Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 02:45 AM EDT

PDB ID	:	6QSW
Title	:	Complement factor B protease domain in complex with the reversible inhibitor N-(2-bromo-4-methylnaphthalen-1-yl)-4,5-dihydro-1H-imidazol-2-amine.
Authors	:	Adams, C.M.; Sellner, H.; Ehara, T.; Mac Sweeney, A.; Crowley, M.; Anderson, K.; Karki, R.; Mainolfi, N.; Valeur, E.; Sirockin, F.; Gerhartz, B.; Erbel, P.; Hughes, N.; Smith, T.M.; Cumin, F.; Argikar, U.; Mogi, M.; Sedrani, R.; Wiesmann, C.; Jaffee, B.; Maibaum, J.; Flohr, S.; Harrison, R.; Eder, J.
Deposited on	:	2019-02-22
Resolution	:	1.64 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:

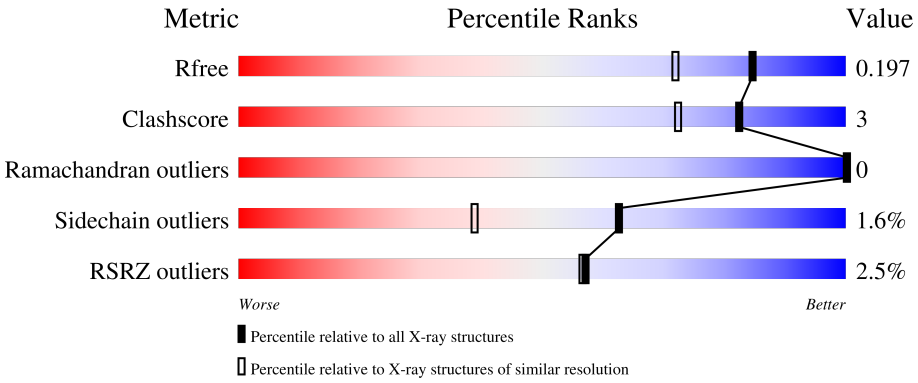
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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 <=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	291	2% 85% 5% 9%
1	BBB	291	% 86% 7% 8%
1	CCC	291	3% 85% 10%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

2 Entry composition

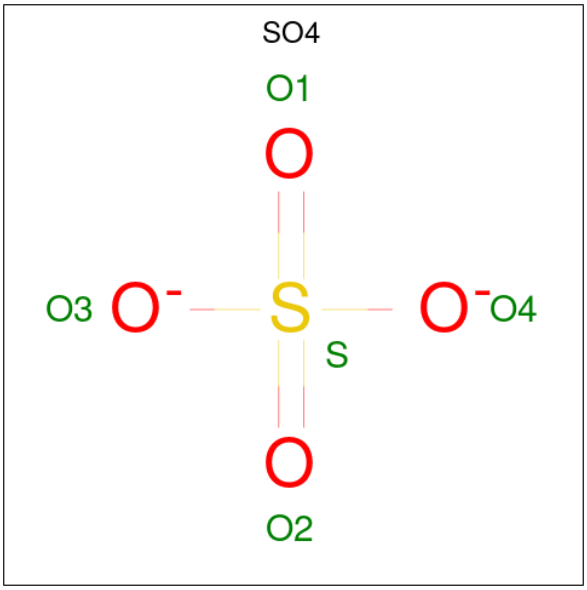
There are 4 unique types of molecules in this entry. The entry contains 13163 atoms, of which 6279 are hydrogens and 0 are deuteriums.

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 Complement factor B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	264	Total	C	H	N	O	S	92	2	0
			4125	1317	2065	351	380	12			
1	BBB	269	Total	C	H	N	O	S	96	4	0
			4227	1355	2108	357	395	12			
1	CCC	263	Total	C	H	N	O	S	86	3	0
			4207	1342	2106	361	386	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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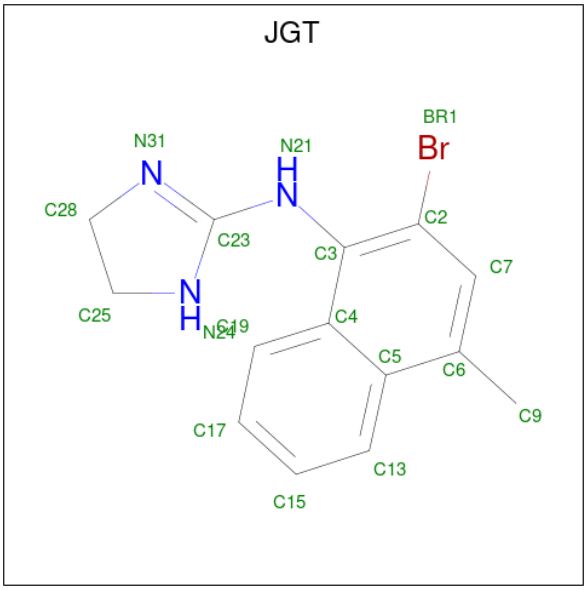
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0
2	CCC	1	Total O S 5 4 1	0	0
2	CCC	1	Total O S 5 4 1	0	0
2	CCC	1	Total O S 5 4 1	0	0

- Molecule 3 is {N}-(2-bromanyl-4-methyl-naphthalen-1-yl)-4,5-dihydro-1 {H}-imidazol-2-amine (three-letter code: JGT) (formula: $C_{14}H_{14}BrN_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Br C N 18 1 14 3	0	0
3	BBB	1	Total Br C N 18 1 14 3	0	0
3	CCC	1	Total Br C N 18 1 14 3	0	0

- Molecule 4 is water.

