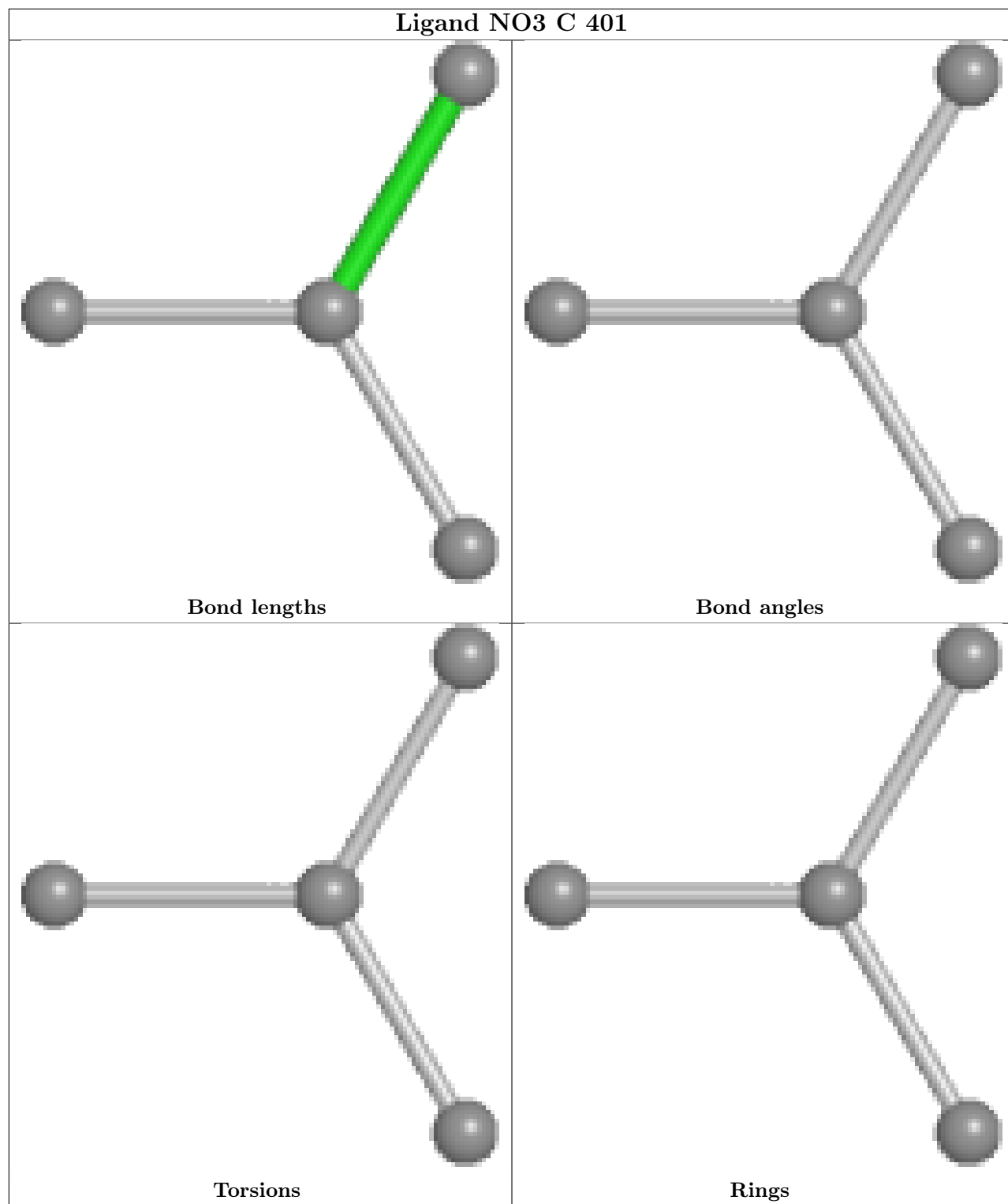
No monomer is involved in short contacts.

