Full wwPDB X-ray Structure Validation Report (i)

Jan 10, 2024 – 04:56 pm GMT

PDB ID	:	7OJM
Title	:	CRYSTAL STRUCTURE OF THE COFACTOR-DEVOID 1-H-3-HYDROXY-4- OXOQUINALDINE 2,4-DIOXYGENASE (HOD) CATALYTICALLY INACTIVE H251A VARIANT COMPLEXED WITH 2-METHYL-QUINOLIN-4(1H)-ONE UNDER NORMOXIC CONDITIONS
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Deposited on	:	2021-05-16
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

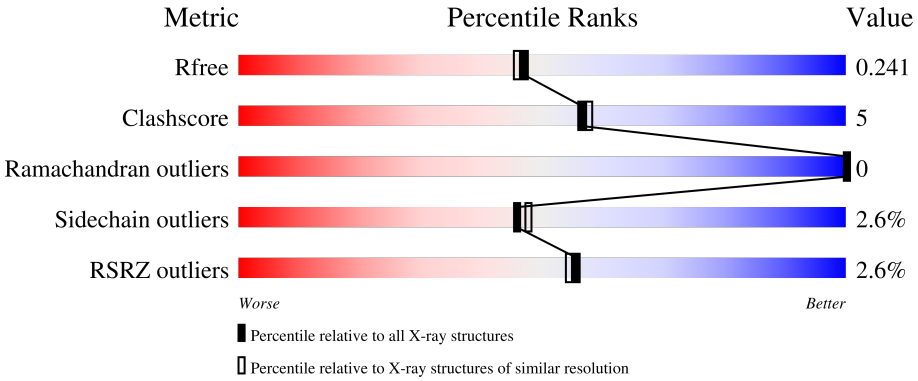
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	288	2% 84% 10% • 5%
1	BBB	288	2% 82% 12% 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4851 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 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	273	Total	C	N	O	S	0	3	0
			2248	1433	394	413	8			
1	BBB	273	Total	C	N	O	S	0	4	0
			2254	1436	394	416	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-11	MET	-	initiating methionine	UNP O31266
AAA	-10	ARG	-	expression tag	UNP O31266
AAA	-9	GLY	-	expression tag	UNP O31266
AAA	-8	SER	-	expression tag	UNP O31266
AAA	-7	HIS	-	expression tag	UNP O31266
AAA	-6	HIS	-	expression tag	UNP O31266
AAA	-5	HIS	-	expression tag	UNP O31266
AAA	-4	HIS	-	expression tag	UNP O31266
AAA	-3	HIS	-	expression tag	UNP O31266
AAA	-2	HIS	-	expression tag	UNP O31266
AAA	-1	GLY	-	expression tag	UNP O31266
AAA	0	SER	-	expression tag	UNP O31266
AAA	69	SER	CYS	engineered mutation	UNP O31266
AAA	251	ALA	HIS	engineered mutation	UNP O31266
BBB	-11	MET	-	initiating methionine	UNP O31266
BBB	-10	ARG	-	expression tag	UNP O31266
BBB	-9	GLY	-	expression tag	UNP O31266
BBB	-8	SER	-	expression tag	UNP O31266
BBB	-7	HIS	-	expression tag	UNP O31266
BBB	-6	HIS	-	expression tag	UNP O31266
BBB	-5	HIS	-	expression tag	UNP O31266
BBB	-4	HIS	-	expression tag	UNP O31266
BBB	-3	HIS	-	expression tag	UNP O31266
BBB	-2	HIS	-	expression tag	UNP O31266
BBB	-1	GLY	-	expression tag	UNP O31266

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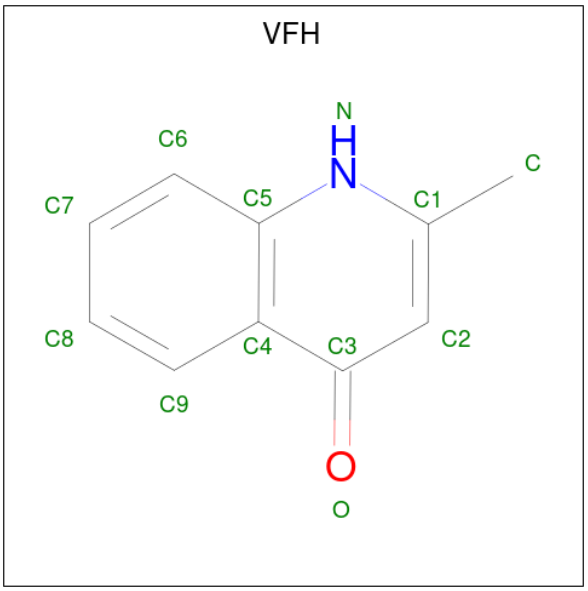
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	SER	-	expression tag	UNP O31266
BBB	69	SER	CYS	engineered mutation	UNP O31266
BBB	251	ALA	HIS	engineered mutation	UNP O31266

- Molecule 2 is 2-methyl-quinolin-4(1H)-one (three-letter code: VFH) (formula: $C_{10}H_9NO$) (labeled as "Ligand of Interest" by depositor).

