



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2022 – 02:46 pm GMT

PDB ID : 6YYR
Title : Structure of Cathepsin S in complex with Compound 20b
Authors : Wagener, M.; Schade, M.; Merla, B.; Hars, U.; Kueckelhaus, S.Q.
Deposited on : 2020-05-05
Resolution : 1.30 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

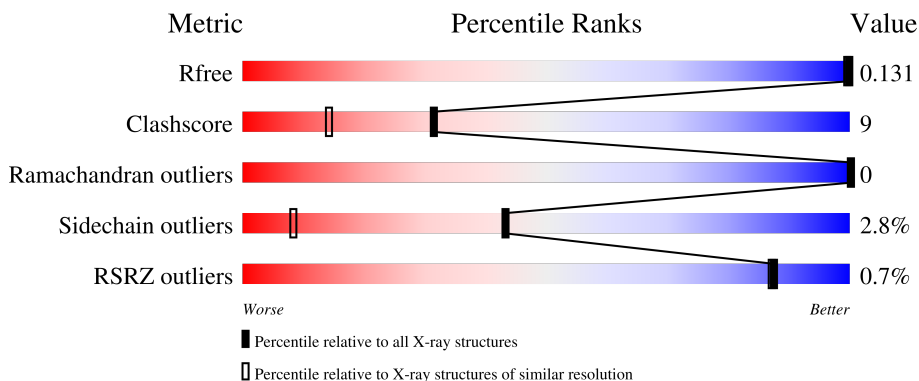
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	AAA	225	90% 6% ..
1	BBB	225	88% 9% .

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	FLC	AAA	1006	-	-	X	-
4	SO4	BBB	1005	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4818 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 Cathepsin S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	220	1861	1173	324	349	15	0	16	0
1	BBB	220	1846	1161	322	349	14	0	15	0

There are 12 discrepancies between the modelled and reference sequences:

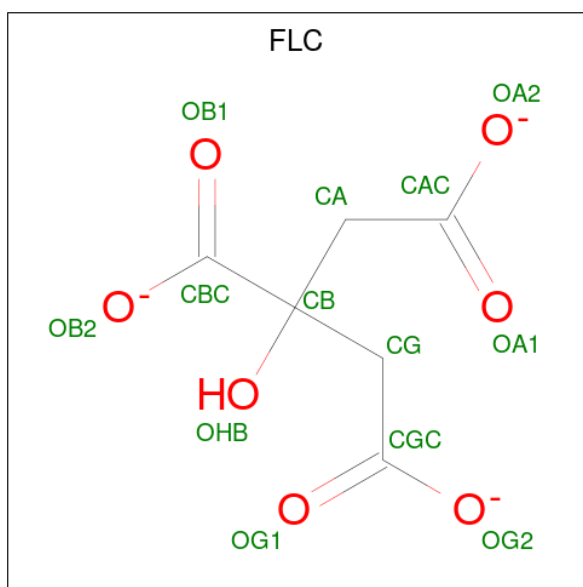
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	218	HIS	-	expression tag	UNP P25774
AAA	219	HIS	-	expression tag	UNP P25774
AAA	220	HIS	-	expression tag	UNP P25774
AAA	221	HIS	-	expression tag	UNP P25774
AAA	222	HIS	-	expression tag	UNP P25774
AAA	223	HIS	-	expression tag	UNP P25774
BBB	218	HIS	-	expression tag	UNP P25774
BBB	219	HIS	-	expression tag	UNP P25774
BBB	220	HIS	-	expression tag	UNP P25774
BBB	221	HIS	-	expression tag	UNP P25774
BBB	222	HIS	-	expression tag	UNP P25774
BBB	223	HIS	-	expression tag	UNP P25774

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 13 6 7	0	0
3	BBB	1	Total C O 13 6 7	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



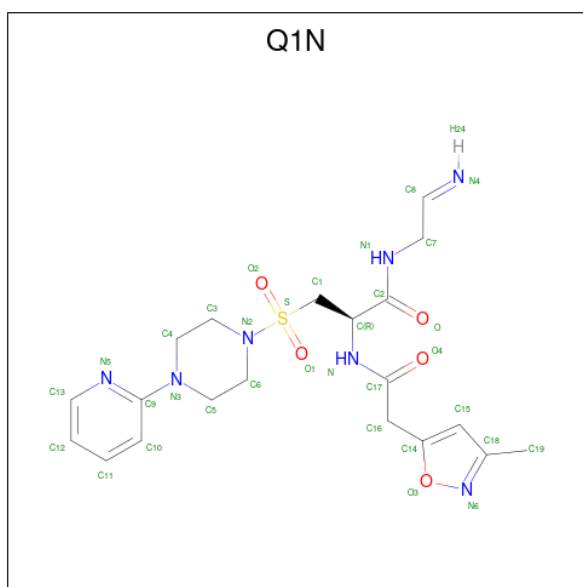
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O S 5 4 1	0	0
4	BBB	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total O S 5 4 1	0	0

- Molecule 5 is (2 {R})- {N}-(2-azanylideneethyl)-2-[2-(3-methyl-1,2-oxazol-5-yl)ethanoylamino]-3-(4-pyridin-2-ylpiperazin-1-yl)sulfonyl-propanamide (three-letter code: Q1N) (formula: C₂₀H₂₇N₇O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C N O S 66 40 14 10 2	0	1
5	BBB	1	Total C N O S 66 40 14 10 2	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	454	Total O 473 473	0	30
6	BBB	424	Total O 437 437	0	29

3 Residue-property plots [i](#)

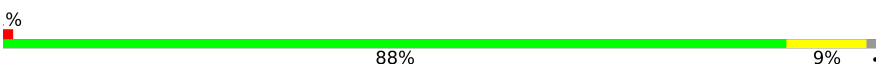
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cathepsin S

Chain AAA:  90% 6% ..



- Molecule 1: Cathepsin S

Chain BBB:  88% 9% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.84Å 85.84Å 151.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 1.30 29.76 – 1.30	Depositor EDS
% Data completeness (in resolution range)	92.9 (29.78-1.30) 92.9 (29.76-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.30Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.097 , 0.131 0.098 , 0.131	Depositor DCC
R_{free} test set	6484 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	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	0.98	EDS
Total number of atoms	4818	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: EDO, FLC, Q1N, SO4

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	AAA	0.75	0/1905	0.93	4/2566 (0.2%)
1	BBB	0.96	6/1891 (0.3%)	1.04	5/2552 (0.2%)
All	All	0.86	6/3796 (0.2%)	0.98	9/5118 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	193	GLU	CD-OE2	20.35	1.48	1.25
1	BBB	193	GLU	CD-OE1	7.86	1.34	1.25
1	BBB	106	ARG	CD-NE	-6.37	1.35	1.46
1	BBB	126	GLU	CD-OE2	-6.06	1.19	1.25
1	BBB	59[A]	GLU	CD-OE1	-5.50	1.19	1.25
1	BBB	59[B]	GLU	CD-OE1	-5.50	1.19	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	106	ARG	NE-CZ-NH1	15.94	128.27	120.30
1	BBB	106	ARG	NE-CZ-NH2	-12.89	113.86	120.30
1	BBB	149	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	AAA	120[A]	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	AAA	120[B]	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	AAA	120[C]	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	AAA	15	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	BBB	122	ASP	CB-CG-OD1	5.01	122.81	118.30
1	BBB	193	GLU	OE1-CD-OE2	5.00	129.30	123.30

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	AAA	1861	0	1790	40	0
1	BBB	1846	0	1754	19	0
2	AAA	20	0	29	0	0
2	BBB	8	0	10	0	0
3	AAA	13	0	5	6	0
3	BBB	13	0	5	0	0
4	AAA	5	0	0	1	0
4	BBB	10	0	0	2	0
5	AAA	66	0	0	6	0
5	BBB	66	0	0	11	0
6	AAA	473	0	0	18	2
6	BBB	437	0	0	19	2
All	All	4818	0	3593	68	3

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 9.