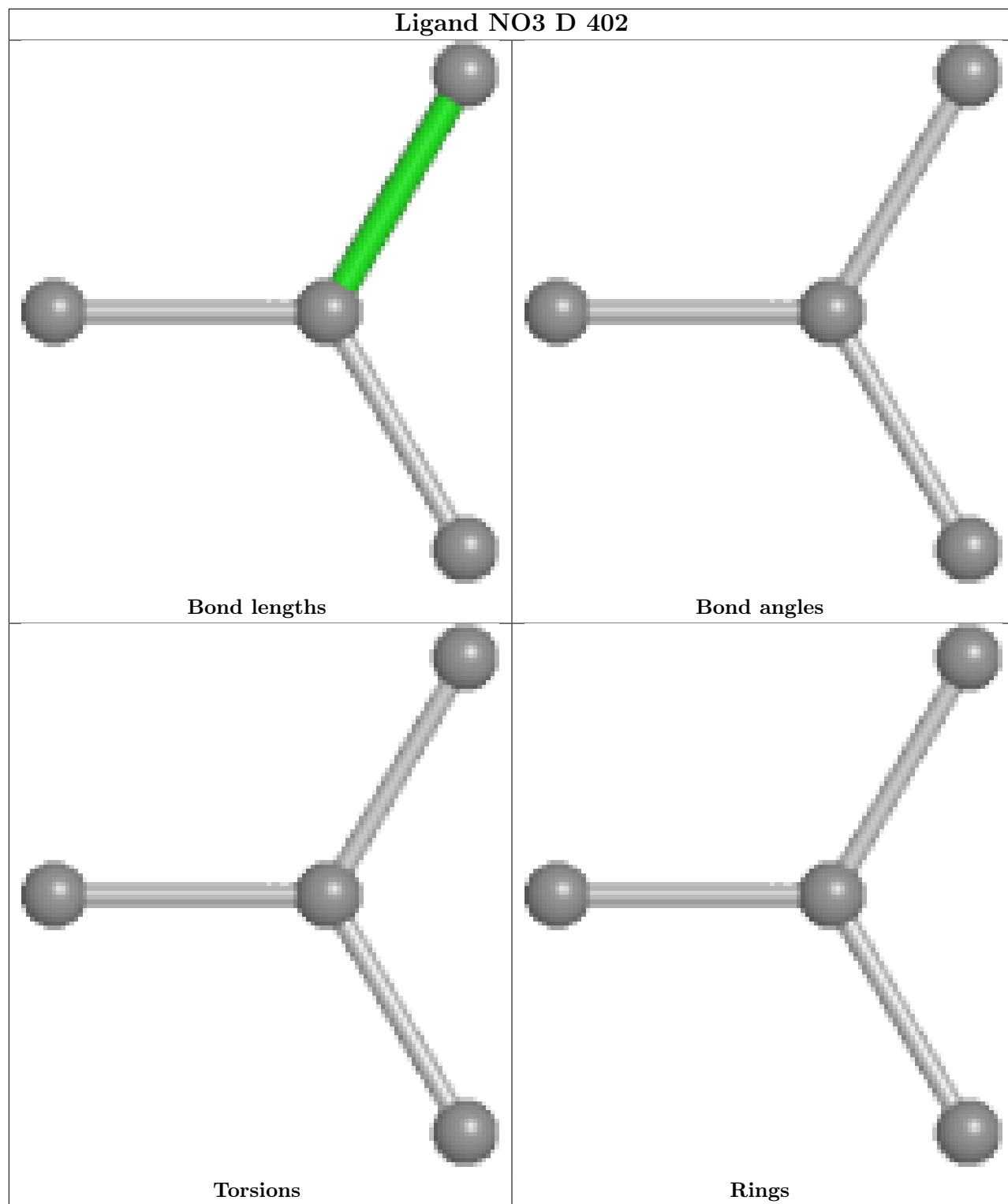
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

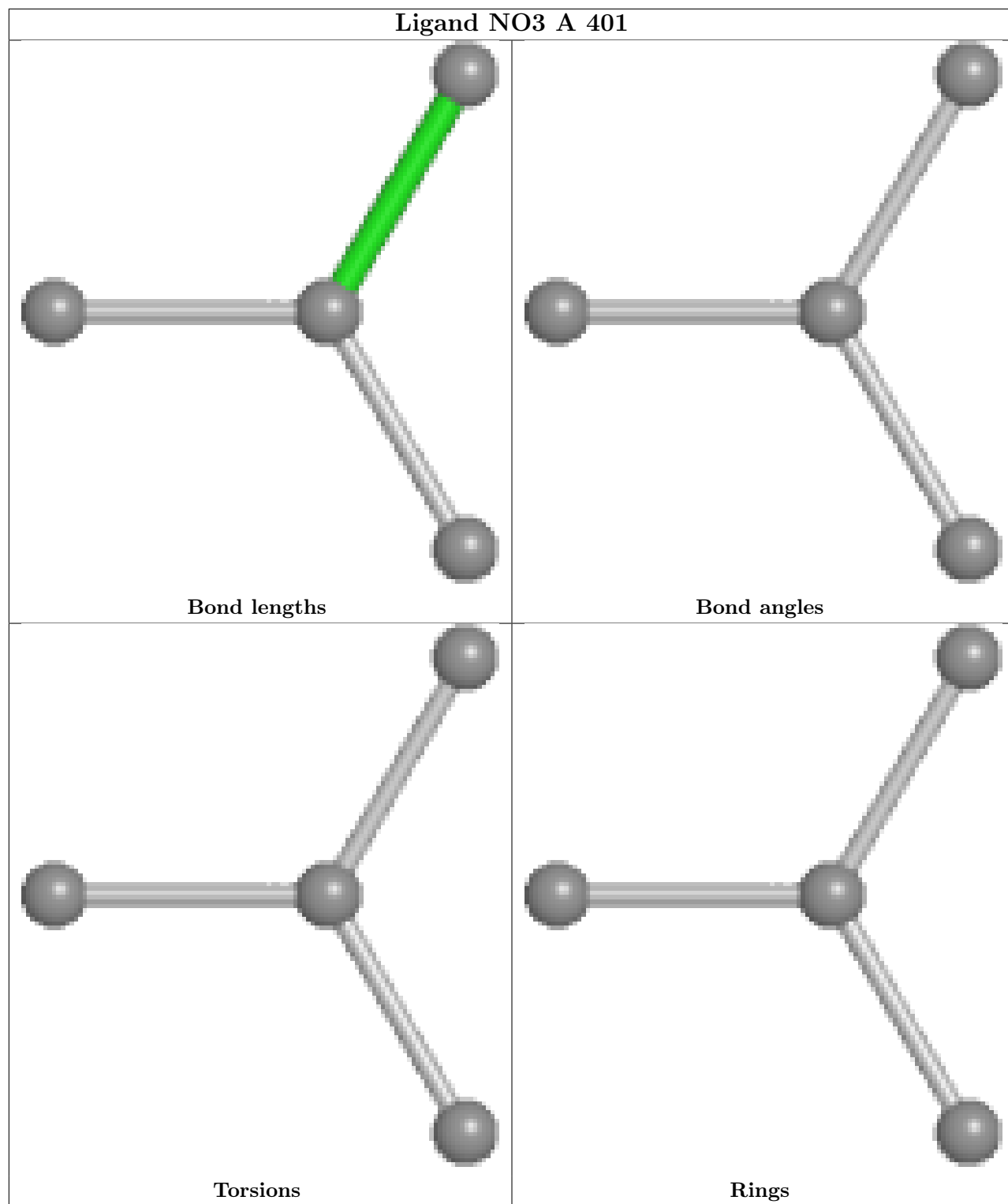
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