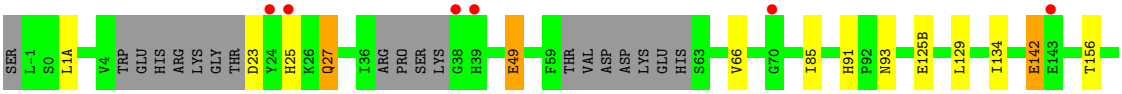
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	173	Total O 173 173	0	0
4	BBB	184	Total O 184 184	0	0
4	CCC	143	Total O 143 143	0	0

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.

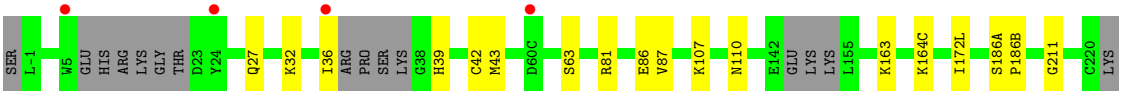
• Molecule 1: Complement factor B

Chain AAA:



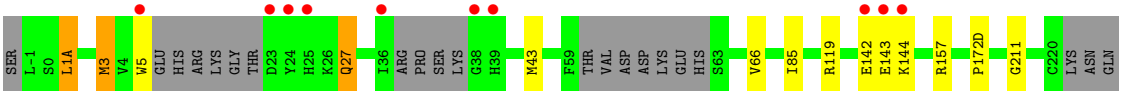
• Molecule 1: Complement factor B

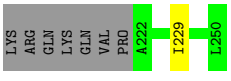
Chain BBB:



• Molecule 1: Complement factor B

Chain CCC:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.28Å 91.28Å 260.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.06 – 1.64 65.06 – 1.64	Depositor EDS
% Data completeness (in resolution range)	95.8 (65.06-1.64) 95.8 (65.06-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0238 2018/15/10	Depositor
R, R_{free}	0.157 , 0.188 0.167 , 0.197	Depositor DCC
R_{free} test set	6478 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	16.4	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13163	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, JGT

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	0.63	0/2105	0.75	0/2846
1	BBB	0.63	0/2177	0.76	0/2947
1	CCC	0.62	0/2151	0.76	0/2904
All	All	0.63	0/6433	0.76	0/8697

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2060	2065	2041	11	0
1	BBB	2119	2108	2092	13	0
1	CCC	2101	2106	2097	9	0
2	AAA	15	0	0	0	0
2	BBB	20	0	0	1	0
2	CCC	15	0	0	0	0
3	AAA	18	0	0	0	0
3	BBB	18	0	0	0	0
3	CCC	18	0	0	1	0
4	AAA	173	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	184	0	0	3	0
4	CCC	143	0	0	0	0
All	All	6884	6279	6230	32	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 3.

All (32) 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:BBB:81:ARG:HG3	4:BBB:531:HOH:O	1.79	0.81
1:AAA:91:HIS:HD2	1:AAA:93:ASN:H	1.29	0.78
1:BBB:43:MET:HE3	4:BBB:427:HOH:O	1.92	0.68
1:BBB:163:LYS:HE2	1:BBB:186(A):SER:O	2.05	0.56
1:BBB:107:LYS:NZ	4:BBB:401:HOH:O	2.31	0.54
1:AAA:91:HIS:CD2	1:AAA:93:ASN:H	2.19	0.54
1:AAA:142:GLU:HG3	1:AAA:156:THR:HG21	1.92	0.52
1:AAA:239:LYS:HE2	4:AAA:449:HOH:O	2.09	0.52
1:CCC:143:GLU:O	1:CCC:144:LYS:HG2	2.10	0.50
1:BBB:110:ASN:ND2	2:BBB:302:SO4:O4	2.29	0.50
1:BBB:42:CYS:O	1:BBB:43:MET:HE2	2.10	0.50
1:CCC:142:GLU:O	1:CCC:142:GLU:HG2	2.10	0.49
1:CCC:27:GLN:OE1	1:CCC:157[A]:ARG:HD3	2.13	0.49
1:CCC:172(D):PRO:HG2	3:CCC:304:JGT:BR1	2.70	0.47
1:CCC:143:GLU:C	1:CCC:144:LYS:HG2	2.35	0.46
1:BBB:36:ILE:HG23	1:BBB:63[B]:SER:OG	2.14	0.46
1:AAA:49[A]:GLU:H	1:AAA:49[A]:GLU:HG2	1.41	0.46
1:AAA:66:VAL:HG23	1:AAA:85:ILE:HD11	1.98	0.45
1:BBB:164(C):LYS:HE2	1:BBB:186(B):PRO:HB3	2.00	0.44
1:CCC:1(A):LEU:HD23	1:CCC:3:MET:HE1	1.98	0.44
1:CCC:66:VAL:HG23	1:CCC:85:ILE:HD11	1.98	0.44
1:AAA:211:GLY:HA2	1:AAA:229:ILE:O	2.18	0.43
1:CCC:5:TRP:HD1	1:CCC:119[A]:ARG:HH12	1.67	0.43
1:CCC:211:GLY:HA2	1:CCC:229:ILE:O	2.18	0.43
1:BBB:211:GLY:HA2	1:BBB:229:ILE:O	2.18	0.43
1:BBB:172(L):ILE:HD13	1:BBB:172(L):ILE:HA	1.92	0.42
1:BBB:32:LYS:HA	1:BBB:43:MET:CE	2.49	0.42
1:AAA:23:ASP:O	1:AAA:27:GLN:NE2	2.53	0.42
1:AAA:25:HIS:ND1	1:AAA:25:HIS:N	2.69	0.41
1:AAA:125(B):GLU:OE1	1:BBB:86:GLU:OE1	2.38	0.41
1:BBB:87:VAL:HG12	1:BBB:107:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:129:LEU:HA	1:AAA:134:ILE:HD13	2.03	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	AAA	256/291 (88%)	253 (99%)	3 (1%)	0	100	100
1	BBB	263/291 (90%)	259 (98%)	4 (2%)	0	100	100
1	CCC	256/291 (88%)	252 (98%)	4 (2%)	0	100	100
All	All	775/873 (89%)	764 (99%)	11 (1%)	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	224/256 (88%)	218 (97%)	6 (3%)	44	18
1	BBB	234/256 (91%)	232 (99%)	2 (1%)	78	63
1	CCC	231/256 (90%)	227 (98%)	4 (2%)	60	36
All	All	689/768 (90%)	677 (98%)	12 (2%)	62	36

