



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:23 PM UTC

PDB ID : 6COE / pdb_00006coe
Title : AtHNL enantioselectivity mutant At-A9-H7 Apo Y13C,Y121L,P126F,L128W
,C131T,F179L,A209I with benzaldehyde, MANDELIC ACID NITRILE
Authors : Jones, B.J.; Kazlauskas, R.J.; Desrouleaux, R.
Deposited on : 2018-03-12
Resolution : 1.84 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

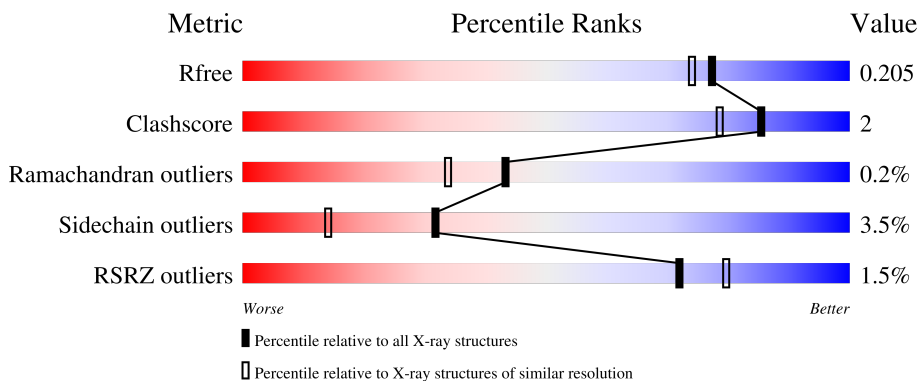
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


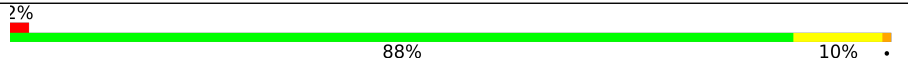
The reported resolution of this entry is 1.84 Å.

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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	260	 2% 85% 12% ..
1	B	260	 2% 88% 10% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4614 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 Alpha-hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	Total	C	N	O	S	0	3	0
			2077	1336	341	383	17			
1	B	259	Total	C	N	O	S	0	8	0
			2119	1359	349	394	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	TYR	engineered mutation	UNP Q9LFT6
A	122	LEU	TYR	engineered mutation	UNP Q9LFT6
A	126	PHE	PRO	engineered mutation	UNP Q9LFT6
A	129	TRP	LEU	engineered mutation	UNP Q9LFT6
A	132	THR	CYS	engineered mutation	UNP Q9LFT6
A	179	LEU	PHE	engineered mutation	UNP Q9LFT6
A	210	ILE	ALA	engineered mutation	UNP Q9LFT6
A	259	GLY	-	expression tag	UNP Q9LFT6
A	260	LEU	-	expression tag	UNP Q9LFT6
B	14	CYS	TYR	engineered mutation	UNP Q9LFT6
B	122	LEU	TYR	engineered mutation	UNP Q9LFT6
B	126	PHE	PRO	engineered mutation	UNP Q9LFT6
B	129	TRP	LEU	engineered mutation	UNP Q9LFT6
B	132	THR	CYS	engineered mutation	UNP Q9LFT6
B	179	LEU	PHE	engineered mutation	UNP Q9LFT6
B	210	ILE	ALA	engineered mutation	UNP Q9LFT6
B	259	GLY	-	expression tag	UNP Q9LFT6
B	260	LEU	-	expression tag	UNP Q9LFT6

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

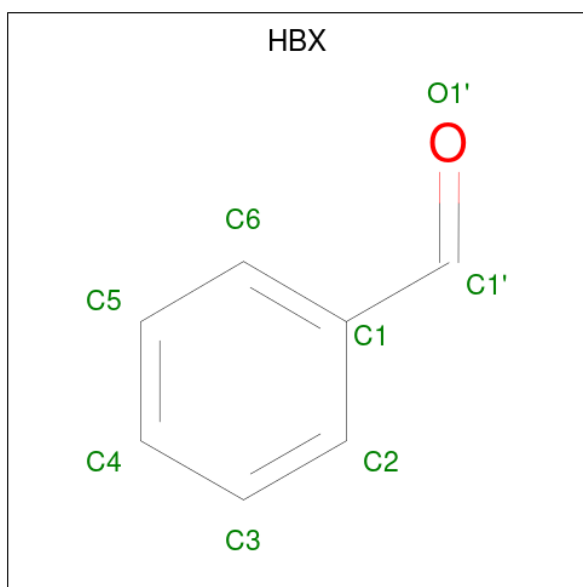


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

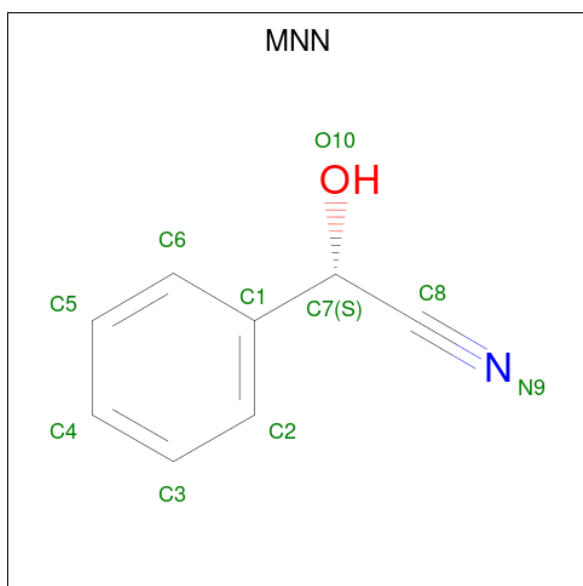
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is benzaldehyde (CCD ID: HBX) (formula: C₇H₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	7	1		
4	B	1	Total	C	O	0	0
			8	7	1		

- Molecule 5 is (S)-MANDELIC ACID NITRILE (CCD ID: MNN) (formula: C_8H_7NO) (labeled as "Ligand of Interest" by depositor).



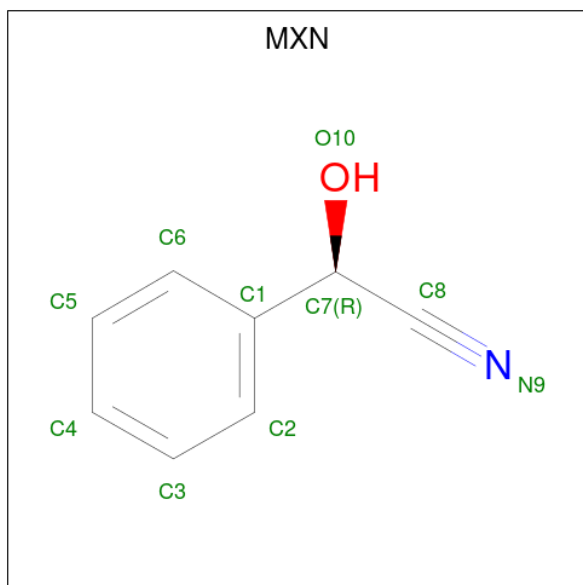
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	8	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	10	8	1	1	0	0