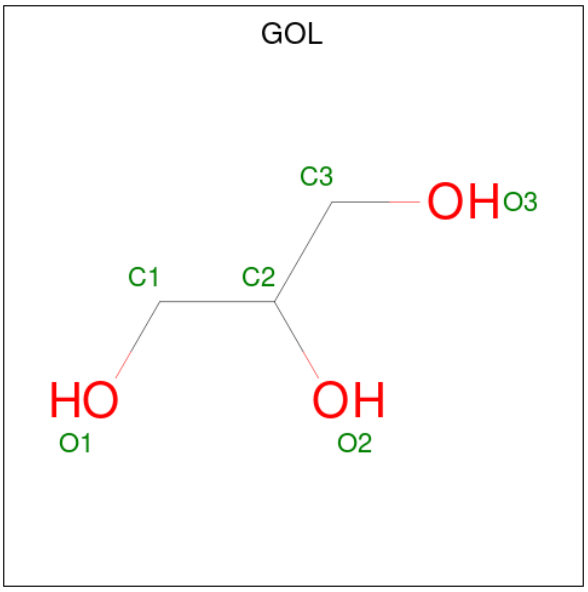


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C N O 12 10 1 1	0	0
2	BBB	1	Total C N O 12 10 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

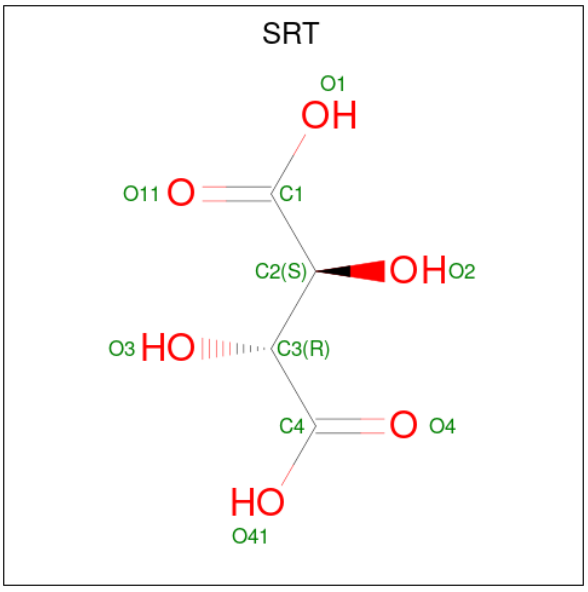
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	2	Total K 2 2	0	0
3	BBB	1	Total K 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 10 4 6	0	0
5	BBB	1	Total C O 10 4 6	0	0
5	BBB	1	Total C O 10 4 6	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	1	Total Na 1 1	0	0

- Molecule 7 is water.

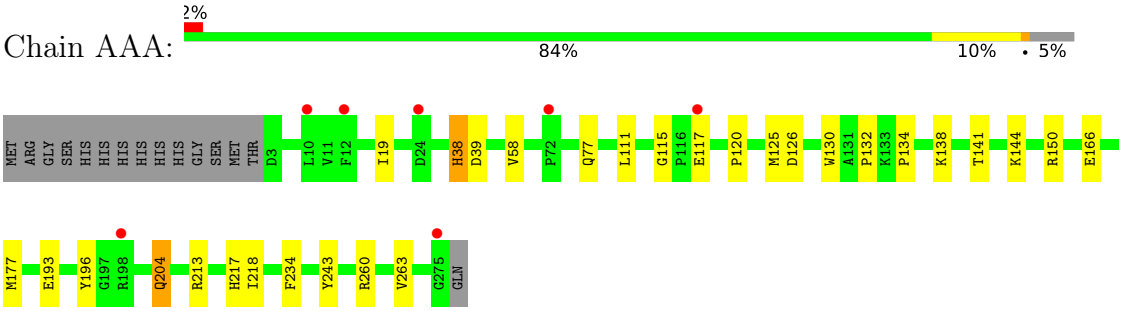
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	150	Total O 157 157	0	7
7	BBB	94	Total O 100 100	0	6

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.