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

Mol	Chain	Res	Type
1	AAA	1(A)	LEU
1	AAA	27	GLN
1	AAA	49[A]	GLU
1	AAA	49[B]	GLU
1	AAA	142	GLU
1	AAA	172(J)	LYS
1	BBB	27	GLN
1	BBB	39	HIS
1	CCC	1(A)	LEU
1	CCC	3	MET
1	CCC	27	GLN
1	CCC	43	MET

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)

13 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	SO4	BBB	303	-	4,4,4	0.42	0	6,6,6	0.12	0
2	SO4	BBB	304	-	4,4,4	0.41	0	6,6,6	0.08	0
2	SO4	BBB	302	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	CCC	303	-	4,4,4	0.40	0	6,6,6	0.05	0
2	SO4	BBB	301	-	4,4,4	0.43	0	6,6,6	0.18	0
2	SO4	AAA	301	-	4,4,4	0.40	0	6,6,6	0.15	0
2	SO4	AAA	303	-	4,4,4	0.43	0	6,6,6	0.06	0
3	JGT	BBB	305	-	19,20,20	1.41	2 (10%)	24,28,28	2.42	11 (45%)
2	SO4	AAA	302	-	4,4,4	0.21	0	6,6,6	0.13	0
3	JGT	CCC	304	-	19,20,20	1.54	3 (15%)	24,28,28	2.00	10 (41%)
3	JGT	AAA	304	-	19,20,20	1.58	2 (10%)	24,28,28	2.01	10 (41%)
2	SO4	CCC	302	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	CCC	301	-	4,4,4	0.50	0	6,6,6	0.10	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
3	JGT	BBB	305	-	-	0/4/11/11	0/3/3/3
3	JGT	AAA	304	-	-	0/4/11/11	0/3/3/3
3	JGT	CCC	304	-	-	0/4/11/11	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	304	JGT	C23-N24	-4.96	1.28	1.35
3	CCC	304	JGT	C23-N24	-4.66	1.28	1.35
3	BBB	305	JGT	BR1-C2	-3.16	1.82	1.89
3	BBB	305	JGT	C23-N24	-3.11	1.30	1.35
3	AAA	304	JGT	BR1-C2	-2.70	1.83	1.89
3	CCC	304	JGT	C17-C19	2.34	1.42	1.36
3	CCC	304	JGT	BR1-C2	-2.21	1.84	1.89