- Molecule 6 is (2R)-hydroxy(phenyl)ethanenitrile (CCD ID: MXN) (formula: C₈H₇NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	10	8	1	1	0	0
6	B	1	10	8	1	1	0	0

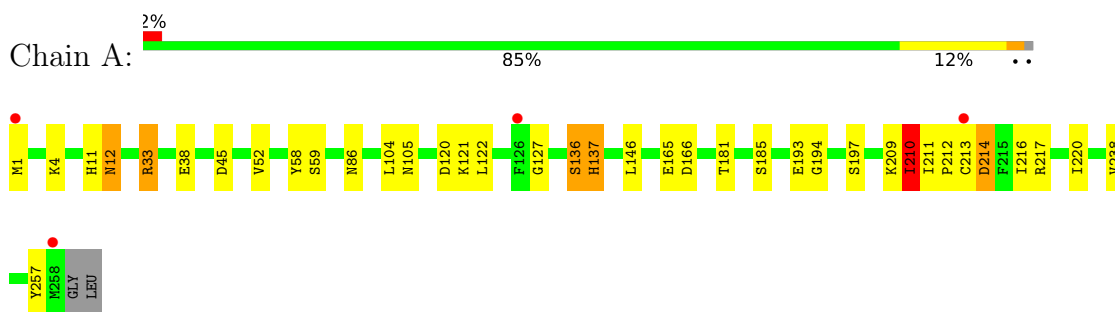
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	163	163	163	0	0
7	B	173	173	173	0	0

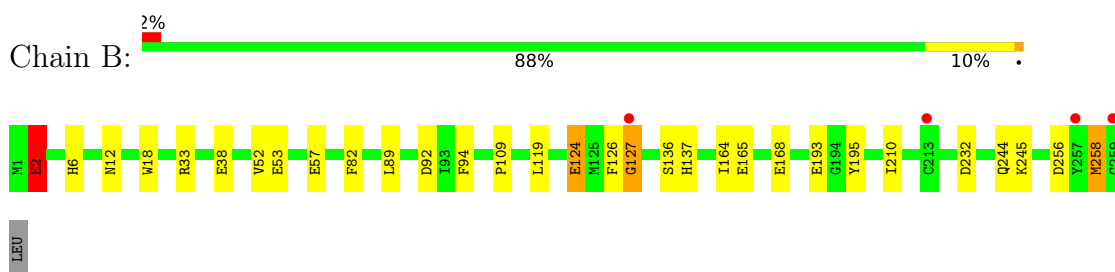
3 Residue-property plots [i](#)

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: Alpha-hydroxynitrile lyase



- Molecule 1: Alpha-hydroxynitrile lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.02Å 87.23Å 123.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.84 50.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-1.84) 95.5 (50.00-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.84Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.154 , 0.199 0.167 , 0.205	Depositor DCC
R_{free} test set	2245 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4614	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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: MNN, MXN, HBX, CL, GOL

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	1.70	19/2128 (0.9%)	1.36	12/2874 (0.4%)
1	B	1.66	12/2173 (0.6%)	1.34	4/2933 (0.1%)
All	All	1.68	31/4301 (0.7%)	1.35	16/5807 (0.3%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	SER	N-CA	9.10	1.57	1.46
1	A	194	GLY	N-CA	8.45	1.51	1.45
1	A	127	GLY	N-CA	7.22	1.55	1.45
1	B	164	ILE	N-CA	-7.04	1.37	1.46
1	B	168	GLU	CA-C	7.03	1.61	1.52
1	A	59	SER	C-O	-6.88	1.15	1.24
1	A	122	LEU	N-CA	-6.56	1.38	1.46
1	B	89	LEU	N-CA	-6.33	1.38	1.46
1	A	197	SER	CA-C	-6.32	1.44	1.52
1	B	109	PRO	CA-C	6.26	1.59	1.52
1	A	257	TYR	N-CA	6.06	1.53	1.46
1	A	12	ASN	N-CA	6.01	1.53	1.45
1	B	195	TYR	C-O	5.94	1.30	1.24
1	A	86	ASN	N-CA	-5.88	1.39	1.46
1	A	4	LYS	N-CA	5.79	1.52	1.45
1	A	33	ARG	CA-C	5.69	1.59	1.52
1	A	146	LEU	C-O	5.66	1.31	1.23
1	B	52	VAL	CA-CB	5.63	1.59	1.53
1	B	94	PHE	CA-CB	5.62	1.59	1.53
1	A	120	ASP	C-O	-5.61	1.17	1.24
1	B	2	GLU	CA-C	5.58	1.59	1.52
1	A	136	SER	CA-C	-5.45	1.46	1.52
1	A	137	HIS	CA-C	-5.42	1.46	1.52
1	B	165	GLU	N-CA	5.35	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	SER	N-CA	5.33	1.52	1.46
1	A	11	HIS	C-O	5.30	1.31	1.23
1	B	89	LEU	CA-C	-5.18	1.46	1.52
1	A	238	VAL	CA-CB	5.16	1.61	1.54
1	B	137	HIS	N-CA	-5.14	1.40	1.46
1	A	181	THR	C-O	-5.01	1.18	1.24
1	A	58	TYR	C-O	5.00	1.29	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ILE	CB-CA-C	-10.14	101.80	111.44
1	B	256	ASP	N-CA-C	7.93	122.05	112.38
1	A	52	VAL	CB-CA-C	-7.79	102.55	111.59
1	A	194	GLY	N-CA-C	-7.23	103.63	110.21
1	A	210	ILE	N-CA-CB	-7.23	105.71	111.64
1	A	166	ASP	N-CA-C	6.26	118.11	111.28
1	B	124	GLU	CB-CA-C	-5.60	102.08	110.88
1	A	136	SER	CB-CA-C	-5.56	98.87	109.66
1	A	209	LYS	CA-C-N	5.55	129.04	123.16
1	A	209	LYS	C-N-CA	5.55	129.04	123.16
1	A	45	ASP	CA-C-O	5.37	125.23	120.02
1	A	209	LYS	N-CA-C	5.34	119.43	113.02
1	A	165	GLU	N-CA-C	-5.28	105.53	111.28
1	A	194	GLY	O-C-N	5.28	124.80	121.85
1	B	18	TRP	N-CA-C	5.27	118.49	111.75
1	A	33	ARG	NE-CZ-NH2	5.16	123.84	119.20

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	2077	0	2059	8	0
1	B	2119	0	2093	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	18	0	24	0	0
2	B	6	0	8	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
4	A	8	0	6	0	0
4	B	8	0	6	0	0
5	A	10	0	4	0	0
5	B	10	0	4	0	0
6	A	10	0	4	0	0
6	B	10	0	4	2	0
7	A	163	0	0	1	0
7	B	173	0	0	2	0
All	All	4614	0	4212	19	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 2.

