Full wwPDB X-ray Structure Validation Report (i)

Jan 10, 2024 – 03:27 pm GMT

PDB ID	:	8ORO
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 HYPEROXYC CONDITIONS
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Deposited on	:	2023-04-15
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:

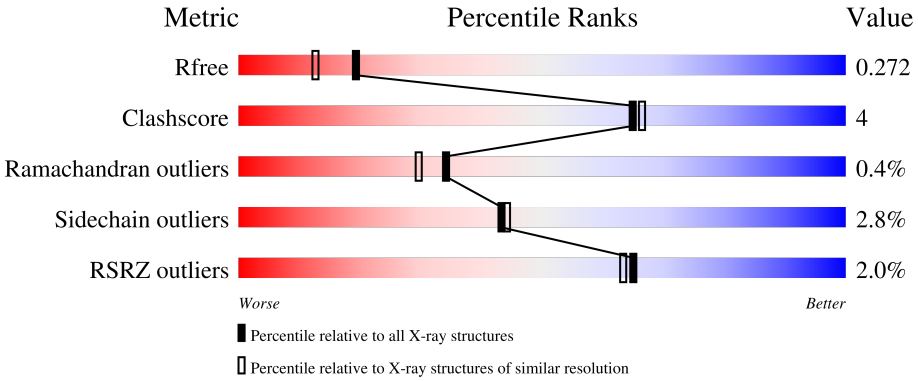
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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	3% 83% 10% • 5%
1	BBB	288	% 86% 8% • 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5018 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	6	0
			2269	1448	398	414	9			
1	BBB	273	Total	C	N	O	S	0	5	0
			2262	1446	396	411	9			

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	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
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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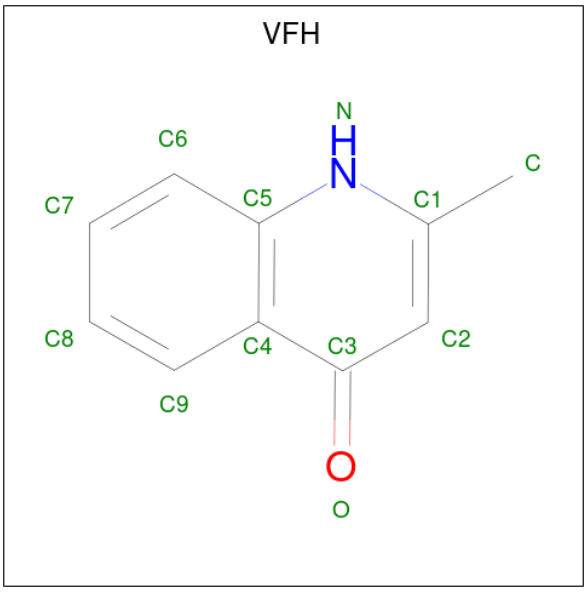
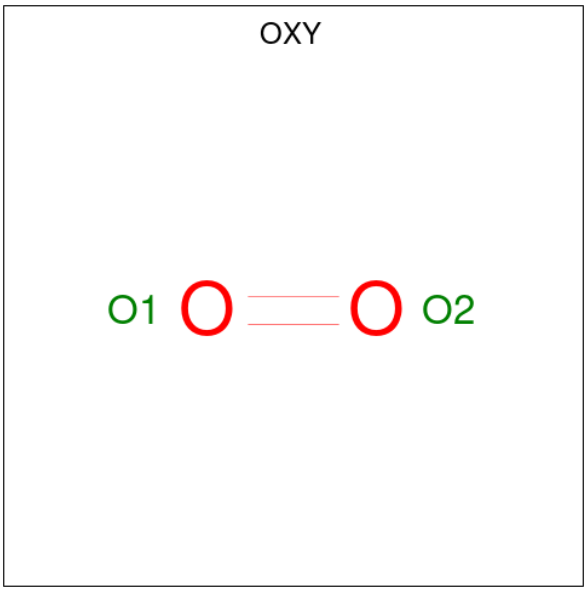
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	SER	-	expression tag	UNP O31266
BBB	69	SER	CYS	engineered mutation	UNP O31266
BBB	101	ALA	SER	engineered mutation	UNP O31266

- 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).