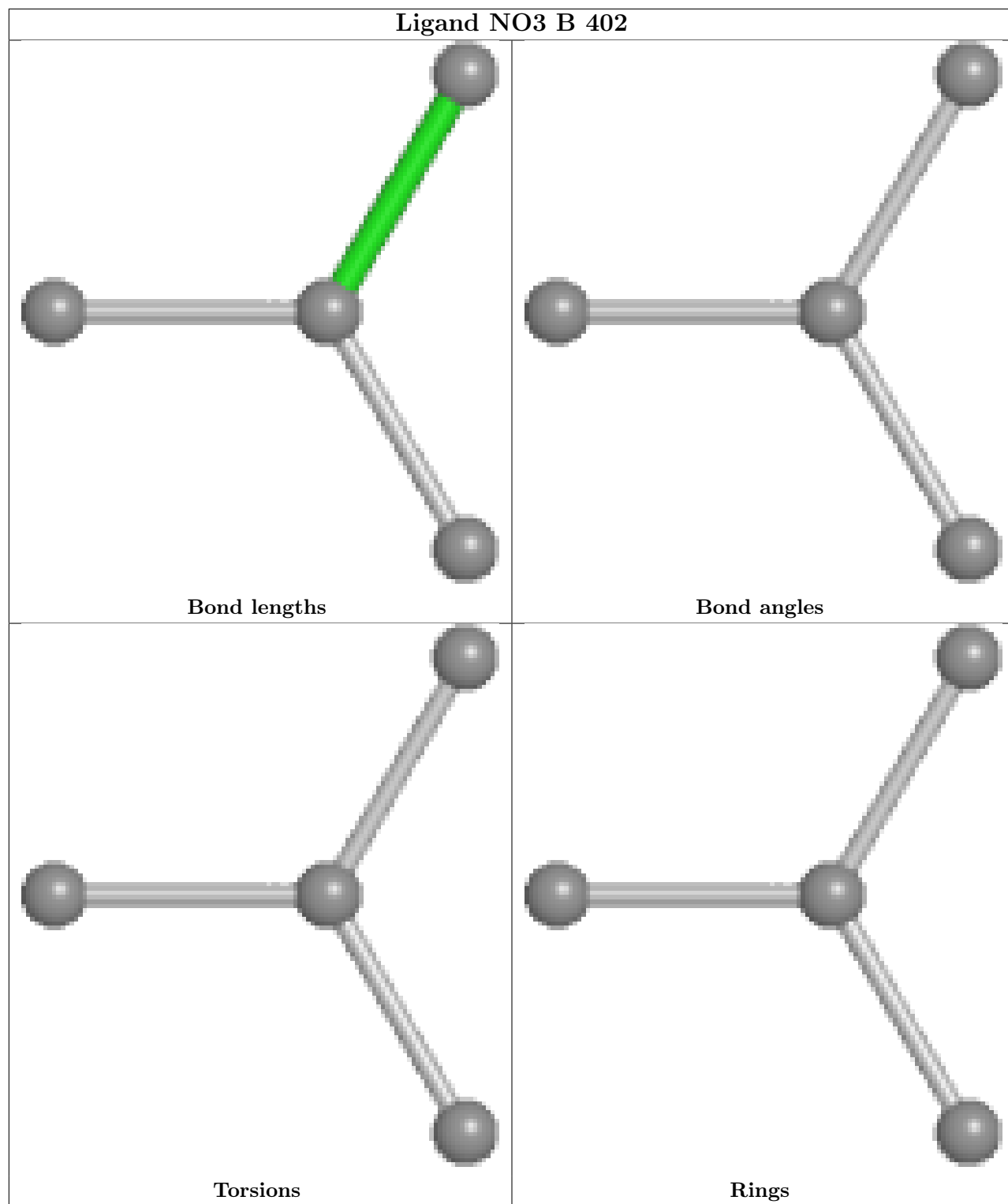


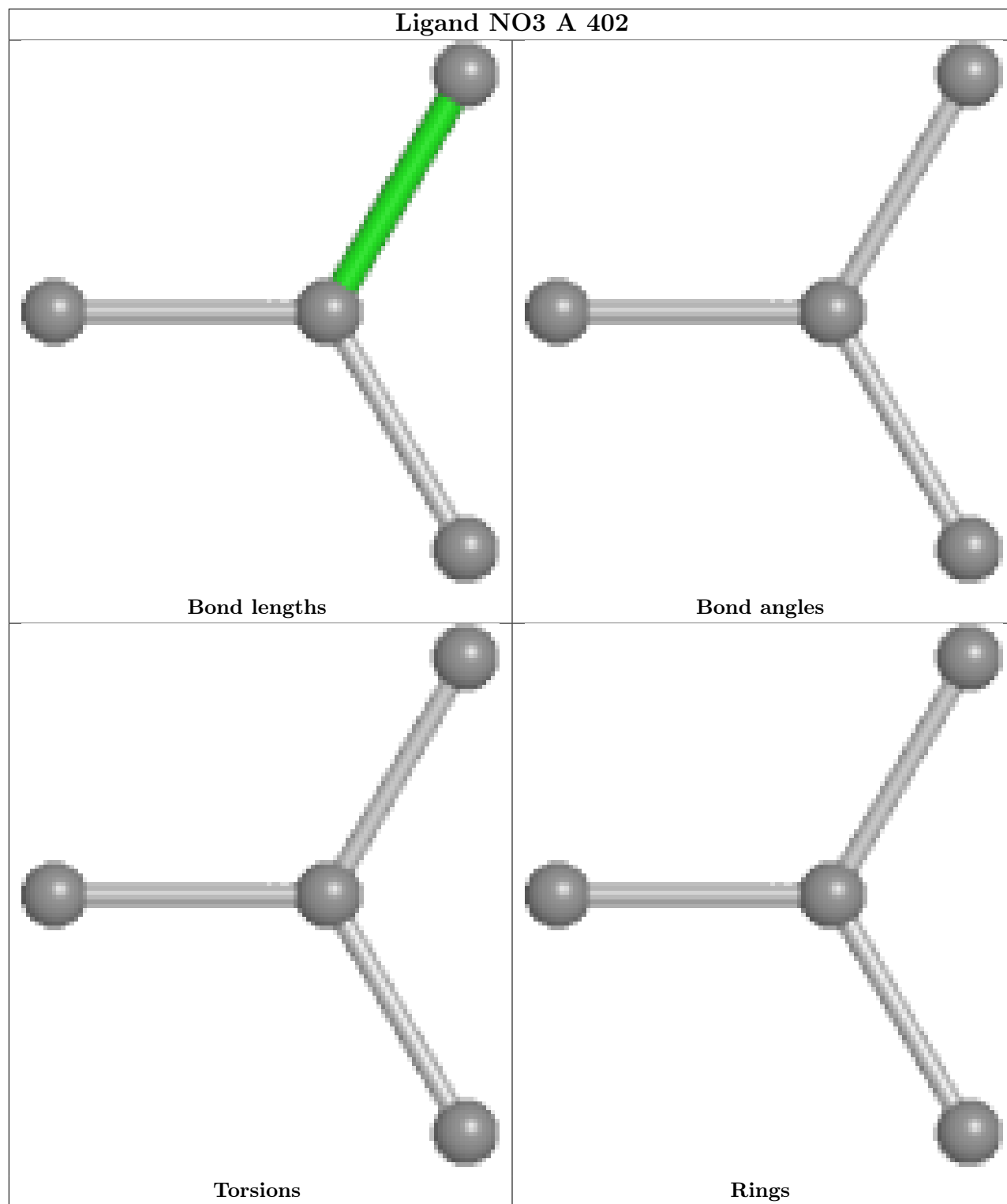


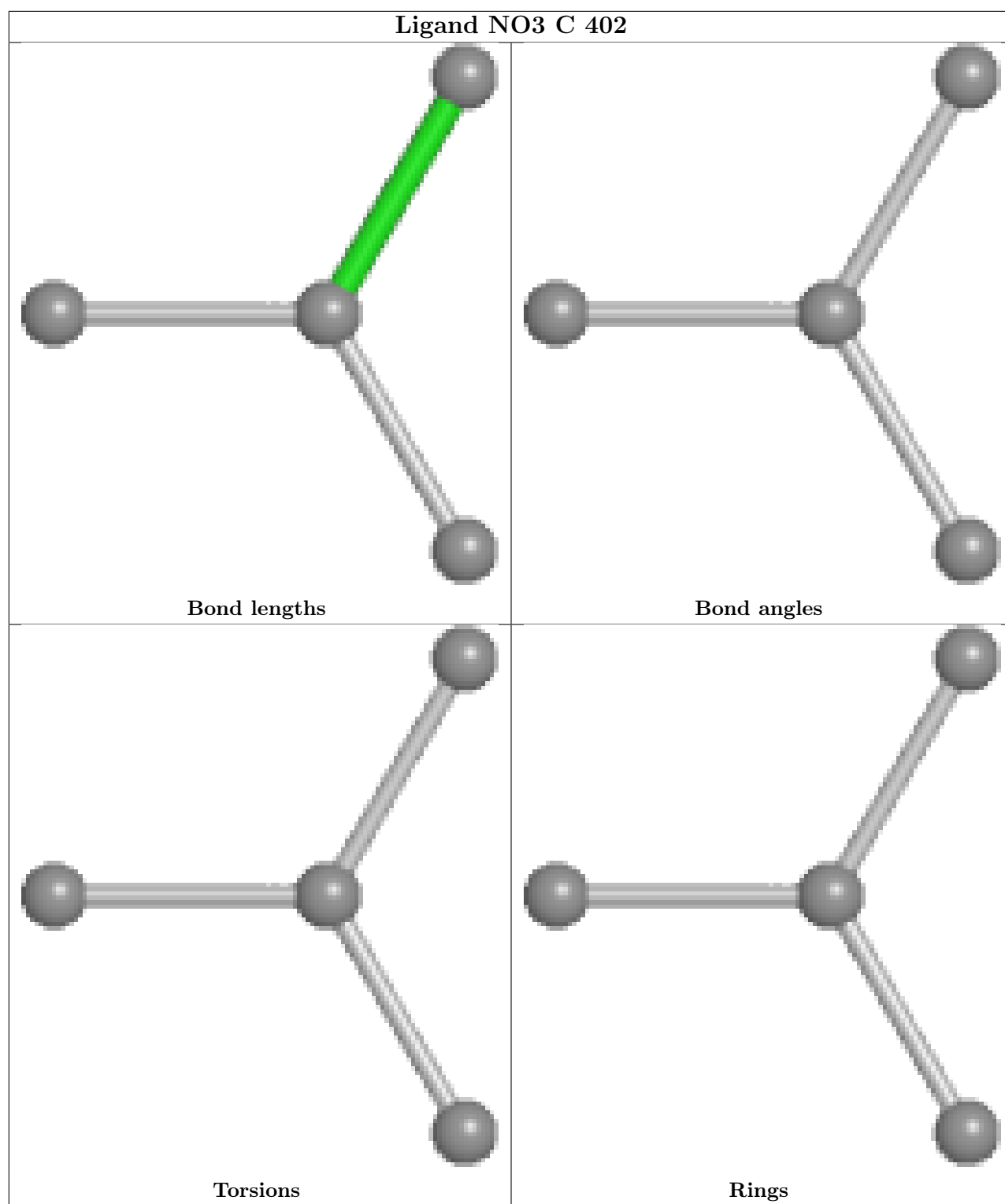












5.7 Other polymers [i](#)

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	342/357 (95%)	0.30	19 (5%) 30 27	37, 54, 84, 110	0
1	B	328/357 (91%)	0.44	19 (5%) 29 25	41, 57, 85, 95	0
1	C	325/357 (91%)	0.08	10 (3%) 51 48	34, 52, 80, 93	0
1	D	333/357 (93%)	0.41	19 (5%) 29 26	34, 58, 95, 110	0
All	All	1328/1428 (92%)	0.31	67 (5%) 34 31	34, 55, 85, 110	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	TRP	7.1
1	D	300	ALA	5.8
1	A	291	LEU	5.7
1	D	302	ALA	5.0
1	A	293	GLY	4.5
1	D	69	ALA	4.5
1	B	47	LEU	4.4
1	A	292	THR	4.4
1	A	294	PRO	4.1
1	A	299	MET	4.1
1	B	290	LEU	3.9
1	D	305	TRP	3.9
1	B	240	TYR	3.9
1	A	300	ALA	3.8