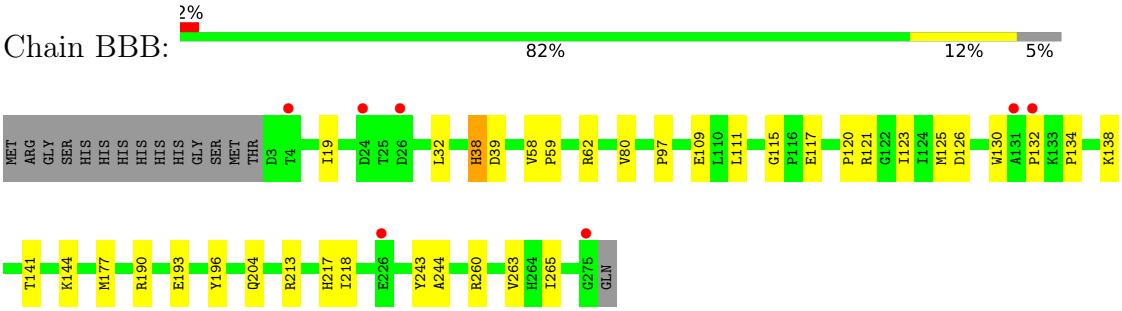
• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain AAA:



• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	119.19Å 119.19Å 44.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.14 – 2.00 42.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.14-2.00) 99.2 (42.14-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.237 0.207 , 0.241	Depositor DCC
R_{free} test set	2117 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 22.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.108 for h,-k,-l	Xtriage
Reported twinning fraction	0.838 for H, K, L 0.162 for -K, -H, -L	Depositor
Outliers	0 of 42344 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4851	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% 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: NA, GOL, VFH, K, SRT

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	0.65	0/2318	0.76	0/3153
1	BBB	0.64	0/2324	0.76	0/3163
All	All	0.65	0/4642	0.76	0/6316

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	2248	0	2137	25	0
1	BBB	2254	0	2137	21	0
2	AAA	12	0	0	1	0
2	BBB	12	0	0	0	0
3	AAA	2	0	0	0	0
3	BBB	1	0	0	0	0
4	AAA	24	0	30	5	0
5	AAA	20	0	8	0	0
5	BBB	20	0	7	1	0
6	BBB	1	0	0	0	0
7	AAA	157	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BBB	100	0	0	4	0
All	All	4851	0	4319	45	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 5.

All (45) 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:AAA:166[B]:GLU:OE1	1:AAA:166[B]:GLU:C	2.21	0.79
1:AAA:204:GLN:HG2	4:AAA:306[A]:GOL:H31	1.66	0.76
1:BBB:62:ARG:NE	7:BBB:403:HOH:O	2.25	0.70
1:AAA:77:GLN:HB2	1:BBB:190:ARG:HD2	1.77	0.66
1:AAA:150:ARG:NH1	7:AAA:407:HOH:O	2.32	0.62
1:AAA:111:LEU:O	1:AAA:213:ARG:NH1	2.36	0.58
1:AAA:120:PRO:O	1:AAA:213:ARG:HG2	2.03	0.58
1:BBB:111:LEU:O	1:BBB:213:ARG:NH1	2.38	0.56
1:BBB:120:PRO:O	1:BBB:213:ARG:HG2	2.06	0.56
1:AAA:38:HIS:HB3	1:AAA:177:MET:HE2	1.91	0.53
1:AAA:204:GLN:HG2	4:AAA:306[A]:GOL:C3	2.38	0.52
1:AAA:132:PRO:HD3	1:AAA:196:TYR:CD1	2.45	0.52
1:BBB:132:PRO:HD3	1:BBB:196:TYR:CD1	2.44	0.52
1:BBB:38:HIS:HB3	1:BBB:177:MET:HE2	1.92	0.52
1:AAA:19:ILE:HB	1:AAA:58:VAL:HB	1.92	0.51
1:AAA:234:PHE:HE1	4:AAA:306[B]:GOL:H32	1.75	0.50
1:BBB:213:ARG:NH2	7:BBB:411:HOH:O	2.45	0.50
1:AAA:204:GLN:HG3	7:AAA:463:HOH:O	2.12	0.49
1:AAA:144:LYS:NZ	1:AAA:193:GLU:OE1	2.34	0.49
1:BBB:217:HIS:O	1:BBB:243:TYR:HA	2.13	0.49
1:BBB:19:ILE:HB	1:BBB:58:VAL:HB	1.96	0.47
1:AAA:217:HIS:O	1:AAA:243:TYR:HA	2.15	0.47
1:BBB:144:LYS:NZ	1:BBB:193:GLU:OE1	2.34	0.47
1:AAA:134:PRO:O	1:AAA:138:LYS:HG3	2.14	0.47
1:BBB:134:PRO:O	1:BBB:138:LYS:HG3	2.16	0.46
1:AAA:234:PHE:CE1	4:AAA:306[B]:GOL:H32	2.50	0.45
1:AAA:138:LYS:O	1:AAA:141:THR:HB	2.17	0.45
1:AAA:204:GLN:CG	4:AAA:306[A]:GOL:H31	2.42	0.44
1:BBB:138:LYS:O	1:BBB:141:THR:HB	2.18	0.44
5:BBB:304:SRT:H2	7:BBB:405:HOH:O	2.17	0.43
1:BBB:115:GLY:HA2	7:BBB:433:HOH:O	2.20	0.42
1:AAA:166[B]:GLU:OE1	1:AAA:166[B]:GLU:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:125:MET:HA	1:BBB:218:ILE:O	2.19	0.41
1:BBB:80:VAL:HG21	1:BBB:109:GLU:HB3	2.02	0.41
1:BBB:260:ARG:O	1:BBB:263:VAL:HG22	2.20	0.41
1:AAA:77:GLN:CB	1:BBB:190:ARG:HD2	2.48	0.41
1:AAA:125:MET:HA	1:AAA:218:ILE:O	2.20	0.41
1:BBB:32:LEU:O	1:BBB:59:PRO:HD2	2.20	0.41
1:AAA:177:MET:HE1	2:AAA:301:VFH:C	2.51	0.41
1:AAA:132:PRO:HD3	1:AAA:196:TYR:CG	2.56	0.41
1:BBB:97:PRO:HD2	1:BBB:121:ARG:O	2.20	0.41
1:BBB:218:ILE:HG22	1:BBB:244:ALA:HB3	2.03	0.41
1:BBB:123:ILE:CD1	1:BBB:265:ILE:HA	2.51	0.41
1:AAA:260:ARG:O	1:AAA:263:VAL:HG22	2.20	0.40
1:AAA:115:GLY:HA2	7:AAA:452:HOH:O	2.20	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	274/288 (95%)	264 (96%)	10 (4%)	0	100	100
1	BBB	275/288 (96%)	264 (96%)	11 (4%)	0	100	100
All	All	549/576 (95%)	528 (96%)	21 (4%)	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	237/247 (96%)	231 (98%)	6 (2%)	47	49
1	BBB	238/247 (96%)	232 (98%)	6 (2%)	47	49
All	All	475/494 (96%)	463 (98%)	12 (2%)	46	49