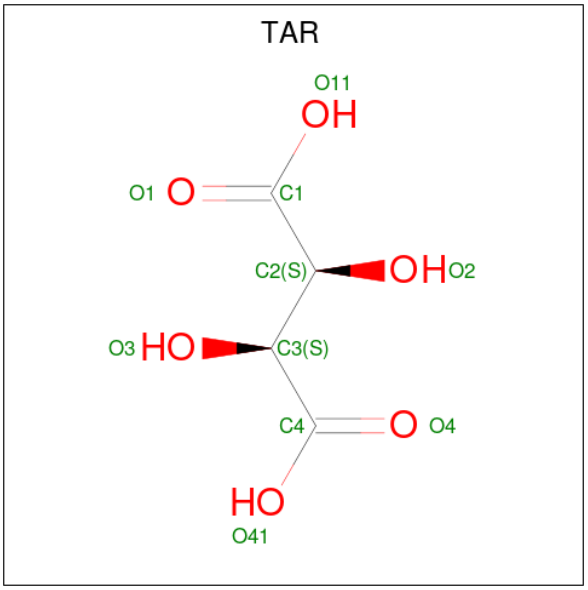
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			12	10	1	1		
2	BBB	1	Total	C	N	O	0	0
			12	10	1	1		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



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

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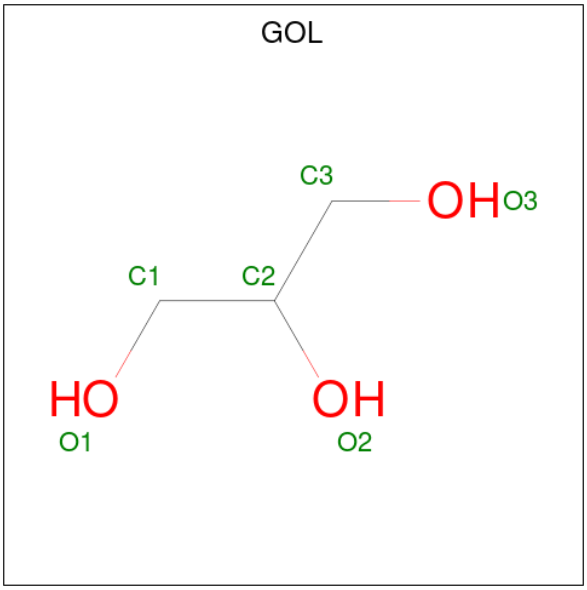
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total C O 10 4 6	0	0
4	BBB	1	Total C O 10 4 6	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C O 6 3 3	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.

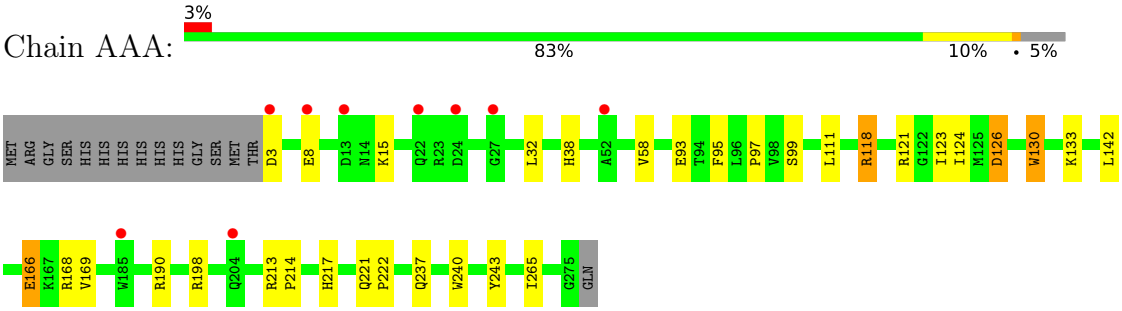
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	225	Total O 227 227	0	2
7	BBB	185	Total O 185 185	0	0

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.

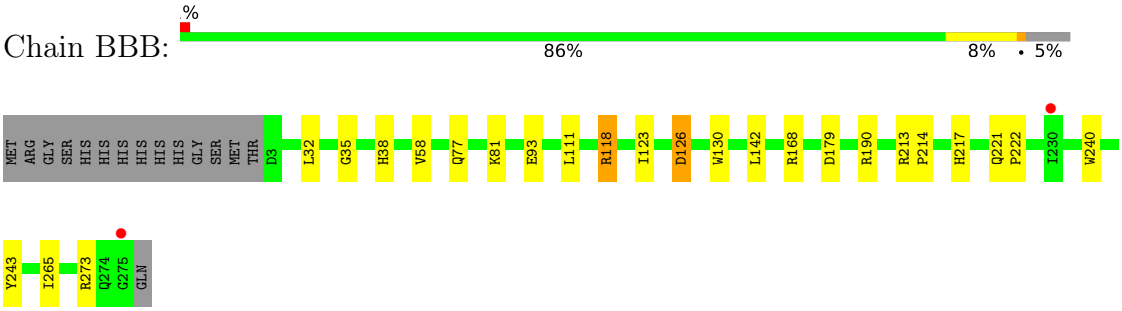
• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain AAA:



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

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	120.11Å 120.11Å 44.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.05 – 2.00 60.05 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (60.05-2.00) 98.9 (60.05-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.269 0.232 , 0.272	Depositor DCC
R_{free} test set	2154 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
Reported twinning fraction	0.854 for H, K, L 0.146 for -K, -H, -L	Depositor
Outliers	0 of 43227 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5018	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.45% 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: TAR, VFH, NA, OXY, 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	0/2352	0.76	0/3198
1	BBB	0.65	0/2342	0.75	0/3185
All	All	0.65	0/4694	0.75	0/6383

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	2269	0	2164	19	0
1	BBB	2262	0	2163	14	0
2	AAA	12	0	0	0	0
2	BBB	12	0	0	0	0
3	AAA	2	0	0	0	0
3	BBB	2	0	0	1	0
4	AAA	20	0	8	3	0
4	BBB	20	0	8	2	0
5	BBB	6	0	8	0	0
6	BBB	1	0	0	0	0
7	AAA	227	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BBB	185	0	0	6	0
All	All	5018	0	4351	37	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 4.

All (37) 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:179:ASP:OD2	7:BBB:401:HOH:O	1.98	0.80
4:AAA:304:TAR:O1	4:AAA:304:TAR:O3	2.05	0.70
1:BBB:168:ARG:NH2	7:BBB:402:HOH:O	2.28	0.65
1:AAA:8:GLU:HG2	1:AAA:15:LYS:HG2	1.79	0.65
4:AAA:303:TAR:O1	4:AAA:303:TAR:O3	2.17	0.63
1:AAA:93:GLU:O	1:AAA:118[B]:ARG:HG2	2.01	0.60
1:BBB:93:GLU:O	1:BBB:118:ARG:HG2	2.03	0.58
1:AAA:237:GLN:NE2	7:AAA:409:HOH:O	2.37	0.57
1:AAA:198:ARG:NH2	7:AAA:412:HOH:O	2.39	0.56
4:BBB:304:TAR:H2	7:BBB:490:HOH:O	2.08	0.52
1:BBB:273:ARG:NH2	7:BBB:409:HOH:O	2.39	0.51
1:AAA:3[A]:ASP:O	1:AAA:3[A]:ASP:OD2	2.29	0.50
1:AAA:130:TRP:CZ2	1:AAA:133:LYS:HE2	2.47	0.50
4:BBB:304:TAR:O11	4:BBB:304:TAR:O3	2.27	0.49
1:AAA:217:HIS:O	1:AAA:243:TYR:HA	2.14	0.47
1:AAA:123:ILE:CD1	1:AAA:265:ILE:HA	2.44	0.47
1:AAA:221:GLN:HA	1:AAA:222:PRO:C	2.35	0.47
1:AAA:190[B]:ARG:HD2	1:BBB:77:GLN:HB2	1.97	0.47
4:AAA:304:TAR:O41	4:AAA:304:TAR:O2	2.33	0.45
1:BBB:32:LEU:HB2	1:BBB:58:VAL:HG22	1.99	0.45
1:BBB:221:GLN:HA	1:BBB:222:PRO:C	2.37	0.45
1:BBB:217:HIS:O	1:BBB:243:TYR:HA	2.16	0.44
1:BBB:214:PRO:HA	1:BBB:240:TRP:O	2.17	0.44
1:AAA:32:LEU:HB2	1:AAA:58:VAL:HG22	1.99	0.44
1:BBB:123:ILE:CD1	1:BBB:265:ILE:HA	2.47	0.44
1:AAA:95:PHE:CE1	1:AAA:118[A]:ARG:HD3	2.53	0.44
1:AAA:214:PRO:HA	1:AAA:240:TRP:O	2.17	0.43
1:AAA:166[A]:GLU:HG3	1:AAA:169:VAL:HG23	2.02	0.42
1:BBB:123:ILE:N	7:BBB:417:HOH:O	2.52	0.42
1:AAA:130:TRP:CH2	1:AAA:133:LYS:HE2	2.55	0.42
1:AAA:99:SER:OG	1:AAA:124:ILE:HG22	2.19	0.41
1:AAA:166[A]:GLU:HG3	1:AAA:169:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:35:GLY:HA3	3:BBB:302:OXY:O1	2.20	0.41
1:BBB:111:LEU:O	1:BBB:213:ARG:NH1	2.50	0.41
1:AAA:111:LEU:O	1:AAA:213:ARG:NH1	2.51	0.40
1:AAA:97:PRO:HD2	1:AAA:121:ARG:O	2.21	0.40
1:BBB:81:LYS:CE	7:BBB:460:HOH:O	2.69	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	276/288 (96%)	270 (98%)	5 (2%)	1 (0%)	34	30
1	BBB	276/288 (96%)	270 (98%)	5 (2%)	1 (0%)	34	30
All	All	552/576 (96%)	540 (98%)	10 (2%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	126	ASP
1	BBB	126	ASP

