



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:40 PM UTC

PDB ID : 7A20 / pdb_00007a20
Title : Azobenzene-Based Inhibitors for Tryptophan Synthase
Authors : Rajendran, C.; Sterner, R.
Deposited on : 2020-08-14
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (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

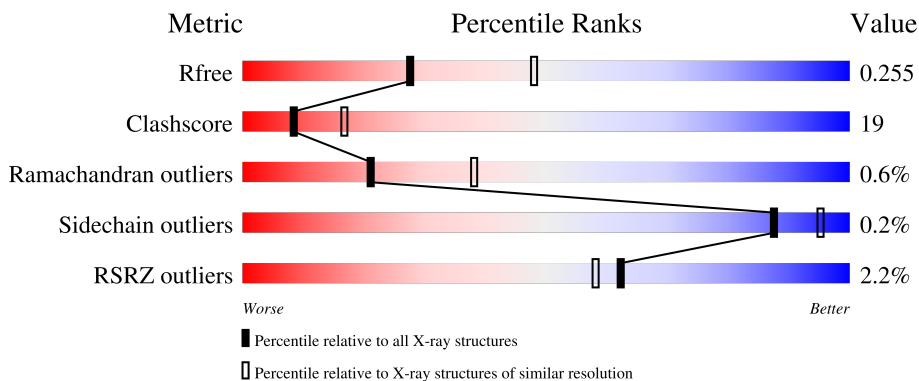
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	709	 23% 13% 64%
1	B	709	 39% 16% 45%
1	C	709	 22% 13% 65%
1	D	709	 42% 13% 44%