All (19) 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:33[B]:ARG:NH1	1:B:33[B]:ARG:HG3	1.51	1.09
1:B:33[B]:ARG:HH11	1:B:33[B]:ARG:CG	1.66	1.07
1:B:33[B]:ARG:HG3	1:B:33[B]:ARG:HH11	0.78	0.91
1:B:53:GLU:OE2	7:B:401:HOH:O	2.02	0.77
1:B:2:GLU:HG3	1:B:258:MET:HE1	1.79	0.64
1:B:6:HIS:CD2	1:B:33[B]:ARG:HD2	2.36	0.61
1:B:126:PHE:O	1:B:127:GLY:O	2.25	0.55
1:A:137:HIS:HE1	7:A:402:HOH:O	1.90	0.54
1:A:210:ILE:O	1:A:212:PRO:HD3	2.07	0.54
1:A:216:ILE:HG22	1:A:220:ILE:HD12	1.93	0.50
1:B:244:GLN:OE1	7:B:402:HOH:O	2.20	0.49
1:A:210:ILE:HG22	1:A:211:ILE:HG12	1.97	0.45
1:B:82:PHE:HB2	6:B:305:MXN:N9	2.34	0.42
1:B:12:ASN:HD22	6:B:305:MXN:H7	1.84	0.42
1:A:213[B]:CYS:SG	1:A:214:ASP:N	2.92	0.42
1:A:213[B]:CYS:SG	1:A:217:ARG:NH1	2.93	0.42
1:A:104:LEU:O	1:A:105:ASN:C	2.63	0.41
1:A:12:ASN:HB2	3:A:304:CL:CL	2.58	0.41
1:B:232:ASP:HB3	1:B:245:LYS:NZ	2.36	0.41

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	259/260 (100%)	253 (98%)	6 (2%)	0	100	100
1	B	265/260 (102%)	259 (98%)	5 (2%)	1 (0%)	30	18
All	All	524/520 (101%)	512 (98%)	11 (2%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	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	229/227 (101%)	221 (96%)	8 (4%)	32	14
1	B	234/227 (103%)	225 (96%)	9 (4%)	29	12
All	All	463/454 (102%)	446 (96%)	17 (4%)	32	13

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	33	ARG
1	A	38	GLU
1	A	121	LYS
1	A	136	SER

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Mol	Chain	Res	Type
1	A	193	GLU
1	A	210	ILE
1	A	214	ASP
1	B	2	GLU
1	B	38	GLU
1	B	57[A]	GLU
1	B	57[B]	GLU
1	B	92	ASP
1	B	119	LEU
1	B	124	GLU
1	B	193	GLU
1	B	258	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	199	GLN
1	B	5	HIS
1	B	137	HIS
1	B	141	ASN
1	B	199	GLN
1	B	224	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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
5	MNN	B	304	6	10,10,10	0.99	1 (10%)	11,12,12	0.99	0
6	MXN	A	307	5	10,10,10	1.08	1 (10%)	11,12,12	1.50	3 (27%)
6	MXN	B	305	5	10,10,10	1.13	1 (10%)	11,12,12	2.11	3 (27%)
2	GOL	A	301	-	5,5,5	0.96	0	5,5,5	1.00	0
4	HBX	A	305	-	8,8,8	0.94	0	9,9,9	1.15	0
2	GOL	B	301	-	5,5,5	0.76	0	5,5,5	0.97	0
4	HBX	B	303	-	8,8,8	0.67	0	9,9,9	0.83	0
5	MNN	A	306	6	10,10,10	0.93	1 (10%)	11,12,12	1.20	1 (9%)
2	GOL	A	303	-	5,5,5	0.77	0	5,5,5	0.43	0
2	GOL	A	302	-	5,5,5	0.72	0	5,5,5	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MNN	B	304	6	-	1/4/6/6	0/1/1/1
6	MXN	A	307	5	-	0/4/6/6	0/1/1/1
6	MXN	B	305	5	-	2/4/6/6	0/1/1/1
2	GOL	A	301	-	-	1/4/4/4	-
4	HBX	A	305	-	-	0/2/2/2	0/1/1/1
2	GOL	B	301	-	-	0/4/4/4	-
4	HBX	B	303	-	-	0/2/2/2	0/1/1/1
5	MNN	A	306	6	-	0/4/6/6	0/1/1/1
2	GOL	A	303	-	-	3/4/4/4	-
2	GOL	A	302	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	307	MXN	C1-C7	-3.20	1.47	1.51
6	B	305	MXN	C1-C7	-3.01	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	304	MNN	C1-C7	-2.58	1.48	1.51
5	A	306	MNN	C1-C7	-2.44	1.48	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	305	MXN	C1-C7-C8	-4.58	104.72	111.91
6	B	305	MXN	C6-C1-C2	3.07	122.11	118.30
6	B	305	MXN	O10-C7-C1	2.76	114.69	110.12
6	A	307	MXN	C6-C1-C2	2.71	121.66	118.30
5	A	306	MNN	C1-C7-C8	-2.40	108.14	111.91
6	A	307	MXN	C1-C7-C8	-2.39	108.15	111.91
6	A	307	MXN	C5-C6-C1	-2.29	117.91	120.65

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	GOL	O1-C1-C2-C3
2	A	303	GOL	O1-C1-C2-C3
2	A	303	GOL	O2-C2-C3-O3
2	A	302	GOL	O1-C1-C2-O2
2	A	303	GOL	O1-C1-C2-O2
2	A	301	GOL	C1-C2-C3-O3
5	B	304	MNN	C6-C1-C7-C8
6	B	305	MXN	C2-C1-C7-C8
6	B	305	MXN	C6-C1-C7-C8

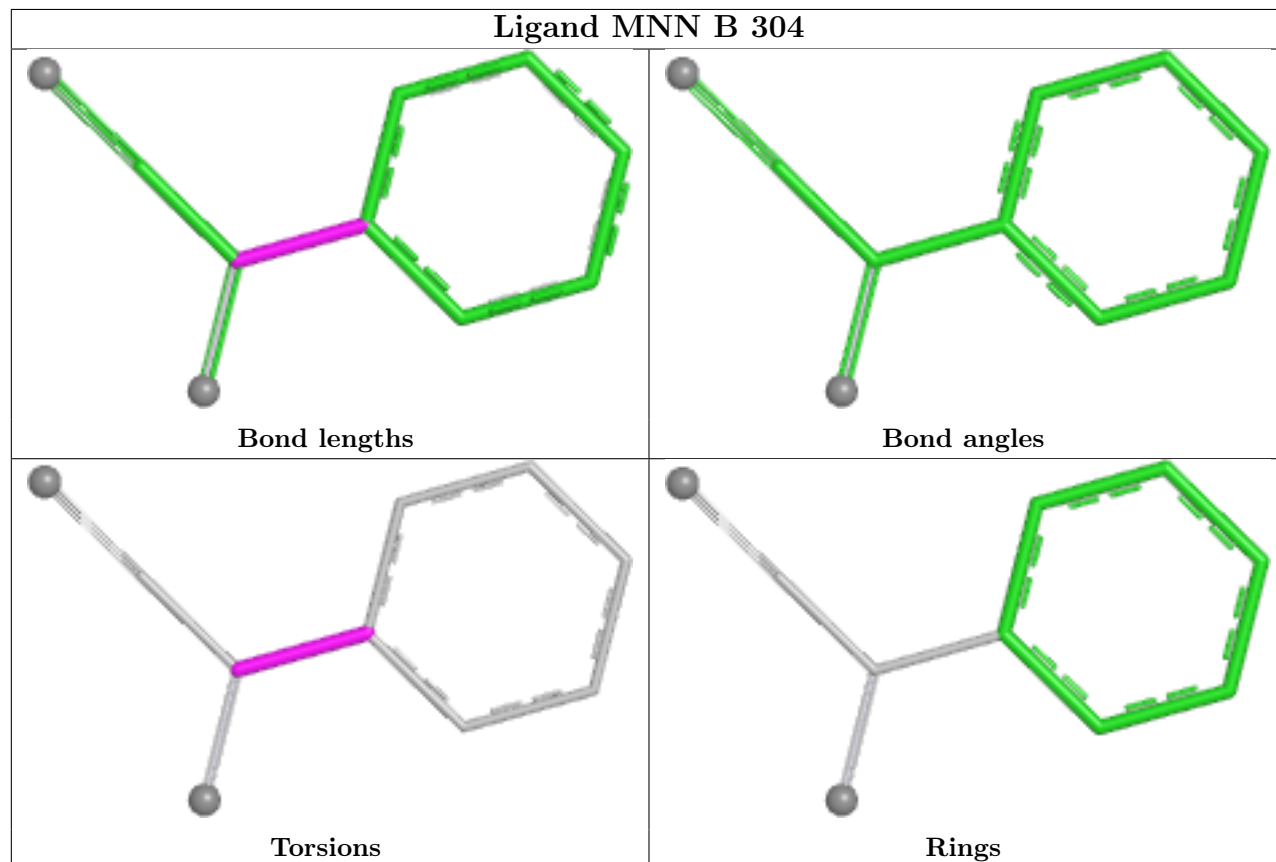
There are no ring outliers.