1	D	307	ASN	3.7
1	D	304	THR	3.6
1	C	47	LEU	3.5
1	D	303	ARG	3.4
1	A	46	PRO	3.4
1	B	390	GLU	3.4
1	A	305	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	292	THR	3.3
1	B	69	ALA	3.1
1	B	291	LEU	3.1
1	C	240	TYR	3.0
1	D	240	TYR	2.9
1	B	264	LEU	2.9
1	A	298	LEU	2.8
1	B	60	ASP	2.7
1	D	68	PRO	2.7
1	C	69	ALA	2.7
1	C	332	ASP	2.7
1	D	301	LEU	2.6
1	B	375	GLN	2.6
1	C	291	LEU	2.6
1	B	58	GLY	2.6
1	A	330	TYR	2.6
1	A	329	GLY	2.5
1	B	124	GLY	2.5
1	A	306	TRP	2.5
1	A	308	GLN	2.4
1	A	301	LEU	2.4
1	D	64	LEU	2.4
1	C	100	TYR	2.3
1	A	240	TYR	2.3
1	B	308	GLN	2.3
1	A	296	ARG	2.2
1	B	241	HIS	2.2
1	D	308	GLN	2.2
1	A	311	VAL	2.2
1	B	289	ASN	2.2
1	B	68	PRO	2.2
1	B	228	ALA	2.1
1	C	73	ALA	2.1
1	B	67	ARG	2.1
1	C	330	TYR	2.1
1	D	73	ALA	2.1
1	B	64	LEU	2.1
1	C	149	VAL	2.1
1	A	333	GLY	2.1