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	144	B	502	-	-	X	-
3	144	D	502	-	-	X	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9806 atoms, of which 12 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 Tryptophan synthase alpha chain, Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	Total 1919	C 1228	N 330	O 353	S 8	0	0	0
1	B	390	Total 2954	C 1858	N 517	O 560	S 19	0	0	0
1	C	249	Total 1876	C 1194	N 322	O 352	S 8	0	1	0
1	D	394	Total 2982	C 1872	N 526	O 565	S 19	0	1	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	SER	-	expression tag	UNP A0A0D6FWC1
A	-24	THR	-	expression tag	UNP A0A0D6FWC1
A	-23	THR	-	expression tag	UNP A0A0D6FWC1
A	-22	ARG	-	expression tag	UNP A0A0D6FWC1
A	-21	PRO	-	expression tag	UNP A0A0D6FWC1
A	-20	ALA	-	expression tag	UNP A0A0D6FWC1
A	-19	MET	-	expression tag	UNP A0A0D6FWC1
A	-18	GLY	-	expression tag	UNP A0A0D6FWC1
A	-17	SER	-	expression tag	UNP A0A0D6FWC1
A	-16	SER	-	expression tag	UNP A0A0D6FWC1
A	-15	HIS	-	expression tag	UNP A0A0D6FWC1
A	-14	HIS	-	expression tag	UNP A0A0D6FWC1
A	-13	HIS	-	expression tag	UNP A0A0D6FWC1
A	-12	HIS	-	expression tag	UNP A0A0D6FWC1
A	-11	HIS	-	expression tag	UNP A0A0D6FWC1
A	-10	HIS	-	expression tag	UNP A0A0D6FWC1
A	-9	SER	-	expression tag	UNP A0A0D6FWC1
A	-8	SER	-	expression tag	UNP A0A0D6FWC1
A	-7	GLY	-	expression tag	UNP A0A0D6FWC1
A	-6	LEU	-	expression tag	UNP A0A0D6FWC1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP A0A0D6FWC1
A	-4	PRO	-	expression tag	UNP A0A0D6FWC1
A	-3	ARG	-	expression tag	UNP A0A0D6FWC1
A	-2	GLY	-	expression tag	UNP A0A0D6FWC1
A	-1	SER	-	expression tag	UNP A0A0D6FWC1
A	0	HIS	-	expression tag	UNP A0A0D6FWC1
A	269	SER	-	linker	UNP A0A0D6FWC1
A	270	THR	-	linker	UNP A0A0D6FWC1
A	271	THR	-	linker	UNP A0A0D6FWC1
A	272	ARG	-	linker	UNP A0A0D6FWC1
A	273	PRO	-	linker	UNP A0A0D6FWC1
A	274	MET	-	linker	UNP A0A0D6FWC1
A	275	THR	-	linker	UNP A0A0D6FWC1
A	276	THR	-	linker	UNP A0A0D6FWC1
A	277	LEU	-	linker	UNP A0A0D6FWC1
A	671	LYS	-	expression tag	UNP A0A0F7J6T4
A	672	LEU	-	expression tag	UNP A0A0F7J6T4
A	673	ALA	-	expression tag	UNP A0A0F7J6T4
A	674	ALA	-	expression tag	UNP A0A0F7J6T4
A	675	ALA	-	expression tag	UNP A0A0F7J6T4
A	676	LEU	-	expression tag	UNP A0A0F7J6T4
A	677	GLU	-	expression tag	UNP A0A0F7J6T4
A	678	HIS	-	expression tag	UNP A0A0F7J6T4
A	679	HIS	-	expression tag	UNP A0A0F7J6T4
A	680	HIS	-	expression tag	UNP A0A0F7J6T4
A	681	HIS	-	expression tag	UNP A0A0F7J6T4
A	682	HIS	-	expression tag	UNP A0A0F7J6T4
A	683	HIS	-	expression tag	UNP A0A0F7J6T4
B	-298	SER	-	expression tag	UNP A0A0D6FWC1
B	-297	THR	-	expression tag	UNP A0A0D6FWC1
B	-296	THR	-	expression tag	UNP A0A0D6FWC1
B	-295	ARG	-	expression tag	UNP A0A0D6FWC1
B	-294	PRO	-	expression tag	UNP A0A0D6FWC1
B	-293	ALA	-	expression tag	UNP A0A0D6FWC1
B	-292	MET	-	expression tag	UNP A0A0D6FWC1
B	-291	GLY	-	expression tag	UNP A0A0D6FWC1
B	-290	SER	-	expression tag	UNP A0A0D6FWC1
B	-289	SER	-	expression tag	UNP A0A0D6FWC1
B	-288	HIS	-	expression tag	UNP A0A0D6FWC1
B	-287	HIS	-	expression tag	UNP A0A0D6FWC1
B	-286	HIS	-	expression tag	UNP A0A0D6FWC1
B	-285	HIS	-	expression tag	UNP A0A0D6FWC1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-284	HIS	-	expression tag	UNP A0A0D6FWC1
B	-283	HIS	-	expression tag	UNP A0A0D6FWC1
B	-282	SER	-	expression tag	UNP A0A0D6FWC1
B	-281	SER	-	expression tag	UNP A0A0D6FWC1
B	-280	GLY	-	expression tag	UNP A0A0D6FWC1
B	-279	LEU	-	expression tag	UNP A0A0D6FWC1
B	-278	VAL	-	expression tag	UNP A0A0D6FWC1
B	-277	PRO	-	expression tag	UNP A0A0D6FWC1
B	-276	ARG	-	expression tag	UNP A0A0D6FWC1
B	-275	GLY	-	expression tag	UNP A0A0D6FWC1
B	-274	SER	-	expression tag	UNP A0A0D6FWC1
B	-273	HIS	-	expression tag	UNP A0A0D6FWC1
B	-4	SER	-	linker	UNP A0A0D6FWC1
B	-3	THR	-	linker	UNP A0A0D6FWC1
B	-2	THR	-	linker	UNP A0A0D6FWC1
B	-1	ARG	-	linker	UNP A0A0D6FWC1
B	0	PRO	-	linker	UNP A0A0D6FWC1
B	1	MET	-	linker	UNP A0A0D6FWC1
B	2	THR	-	linker	UNP A0A0D6FWC1
B	3	THR	-	linker	UNP A0A0D6FWC1
B	4	LEU	-	linker	UNP A0A0D6FWC1
B	398	LYS	-	expression tag	UNP A0A0F7J6T4
B	399	LEU	-	expression tag	UNP A0A0F7J6T4
B	400	ALA	-	expression tag	UNP A0A0F7J6T4
B	401	ALA	-	expression tag	UNP A0A0F7J6T4
B	402	ALA	-	expression tag	UNP A0A0F7J6T4
B	403	LEU	-	expression tag	UNP A0A0F7J6T4
B	404	GLU	-	expression tag	UNP A0A0F7J6T4
B	405	HIS	-	expression tag	UNP A0A0F7J6T4
B	406	HIS	-	expression tag	UNP A0A0F7J6T4
B	407	HIS	-	expression tag	UNP A0A0F7J6T4
B	408	HIS	-	expression tag	UNP A0A0F7J6T4
B	409	HIS	-	expression tag	UNP A0A0F7J6T4
B	410	HIS	-	expression tag	UNP A0A0F7J6T4
C	-25	SER	-	expression tag	UNP A0A0D6FWC1
C	-24	THR	-	expression tag	UNP A0A0D6FWC1
C	-23	THR	-	expression tag	UNP A0A0D6FWC1
C	-22	ARG	-	expression tag	UNP A0A0D6FWC1
C	-21	PRO	-	expression tag	UNP A0A0D6FWC1
C	-20	ALA	-	expression tag	UNP A0A0D6FWC1
C	-19	MET	-	expression tag	UNP A0A0D6FWC1
C	-18	GLY	-	expression tag	UNP A0A0D6FWC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP A0A0D6FWC1
C	-16	SER	-	expression tag	UNP A0A0D6FWC1
C	-15	HIS	-	expression tag	UNP A0A0D6FWC1
C	-14	HIS	-	expression tag	UNP A0A0D6FWC1
C	-13	HIS	-	expression tag	UNP A0A0D6FWC1
C	-12	HIS	-	expression tag	UNP A0A0D6FWC1
C	-11	HIS	-	expression tag	UNP A0A0D6FWC1
C	-10	HIS	-	expression tag	UNP A0A0D6FWC1
C	-9	SER	-	expression tag	UNP A0A0D6FWC1
C	-8	SER	-	expression tag	UNP A0A0D6FWC1
C	-7	GLY	-	expression tag	UNP A0A0D6FWC1
C	-6	LEU	-	expression tag	UNP A0A0D6FWC1
C	-5	VAL	-	expression tag	UNP A0A0D6FWC1
C	-4	PRO	-	expression tag	UNP A0A0D6FWC1
C	-3	ARG	-	expression tag	UNP A0A0D6FWC1
C	-2	GLY	-	expression tag	UNP A0A0D6FWC1
C	-1	SER	-	expression tag	UNP A0A0D6FWC1
C	0	HIS	-	expression tag	UNP A0A0D6FWC1
C	269	SER	-	linker	UNP A0A0D6FWC1
C	270	THR	-	linker	UNP A0A0D6FWC1
C	271	THR	-	linker	UNP A0A0D6FWC1
C	272	ARG	-	linker	UNP A0A0D6FWC1
C	273	PRO	-	linker	UNP A0A0D6FWC1
C	274	MET	-	linker	UNP A0A0D6FWC1
C	275	THR	-	linker	UNP A0A0D6FWC1
C	276	THR	-	linker	UNP A0A0D6FWC1
C	277	LEU	-	linker	UNP A0A0D6FWC1
C	671	LYS	-	expression tag	UNP A0A0F7J6T4
C	672	LEU	-	expression tag	UNP A0A0F7J6T4
C	673	ALA	-	expression tag	UNP A0A0F7J6T4
C	674	ALA	-	expression tag	UNP A0A0F7J6T4
C	675	ALA	-	expression tag	UNP A0A0F7J6T4
C	676	LEU	-	expression tag	UNP A0A0F7J6T4
C	677	GLU	-	expression tag	UNP A0A0F7J6T4
C	678	HIS	-	expression tag	UNP A0A0F7J6T4
C	679	HIS	-	expression tag	UNP A0A0F7J6T4
C	680	HIS	-	expression tag	UNP A0A0F7J6T4
C	681	HIS	-	expression tag	UNP A0A0F7J6T4
C	682	HIS	-	expression tag	UNP A0A0F7J6T4
C	683	HIS	-	expression tag	UNP A0A0F7J6T4
D	-298	SER	-	expression tag	UNP A0A0D6FWC1
D	-297	THR	-	expression tag	UNP A0A0D6FWC1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-296	THR	-	expression tag	UNP A0A0D6FWC1
D	-295	ARG	-	expression tag	UNP A0A0D6FWC1
D	-294	PRO	-	expression tag	UNP A0A0D6FWC1
D	-293	ALA	-	expression tag	UNP A0A0D6FWC1
D	-292	MET	-	expression tag	UNP A0A0D6FWC1
D	-291	GLY	-	expression tag	UNP A0A0D6FWC1
D	-290	SER	-	expression tag	UNP A0A0D6FWC1
D	-289	SER	-	expression tag	UNP A0A0D6FWC1
D	-288	HIS	-	expression tag	UNP A0A0D6FWC1
D	-287	HIS	-	expression tag	UNP A0A0D6FWC1
D	-286	HIS	-	expression tag	UNP A0A0D6FWC1
D	-285	HIS	-	expression tag	UNP A0A0D6FWC1
D	-284	HIS	-	expression tag	UNP A0A0D6FWC1
D	-283	HIS	-	expression tag	UNP A0A0D6FWC1
D	-282	SER	-	expression tag	UNP A0A0D6FWC1
D	-281	SER	-	expression tag	UNP A0A0D6FWC1
D	-280	GLY	-	expression tag	UNP A0A0D6FWC1
D	-279	LEU	-	expression tag	UNP A0A0D6FWC1
D	-278	VAL	-	expression tag	UNP A0A0D6FWC1
D	-277	PRO	-	expression tag	UNP A0A0D6FWC1
D	-276	ARG	-	expression tag	UNP A0A0D6FWC1
D	-275	GLY	-	expression tag	UNP A0A0D6FWC1
D	-274	SER	-	expression tag	UNP A0A0D6FWC1
D	-273	HIS	-	expression tag	UNP A0A0D6FWC1
D	-4	SER	-	linker	UNP A0A0D6FWC1
D	-3	THR	-	linker	UNP A0A0D6FWC1
D	-2	THR	-	linker	UNP A0A0D6FWC1
D	-1	ARG	-	linker	UNP A0A0D6FWC1
D	0	PRO	-	linker	UNP A0A0D6FWC1
D	1	MET	-	linker	UNP A0A0D6FWC1
D	2	THR	-	linker	UNP A0A0D6FWC1
D	3	THR	-	linker	UNP A0A0D6FWC1
D	4	LEU	-	linker	UNP A0A0D6FWC1
D	398	LYS	-	expression tag	UNP A0A0F7J6T4
D	399	LEU	-	expression tag	UNP A0A0F7J6T4
D	400	ALA	-	expression tag	UNP A0A0F7J6T4
D	401	ALA	-	expression tag	UNP A0A0F7J6T4
D	402	ALA	-	expression tag	UNP A0A0F7J6T4
D	403	LEU	-	expression tag	UNP A0A0F7J6T4
D	404	GLU	-	expression tag	UNP A0A0F7J6T4
D	405	HIS	-	expression tag	UNP A0A0F7J6T4
D	406	HIS	-	expression tag	UNP A0A0F7J6T4