All (68) 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)
5:AAA:1008[A]:Q1N:C19	5:BBB:1006[A]:Q1N:N6	1.99	1.26
1:AAA:70[A]:PHE:CE2	5:BBB:1006[A]:Q1N:C11	2.19	1.24
4:BBB:1005:SO4:O3	6:BBB:1101:HOH:O	1.59	1.17
1:BBB:141[B]:ARG:HD2	6:BBB:1348:HOH:O	1.59	1.02
1:AAA:10[B]:LYS:HE2	6:BBB:1219[B]:HOH:O	1.63	0.97
4:BBB:1005:SO4:O4	6:BBB:1102:HOH:O	1.81	0.97
1:AAA:70[A]:PHE:CZ	5:BBB:1006[A]:Q1N:C11	2.49	0.94
1:AAA:70[A]:PHE:HE2	5:BBB:1006[A]:Q1N:C11	1.75	0.93
1:AAA:120[C]:ARG:HG2	1:AAA:120[C]:ARG:HH11	1.41	0.85
1:AAA:44[A]:LYS:HE3	6:AAA:1321:HOH:O	1.77	0.84
1:BBB:112[B]:LYS:HE2	6:BBB:1280:HOH:O	1.75	0.84
1:AAA:120[A]:ARG:CZ	6:AAA:1113:HOH:O	2.29	0.80
1:AAA:44[A]:LYS:CE	6:AAA:1321:HOH:O	2.30	0.76
1:AAA:70[A]:PHE:CE2	5:BBB:1006[A]:Q1N:C12	2.70	0.75
5:AAA:1008[A]:Q1N:C19	5:BBB:1006[A]:Q1N:C18	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:10[A]:LYS:NZ	6:AAA:1101:HOH:O	2.15	0.74
1:AAA:44[B]:LYS:NZ	3:AAA:1006:FLC:HG2	2.04	0.72
1:AAA:60[A]:LYS:NZ	6:AAA:1103:HOH:O	2.24	0.70
5:AAA:1008[B]:Q1N:N6	5:BBB:1006[B]:Q1N:C19	2.57	0.68
1:AAA:116[B]:LEU:CD2	6:AAA:1495:HOH:O	2.44	0.66
5:AAA:1008[B]:Q1N:C19	5:BBB:1006[B]:Q1N:N6	2.59	0.64
1:AAA:10[B]:LYS:CE	6:BBB:1219[B]:HOH:O	2.34	0.63
1:AAA:70[A]:PHE:HE2	5:BBB:1006[A]:Q1N:C12	2.10	0.62
1:BBB:141[A]:ARG:HD3	6:BBB:1102:HOH:O	1.99	0.61
1:BBB:173[B]:ASP:OD2	6:BBB:1103:HOH:O	2.16	0.61
1:BBB:141[A]:ARG:CD	6:BBB:1102:HOH:O	2.49	0.60
1:AAA:120[B]:ARG:NH1	6:AAA:1106:HOH:O	2.35	0.60
5:AAA:1008[A]:Q1N:C13	6:AAA:1251[A]:HOH:O	2.49	0.60
1:AAA:177[B]:LYS:HG2	6:AAA:1402:HOH:O	2.01	0.60
5:BBB:1006[B]:Q1N:C13	6:BBB:1250[B]:HOH:O	2.49	0.59
1:AAA:120[C]:ARG:NH1	6:AAA:1102:HOH:O	2.24	0.59
1:BBB:9:GLU:OE1	6:BBB:1104:HOH:O	2.17	0.59
1:BBB:116[B]:LEU:CD2	6:BBB:1134[B]:HOH:O	2.49	0.59
1:BBB:112[A]:LYS:NZ	1:BBB:216:GLU:OE2	2.37	0.58
1:BBB:112[A]:LYS:NZ	1:BBB:216:GLU:CD	2.57	0.58
1:AAA:44[B]:LYS:HZ2	3:AAA:1006:FLC:HG2	1.71	0.54
1:BBB:104:LYS:HE3	1:BBB:105:TYR:CZ	2.46	0.51
1:AAA:120[C]:ARG:HH11	1:AAA:120[C]:ARG:CG	2.19	0.51
1:BBB:120[B]:ARG:NH2	6:BBB:1112:HOH:O	2.44	0.51
1:AAA:116[B]:LEU:HD21	6:AAA:1495:HOH:O	2.07	0.50
1:AAA:120[A]:ARG:NH2	6:AAA:1113:HOH:O	2.43	0.49
1:AAA:120[C]:ARG:HG2	1:AAA:120[C]:ARG:NH1	2.19	0.49
1:AAA:5:VAL:HG13	6:AAA:1424[B]:HOH:O	2.13	0.48
1:AAA:44[B]:LYS:HE3	3:AAA:1006:FLC:OG1	2.13	0.48
1:BBB:116[B]:LEU:HD21	6:BBB:1134[B]:HOH:O	2.11	0.47
5:AAA:1008[A]:Q1N:C19	5:BBB:1006[A]:Q1N:C19	2.92	0.47
1:BBB:9:GLU:OE2	6:BBB:1105:HOH:O	2.20	0.47
1:AAA:44[B]:LYS:CE	3:AAA:1006:FLC:HG2	2.46	0.46
1:AAA:117:PRO:HB2	1:AAA:120[B]:ARG:HD3	1.98	0.46
1:BBB:141[A]:ARG:NE	6:BBB:1102:HOH:O	2.48	0.46
1:AAA:44[B]:LYS:HG2	1:AAA:46:VAL:HG23	1.98	0.46
1:AAA:60[B]:LYS:HE3	6:AAA:1389:HOH:O	2.17	0.45
1:AAA:177[A]:LYS:HD3	6:AAA:1402:HOH:O	2.17	0.45
1:BBB:218:HIS:ND1	1:BBB:218:HIS:C	2.69	0.44
1:AAA:44[B]:LYS:HG2	1:AAA:46:VAL:CG2	2.48	0.44
1:AAA:116[B]:LEU:HB3	1:AAA:117:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:44[B]:LYS:HZ2	3:AAA:1006:FLC:CG	2.31	0.43
1:BBB:104:LYS:HE2	6:BBB:1143:HOH:O	2.19	0.43
1:AAA:120[A]:ARG:NH1	6:AAA:1113:HOH:O	2.47	0.42
4:AAA:1007:SO4:O2	6:BBB:1219[B]:HOH:O	2.20	0.42
1:AAA:112[A]:LYS:HZ2	1:AAA:112[A]:LYS:HB2	1.84	0.42
1:AAA:116[B]:LEU:HD22	6:AAA:1495:HOH:O	2.12	0.42
1:AAA:44[A]:LYS:NZ	3:AAA:1006:FLC:OG1	2.44	0.41
1:AAA:67:ASN:HB3	6:AAA:1120:HOH:O	2.20	0.41
1:AAA:73:THR:HG22	1:BBB:118:TYR:CD2	2.56	0.41
1:AAA:112[A]:LYS:HB2	1:AAA:112[A]:LYS:NZ	2.36	0.41
1:BBB:112[A]:LYS:HZ2	1:BBB:216:GLU:CD	2.24	0.41
1:BBB:112[A]:LYS:HE3	6:BBB:1331[A]:HOH:O	2.20	0.41