1	A	297	ASN	2.1
1	C	308	GLN	2.1
1	B	309	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	333	GLY	2.1
1	D	67	ARG	2.1
1	D	121	VAL	2.0
1	D	71	PRO	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](#)

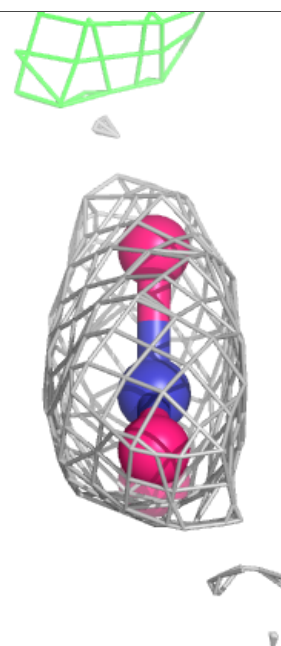
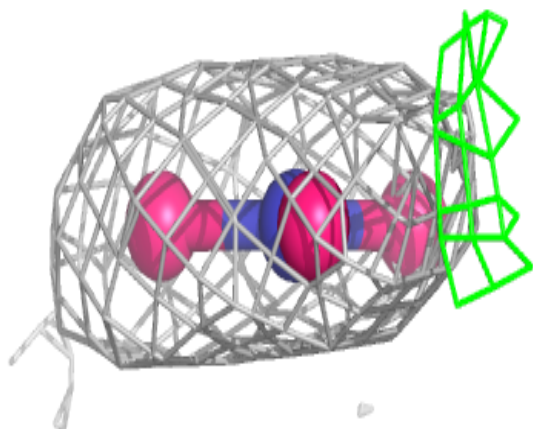
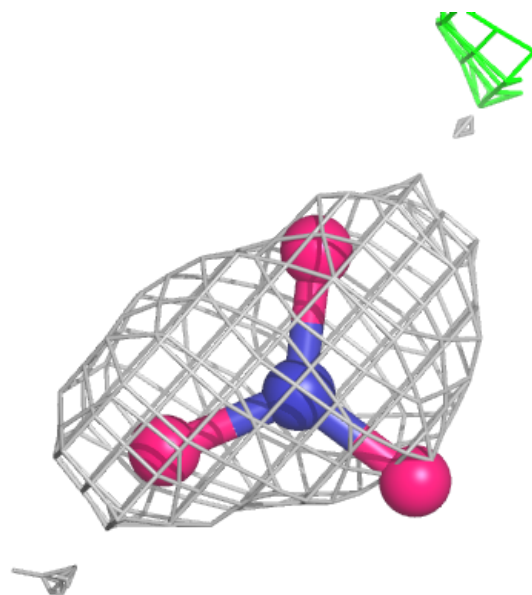
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NO3	D	402	4/4	0.76	0.20	112,113,113,113	0
2	NO3	B	401	4/4	0.77	0.19	104,105,105,106	0
2	NO3	B	402	4/4	0.86	0.14	96,96,96,97	0
2	NO3	D	401	4/4	0.87	0.17	73,75,76,76	0
2	NO3	C	402	4/4	0.88	0.11	99,100,100,100	0
2	NO3	A	401	4/4	0.89	0.13	74,77,77,79	0
2	NO3	A	402	4/4	0.91	0.18	63,63,64,66	0
2	NO3	C	401	4/4	0.94	0.17	60,63,64,64	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.

