Full wwPDB X-ray Structure Validation Report (i)

Jan 10, 2024 – 03:39 pm GMT

PDB ID	:	8OXN
Title	:	CRYSTAL STRUCTURE OF THE COFACTOR-DEVOID 1-H-3-HYDROXY-4- OXOQUINALDINE 2,4-DIOXYGENASE (HOD) S101A VARIANT COMPLEXED WITH 2-METHYL-QUINOLIN-4(1H)-ONE UNDER NORMOXYC CONDITIONS
Authors	:	Bui, S.; Steiner, R.A.
Deposited on	:	2023-05-02
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:

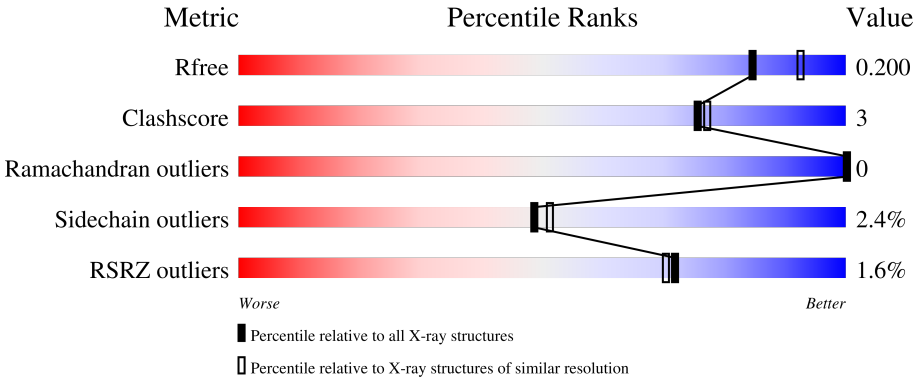
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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% 86% 8% 5%
1	BBB	288	% 88% 7% 5%
1	CCC	288	% 89% 6% 5%
1	DDD	288	2% 86% 8% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9196 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	2	0
			2243	1432	393	409	9			
1	BBB	273	Total	C	N	O	S	0	2	0
			2243	1433	393	409	8			
1	CCC	273	Total	C	N	O	S	0	2	0
			2243	1432	393	410	8			
1	DDD	273	Total	C	N	O	S	0	1	0
			2233	1427	391	407	8			

There are 56 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	101	ALA	SER	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

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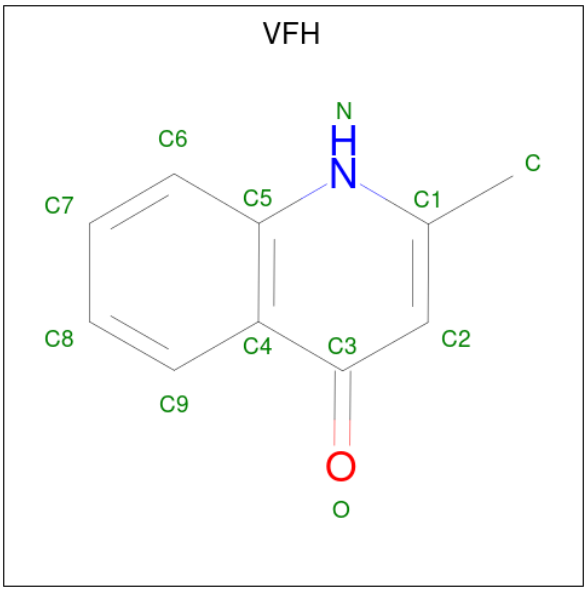
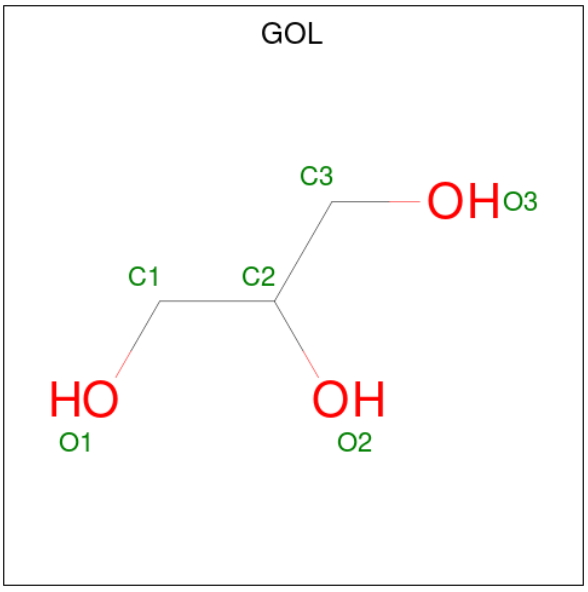
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-4	HIS	-	expression tag	UNP O31266
BBB	-3	HIS	-	expression tag	UNP O31266
BBB	-2	HIS	-	expression tag	UNP O31266
BBB	-1	GLY	-	expression tag	UNP O31266
BBB	0	SER	-	expression tag	UNP O31266
BBB	69	SER	CYS	engineered mutation	UNP O31266
BBB	101	ALA	SER	engineered mutation	UNP O31266
CCC	-11	MET	-	initiating methionine	UNP O31266
CCC	-10	ARG	-	expression tag	UNP O31266
CCC	-9	GLY	-	expression tag	UNP O31266
CCC	-8	SER	-	expression tag	UNP O31266
CCC	-7	HIS	-	expression tag	UNP O31266
CCC	-6	HIS	-	expression tag	UNP O31266
CCC	-5	HIS	-	expression tag	UNP O31266
CCC	-4	HIS	-	expression tag	UNP O31266
CCC	-3	HIS	-	expression tag	UNP O31266
CCC	-2	HIS	-	expression tag	UNP O31266
CCC	-1	GLY	-	expression tag	UNP O31266
CCC	0	SER	-	expression tag	UNP O31266
CCC	69	SER	CYS	engineered mutation	UNP O31266
CCC	101	ALA	SER	engineered mutation	UNP O31266
DDD	-11	MET	-	initiating methionine	UNP O31266
DDD	-10	ARG	-	expression tag	UNP O31266
DDD	-9	GLY	-	expression tag	UNP O31266
DDD	-8	SER	-	expression tag	UNP O31266
DDD	-7	HIS	-	expression tag	UNP O31266
DDD	-6	HIS	-	expression tag	UNP O31266
DDD	-5	HIS	-	expression tag	UNP O31266
DDD	-4	HIS	-	expression tag	UNP O31266
DDD	-3	HIS	-	expression tag	UNP O31266
DDD	-2	HIS	-	expression tag	UNP O31266
DDD	-1	GLY	-	expression tag	UNP O31266
DDD	0	SER	-	expression tag	UNP O31266
DDD	69	SER	CYS	engineered mutation	UNP O31266
DDD	101	ALA	SER	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).