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BBB	305	JGT	BR1-C2-C7	-5.27	109.40	118.39
3	AAA	304	JGT	C4-C3-N21	4.34	124.90	119.13
3	BBB	305	JGT	BR1-C2-C3	4.09	124.51	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CCC	304	JGT	C4-C3-N21	3.78	124.14	119.13
3	CCC	304	JGT	C25-C28-N31	-3.76	98.00	105.26
3	BBB	305	JGT	C4-C3-N21	3.75	124.11	119.13
3	CCC	304	JGT	BR1-C2-C3	3.37	123.66	119.73
3	BBB	305	JGT	C2-C3-C4	-3.36	114.14	117.61
3	AAA	304	JGT	BR1-C2-C7	-3.24	112.86	118.39
3	AAA	304	JGT	C6-C7-C2	-3.02	119.65	121.30
3	BBB	305	JGT	C25-C28-N31	-3.02	99.43	105.26
3	CCC	304	JGT	BR1-C2-C7	-3.01	113.25	118.39
3	BBB	305	JGT	C19-C4-C3	-2.95	119.46	124.78
3	BBB	305	JGT	C3-C4-C5	2.94	121.17	117.66
3	CCC	304	JGT	C9-C6-C7	-2.64	116.89	120.74
3	AAA	304	JGT	C13-C5-C6	-2.57	118.76	123.66
3	AAA	304	JGT	C25-C28-N31	-2.57	100.31	105.26
3	AAA	304	JGT	C3-C4-C5	2.56	120.71	117.66
3	BBB	305	JGT	C9-C6-C5	2.54	125.01	121.08
3	CCC	304	JGT	C28-C25-N24	2.51	104.60	101.69
3	AAA	304	JGT	BR1-C2-C3	2.48	122.62	119.73
3	CCC	304	JGT	C28-N31-C23	2.45	112.67	106.53
3	CCC	304	JGT	C13-C5-C6	-2.36	119.15	123.66
3	BBB	305	JGT	C7-C2-C3	2.34	125.95	121.85
3	BBB	305	JGT	C6-C5-C4	2.29	121.33	119.76
3	BBB	305	JGT	C13-C5-C6	-2.28	119.31	123.66
3	CCC	304	JGT	C9-C6-C5	2.12	124.35	121.08
3	CCC	304	JGT	C6-C5-C4	2.09	121.19	119.76
3	AAA	304	JGT	C19-C4-C3	-2.04	121.11	124.78
3	AAA	304	JGT	C28-N31-C23	2.03	111.63	106.53
3	AAA	304	JGT	C9-C6-C7	-2.01	117.80	120.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

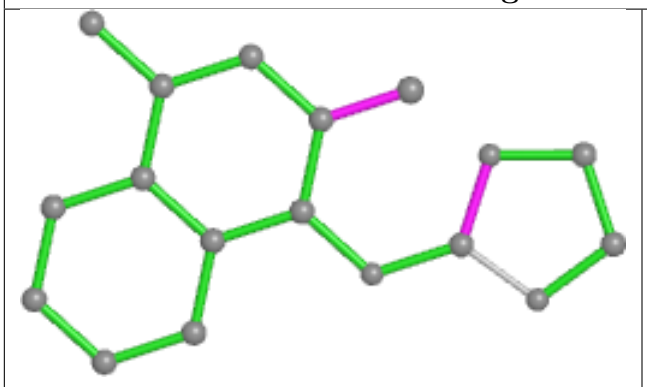
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	302	SO4	1	0
3	CCC	304	JGT	1	0

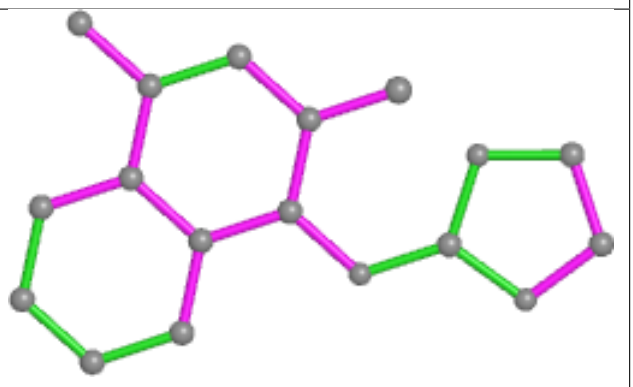
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