All (3) 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)
6:BBB:1351:HOH:O	6:BBB:1351:HOH:O[6_565]	1.60	0.60
6:AAA:1185:HOH:O	6:BBB:1403:HOH:O[8_655]	2.12	0.08
6:AAA:1238:HOH:O	6:AAA:1238:HOH:O[5_555]	2.19	0.01

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	AAA	235/225 (104%)	230 (98%)	5 (2%)	0	100	100
1	BBB	233/225 (104%)	230 (99%)	3 (1%)	0	100	100
All	All	468/450 (104%)	460 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	198/186 (106%)	191 (96%)	7 (4%)	36 5
1	BBB	196/186 (105%)	191 (97%)	5 (3%)	46 10
All	All	394/372 (106%)	382 (97%)	12 (3%)	43 7

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	52	ASN
1	AAA	90	TYR
1	AAA	112[A]	LYS
1	AAA	112[B]	LYS
1	AAA	158	CYS
1	AAA	177[A]	LYS
1	AAA	177[B]	LYS
1	BBB	0	ILE
1	BBB	52	ASN
1	BBB	90	TYR
1	BBB	158	CYS
1	BBB	218	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	EDO	AAA	1001	-	3,3,3	1.38	1 (33%)	2,2,2	0.90	0
2	EDO	AAA	1005	-	3,3,3	0.80	0	2,2,2	0.61	0
2	EDO	AAA	1004	-	3,3,3	1.33	0	2,2,2	0.26	0
5	Q1N	BBB	1006[A]	1	32,35,35	1.24	3 (9%)	39,48,48	2.44	13 (33%)
4	SO4	AAA	1007	-	4,4,4	0.37	0	6,6,6	0.76	0
3	FLC	AAA	1006	-	12,12,12	1.39	1 (8%)	17,17,17	2.74	6 (35%)
3	FLC	BBB	1003	-	12,12,12	1.56	3 (25%)	17,17,17	1.38	3 (17%)
5	Q1N	BBB	1006[B]	1	32,35,35	1.77	12 (37%)	39,48,48	2.22	12 (30%)
2	EDO	AAA	1002	-	3,3,3	0.91	0	2,2,2	0.12	0
2	EDO	AAA	1003	-	3,3,3	0.62	0	2,2,2	0.61	0
2	EDO	BBB	1002	-	3,3,3	0.87	0	2,2,2	0.26	0
4	SO4	BBB	1005	-	4,4,4	0.40	0	6,6,6	0.46	0
5	Q1N	AAA	1008[A]	1	32,35,35	1.58	8 (25%)	39,48,48	3.01	16 (41%)
4	SO4	BBB	1004	-	4,4,4	0.36	0	6,6,6	0.31	0
5	Q1N	AAA	1008[B]	1	32,35,35	1.94	7 (21%)	39,48,48	2.40	13 (33%)
2	EDO	BBB	1001	-	3,3,3	1.24	0	2,2,2	0.42	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	AAA	1001	-	-	0/1/1/1	-
2	EDO	AAA	1005	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	AAA	1004	-	-	1/1/1/1	-
5	Q1N	BBB	1006[A]	1	-	3/28/41/41	0/3/3/3
3	FLC	AAA	1006	-	-	3/16/16/16	-
3	FLC	BBB	1003	-	-	2/16/16/16	-
5	Q1N	BBB	1006[B]	1	-	5/28/41/41	0/3/3/3
2	EDO	AAA	1002	-	-	1/1/1/1	-
2	EDO	AAA	1003	-	-	0/1/1/1	-
2	EDO	BBB	1002	-	-	0/1/1/1	-
5	Q1N	AAA	1008[A]	1	-	5/28/41/41	0/3/3/3
5	Q1N	AAA	1008[B]	1	-	3/28/41/41	0/3/3/3
2	EDO	BBB	1001	-	-	1/1/1/1	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	1008[B]	Q1N	O2-S	-6.49	1.35	1.43
5	AAA	1008[B]	Q1N	O1-S	5.26	1.49	1.43
5	AAA	1008[A]	Q1N	C6-N2	-3.90	1.43	1.47
5	AAA	1008[A]	Q1N	C16-C14	-3.68	1.48	1.51
3	AAA	1006	FLC	OA2-CAC	-3.65	1.18	1.30
5	BBB	1006[B]	Q1N	C15-C14	-3.51	1.34	1.39
5	BBB	1006[A]	Q1N	C16-C14	-3.24	1.49	1.51
5	BBB	1006[B]	Q1N	C13-N5	-2.98	1.28	1.34
5	AAA	1008[B]	Q1N	S-N2	-2.97	1.59	1.63
5	BBB	1006[B]	Q1N	C3-N2	-2.93	1.44	1.47
5	BBB	1006[B]	Q1N	C7-C8	2.93	1.59	1.49
5	BBB	1006[B]	Q1N	C11-C10	2.92	1.45	1.38
5	BBB	1006[A]	Q1N	C6-N2	2.83	1.50	1.47
5	AAA	1008[B]	Q1N	C16-C14	-2.72	1.49	1.51
3	BBB	1003	FLC	OG2-CGC	-2.63	1.21	1.30
5	BBB	1006[B]	Q1N	C6-N2	2.56	1.50	1.47
5	AAA	1008[A]	Q1N	O2-S	-2.55	1.40	1.43
3	BBB	1003	FLC	OB2-CBC	-2.55	1.20	1.30
3	BBB	1003	FLC	OA2-CAC	-2.52	1.22	1.30
5	BBB	1006[B]	Q1N	C1-C	2.52	1.56	1.53
5	BBB	1006[B]	Q1N	C1-S	-2.41	1.70	1.78
5	AAA	1008[B]	Q1N	C3-N2	-2.40	1.45	1.47
5	AAA	1008[A]	Q1N	S-N2	-2.39	1.59	1.63
5	AAA	1008[A]	Q1N	C19-C18	2.35	1.55	1.50
5	AAA	1008[A]	Q1N	C5-N3	2.34	1.50	1.46
5	BBB	1006[B]	Q1N	O2-S	2.33	1.45	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	1001	EDO	O1-C1	-2.32	1.30	1.42
5	BBB	1006[B]	Q1N	C12-C13	2.31	1.44	1.37
5	BBB	1006[A]	Q1N	C3-N2	-2.31	1.45	1.47
5	AAA	1008[B]	Q1N	C11-C10	-2.24	1.34	1.38
5	AAA	1008[A]	Q1N	C11-C10	2.21	1.43	1.38
5	AAA	1008[A]	Q1N	C1-S	-2.20	1.71	1.78
5	BBB	1006[B]	Q1N	C16-C14	-2.15	1.49	1.51
5	BBB	1006[B]	Q1N	C4-N3	2.08	1.50	1.46
5	AAA	1008[B]	Q1N	C15-C14	-2.02	1.36	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	1008[A]	Q1N	C5-C6-N2	-12.28	99.53	108.91
5	BBB	1006[A]	Q1N	C4-C3-N2	-6.68	103.81	108.91