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

Mol	Chain	Res	Type
1	AAA	38	HIS
1	AAA	39	ASP
1	AAA	117	GLU
1	AAA	126	ASP
1	AAA	130	TRP
1	AAA	204	GLN
1	BBB	38	HIS
1	BBB	39	ASP
1	BBB	117	GLU
1	BBB	126	ASP
1	BBB	130	TRP
1	BBB	204	GLN

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)

Of 14 ligands modelled in this entry, 4 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	SRT	AAA	308	3	9,9,9	1.00	0	12,12,12	1.12	1 (8%)
5	SRT	AAA	307	-	9,9,9	0.97	0	12,12,12	1.24	2 (16%)
2	VFH	BBB	301	-	13,13,13	0.29	0	18,18,18	0.36	0
4	GOL	AAA	305	-	5,5,5	0.08	0	5,5,5	0.24	0
4	GOL	AAA	306[B]	-	5,5,5	0.10	0	5,5,5	0.29	0
5	SRT	BBB	305	3	9,9,9	1.22	1 (11%)	12,12,12	1.03	0
5	SRT	BBB	304	-	9,9,9	1.15	1 (11%)	12,12,12	0.98	0
2	VFH	AAA	301	-	13,13,13	0.33	0	18,18,18	0.36	0
4	GOL	AAA	306[A]	-	5,5,5	0.07	0	5,5,5	0.31	0
4	GOL	AAA	304	3	5,5,5	0.12	0	5,5,5	0.36	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	SRT	AAA	308	3	-	6/12/12/12	-
5	SRT	AAA	307	-	-	11/12/12/12	-
2	VFH	BBB	301	-	-	-	0/2/2/2
4	GOL	AAA	305	-	-	2/4/4/4	-
4	GOL	AAA	306[B]	-	-	2/4/4/4	-
5	SRT	BBB	305	3	-	2/12/12/12	-
5	SRT	BBB	304	-	-	12/12/12/12	-
2	VFH	AAA	301	-	-	-	0/2/2/2
4	GOL	AAA	306[A]	-	-	2/4/4/4	-
4	GOL	AAA	304	3	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	BBB	305	SRT	O41-C4	-2.22	1.23	1.30
5	BBB	304	SRT	O1-C1	-2.09	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AAA	307	SRT	O11-C1-C2	-2.38	115.37	121.63
5	AAA	307	SRT	O1-C1-C2	2.38	119.70	113.27
5	AAA	308	SRT	O11-C1-C2	-2.03	116.30	121.63