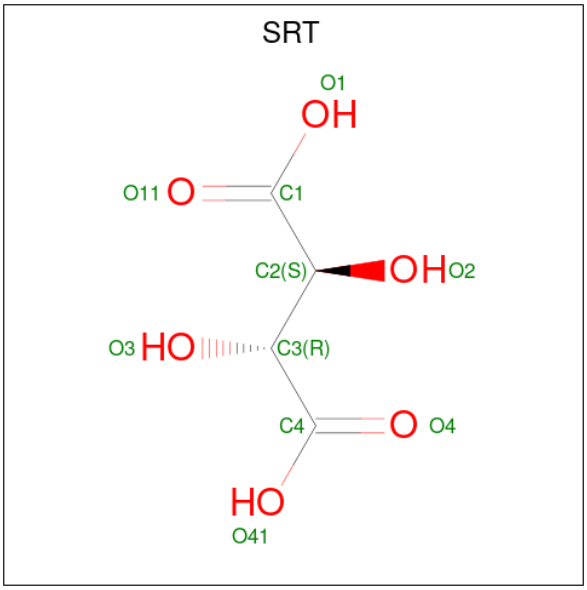
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			12	10	1	1		
2	BBB	1	Total	C	N	O	0	0
			12	10	1	1		
2	CCC	1	Total	C	N	O	0	0
			12	10	1	1		
2	DDD	1	Total	C	N	O	0	0
			12	10	1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 6 3 3	0	0
3	CCC	1	Total C O 6 3 3	0	0
3	DDD	1	Total C O 6 3 3	0	0

- Molecule 4 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: $C_4H_6O_6$).



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

- Molecule 5 is water.

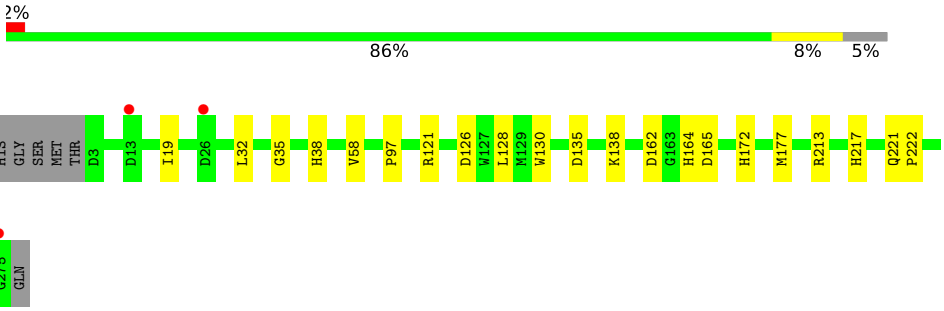
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	39	Total O 39 39	0	0
5	BBB	46	Total O 46 46	0	0
5	CCC	35	Total O 35 35	0	0
5	DDD	38	Total O 38 38	0	0

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.

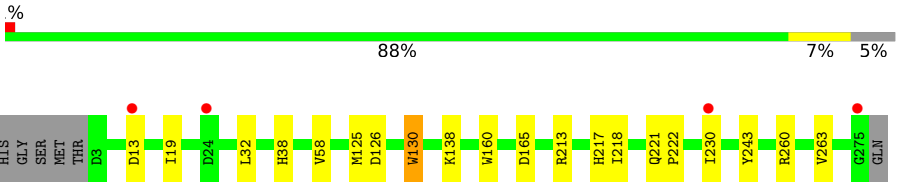
• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain AAA:



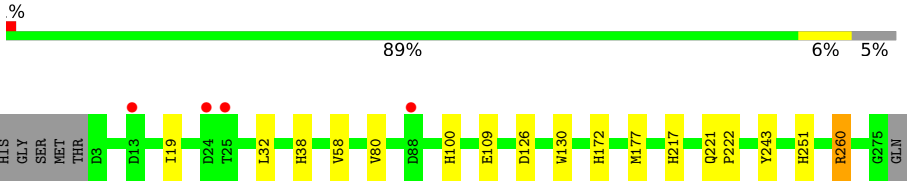
• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain BBB:



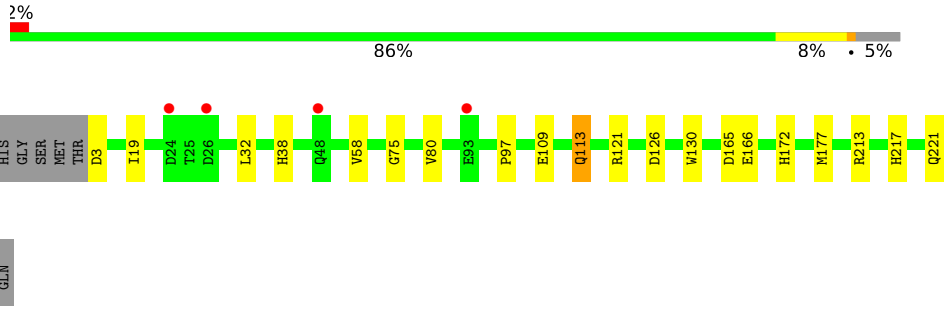
• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain CCC:



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

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.80Å 167.79Å 167.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.56 – 2.00 46.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.56-2.00) 99.8 (46.56-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.173 , 0.194 0.179 , 0.200	Depositor DCC
R_{free} test set	4298 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 23.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.457 for -h,l,k	Xtriage
Reported twinning fraction	0.529 for H, K, L 0.471 for -H, -L, -K	Depositor
Outliers	0 of 86660 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9196	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0318e-03.*

[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: VFH, SRT, 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	AAA	0.65	0/2314	0.76	0/3149
1	BBB	0.67	0/2314	0.76	1/3149 (0.0%)
1	CCC	0.66	0/2314	0.76	1/3149 (0.0%)
1	DDD	0.65	0/2304	0.76	0/3136
All	All	0.66	0/9246	0.76	2/12583 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	260	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	BBB	260	ARG	NE-CZ-NH2	-5.49	117.56	120.30