5	AAA	1008[B]	Q1N	C19-C18-N6	6.58	133.10	120.06
3	AAA	1006	FLC	OB1-CBC-CB	-6.58	112.93	122.25
5	BBB	1006[B]	Q1N	C13-N5-C9	6.11	124.93	116.86
5	AAA	1008[A]	Q1N	O2-S-O1	-5.92	112.90	118.98
3	AAA	1006	FLC	OHB-CB-CG	-5.68	96.12	109.40
5	BBB	1006[A]	Q1N	C5-C6-N2	-5.43	104.76	108.91
5	BBB	1006[A]	Q1N	C19-C18-N6	5.13	130.22	120.06
5	AAA	1008[B]	Q1N	C1-S-N2	5.04	112.66	106.10
5	AAA	1008[A]	Q1N	C13-N5-C9	4.91	123.35	116.86
5	AAA	1008[B]	Q1N	C19-C18-C15	-4.75	116.47	129.06
5	BBB	1006[B]	Q1N	C12-C13-N5	-4.59	115.93	123.43
5	BBB	1006[B]	Q1N	C3-N2-S	4.41	126.89	118.61
5	BBB	1006[A]	Q1N	C3-N2-C6	4.31	116.94	112.17
5	BBB	1006[A]	Q1N	C6-C5-N3	-4.28	102.39	110.70
5	AAA	1008[B]	Q1N	O2-S-O1	4.19	123.28	118.98
5	AAA	1008[B]	Q1N	C3-N2-C6	4.13	116.74	112.17
5	AAA	1008[A]	Q1N	C3-N2-S	4.06	126.23	118.61
5	AAA	1008[A]	Q1N	C12-C13-N5	-3.98	116.92	123.43
3	AAA	1006	FLC	OHB-CB-CBC	3.98	114.45	108.86
5	BBB	1006[A]	Q1N	C19-C18-C15	-3.95	118.60	129.06
5	BBB	1006[B]	Q1N	C14-C16-C17	-3.93	105.58	113.39
5	AAA	1008[A]	Q1N	O1-S-N2	3.92	110.55	107.23
5	AAA	1008[B]	Q1N	O1-S-N2	-3.72	104.08	107.23
5	AAA	1008[A]	Q1N	C3-N2-C6	3.56	116.11	112.17
5	BBB	1006[A]	Q1N	O1-S-N2	3.56	110.24	107.23
5	AAA	1008[A]	Q1N	C1-S-N2	3.47	110.61	106.10
5	BBB	1006[B]	Q1N	C1-S-N2	3.38	110.50	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	BBB	1006[B]	Q1N	C3-N2-C6	3.32	115.84	112.17
5	BBB	1006[A]	Q1N	C14-C16-C17	-3.31	106.81	113.39
5	AAA	1008[B]	Q1N	O2-S-C1	-3.26	102.56	107.96
5	AAA	1008[B]	Q1N	C12-C13-N5	-3.25	118.11	123.43
5	AAA	1008[B]	Q1N	C4-C3-N2	-3.20	106.47	108.91
5	BBB	1006[A]	Q1N	C4-N3-C9	-2.99	113.44	120.39
5	BBB	1006[B]	Q1N	N5-C9-N3	-2.99	112.31	116.79
3	AAA	1006	FLC	OG1-CGC-CG	-2.93	114.38	122.94
5	BBB	1006[B]	Q1N	C4-N3-C9	-2.81	113.87	120.39
3	AAA	1006	FLC	OG2-CGC-CG	2.65	122.85	114.35
5	BBB	1006[A]	Q1N	C1-S-N2	2.59	109.47	106.10
5	BBB	1006[B]	Q1N	C4-C3-N2	2.56	110.87	108.91
5	AAA	1008[A]	Q1N	C6-C5-N3	-2.53	105.78	110.70
5	BBB	1006[B]	Q1N	C11-C10-C9	-2.48	114.31	117.66
3	AAA	1006	FLC	OB2-CBC-CB	2.46	117.32	113.05
3	BBB	1003	FLC	OA1-CAC-CA	-2.44	115.82	122.94
5	AAA	1008[A]	Q1N	C19-C18-N6	2.37	124.76	120.06
5	BBB	1006[A]	Q1N	C11-C10-C9	2.35	120.84	117.66
5	AAA	1008[B]	Q1N	C14-C16-C17	-2.29	108.83	113.39
3	BBB	1003	FLC	OG2-CGC-CG	2.26	121.62	114.35
5	AAA	1008[A]	Q1N	C-C2-N1	-2.21	112.09	116.54
5	BBB	1006[A]	Q1N	C12-C11-C10	-2.20	116.84	120.19
5	AAA	1008[B]	Q1N	C3-C4-N3	-2.20	106.43	110.70
5	AAA	1008[A]	Q1N	C14-C16-C17	-2.18	109.05	113.39
5	BBB	1006[B]	Q1N	C19-C18-N6	2.18	124.38	120.06
3	BBB	1003	FLC	OB1-CBC-CB	-2.14	119.22	122.25
5	AAA	1008[A]	Q1N	O4-C17-C16	2.12	126.87	122.03
5	AAA	1008[B]	Q1N	C5-N3-C9	-2.12	115.47	120.39
5	AAA	1008[A]	Q1N	C4-N3-C9	-2.11	115.49	120.39
5	BBB	1006[A]	Q1N	C10-C9-N3	-2.10	117.93	121.70
5	AAA	1008[B]	Q1N	O-C2-C	2.08	124.82	120.45
5	AAA	1008[A]	Q1N	C11-C10-C9	-2.04	114.90	117.66
5	BBB	1006[B]	Q1N	C11-C12-C13	2.03	122.55	118.62
5	AAA	1008[A]	Q1N	C11-C12-C13	2.03	122.54	118.62

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	BBB	1006[A]	Q1N	C3-N2-S-O2
5	AAA	1008[A]	Q1N	C3-N2-S-O2
5	AAA	1008[B]	Q1N	C3-N2-S-O1

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Mol	Chain	Res	Type	Atoms
5	BBB	1006[A]	Q1N	C3-N2-S-C1
5	BBB	1006[A]	Q1N	C3-N2-S-O1
5	BBB	1006[B]	Q1N	C3-N2-S-C1
5	BBB	1006[B]	Q1N	C3-N2-S-O1
5	BBB	1006[B]	Q1N	N5-C9-N3-C5
5	BBB	1006[B]	Q1N	C10-C9-N3-C5
5	AAA	1008[A]	Q1N	C3-N2-S-O1
5	AAA	1008[B]	Q1N	C3-N2-S-O2
5	BBB	1006[B]	Q1N	C3-N2-S-O2
3	AAA	1006	FLC	CA-CB-CBC-OB2
2	BBB	1001	EDO	O1-C1-C2-O2
5	AAA	1008[A]	Q1N	C3-N2-S-C1
5	AAA	1008[B]	Q1N	C3-N2-S-C1
3	BBB	1003	FLC	CB-CA-CAC-OA2
3	BBB	1003	FLC	CB-CA-CAC-OA1
2	AAA	1004	EDO	O1-C1-C2-O2
2	AAA	1005	EDO	O1-C1-C2-O2
2	AAA	1002	EDO	O1-C1-C2-O2
5	AAA	1008[A]	Q1N	N5-C9-N3-C5
3	AAA	1006	FLC	CB-CA-CAC-OA1
3	AAA	1006	FLC	CB-CA-CAC-OA2
5	AAA	1008[A]	Q1N	C10-C9-N3-C5