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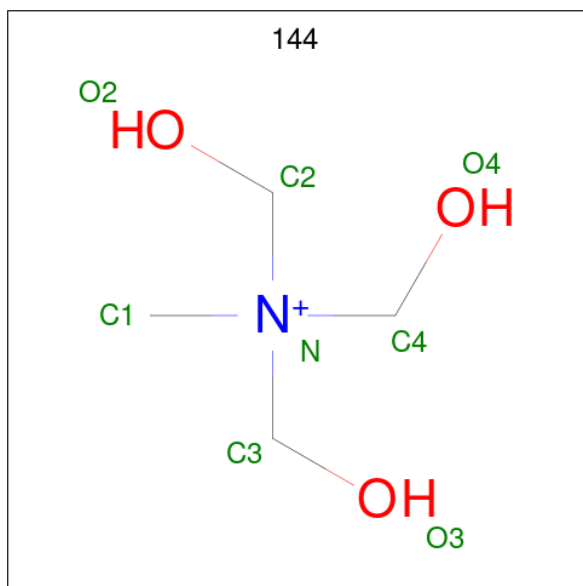
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Chain	Residue	Modelled	Actual	Comment	Reference
D	407	HIS	-	expression tag	UNP A0A0F7J6T4
D	408	HIS	-	expression tag	UNP A0A0F7J6T4
D	409	HIS	-	expression tag	UNP A0A0F7J6T4
D	410	HIS	-	expression tag	UNP A0A0F7J6T4