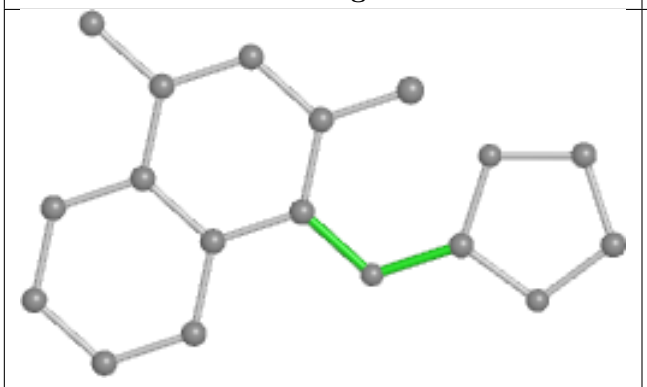
Ligand JGT BBB 305



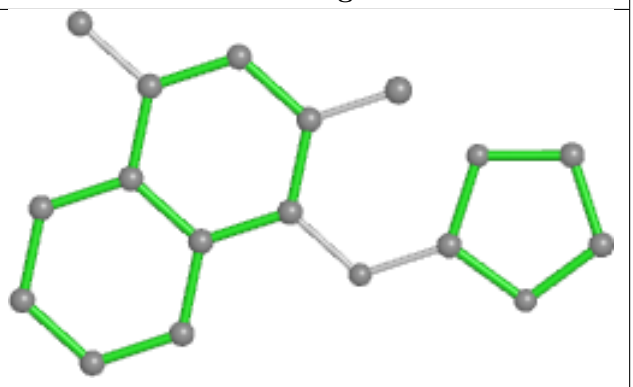
Bond lengths



Bond angles

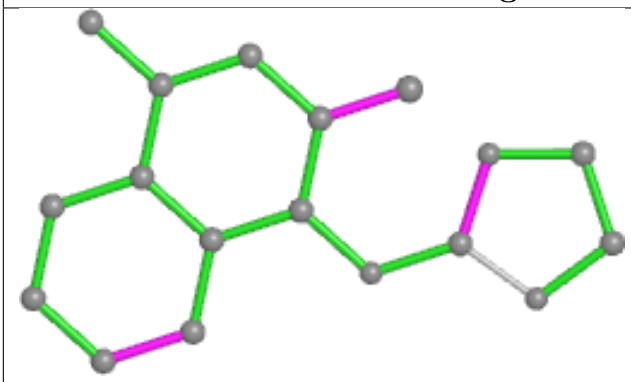


Torsions

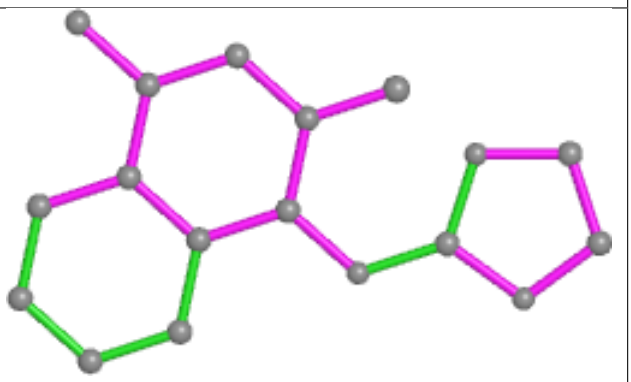


Rings

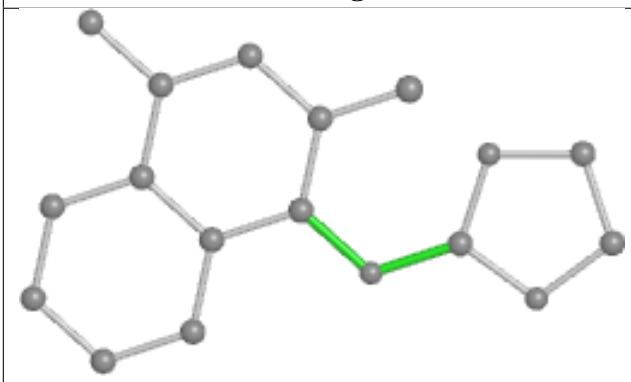
Ligand JGT CCC 304



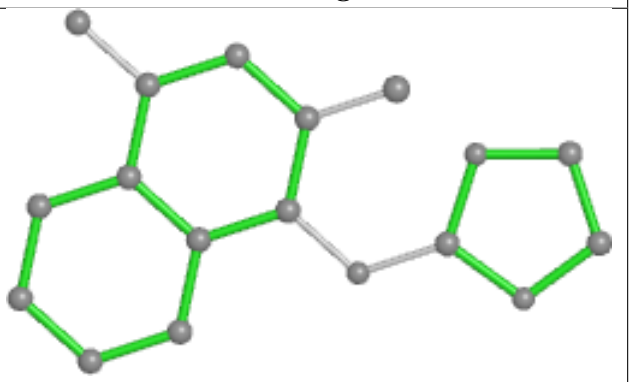
Bond lengths



Bond angles

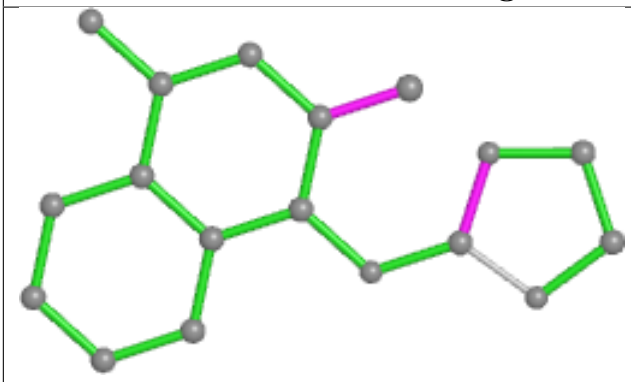


Torsions

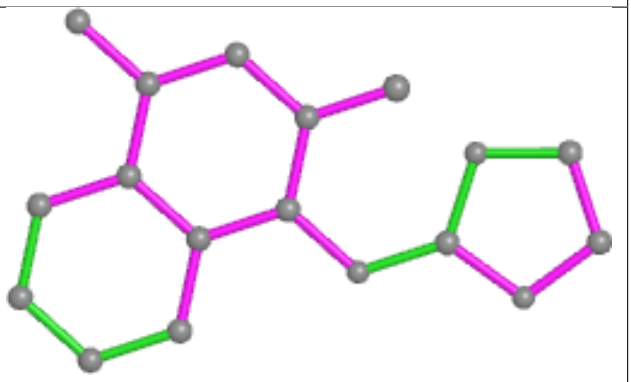


Rings

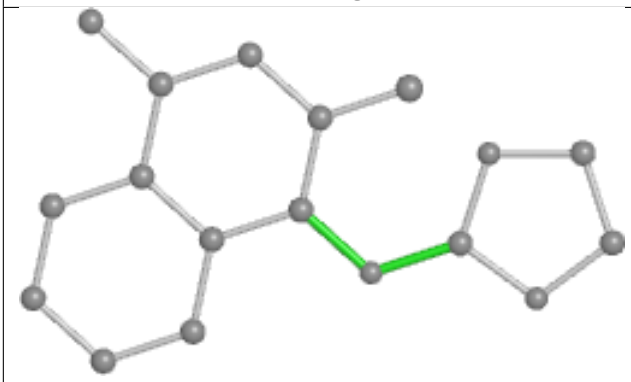
Ligand JGT AAA 304



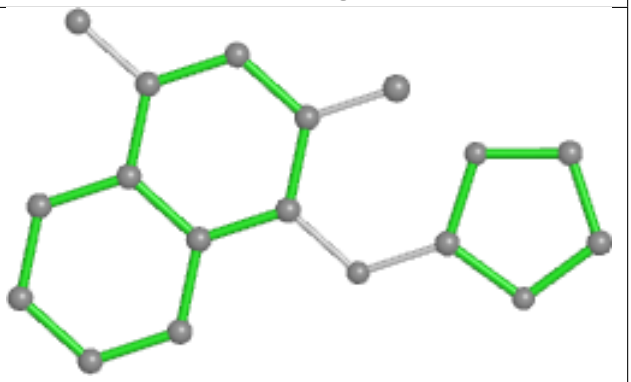
Bond lengths



Bond angles



Torsions



Rings

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

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, 95^{th} 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	264/291 (90%)	-0.17	6 (2%)	60	60	12, 19, 43, 125	0
1	BBB	269/291 (92%)	-0.13	4 (1%)	73	74	11, 18, 39, 62	0
1	CCC	263/291 (90%)	-0.06	10 (3%)	40	38	13, 21, 48, 81	0
All	All	796/873 (91%)	-0.12	20 (2%)	57	56	11, 19, 45, 125	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	5	TRP	9.2