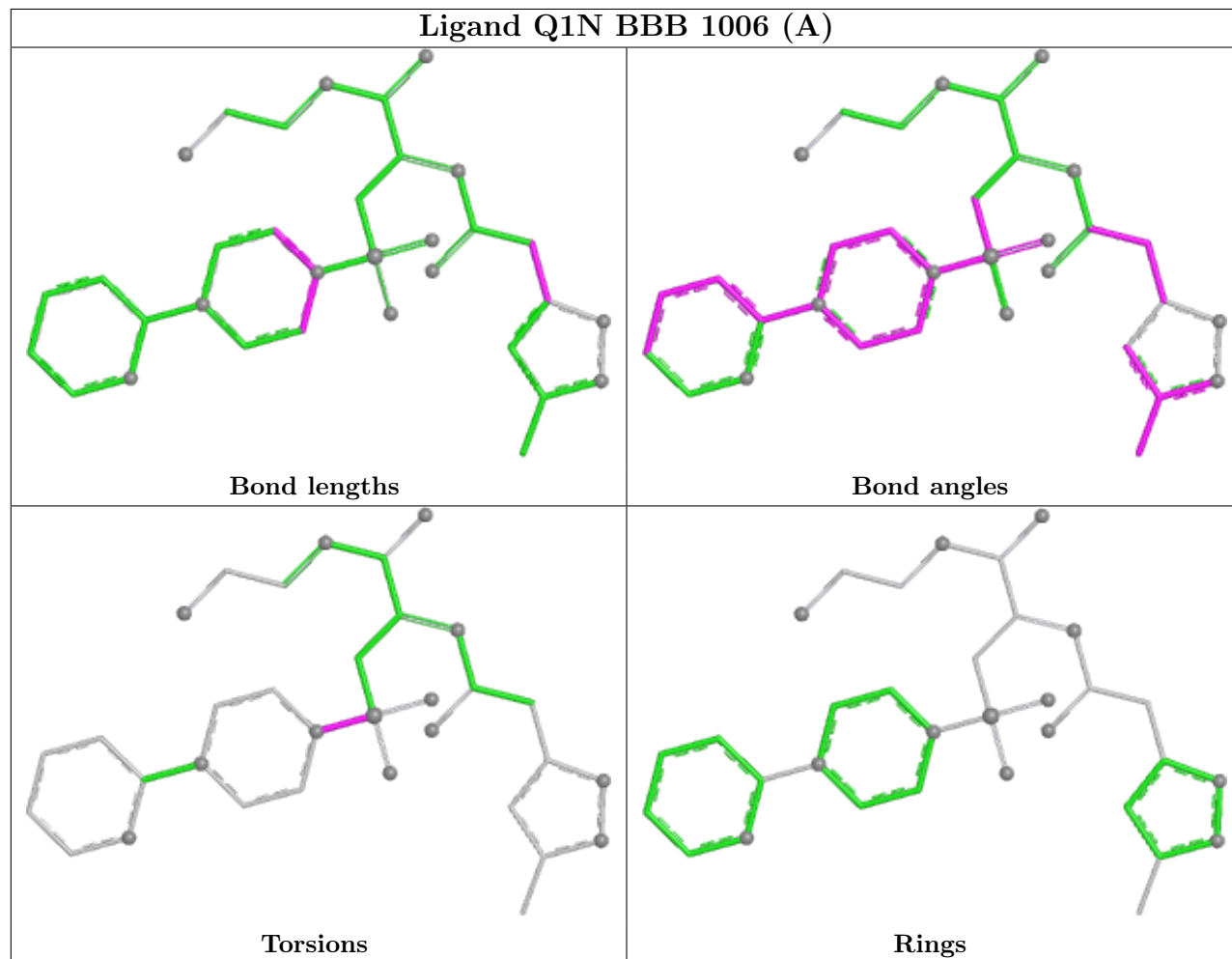
There are no ring outliers.

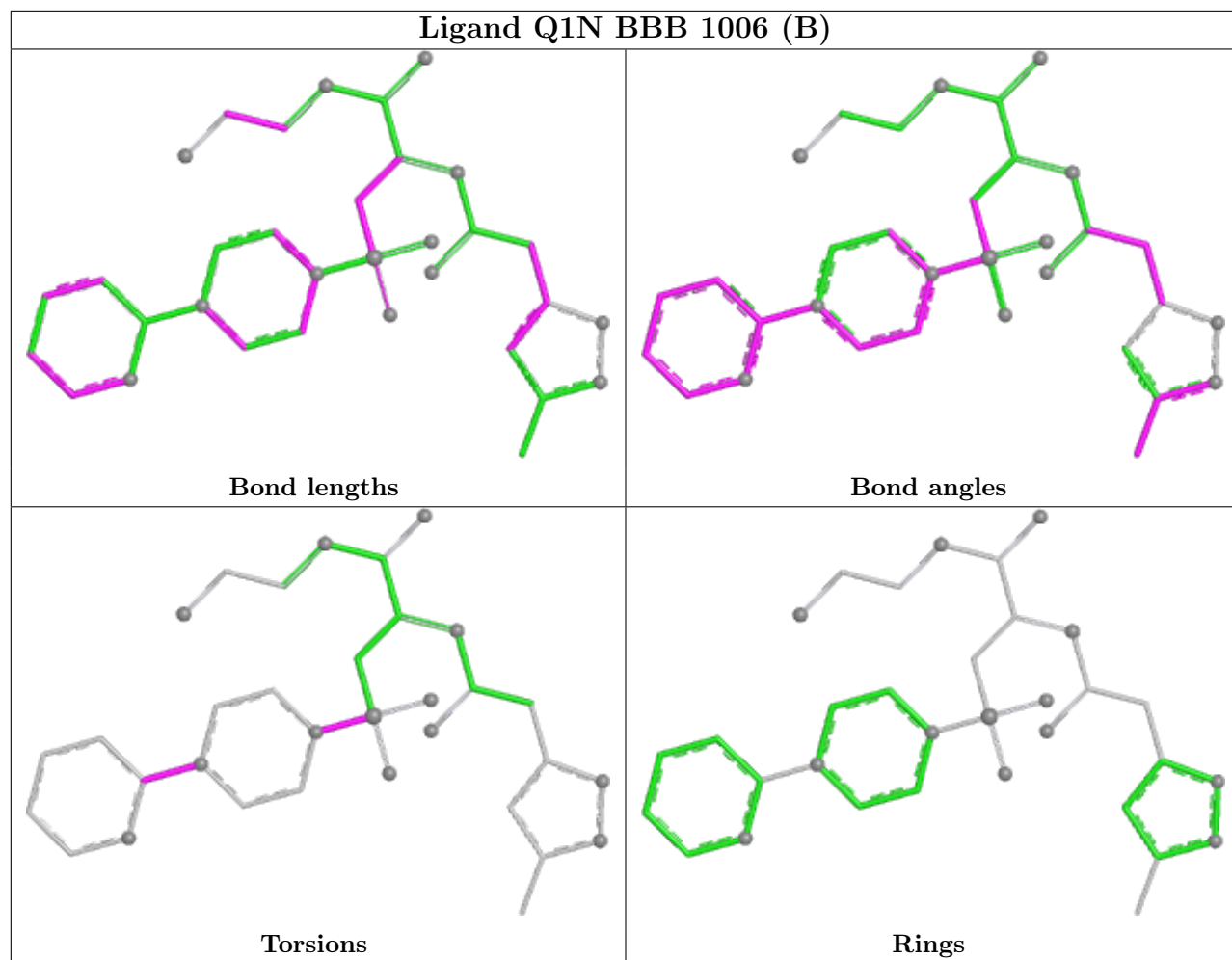
7 monomers are involved in 21 short contacts:

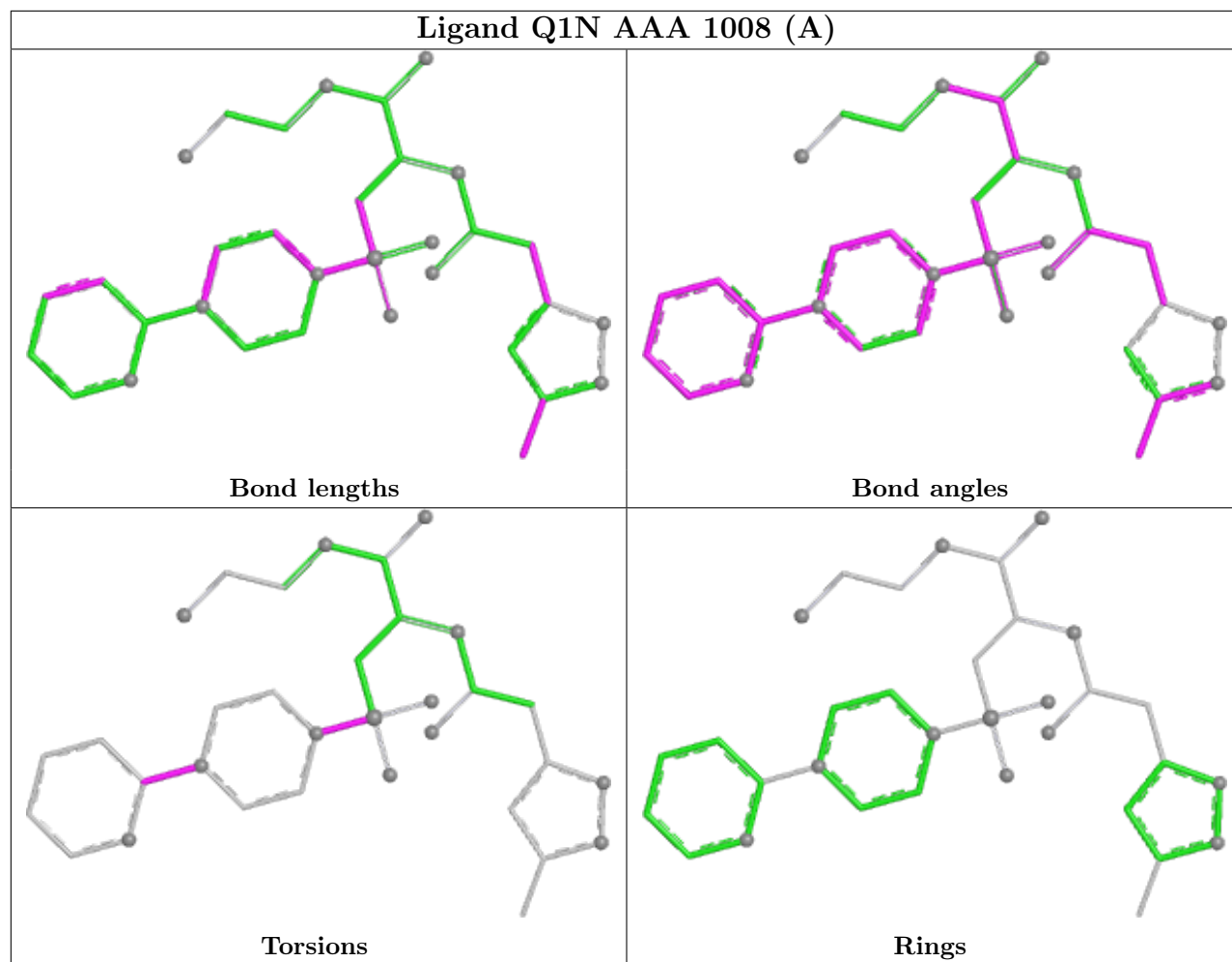
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	1006[A]	Q1N	8	0
4	AAA	1007	SO4	1	0
3	AAA	1006	FLC	6	0
5	BBB	1006[B]	Q1N	3	0
4	BBB	1005	SO4	2	0
5	AAA	1008[A]	Q1N	4	0
5	AAA	1008[B]	Q1N	2	0