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	2243	0	2134	19	0
1	BBB	2243	0	2135	11	0
1	CCC	2243	0	2134	11	0
1	DDD	2233	0	2126	16	0
2	AAA	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	12	0	0	1	0
2	CCC	12	0	0	0	0
2	DDD	12	0	0	0	0
3	BBB	6	0	8	3	0
3	CCC	6	0	8	1	0
3	DDD	6	0	8	1	0
4	CCC	10	0	4	1	0
5	AAA	39	0	0	2	0
5	BBB	46	0	0	3	0
5	CCC	35	0	0	2	0
5	DDD	38	0	0	5	0
All	All	9196	0	8557	55	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 (55) 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:DDD:166:GLU:HG3	5:DDD:411:HOH:O	1.42	1.18
3:BBB:302:GOL:H11	5:BBB:415:HOH:O	1.76	0.84
1:AAA:165:ASP:OD2	1:CCC:260:ARG:HD3	1.90	0.70
1:AAA:263:VAL:HG21	3:DDD:302:GOL:H2	1.76	0.67
3:CCC:303:GOL:H12	5:CCC:431:HOH:O	1.94	0.65
1:AAA:165:ASP:OD2	1:CCC:260:ARG:CD	2.45	0.65
1:AAA:260:ARG:HD3	1:DDD:165:ASP:OD2	1.98	0.62
1:DDD:109:GLU:O	1:DDD:113:GLN:HG2	2.02	0.60
1:AAA:164:HIS:HD2	4:CCC:302:SRT:O41	1.87	0.57
1:BBB:130:TRP:HE3	1:BBB:230[B]:ILE:HD12	1.69	0.57
1:DDD:80:VAL:HG11	1:DDD:113:GLN:HG3	1.86	0.57
1:AAA:162:ASP:HB2	1:AAA:221[A]:GLN:HE22	1.70	0.56
1:AAA:172:HIS:NE2	1:AAA:177[A]:MET:HE2	2.21	0.56
1:CCC:260:ARG:NH2	5:CCC:402:HOH:O	2.38	0.55
1:DDD:172:HIS:NE2	1:DDD:177:MET:HE2	2.23	0.54
1:BBB:32:LEU:HB2	1:BBB:58:VAL:HG22	1.90	0.53
1:AAA:162:ASP:CB	1:AAA:221[A]:GLN:HE22	2.21	0.53
1:AAA:32:LEU:HB2	1:AAA:58:VAL:HG22	1.91	0.53
1:CCC:172:HIS:NE2	1:CCC:177:MET:HE2	2.24	0.53
1:DDD:32:LEU:HB2	1:DDD:58:VAL:HG22	1.91	0.53
1:CCC:32:LEU:HB2	1:CCC:58:VAL:HG22	1.92	0.51
1:BBB:165:ASP:O	3:BBB:302:GOL:O3	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:13:ASP:HB3	5:BBB:444:HOH:O	2.12	0.49
1:BBB:130:TRP:HE3	1:BBB:230[B]:ILE:CD1	2.25	0.49
1:CCC:221:GLN:HA	1:CCC:222:PRO:C	2.33	0.49
1:BBB:130:TRP:CE3	1:BBB:230[B]:ILE:HD12	2.47	0.49
3:BBB:302:GOL:C1	5:BBB:415:HOH:O	2.45	0.48
1:DDD:3:ASP:O	5:DDD:401:HOH:O	2.20	0.48
1:DDD:221:GLN:HA	1:DDD:222:PRO:C	2.34	0.48
1:AAA:221[B]:GLN:HA	1:AAA:222:PRO:C	2.34	0.48
1:AAA:260:ARG:CD	1:DDD:165:ASP:OD2	2.60	0.48
1:BBB:221:GLN:HA	1:BBB:222:PRO:C	2.35	0.45
1:AAA:165:ASP:OD2	1:CCC:260:ARG:HD2	2.17	0.45
1:BBB:217:HIS:O	1:BBB:243:TYR:HA	2.17	0.44
1:AAA:35:GLY:HA3	5:AAA:405:HOH:O	2.17	0.44
1:BBB:160:TRP:CZ2	2:BBB:301:VFH:C3	3.01	0.44
1:AAA:221[A]:GLN:HA	1:AAA:222:PRO:C	2.36	0.43
1:CCC:217:HIS:O	1:CCC:243:TYR:HA	2.18	0.43
1:AAA:177[A]:MET:HE1	2:AAA:301:VFH:C	2.48	0.43
1:DDD:217:HIS:O	1:DDD:243:TYR:HA	2.18	0.43
1:DDD:19:ILE:HB	1:DDD:58:VAL:HB	2.01	0.43
1:DDD:75:GLY:HA3	5:DDD:426:HOH:O	2.17	0.43
1:AAA:19:ILE:HB	1:AAA:58:VAL:HB	2.01	0.43
1:CCC:100:HIS:HE1	1:CCC:251:HIS:O	2.00	0.43
1:DDD:263[B]:VAL:HG23	5:DDD:418:HOH:O	2.18	0.42
1:AAA:217:HIS:O	1:AAA:243:TYR:HA	2.19	0.42
1:DDD:97:PRO:HD2	1:DDD:121:ARG:O	2.20	0.42
1:BBB:19:ILE:HB	1:BBB:58:VAL:HB	2.02	0.41
1:BBB:125:MET:HA	1:BBB:218:ILE:O	2.20	0.41
1:DDD:228:GLU:OE2	5:DDD:402:HOH:O	2.21	0.41
1:AAA:97:PRO:HD2	1:AAA:121:ARG:O	2.21	0.41
1:CCC:19:ILE:HB	1:CCC:58:VAL:HB	2.03	0.41
1:DDD:80:VAL:HG21	1:DDD:109:GLU:HB3	2.03	0.41
1:CCC:80:VAL:HG21	1:CCC:109:GLU:HB3	2.03	0.40
1:AAA:135:ASP:HB2	5:AAA:434: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	273/288 (95%)	267 (98%)	6 (2%)	0	100	100
1	BBB	273/288 (95%)	266 (97%)	7 (3%)	0	100	100
1	CCC	273/288 (95%)	266 (97%)	7 (3%)	0	100	100
1	DDD	272/288 (94%)	265 (97%)	7 (3%)	0	100	100
All	All	1091/1152 (95%)	1064 (98%)	27 (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	236/247 (96%)	229 (97%)	7 (3%)	41	41
1	BBB	236/247 (96%)	230 (98%)	6 (2%)	47	49
1	CCC	236/247 (96%)	233 (99%)	3 (1%)	69	74
1	DDD	235/247 (95%)	228 (97%)	7 (3%)	41	41
All	All	943/988 (95%)	920 (98%)	23 (2%)	49	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	38	HIS
1	AAA	126	ASP

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Mol	Chain	Res	Type
1	AAA	128	LEU
1	AAA	130	TRP
1	AAA	138	LYS
1	AAA	213	ARG
1	AAA	263	VAL
1	BBB	38	HIS
1	BBB	126	ASP
1	BBB	130	TRP
1	BBB	138	LYS
1	BBB	213	ARG
1	BBB	263	VAL
1	CCC	38	HIS
1	CCC	126	ASP
1	CCC	130	TRP
1	DDD	38	HIS
1	DDD	113	GLN
1	DDD	126	ASP
1	DDD	130	TRP
1	DDD	213	ARG
1	DDD	263[A]	VAL
1	DDD	263[B]	VAL

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)