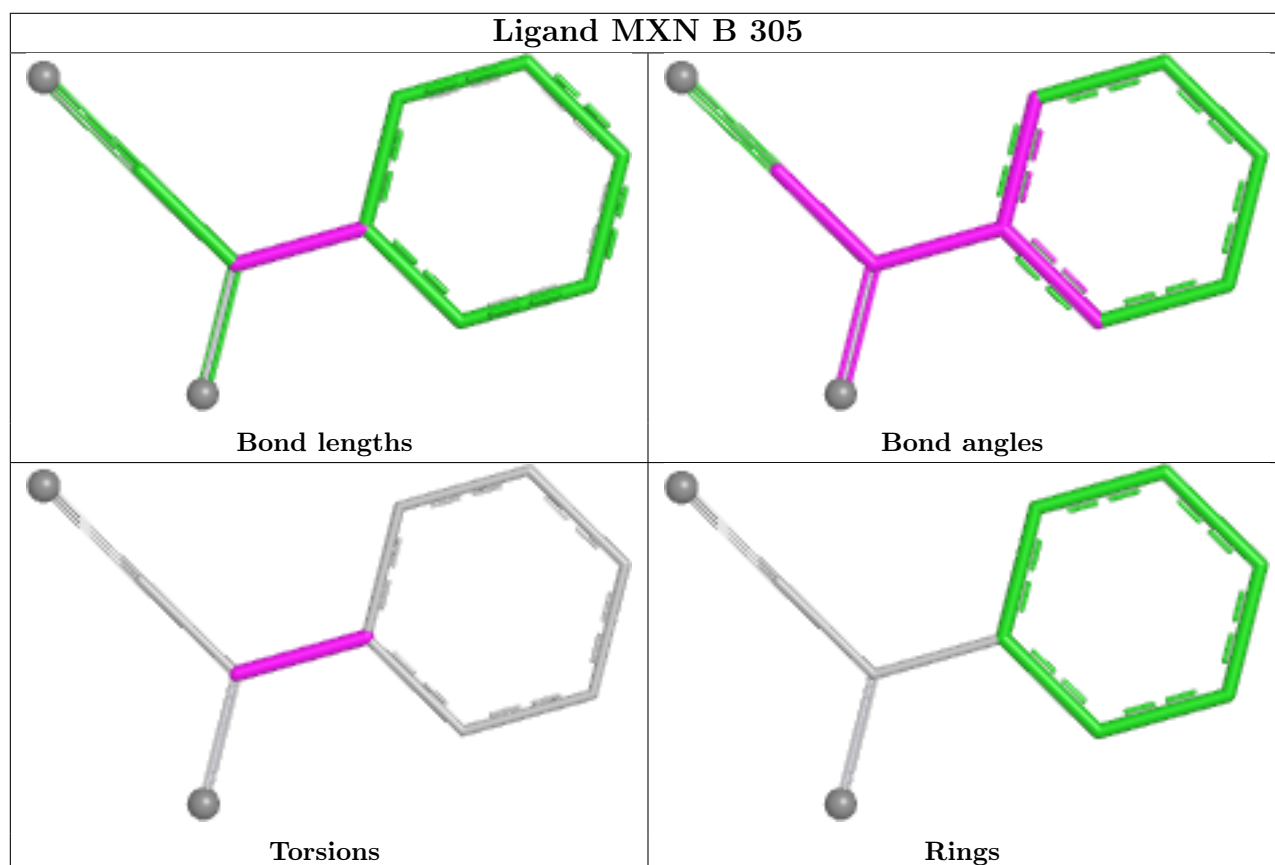
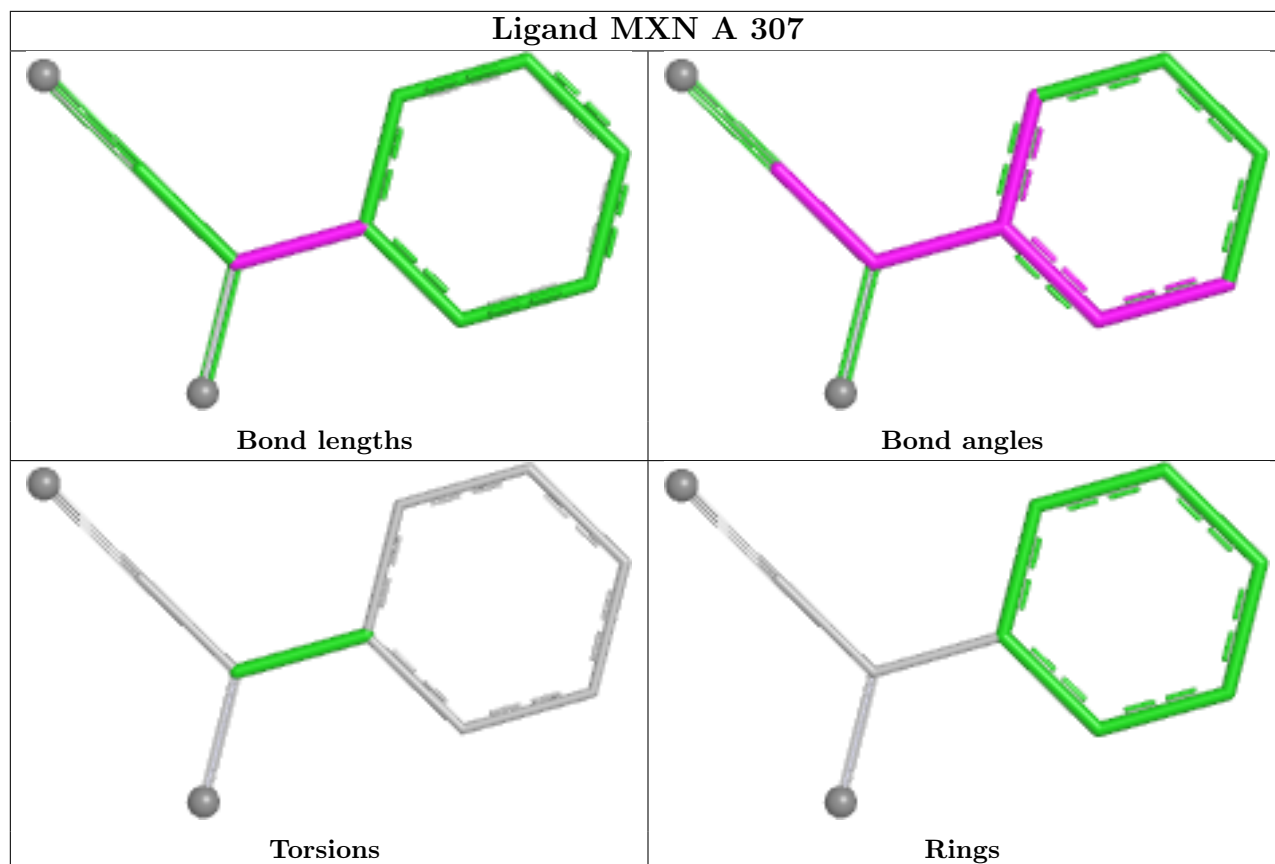
1 monomer is involved in 2 short contacts:

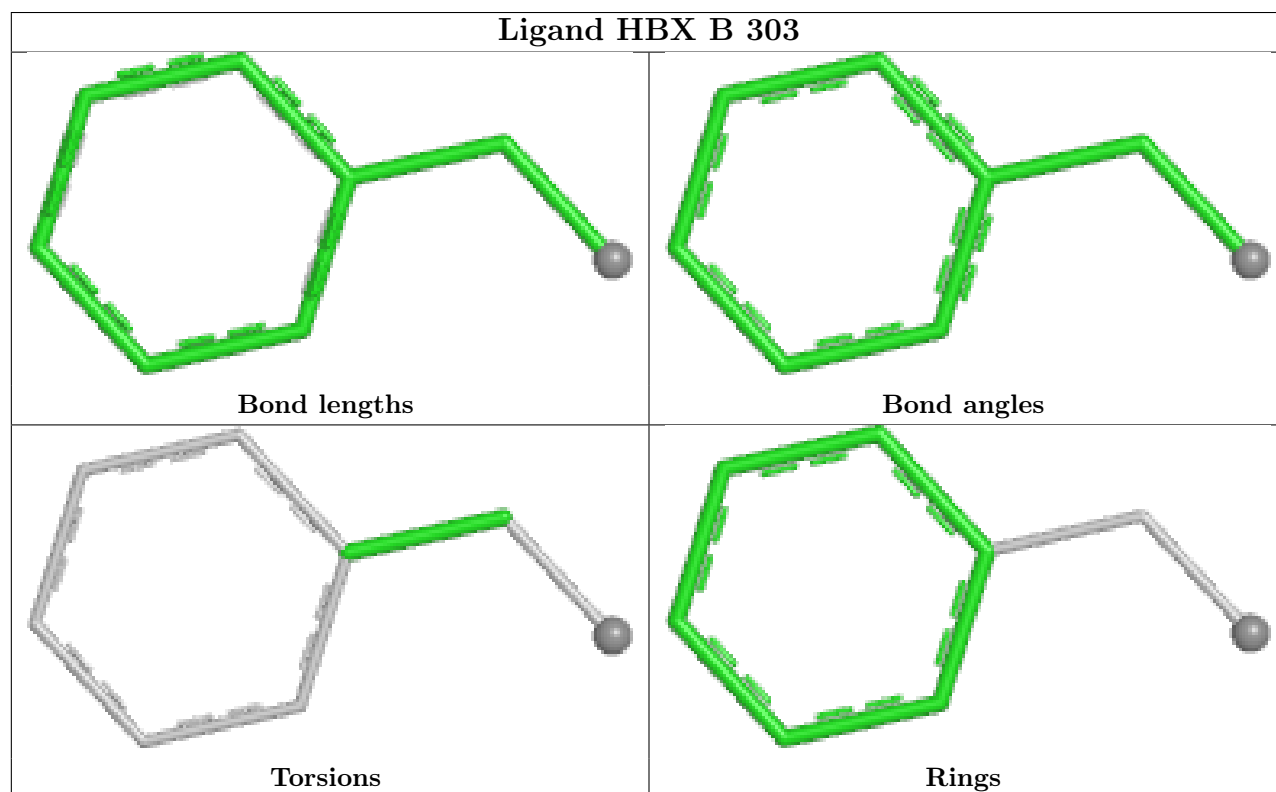
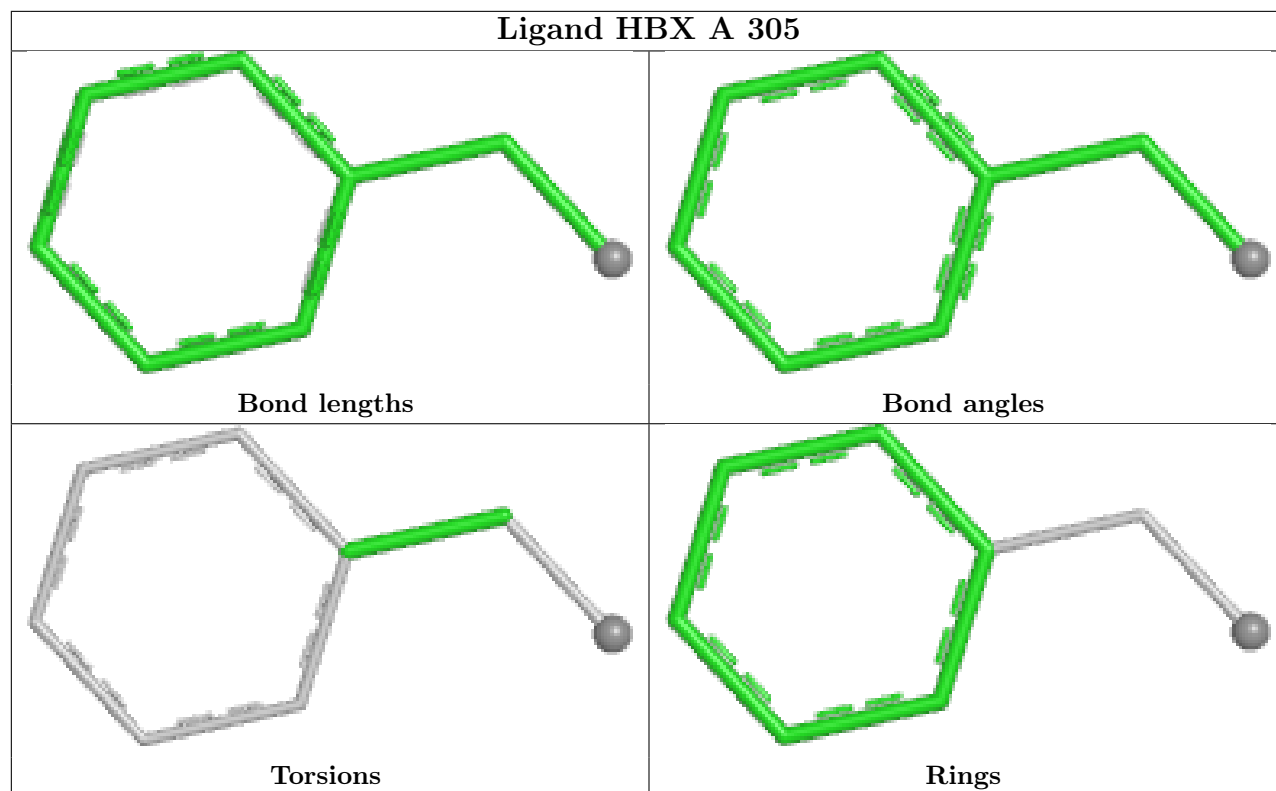
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	305	MXN	2	0