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (CCD ID: 144) (formula: C₄H₁₂NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 8 4 1 3	0	0
3	D	1	Total C H N O 20 4 12 1 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	15	Total 15	O 15	0	0
4	C	6	Total 6	O 6	0	0
4	D	14	Total 14	O 14	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.37Å 95.97Å 184.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 2.50 47.10 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.10-2.50) 99.7 (47.10-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.190 , 0.250 0.197 , 0.255	Depositor DCC
R_{free} test set	2911 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtrriage
Anisotropy	0.496	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.005 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9806	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: NA, 144

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	0/1958	0.60	0/2663
1	B	0.43	0/3012	0.64	4/4069 (0.1%)
1	C	0.36	0/1912	0.55	0/2598
1	D	0.45	1/3040 (0.0%)	0.62	0/4108
All	All	0.42	1/9922 (0.0%)	0.61	4/13438 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	101	MET	CA-C	7.17	1.62	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	MET	CB-CG-SD	-7.16	91.21	112.70
1	B	152	MET	CA-C-N	5.32	131.83	121.41
1	B	152	MET	C-N-CA	5.32	131.83	121.41
1	B	153	GLY	N-CA-C	5.25	125.62	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	153	GLY	Peptide

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	1919	0	1928	81	0
1	B	2954	0	2931	104	2
1	C	1876	0	1869	94	0
1	D	2982	0	2944	84	2
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	B	8	0	12	14	0
3	D	8	12	12	10	0
4	A	10	0	0	2	0
4	B	15	0	0	2	0
4	C	6	0	0	5	0
4	D	14	0	0	2	0
All	All	9794	12	9696	371	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 19.

The worst 5 of 371 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)
3:B:502:144:N	3:B:502:144:C2	1.77	1.46
3:D:502:144:N	3:D:502:144:C2	1.86	1.37
1:B:137:LYS:HB2	1:B:164:ALA:HB3	1.33	1.08
1:C:140:ARG:HD3	1:C:169:TYR:HB3	1.42	1.00
1:C:40:LEU:HD23	1:C:259:VAL:HG21	1.49	0.95

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)
1:B:60:THR:OG1	1:D:51:ASN:O[3_544]	2.07	0.13
1:B:153:GLY:O	1:D:341:ARG:NH2[3_544]	2.15	0.05

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	252/709 (36%)	239 (95%)	10 (4%)	3 (1%)	10	20
1	B	388/709 (55%)	365 (94%)	21 (5%)	2 (0%)	24	43
1	C	246/709 (35%)	230 (94%)	16 (6%)	0	100	100
1	D	393/709 (55%)	366 (93%)	24 (6%)	3 (1%)	16	31
All	All	1279/2836 (45%)	1200 (94%)	71 (6%)	8 (1%)	21	38

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	SER
1	D	163	SER
1	A	15	ARG
1	A	59	ALA
1	B	153	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/556 (35%)	196 (100%)	0	100	100
1	B	306/556 (55%)	306 (100%)	0	100	100
1	C	192/556 (34%)	190 (99%)	2 (1%)	68	86
1	D	306/556 (55%)	305 (100%)	1 (0%)	86	94
All	All	1000/2224 (45%)	997 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	198[A]	GLU
1	C	198[B]	GLU
1	D	63	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	26	ASN
1	D	94	GLN
1	D	317	ASN
1	D	260	HIS
1	C	12	ASN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	144	B	502	-	1,7,7	0.38	0	3,9,9	2.86	2 (66%)
3	144	D	502	-	1,7,7	0.15	0	3,9,9	1.75	1 (33%)

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	144	B	502	-	-	0/0/9/9	-
3	144	D	502	-	-	0/0/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	144	C1-N-C2	-3.97	99.17	109.30
3	D	502	144	C1-N-C3	2.46	115.57	109.30
3	B	502	144	C1-N-C3	2.39	115.41	109.30

There are no chirality outliers.

There are no torsion outliers.