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	306[B]	GOL	O1-C1-C2-C3
5	BBB	304	SRT	O11-C1-C2-O2
5	BBB	304	SRT	O2-C2-C3-O3
5	BBB	304	SRT	C1-C2-C3-O3
5	AAA	308	SRT	C1-C2-C3-C4
5	BBB	304	SRT	C1-C2-C3-C4
5	AAA	308	SRT	O2-C2-C3-C4
5	BBB	304	SRT	O2-C2-C3-C4
5	AAA	307	SRT	O1-C1-C2-O2
5	AAA	307	SRT	O11-C1-C2-O2
5	BBB	304	SRT	O1-C1-C2-O2
5	AAA	307	SRT	O1-C1-C2-C3
5	AAA	307	SRT	O2-C2-C3-O3
5	AAA	307	SRT	O11-C1-C2-C3
5	BBB	305	SRT	O2-C2-C3-C4
5	BBB	304	SRT	O11-C1-C2-C3
4	AAA	306[B]	GOL	O1-C1-C2-O2
5	BBB	305	SRT	C1-C2-C3-C4
5	AAA	307	SRT	O2-C2-C3-C4
5	AAA	308	SRT	C1-C2-C3-O3
5	AAA	307	SRT	O3-C3-C4-O41
5	AAA	307	SRT	O3-C3-C4-O4
5	AAA	308	SRT	C2-C3-C4-O4
5	BBB	304	SRT	O1-C1-C2-C3
5	AAA	308	SRT	O2-C2-C3-O3
5	AAA	308	SRT	C2-C3-C4-O41
4	AAA	306[A]	GOL	O1-C1-C2-O2
4	AAA	306[A]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	AAA	307	SRT	C1-C2-C3-O3
5	BBB	304	SRT	C2-C3-C4-O4
5	AAA	307	SRT	C2-C3-C4-O4
5	BBB	304	SRT	O3-C3-C4-O41
5	BBB	304	SRT	C2-C3-C4-O41
5	AAA	307	SRT	C2-C3-C4-O41
5	BBB	304	SRT	O3-C3-C4-O4
4	AAA	305	GOL	O1-C1-C2-C3
4	AAA	305	GOL	O1-C1-C2-O2

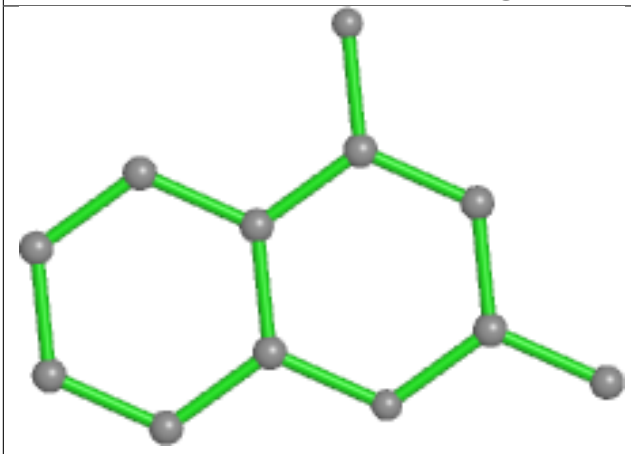
There are no ring outliers.

4 monomers are involved in 7 short contacts:

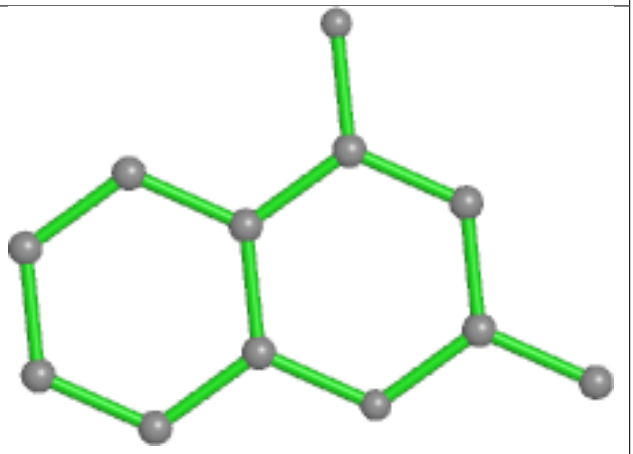
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	306[B]	GOL	2	0
5	BBB	304	SRT	1	0
2	AAA	301	VFH	1	0
4	AAA	306[A]	GOL	3	0

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.