1	AAA	24	TYR	7.3
1	CCC	24	TYR	7.1
1	BBB	5	TRP	5.5
1	CCC	38	GLY	5.5
1	AAA	39	HIS	5.1
1	CCC	23	ASP	4.3
1	CCC	36	ILE	4.3
1	BBB	60(C)	ASP	4.3
1	AAA	38	GLY	3.9
1	CCC	39	HIS	3.4
1	AAA	143	GLU	3.4
1	BBB	36	ILE	3.2
1	CCC	144	LYS	3.1
1	CCC	143	GLU	2.9
1	CCC	25	HIS	2.6
1	BBB	24	TYR	2.4
1	AAA	25	HIS	2.3
1	AAA	70	GLY	2.3
1	CCC	142	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

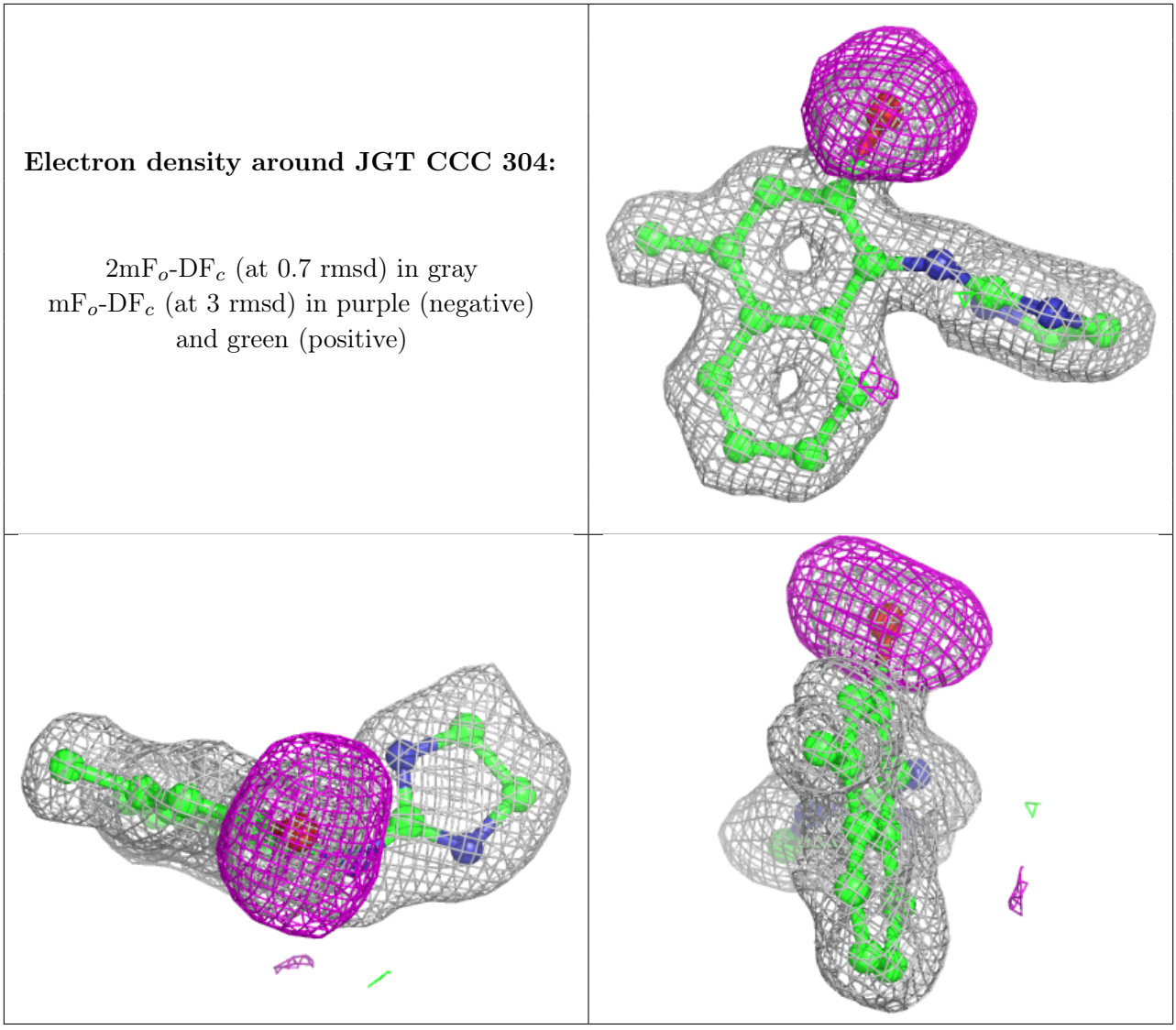
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	JGT	CCC	304	18/18	0.90	0.09	17,20,27,52	0
3	JGT	BBB	305	18/18	0.92	0.10	12,14,17,37	0
3	JGT	AAA	304	18/18	0.92	0.09	13,14,18,38	0
2	SO4	BBB	302	5/5	0.97	0.06	29,30,33,40	0
2	SO4	AAA	302	5/5	0.97	0.10	31,35,41,50	0
2	SO4	CCC	303	5/5	0.98	0.07	47,58,60,71	0
2	SO4	AAA	303	5/5	0.98	0.08	38,40,44,53	0
2	SO4	BBB	304	5/5	0.98	0.08	40,41,49,51	0
2	SO4	CCC	302	5/5	0.98	0.06	26,27,28,31	0
2	SO4	CCC	301	5/5	0.99	0.08	35,36,43,45	0
2	SO4	BBB	303	5/5	0.99	0.07	31,33,44,47	0
2	SO4	BBB	301	5/5	0.99	0.06	25,26,31,32	0
2	SO4	AAA	301	5/5	1.00	0.07	23,24,32,32	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.