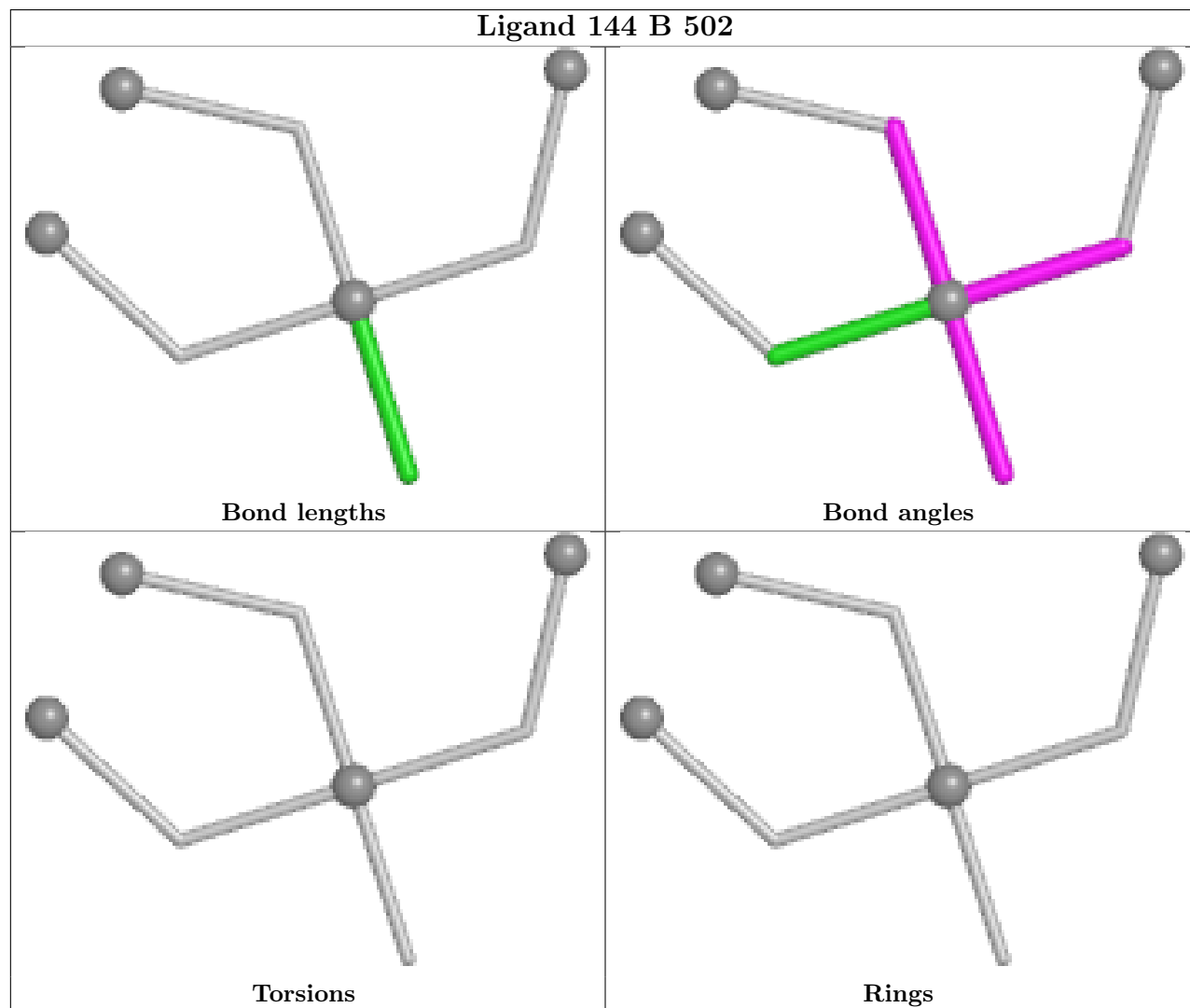
There are no ring outliers.

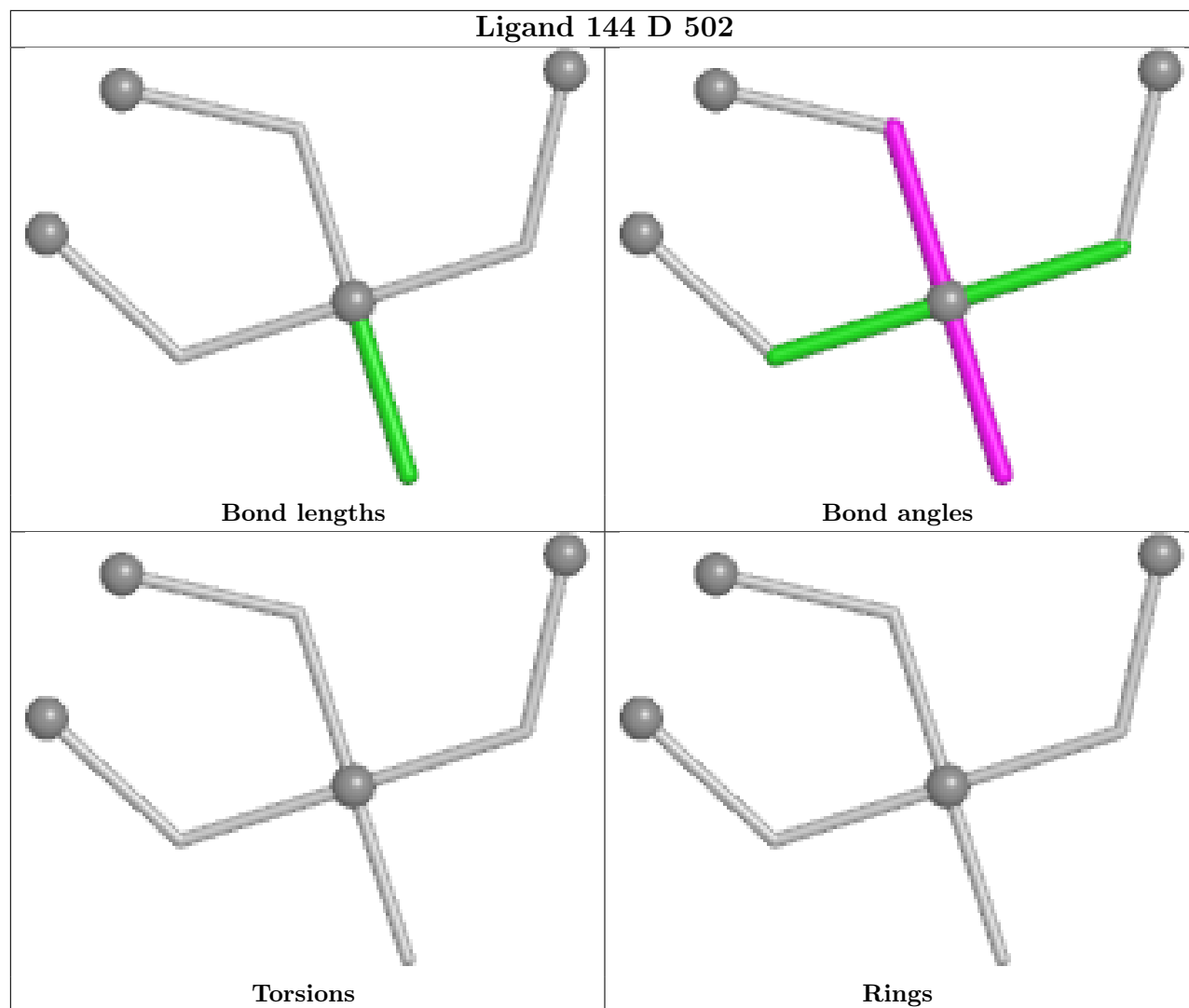
2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	144	14	0
3	D	502	144	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	256/709 (36%)	0.10	9 (3%) 47 42	44, 66, 91, 123	0
1	B	390/709 (55%)	0.04	5 (1%) 75 71	44, 59, 85, 109	0
1	C	249/709 (35%)	0.47	8 (3%) 50 46	41, 79, 98, 113	1 (0%)
1	D	394/709 (55%)	-0.05	7 (1%) 67 64	29, 59, 85, 105	1 (0%)
All	All	1289/2836 (45%)	0.11	29 (2%) 62 58	29, 64, 92, 123	2 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	197	ILE	5.4
1	A	268	ALA	4.7
1	C	198[A]	GLU	4.6
1	D	166	LEU	4.1
1	C	58	LEU	3.8