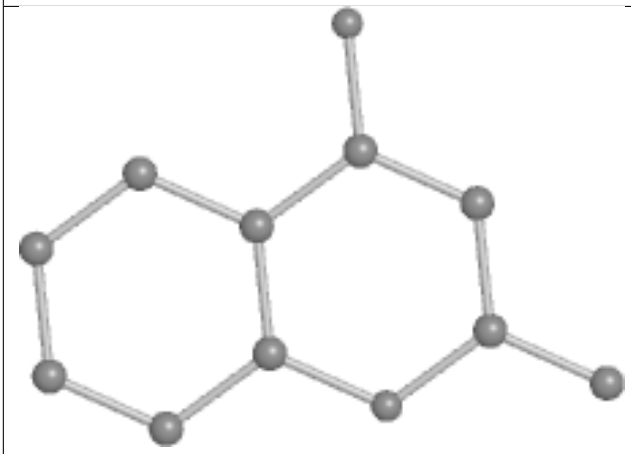
Ligand VFH BBB 301



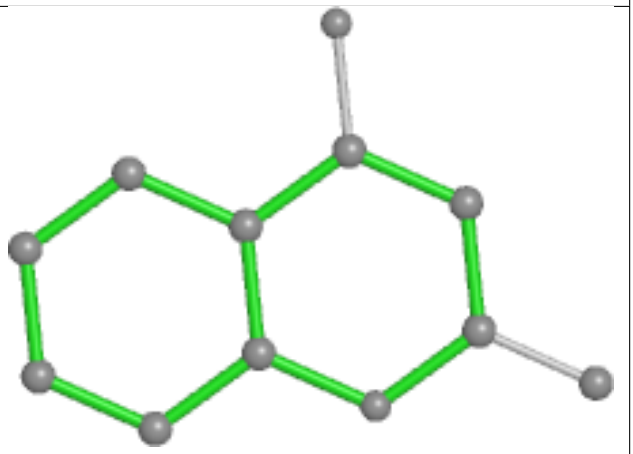
Bond lengths



Bond angles

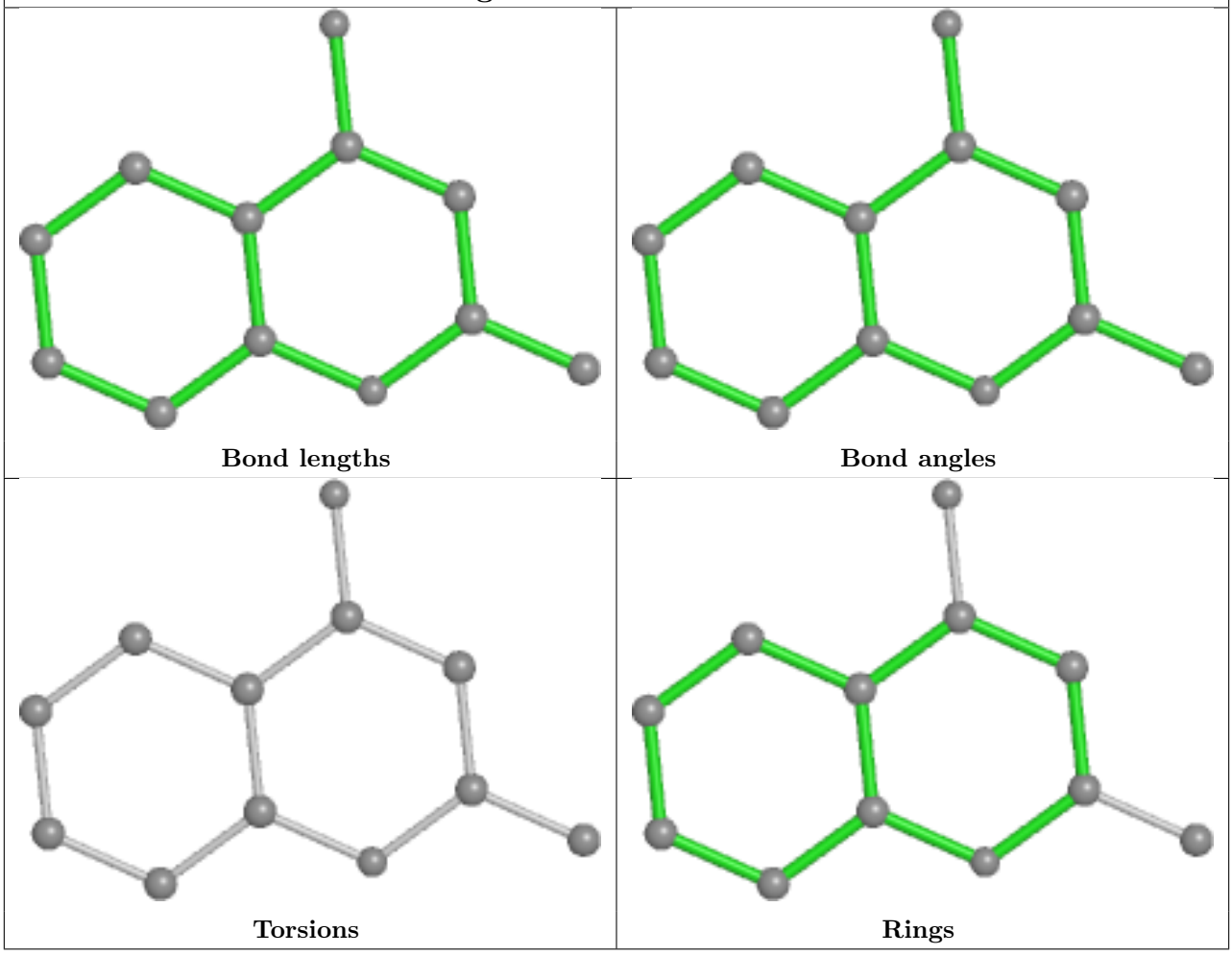


Torsions



Rings

Ligand VFH AAA 301



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	273/288 (94%)	0.31	7 (2%)	56	54	17, 31, 54, 80	0
1	BBB	273/288 (94%)	0.41	7 (2%)	56	54	20, 36, 53, 74	0
All	All	546/576 (94%)	0.36	14 (2%)	56	54	17, 34, 54, 80	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	275	GLY	7.5
1	BBB	24	ASP	5.5
1	AAA	24	ASP	3.9
1	AAA	12	PHE	3.8
1	BBB	131	ALA	2.8
1	BBB	4	THR	2.6
1	BBB	132	PRO	2.5
1	AAA	72	PRO	2.3
1	BBB	226	GLU	2.3
1	BBB	26	ASP	2.2
1	AAA	10	LEU	2.2
1	AAA	117	GLU	2.1
1	AAA	198	ARG	2.1
1	AAA	275	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