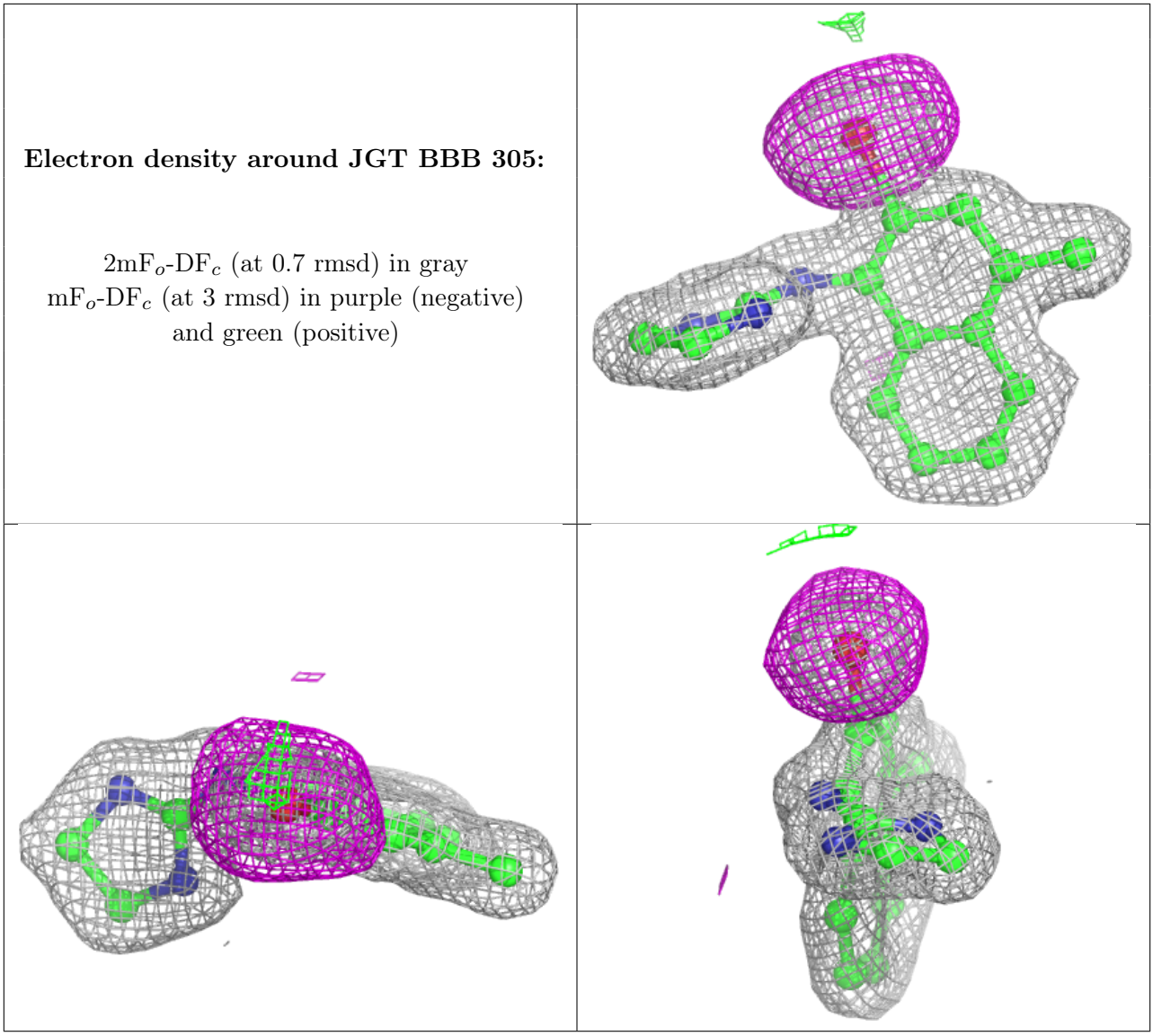
Electron density around JGT CCC 304:

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



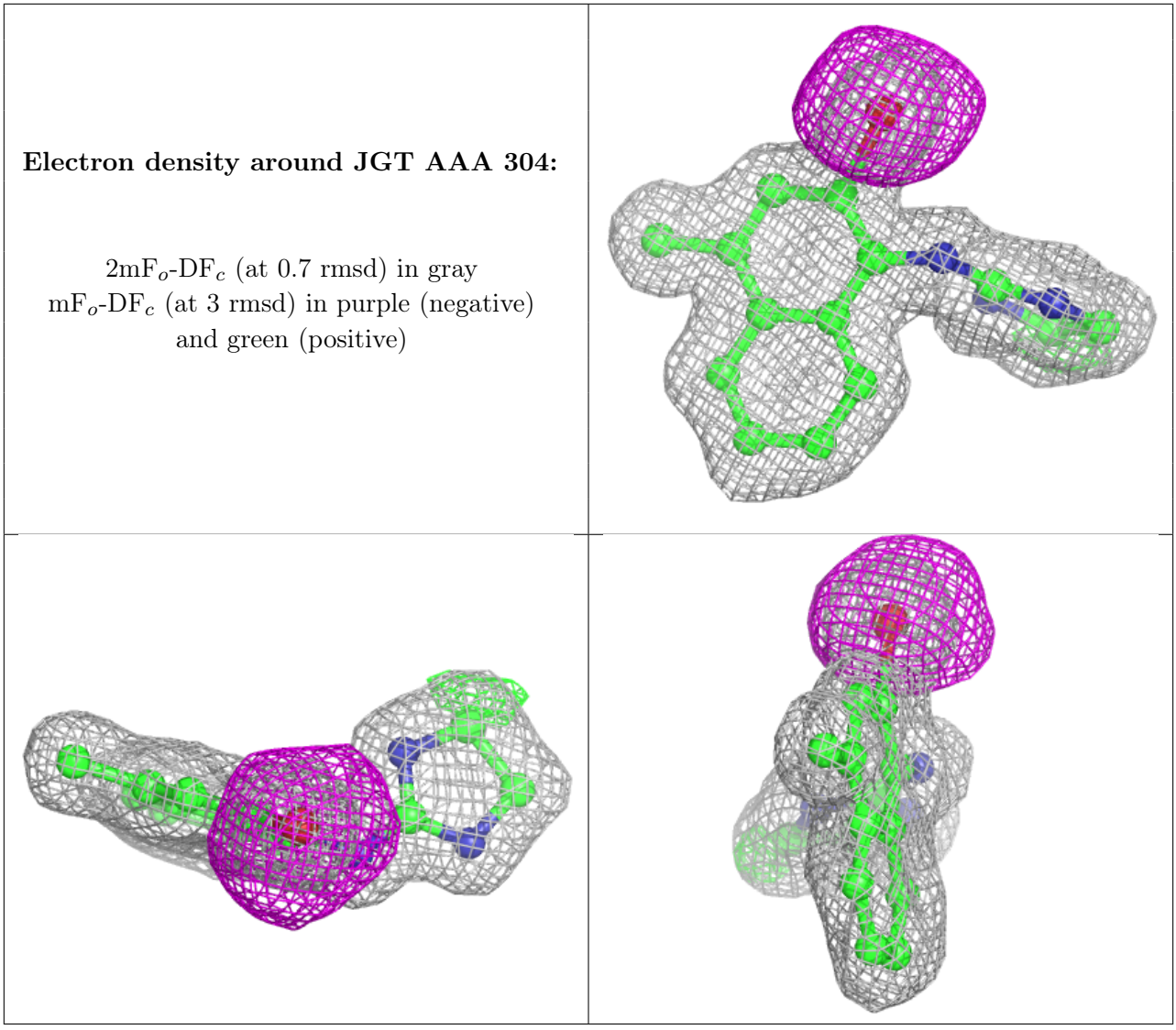
Electron density around JGT BBB 305:

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



Electron density around JGT AAA 304:

$2mF_o$-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.