8 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	VFH	BBB	301	-	13,13,13	0.48	0	18,18,18	0.45	0
3	GOL	BBB	302	-	5,5,5	0.33	0	5,5,5	0.36	0
2	VFH	CCC	301	-	13,13,13	0.42	0	18,18,18	0.38	0
2	VFH	AAA	301	-	13,13,13	0.29	0	18,18,18	0.41	0
2	VFH	DDD	301	-	13,13,13	0.38	0	18,18,18	0.51	0
3	GOL	DDD	302	-	5,5,5	0.14	0	5,5,5	0.32	0
3	GOL	CCC	303	-	5,5,5	0.30	0	5,5,5	0.38	0
4	SRT	CCC	302	-	9,9,9	1.09	1 (11%)	12,12,12	0.95	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
2	VFH	BBB	301	-	-	-	0/2/2/2
3	GOL	BBB	302	-	-	2/4/4/4	-
2	VFH	CCC	301	-	-	-	0/2/2/2
2	VFH	AAA	301	-	-	-	0/2/2/2
2	VFH	DDD	301	-	-	-	0/2/2/2
3	GOL	DDD	302	-	-	2/4/4/4	-
3	GOL	CCC	303	-	-	4/4/4/4	-
4	SRT	CCC	302	-	-	5/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	CCC	302	SRT	O41-C4	-2.39	1.22	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	302	GOL	C1-C2-C3-O3
3	CCC	303	GOL	O1-C1-C2-C3
3	CCC	303	GOL	C1-C2-C3-O3
3	BBB	302	GOL	O2-C2-C3-O3
4	CCC	302	SRT	O11-C1-C2-O2
3	DDD	302	GOL	O1-C1-C2-C3
3	CCC	303	GOL	O1-C1-C2-O2
3	CCC	303	GOL	O2-C2-C3-O3
4	CCC	302	SRT	O1-C1-C2-O2
3	DDD	302	GOL	O1-C1-C2-O2
4	CCC	302	SRT	O2-C2-C3-O3
4	CCC	302	SRT	O11-C1-C2-C3
4	CCC	302	SRT	O1-C1-C2-C3

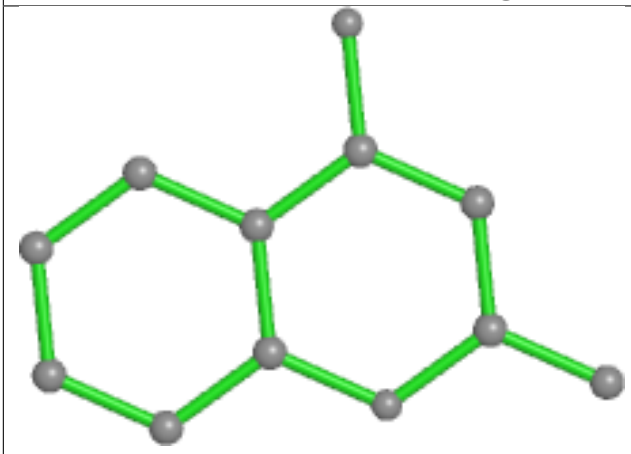
There are no ring outliers.

6 monomers are involved in 8 short contacts:

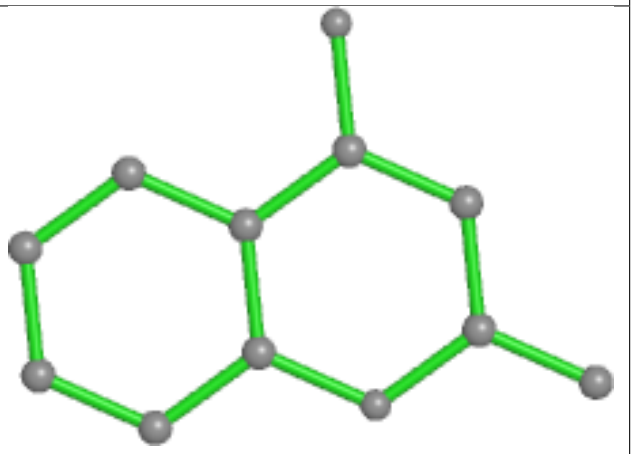
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	301	VFH	1	0
3	BBB	302	GOL	3	0
2	AAA	301	VFH	1	0
3	DDD	302	GOL	1	0
3	CCC	303	GOL	1	0
4	CCC	302	SRT	1	0

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.