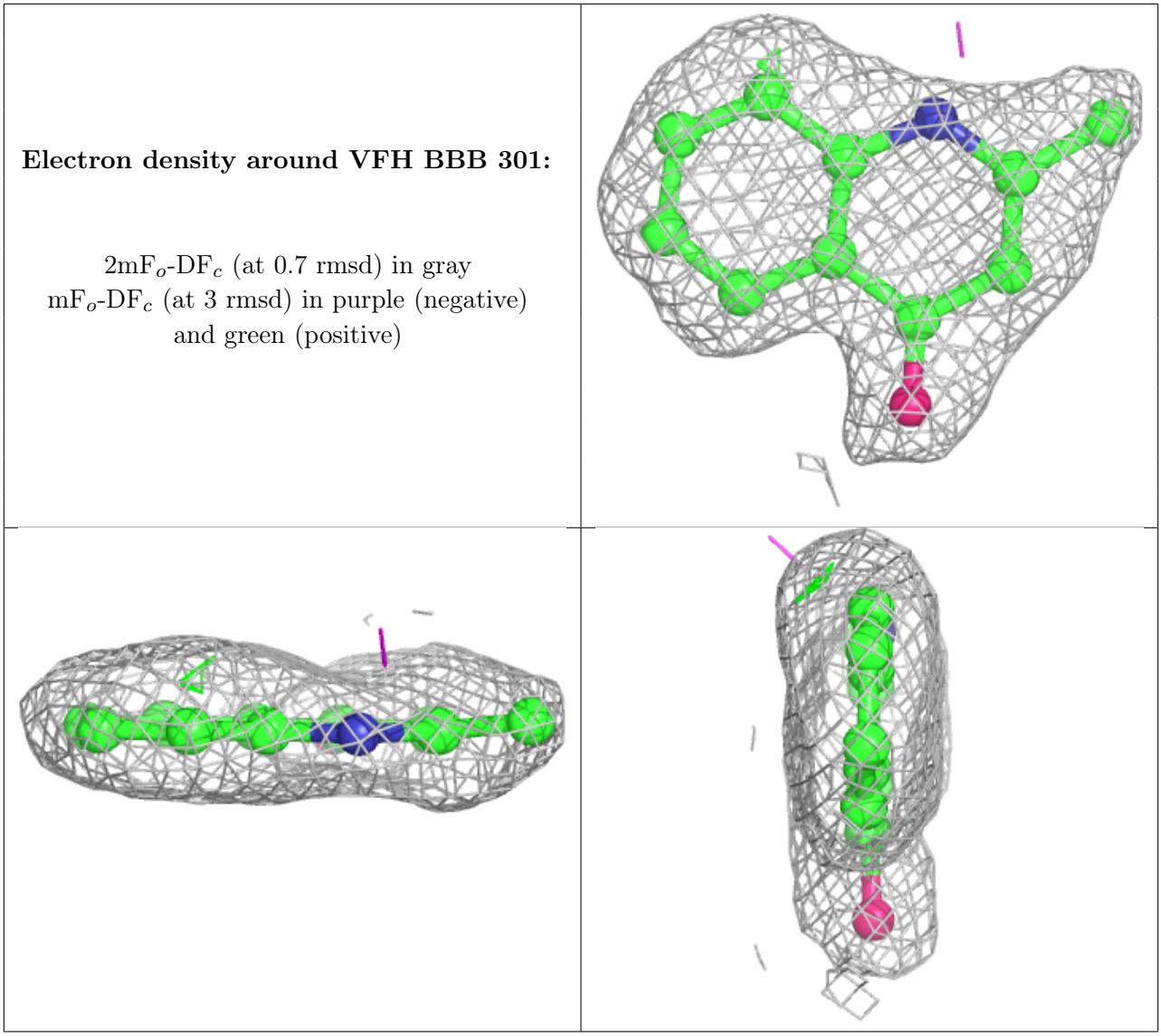
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GOL	AAA	306[A]	6/6	0.79	0.22	25,25,26,27	6
4	GOL	AAA	306[B]	6/6	0.79	0.22	30,32,32,32	6
5	SRT	AAA	308	10/10	0.81	0.19	26,33,38,40	0
5	SRT	BBB	305	10/10	0.83	0.25	33,36,41,44	0
2	VFH	BBB	301	12/12	0.85	0.16	26,30,32,33	12
5	SRT	BBB	304	10/10	0.87	0.17	34,39,47,48	0
4	GOL	AAA	305	6/6	0.88	0.13	42,46,49,50	0
4	GOL	AAA	304	6/6	0.88	0.30	42,44,45,46	0
5	SRT	AAA	307	10/10	0.91	0.17	29,37,40,47	0
2	VFH	AAA	301	12/12	0.91	0.17	20,25,26,27	12
3	K	BBB	302	1/1	0.95	0.07	35,35,35,35	0
6	NA	BBB	303	1/1	0.96	0.09	26,26,26,26	0
3	K	AAA	303	1/1	0.97	0.07	32,32,32,32	0
3	K	AAA	302	1/1	1.00	0.04	30,30,30,30	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.