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](#)

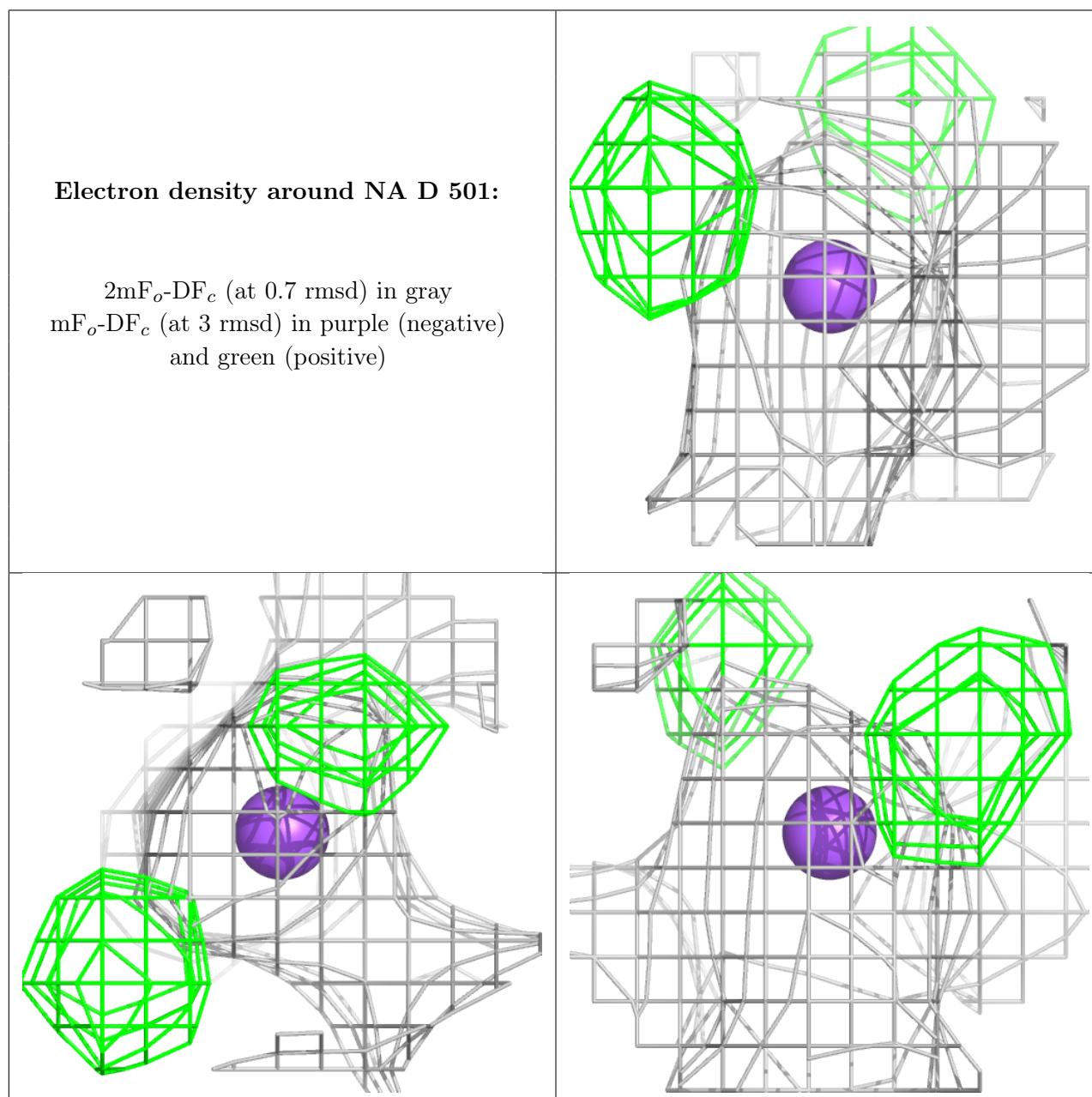
There are no oligosaccharides in this entry.