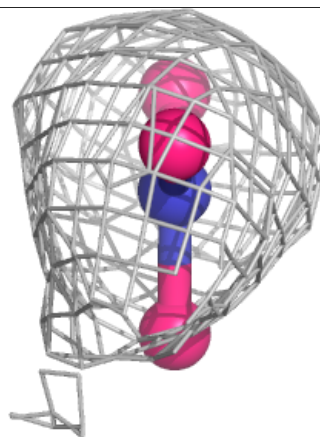
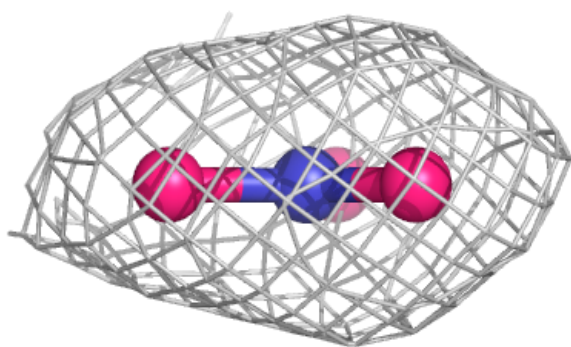
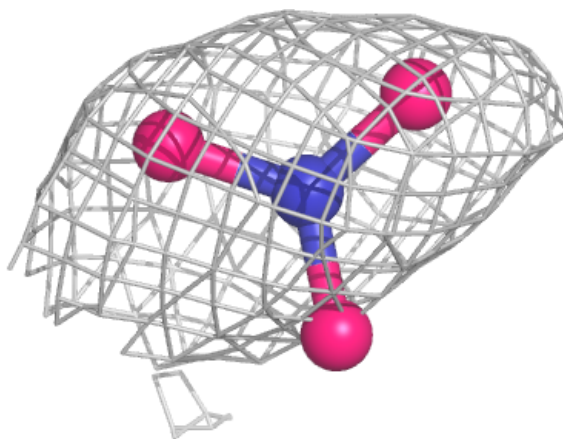
Electron density around NO3 D 402:

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



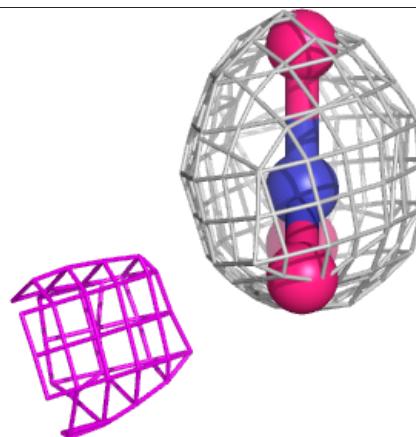
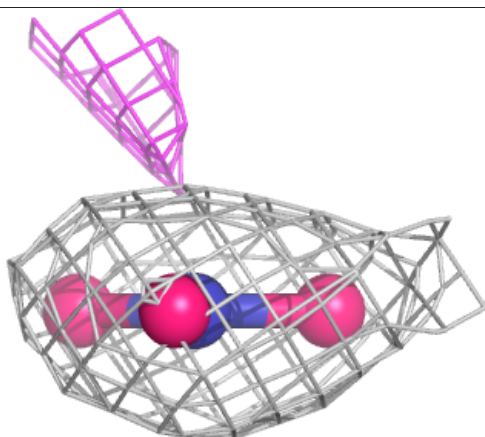
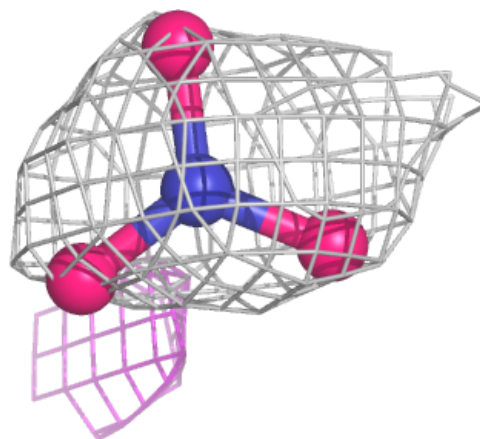
Electron density around NO3 B 401:

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



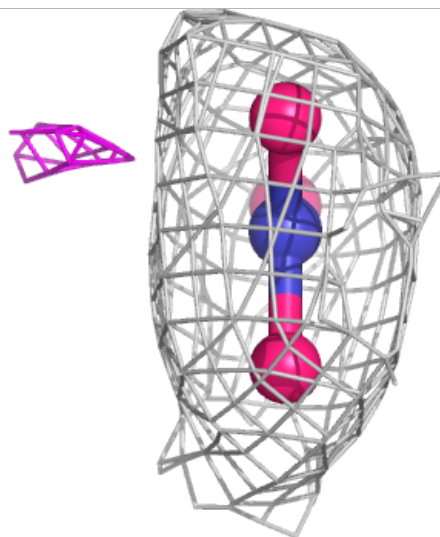
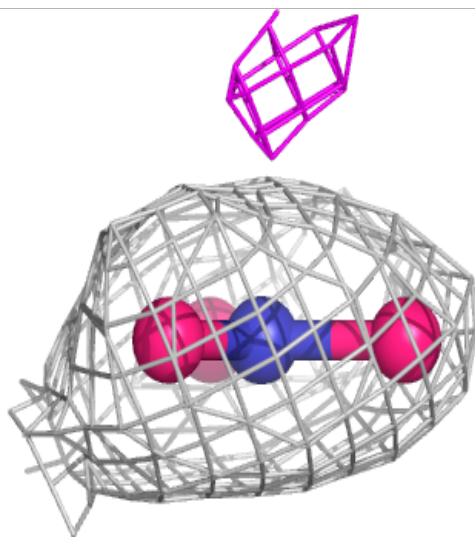
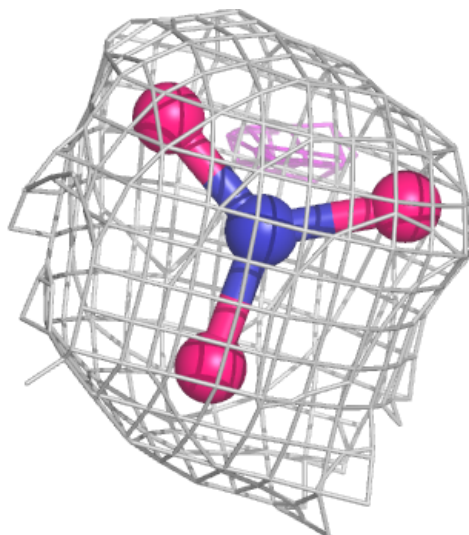
Electron density around NO3 B 402:

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



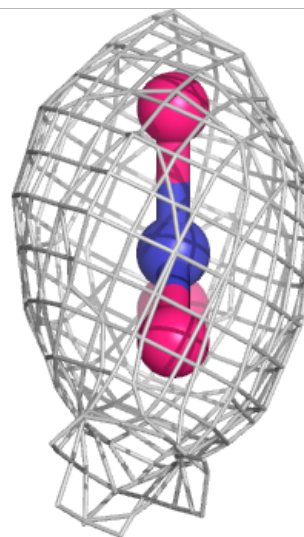
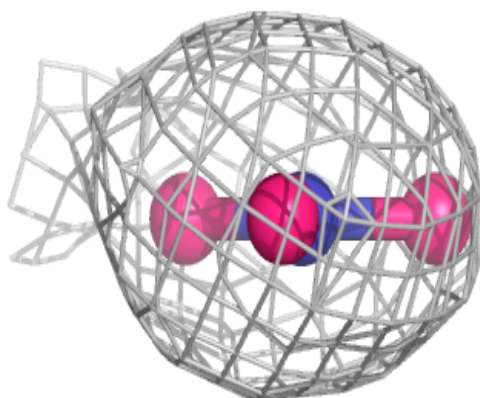
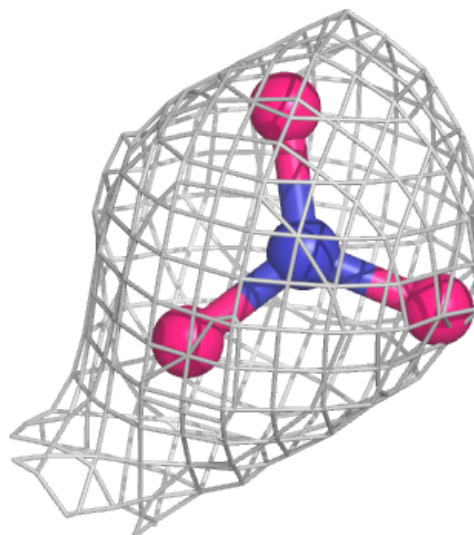
Electron density around NO3 D 401:

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



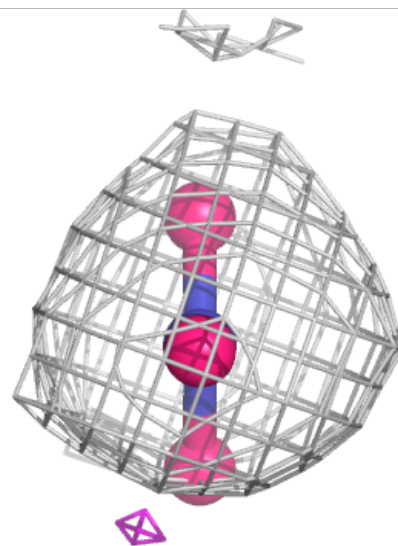
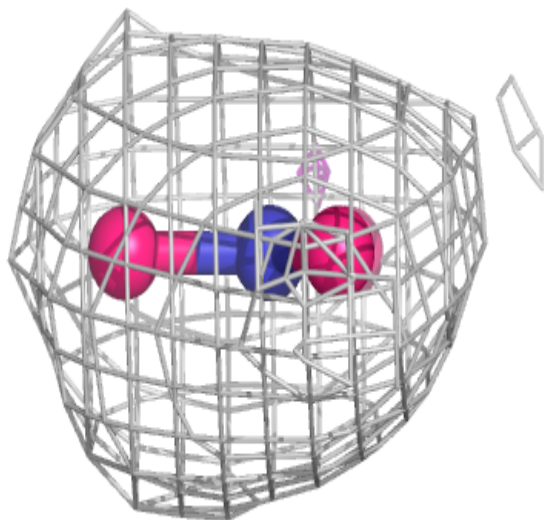
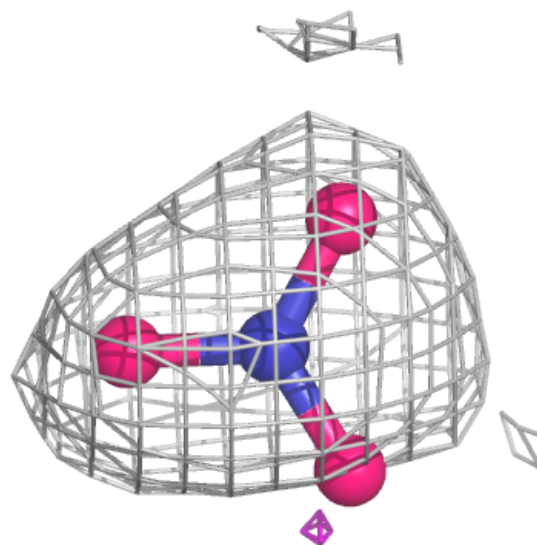
Electron density around NO3 C 402:

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



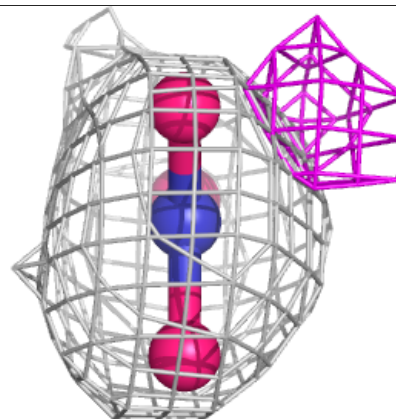
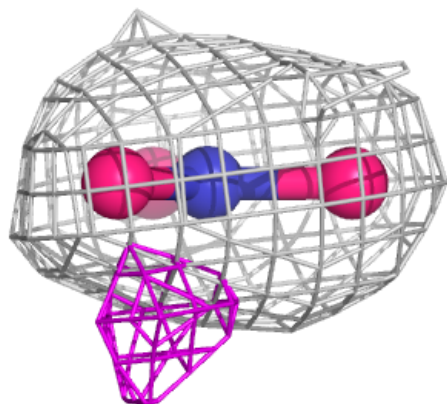
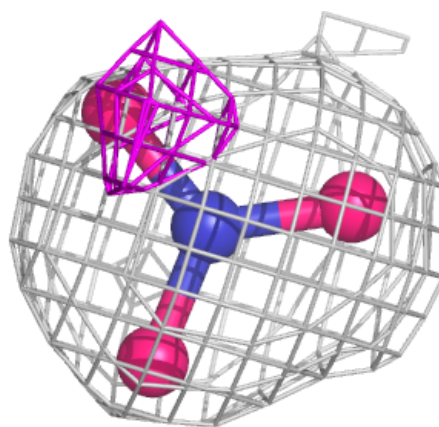
Electron density around NO3 A 401:

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



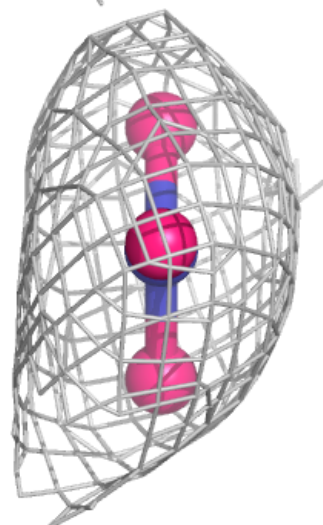
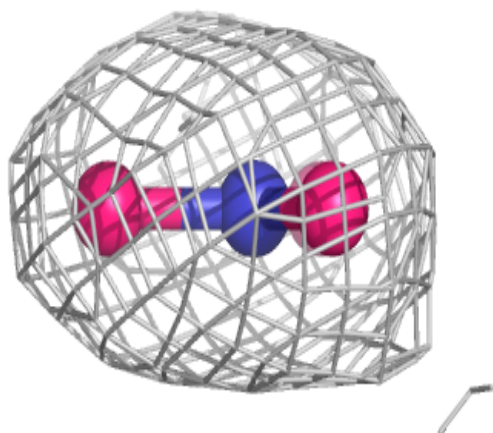
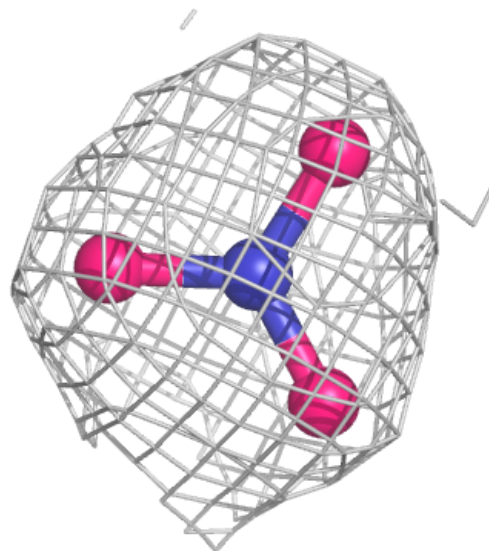
Electron density around NO3 A 402:

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



Electron density around NO3 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.