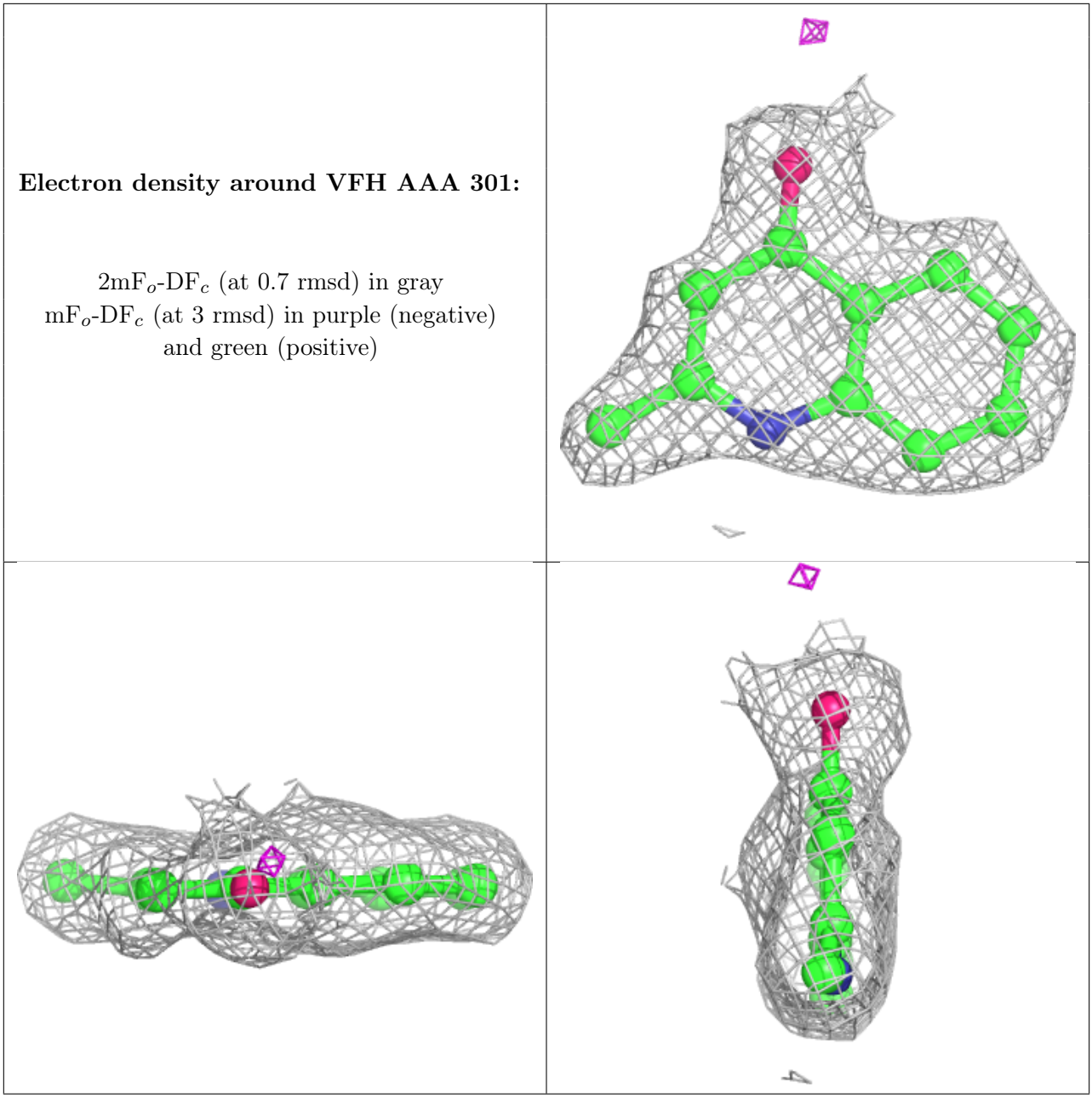
Electron density around VFH BBB 301:

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



Electron density around VFH AAA 301:

$2mF_o$-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.