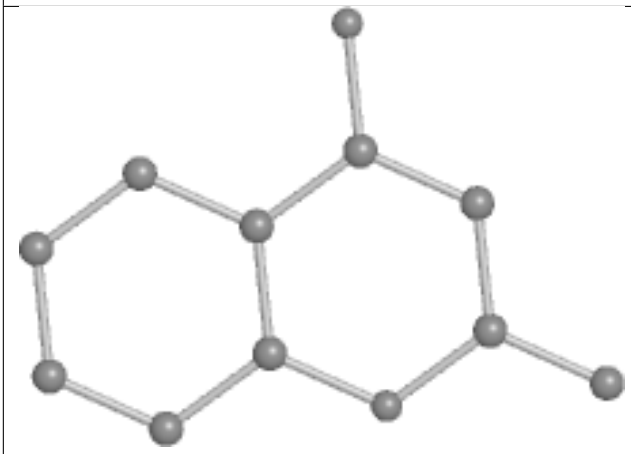
Ligand VFH BBB 301



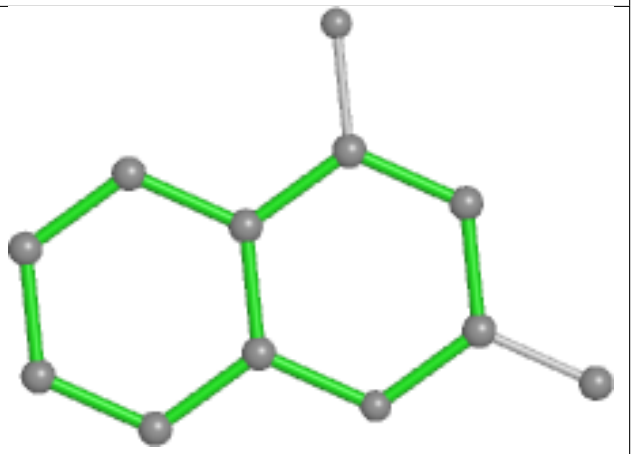
Bond lengths



Bond angles

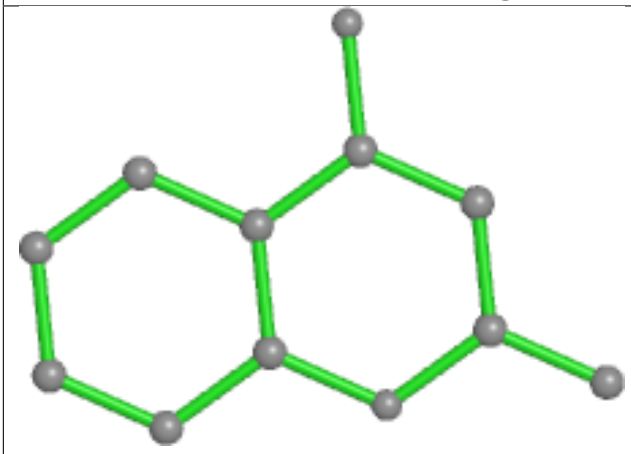


Torsions

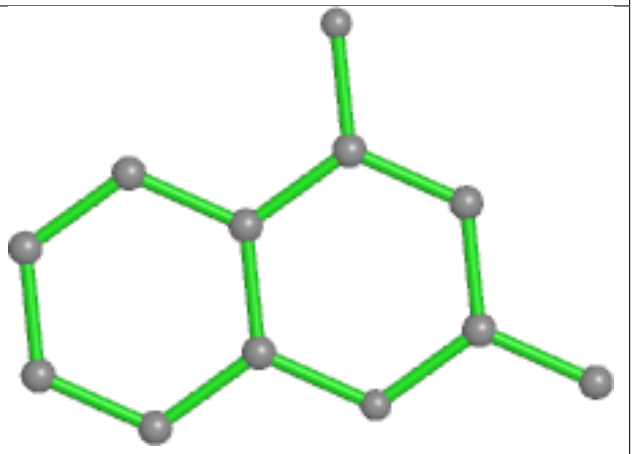


Rings

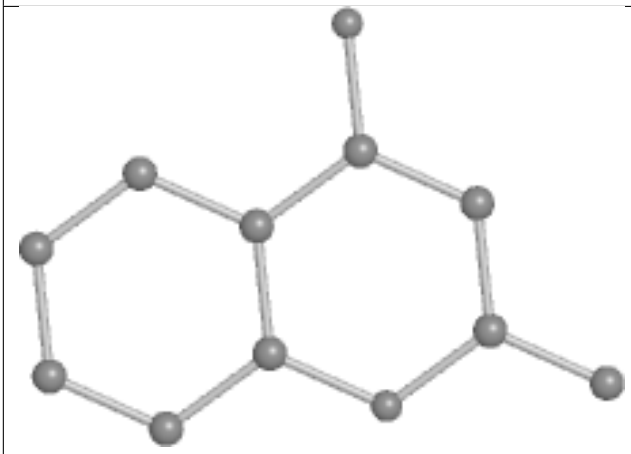
Ligand VFH CCC 301



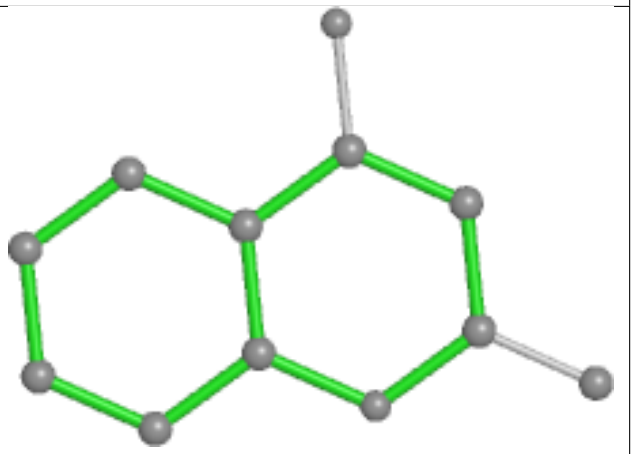
Bond lengths



Bond angles

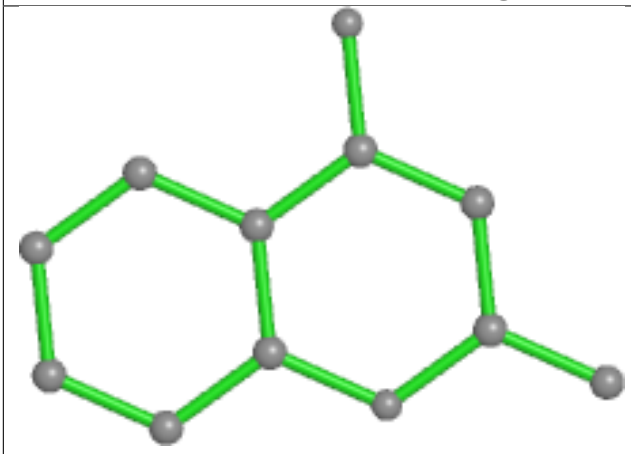


Torsions

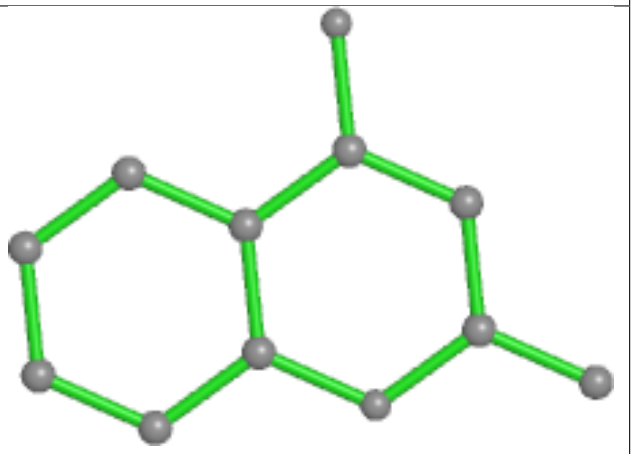


Rings

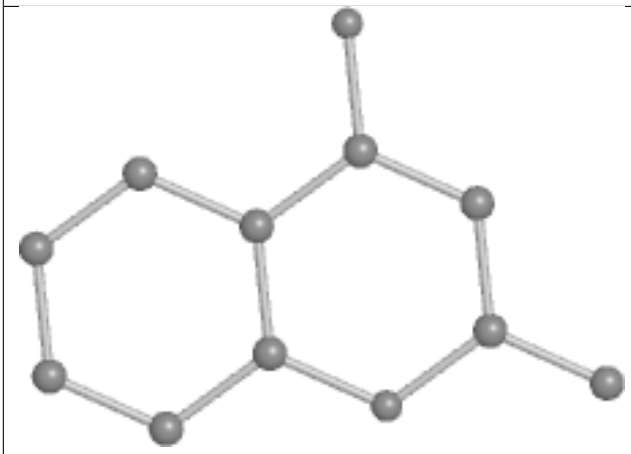
Ligand VFH AAA 301



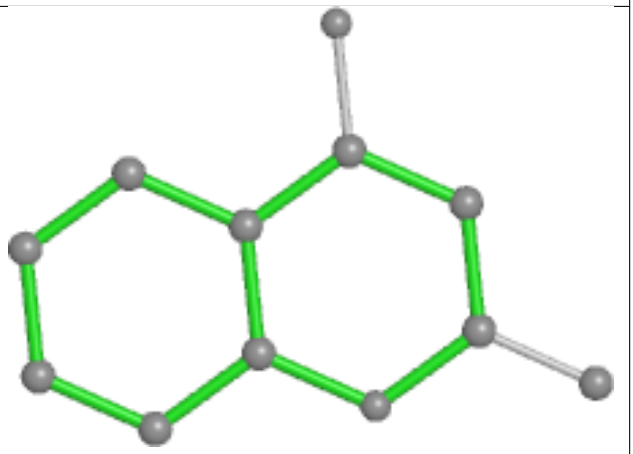
Bond lengths



Bond angles

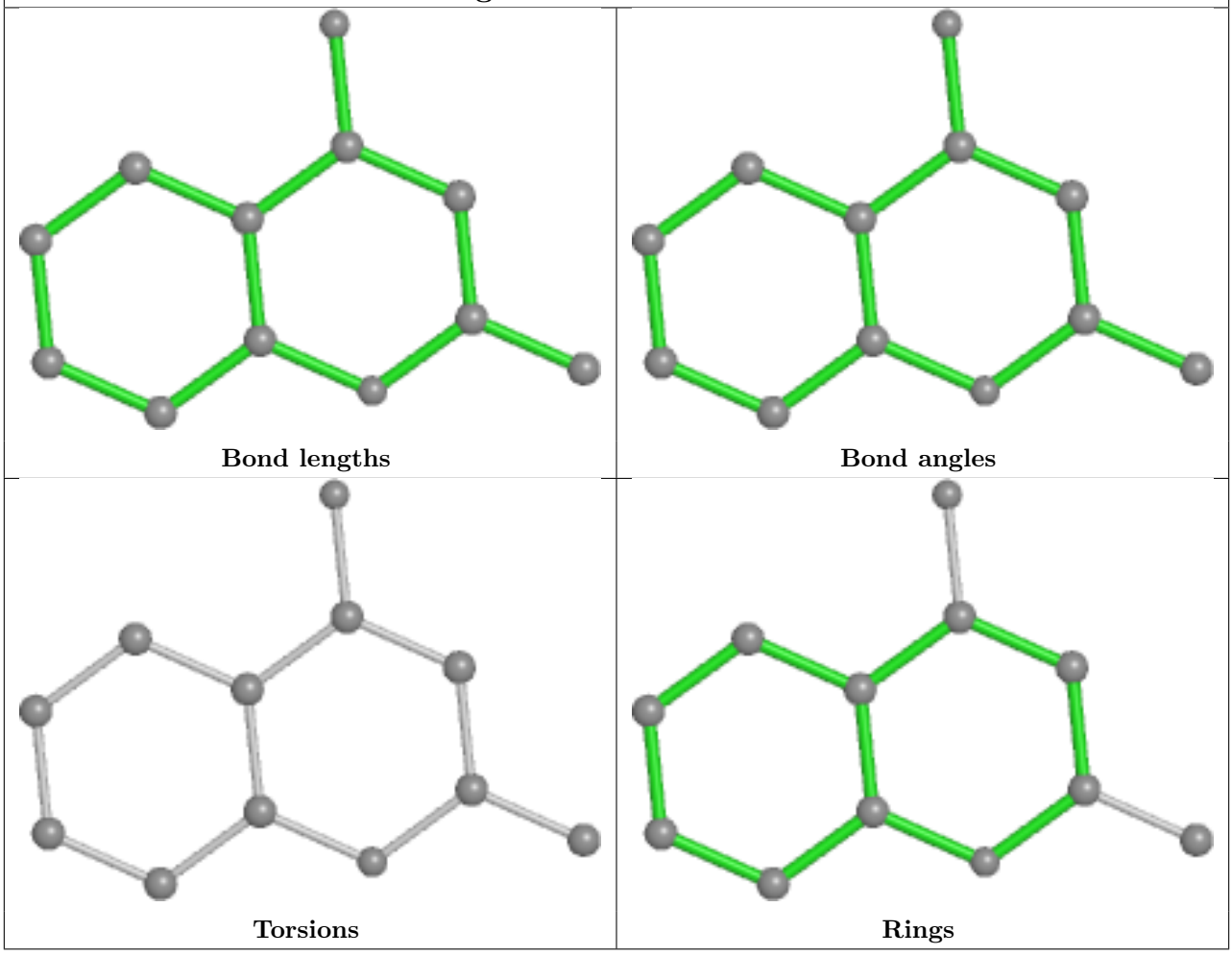


Torsions



Rings

Ligand VFH DDD 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%)	0.18	5 (1%)	68	66	24, 36, 54, 95	0