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.

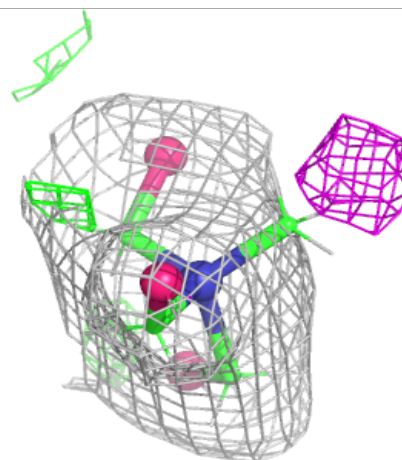
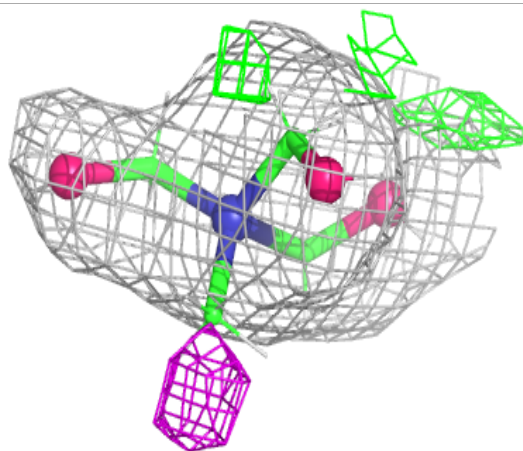
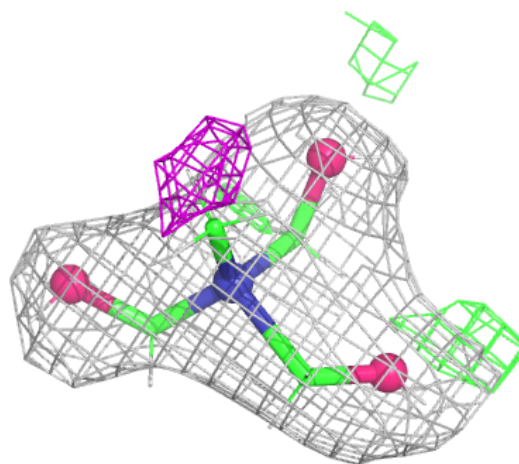
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	D	501	1/1	0.83	0.18	66,66,66,66	0
3	144	D	502	8/8	0.86	0.14	61,78,94,94	0
2	NA	B	501	1/1	0.87	0.18	65,65,65,65	0
3	144	B	502	8/8	0.89	0.12	57,62,67,67	0

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.



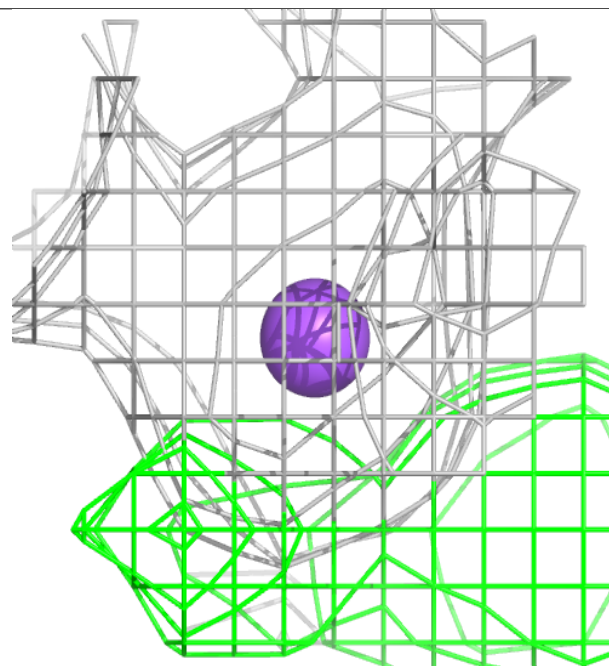
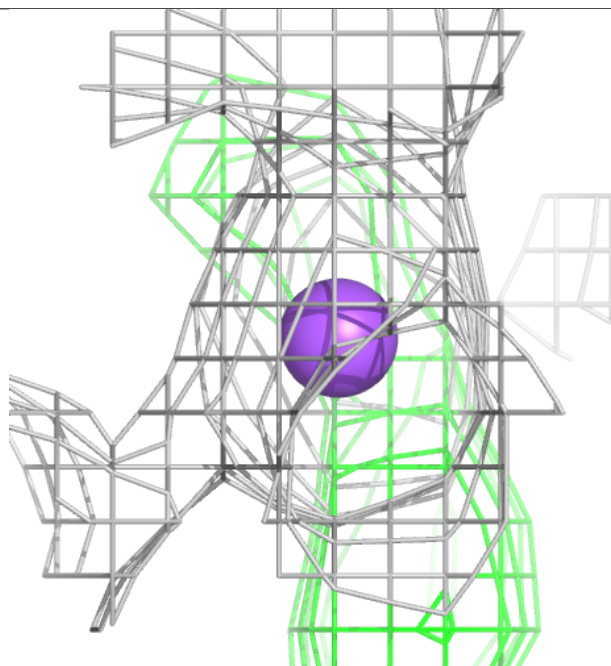
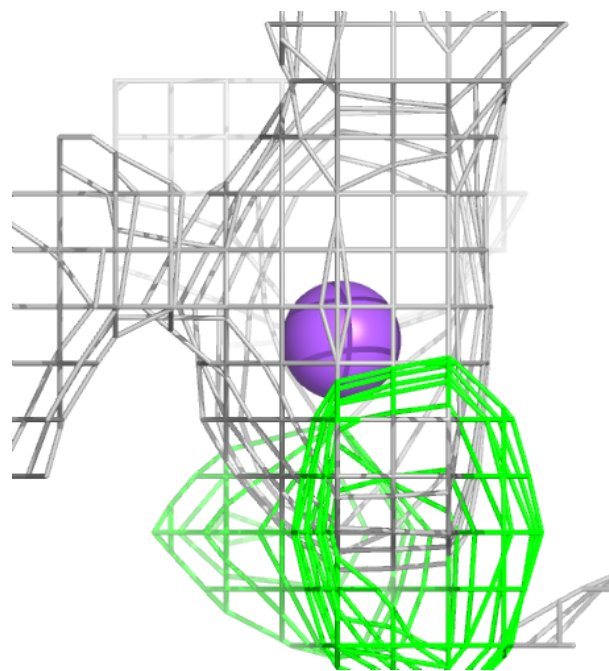
Electron density around 144 D 502:

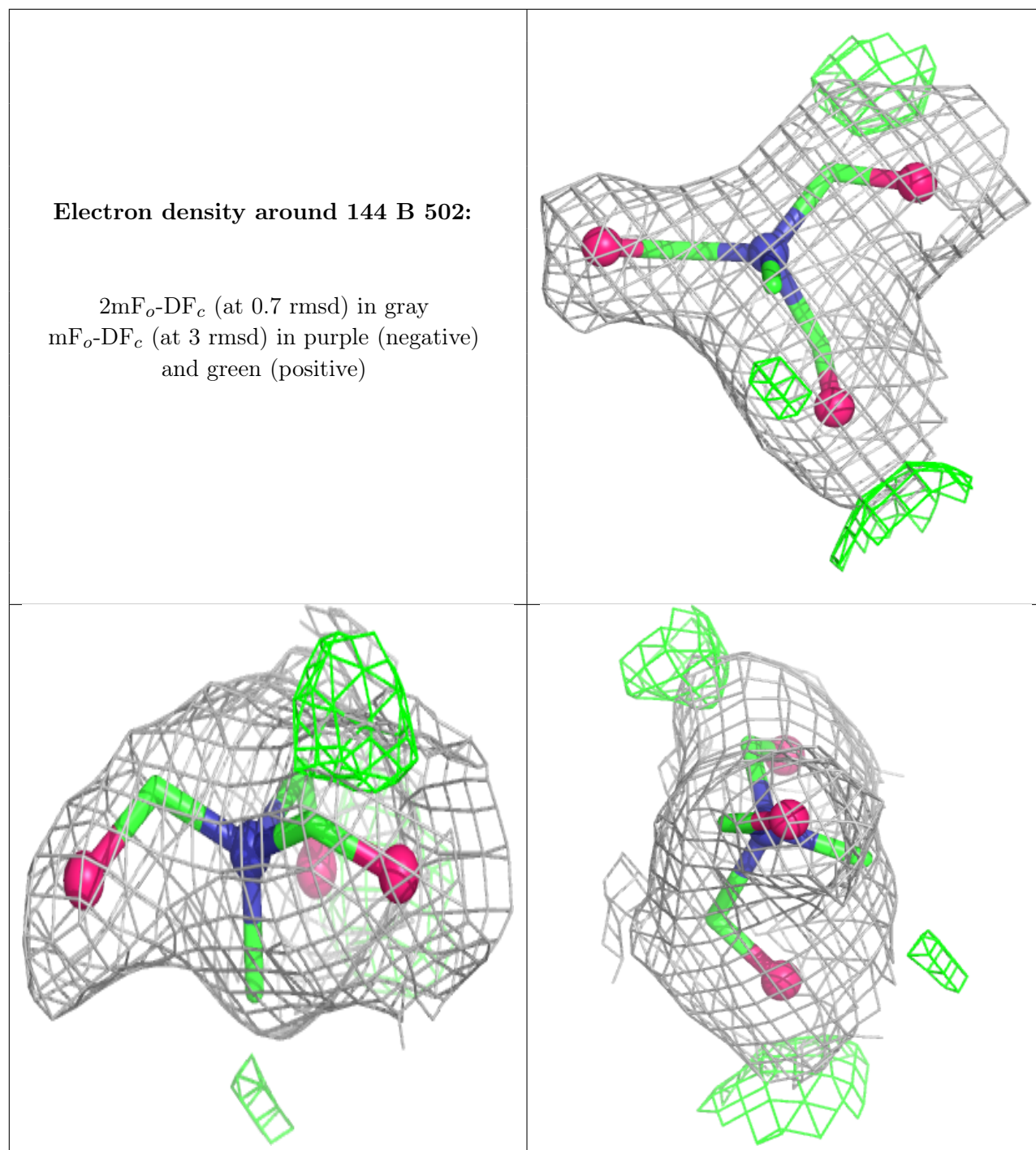
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NA B 501:

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





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.