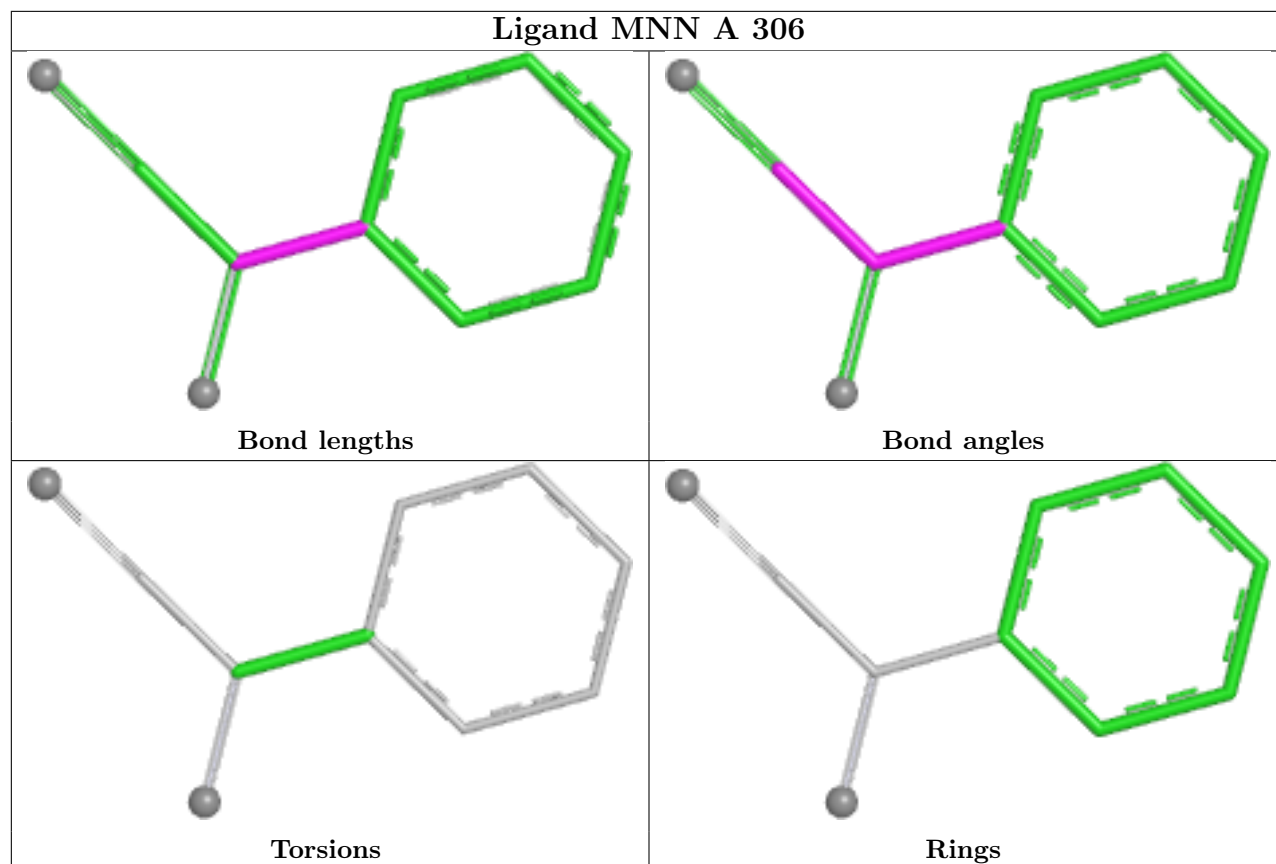
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	258/260 (99%)	-0.12	4 (1%) 70 78	10, 31, 51, 93	3 (1%)
1	B	259/260 (99%)	-0.31	4 (1%) 72 79	10, 26, 51, 89	8 (3%)
All	All	517/520 (99%)	-0.21	8 (1%) 72 79	10, 28, 51, 93	11 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	GLY	2.6
1	A	258	MET	2.6
1	A	126	PHE	2.5
1	B	257	TYR	2.4
1	B	259	GLY	2.4
1	A	1	MET	2.2
1	B	213[A]	CYS	2.1
1	A	213[A]	CYS	2.1

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,

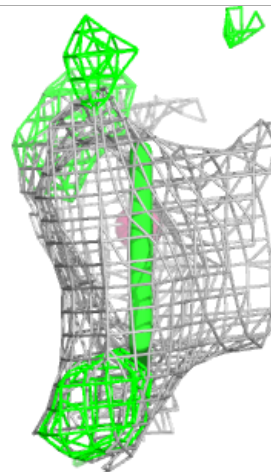
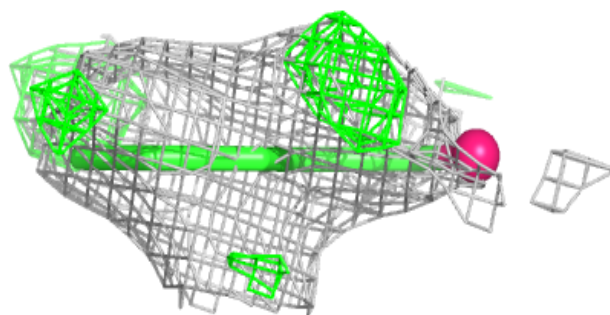
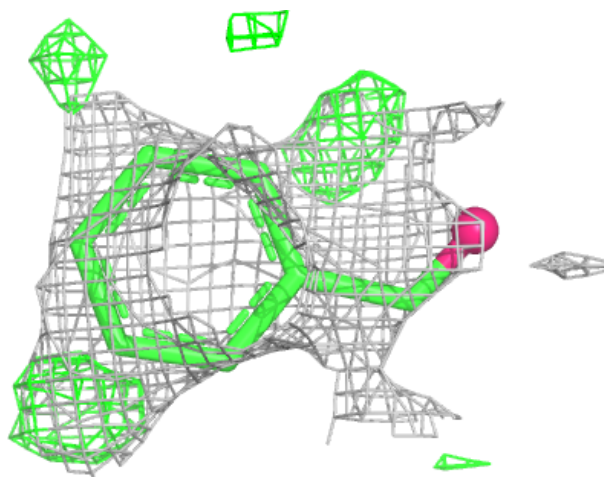
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	303	6/6	0.75	0.17	56,69,75,78	0
4	HBX	A	305	8/8	0.76	0.19	75,84,86,91	0
4	HBX	B	303	8/8	0.81	0.16	76,83,85,90	0
5	MNN	A	306	10/10	0.85	0.22	39,48,53,54	10
2	GOL	A	301	6/6	0.87	0.11	38,47,50,53	0
5	MNN	B	304	10/10	0.87	0.18	39,44,58,60	10
2	GOL	A	302	6/6	0.88	0.13	56,73,74,75	0
6	MXN	B	305	10/10	0.92	0.11	28,39,43,43	10
6	MXN	A	307	10/10	0.94	0.10	25,34,36,38	10
2	GOL	B	301	6/6	0.94	0.08	28,37,39,45	0
3	CL	A	304	1/1	0.99	0.02	23,23,23,23	1
3	CL	B	302	1/1	0.99	0.03	20,20,20,20	1

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.