1	BBB	273/288 (94%)	0.05	4 (1%)	73	72	20, 32, 51, 77	0
1	CCC	273/288 (94%)	0.18	4 (1%)	73	72	20, 35, 55, 75	0
1	DDD	273/288 (94%)	0.19	5 (1%)	68	66	18, 34, 54, 74	0
All	All	1092/1152 (94%)	0.15	18 (1%)	72	70	18, 34, 54, 95	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	275	GLY	14.8
1	BBB	275	GLY	5.2
1	CCC	24	ASP	3.5
1	DDD	26	ASP	3.4
1	BBB	230[A]	ILE	3.3
1	DDD	275	GLY	3.0
1	BBB	13	ASP	2.9
1	BBB	24	ASP	2.7
1	CCC	13	ASP	2.5
1	DDD	93	GLU	2.5
1	CCC	88	ASP	2.4
1	AAA	13	ASP	2.4
1	AAA	237	GLN	2.3
1	DDD	48	GLN	2.2
1	AAA	274	GLN	2.1
1	DDD	24	ASP	2.1
1	AAA	26	ASP	2.1
1	CCC	25	THR	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)

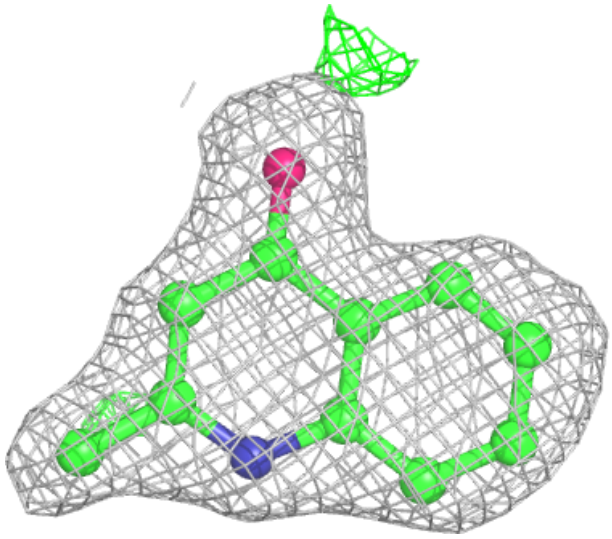
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