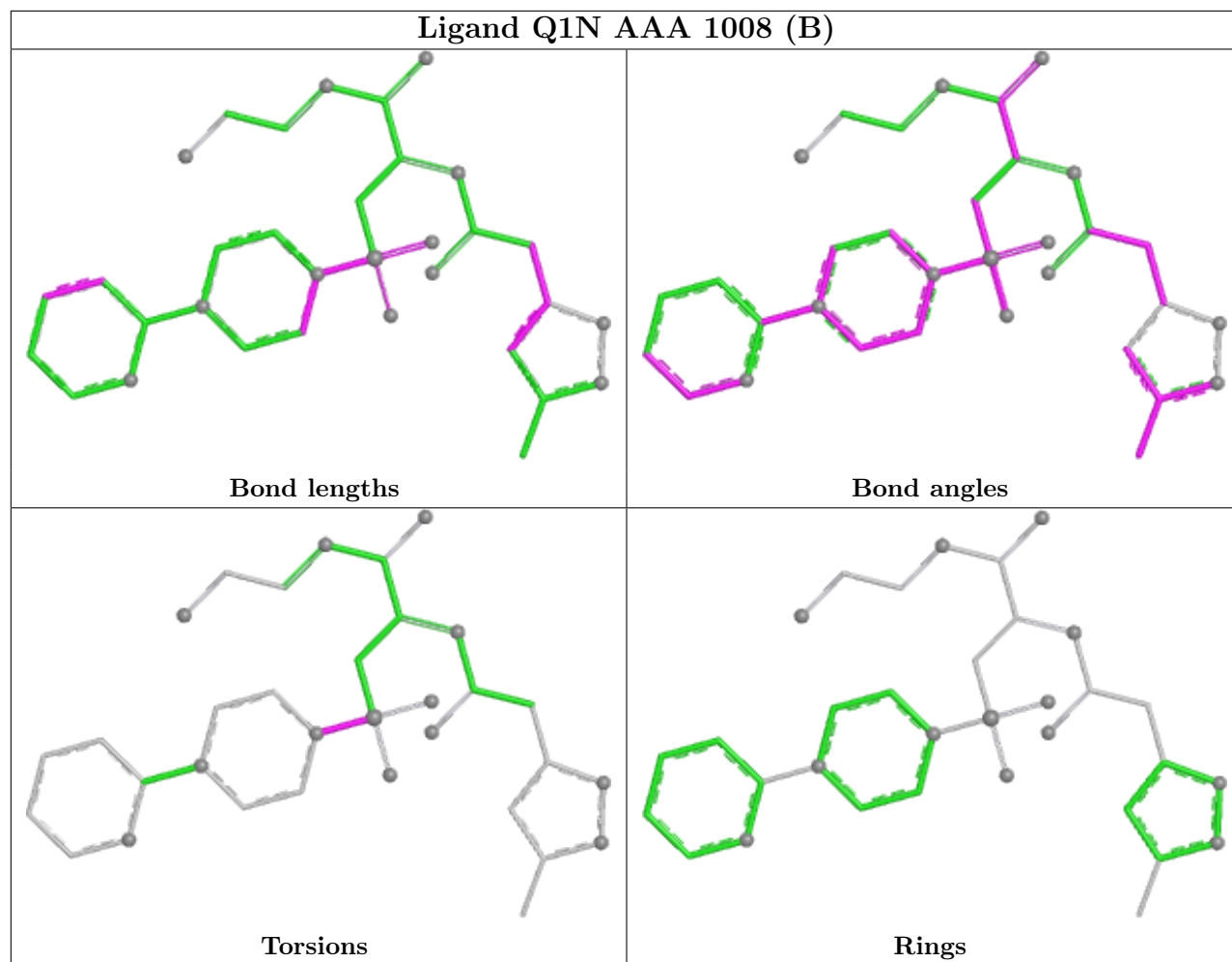
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	AAA	220/225 (97%)	-0.59	0 100 100	9, 12, 23, 53	0
1	BBB	220/225 (97%)	-0.54	3 (1%) 75 77	9, 12, 23, 60	0
All	All	440/450 (97%)	-0.57	3 (0%) 87 87	9, 12, 23, 60	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	0	ILE	4.4
1	BBB	-1	ARG	3.6
1	BBB	218	HIS	3.6

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 monosaccharides 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.

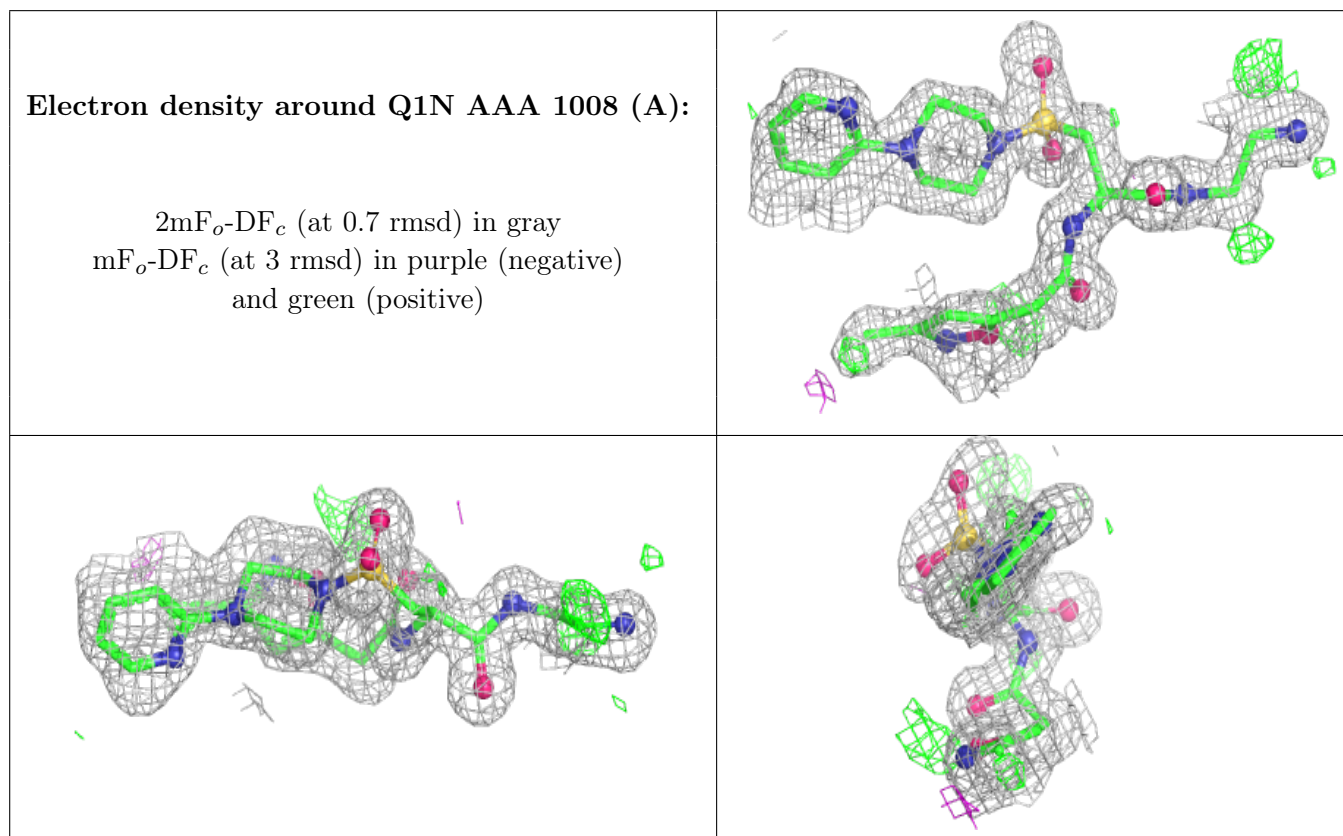
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	AAA	1002	4/4	0.88	0.14	26,30,33,40	0
2	EDO	AAA	1004	4/4	0.89	0.08	23,24,25,28	0