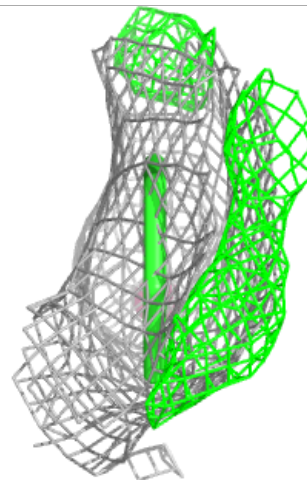
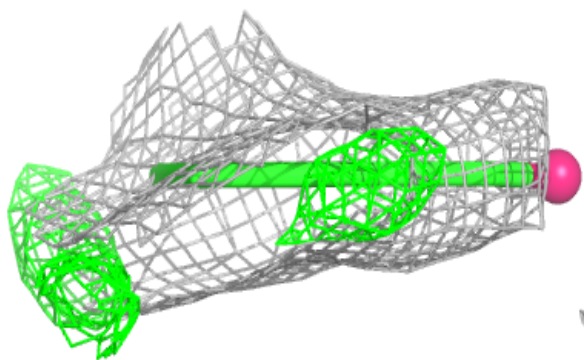
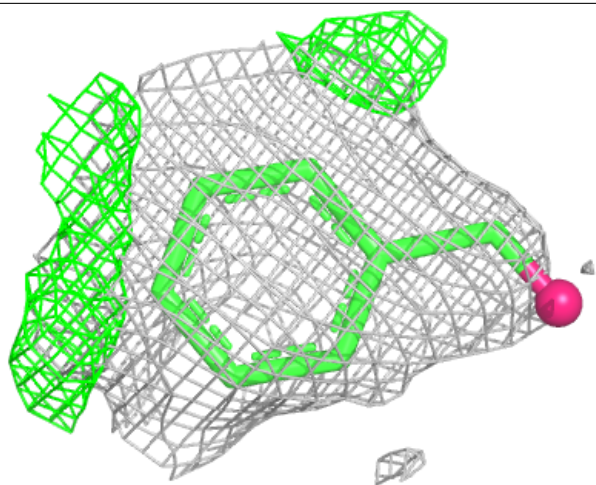
Electron density around HBX A 305:

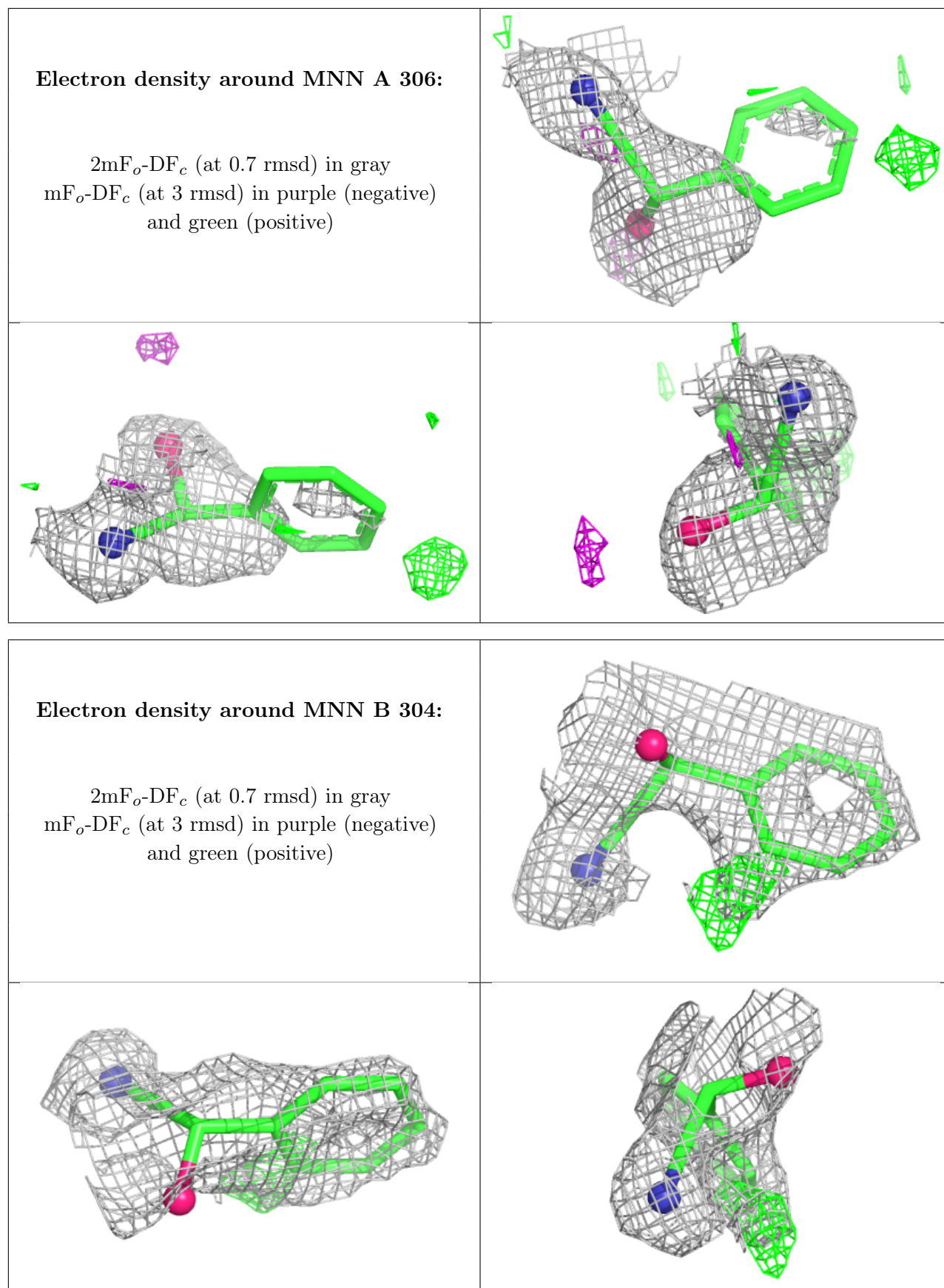
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