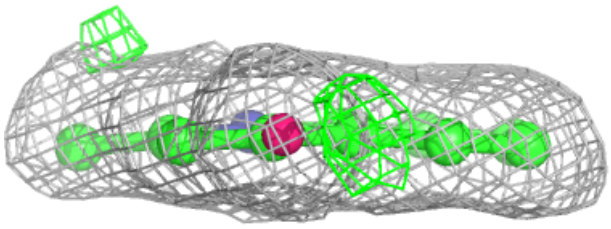
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	CCC	303	6/6	0.92	0.17	33,36,39,39	0
2	VFH	DDD	301	12/12	0.94	0.12	23,25,27,27	0
2	VFH	CCC	301	12/12	0.94	0.10	25,29,31,34	0
3	GOL	DDD	302	6/6	0.94	0.15	31,42,43,51	0
4	SRT	CCC	302	10/10	0.94	0.09	24,29,34,35	0
3	GOL	BBB	302	6/6	0.96	0.10	21,24,24,25	0
2	VFH	BBB	301	12/12	0.97	0.12	16,18,21,21	0
2	VFH	AAA	301	12/12	0.98	0.10	18,20,22,23	0

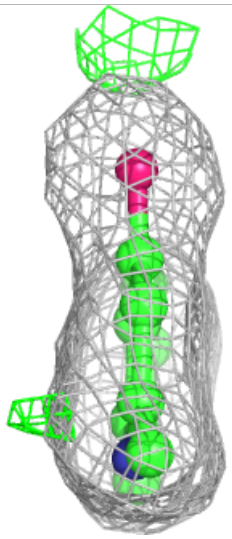
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around VFH DDD 301:

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

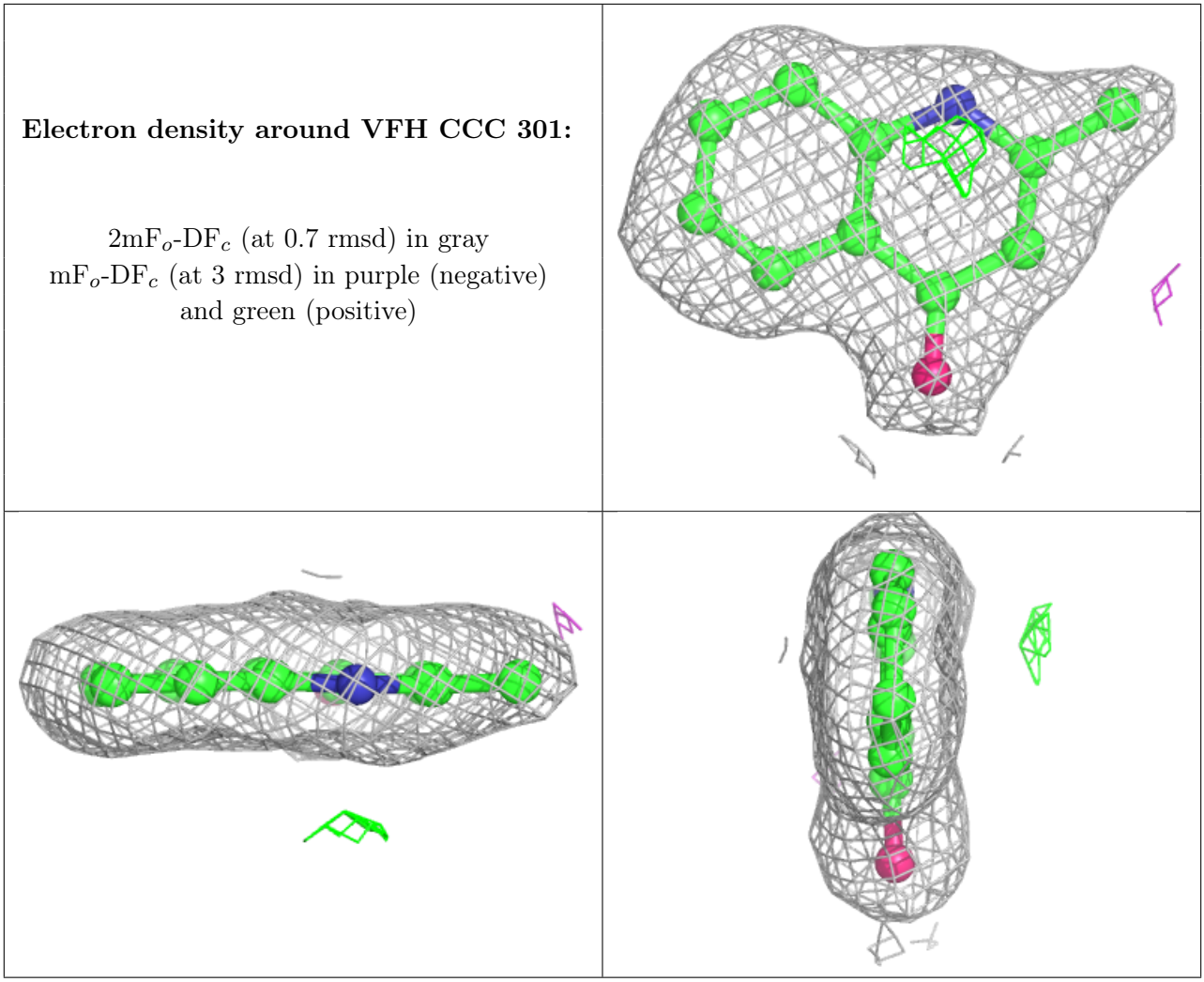






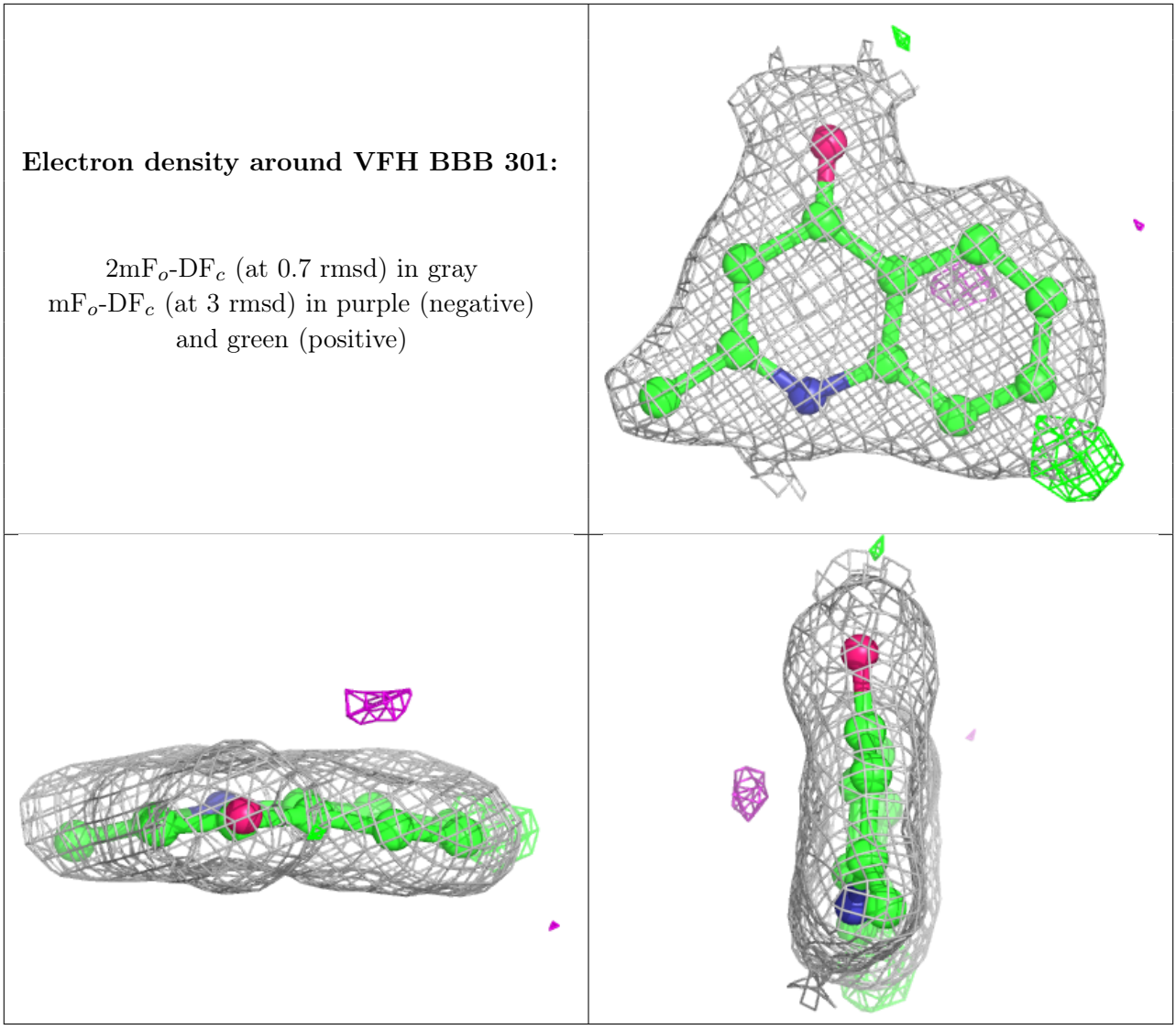
Electron density around VFH CCC 301:

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



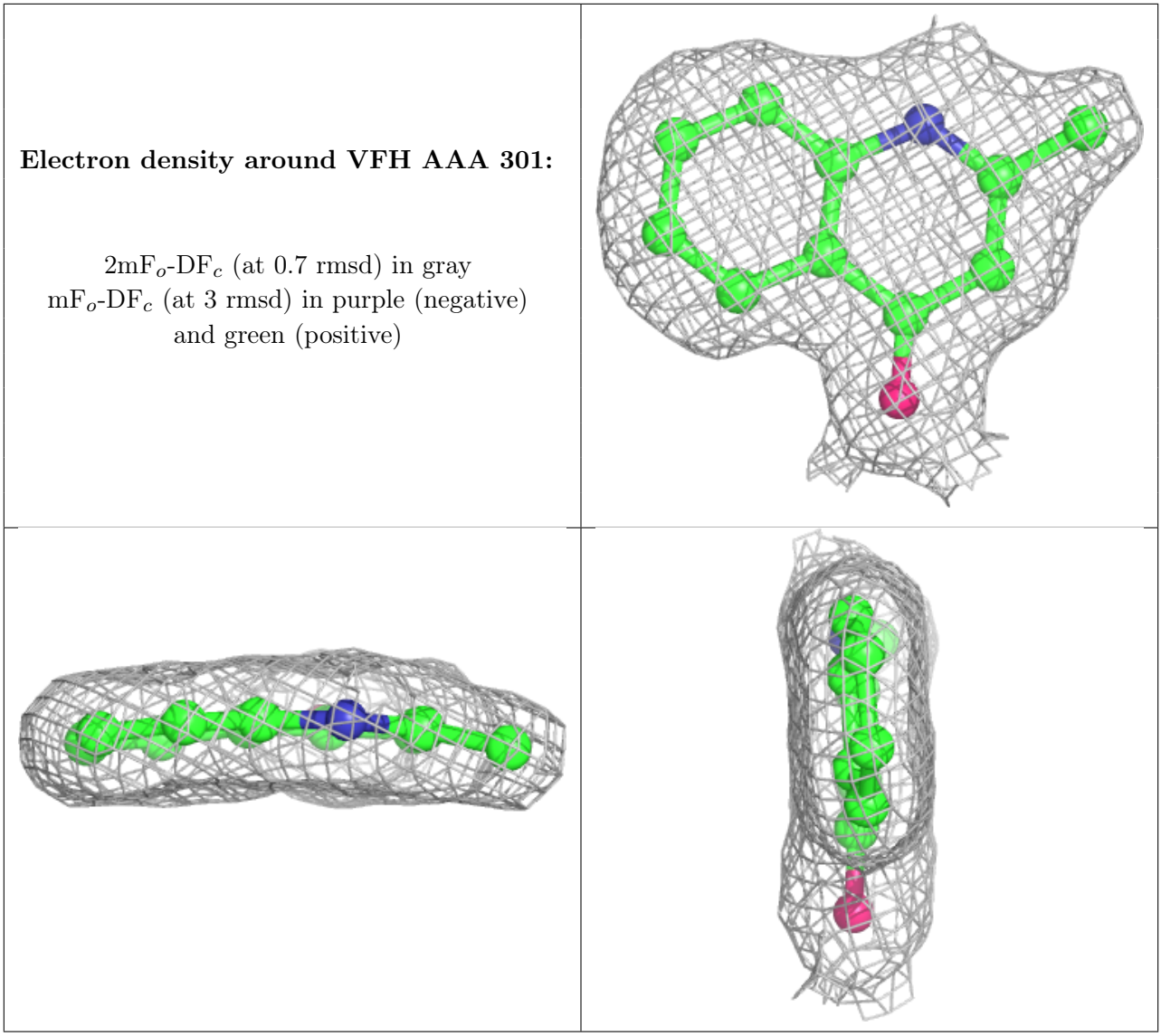
Electron density around VFH BBB 301:

$2mF_o$-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

There are no such residues in this entry.