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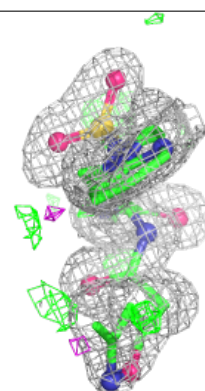
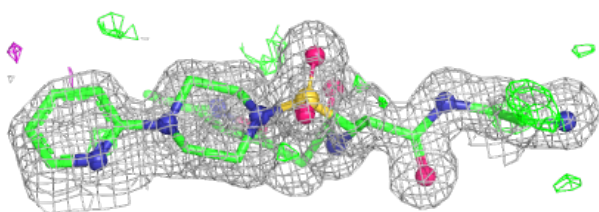
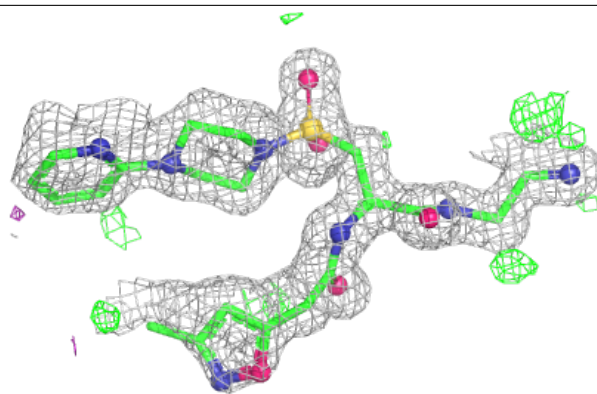
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FLC	AAA	1006	13/13	0.94	0.10	13,22,31,36	13
3	FLC	BBB	1003	13/13	0.94	0.09	13,17,35,40	13
4	SO4	AAA	1007	5/5	0.95	0.11	11,16,23,23	5
2	EDO	AAA	1001	4/4	0.96	0.05	21,23,32,35	0
2	EDO	BBB	1001	4/4	0.96	0.06	23,26,30,31	4
2	EDO	BBB	1002	4/4	0.96	0.07	17,18,19,20	0
2	EDO	AAA	1005	4/4	0.97	0.11	23,29,30,36	0
2	EDO	AAA	1003	4/4	0.97	0.05	16,17,17,19	0
4	SO4	BBB	1004	5/5	0.98	0.10	22,23,26,28	5
4	SO4	BBB	1005	5/5	0.98	0.06	19,20,21,28	5
5	Q1N	AAA	1008[A]	33/33	0.98	0.06	14,16,20,23	33
5	Q1N	AAA	1008[B]	33/33	0.98	0.06	10,14,28,41	33
5	Q1N	BBB	1006[A]	33/33	0.98	0.07	9,16,28,33	33
5	Q1N	BBB	1006[B]	33/33	0.98	0.07	8,11,17,20	33

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.

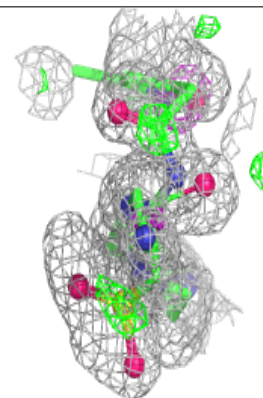
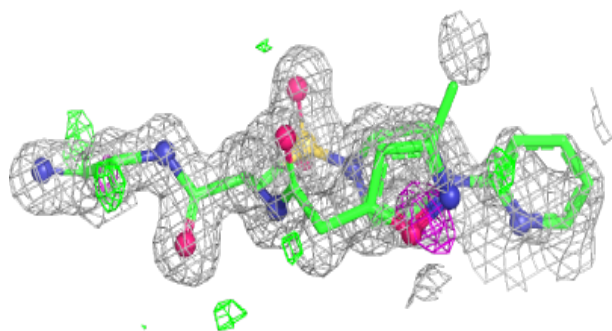
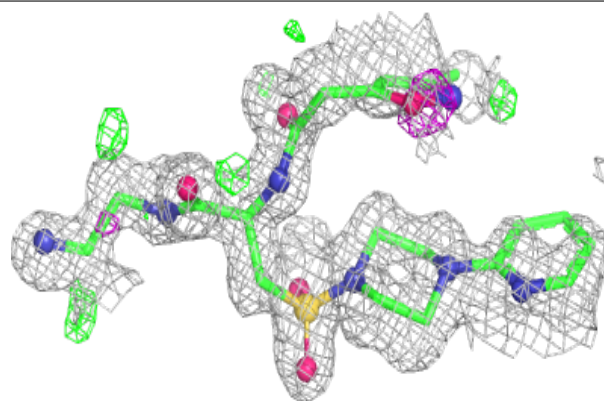


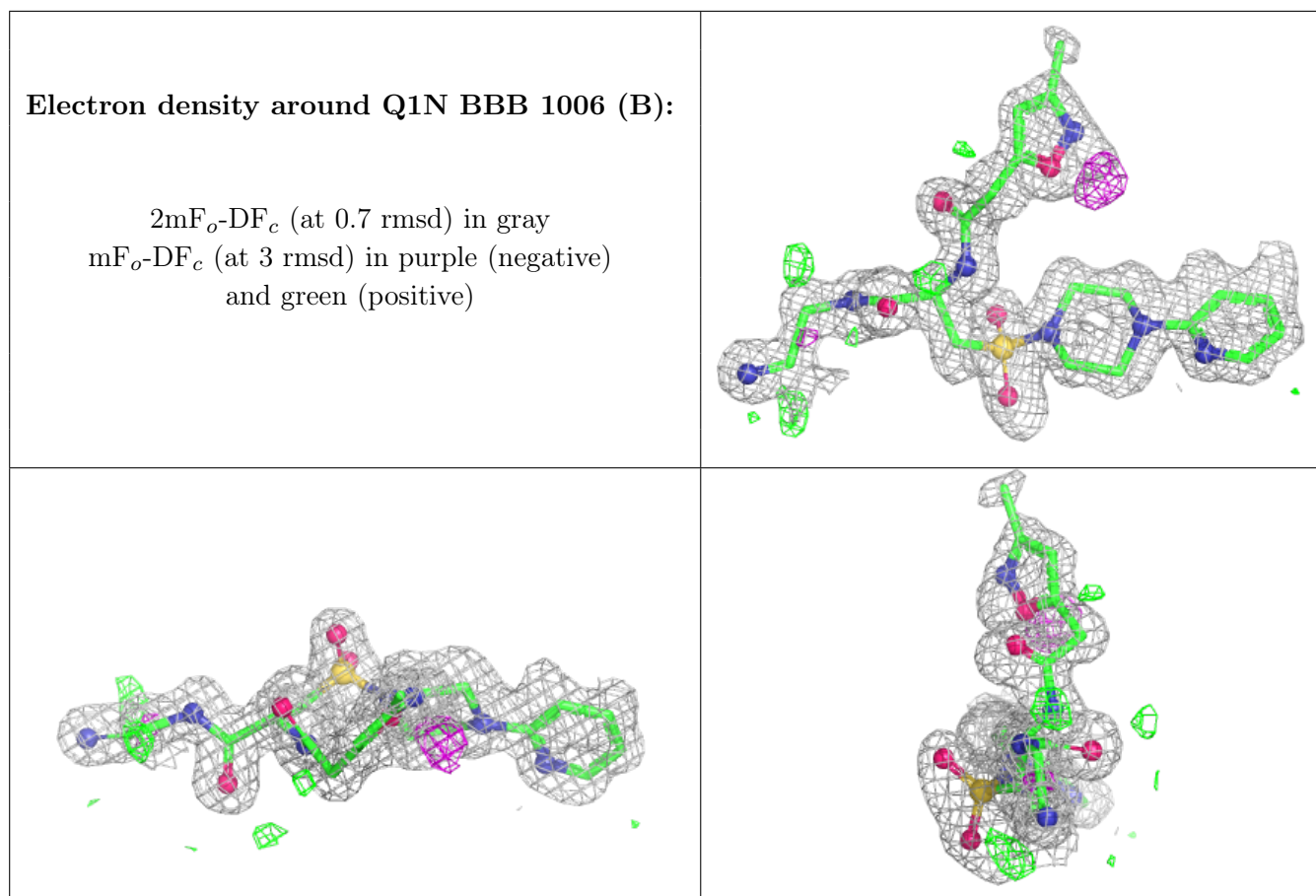
Electron density around Q1N AAA 1008 (B):

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

**Electron density around Q1N BBB 1006 (A):**

$2mF_o-DF_c$ (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.