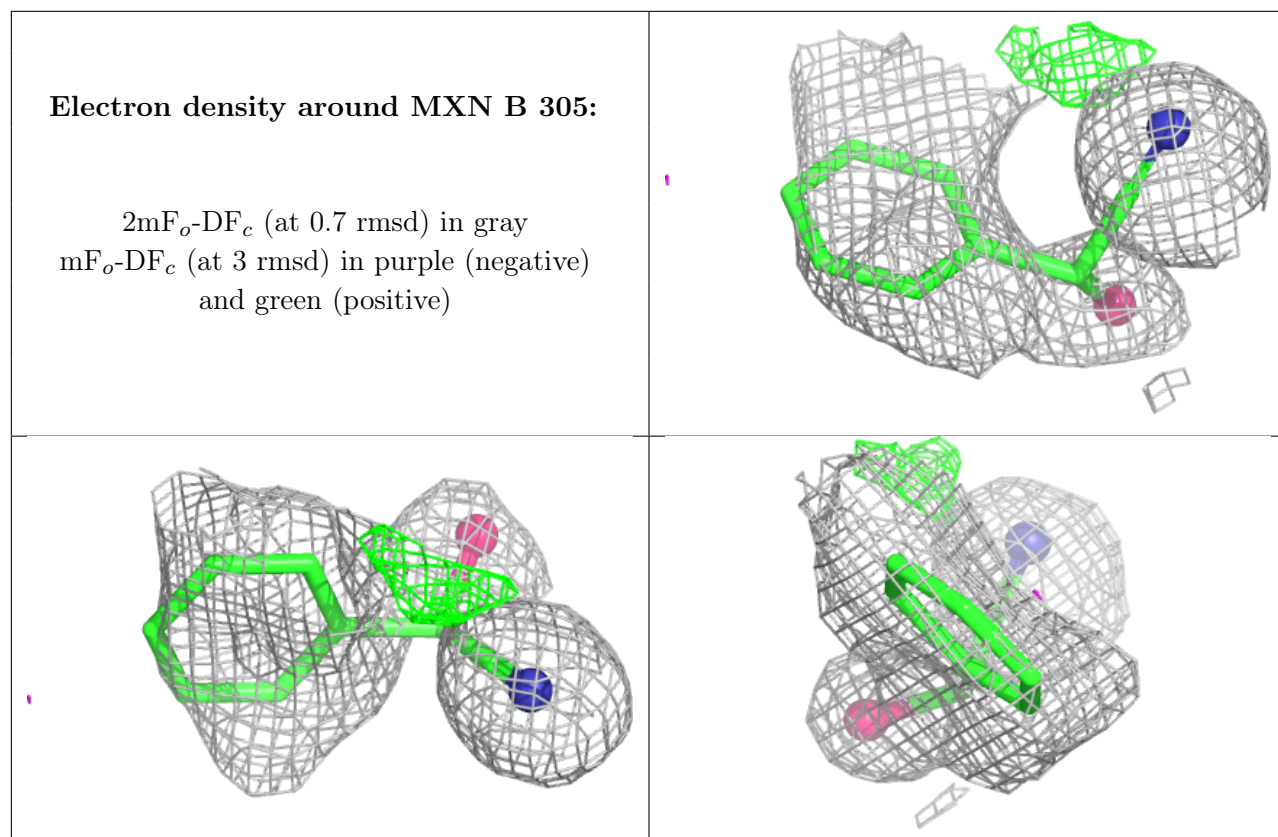


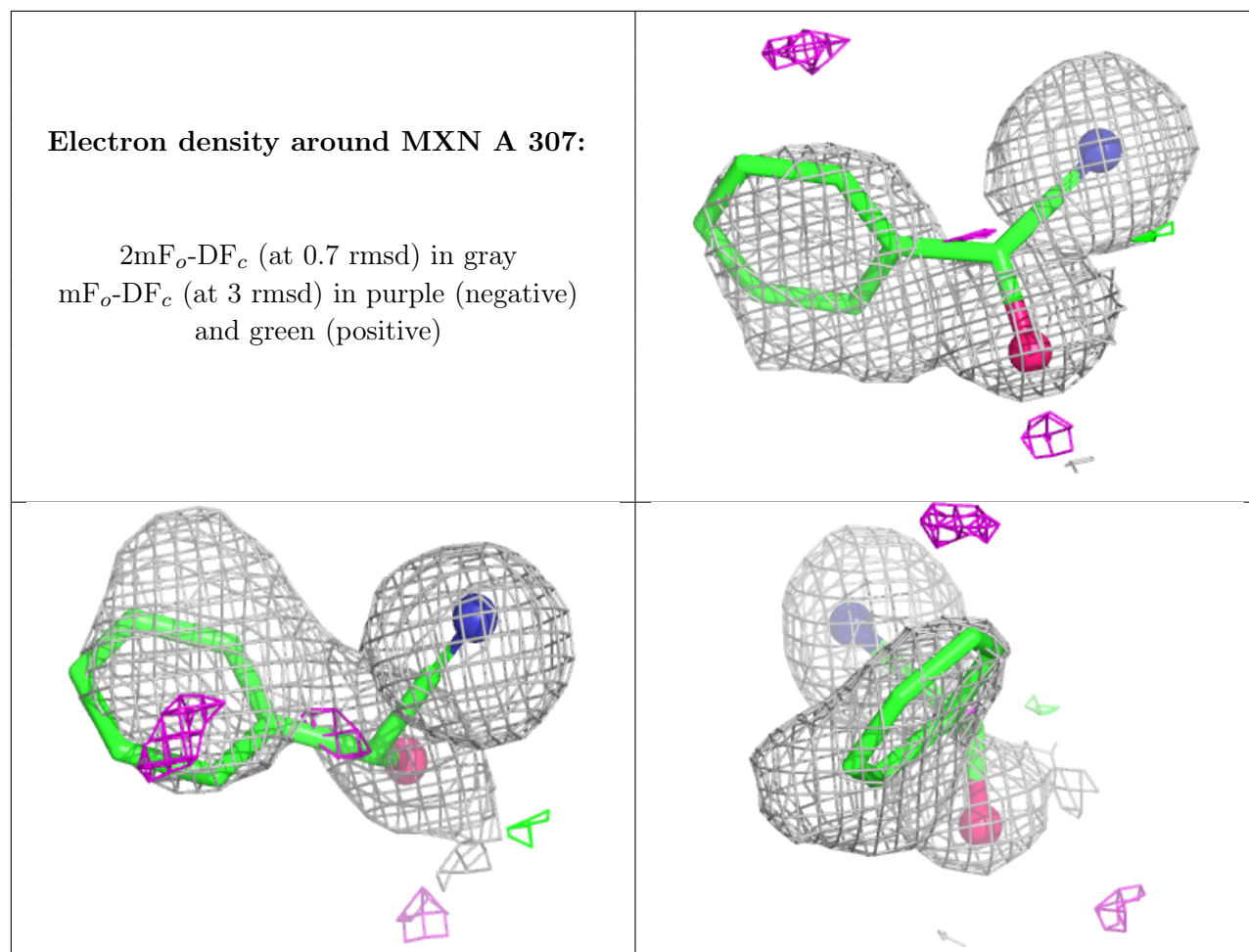
Electron density around HBX B 303:

$2mF_o-DF_c$ (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.