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	240/247 (97%)	231 (96%)	9 (4%)	33	31
1	BBB	239/247 (97%)	233 (98%)	6 (2%)	47	49
All	All	479/494 (97%)	464 (97%)	15 (3%)	43	40

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	38	HIS
1	AAA	118[A]	ARG
1	AAA	118[B]	ARG
1	AAA	126	ASP
1	AAA	130	TRP
1	AAA	142	LEU
1	AAA	166[A]	GLU
1	AAA	166[B]	GLU
1	AAA	168	ARG
1	BBB	38	HIS
1	BBB	118	ARG
1	BBB	126	ASP
1	BBB	130	TRP
1	BBB	142	LEU
1	BBB	190	ARG

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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	OXY	AAA	302	-	1,1,1	0.23	0	-		
4	TAR	BBB	304	-	9,9,9	1.14	0	12,12,12	1.08	0
4	TAR	AAA	303	-	9,9,9	0.94	0	12,12,12	1.02	0
4	TAR	AAA	304	-	9,9,9	1.18	1 (11%)	12,12,12	1.09	0
5	GOL	BBB	305	-	5,5,5	0.09	0	5,5,5	0.28	0
2	VFH	AAA	301	-	13,13,13	0.33	0	18,18,18	0.36	0
4	TAR	BBB	303	-	9,9,9	1.06	1 (11%)	12,12,12	0.90	0
2	VFH	BBB	301	-	13,13,13	0.24	0	18,18,18	0.32	0
3	OXY	BBB	302	-	1,1,1	0.24	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
4	TAR	BBB	304	-	-	8/12/12/12	-
4	TAR	AAA	303	-	-	8/12/12/12	-
4	TAR	AAA	304	-	-	12/12/12/12	-
5	GOL	BBB	305	-	-	2/4/4/4	-
2	VFH	AAA	301	-	-	-	0/2/2/2
4	TAR	BBB	303	-	-	4/12/12/12	-
2	VFH	BBB	301	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	304	TAR	O11-C1	-2.22	1.23	1.30
4	BBB	303	TAR	O11-C1	-2.08	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

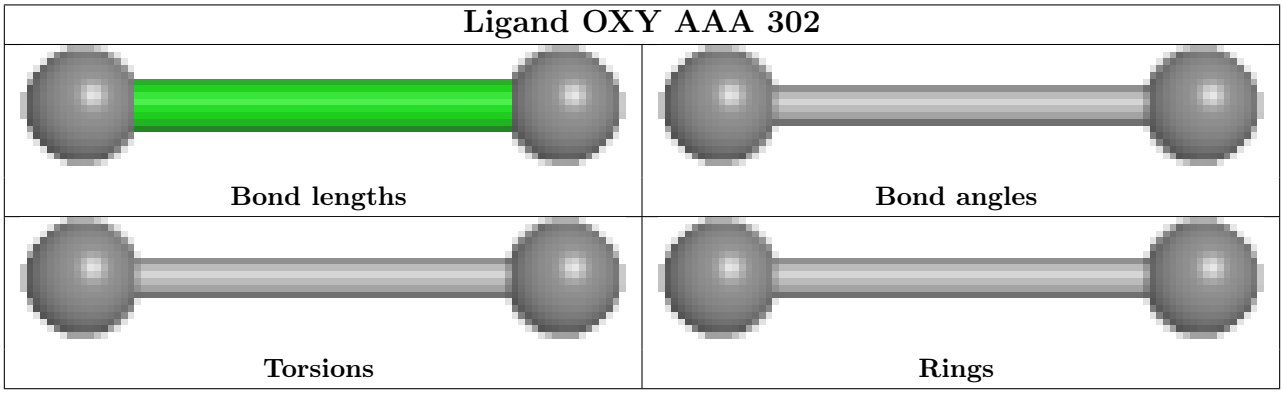
Mol	Chain	Res	Type	Atoms
4	AAA	303	TAR	O1-C1-C2-O2
4	AAA	303	TAR	O11-C1-C2-O2
4	AAA	304	TAR	C1-C2-C3-C4
4	AAA	304	TAR	O2-C2-C3-O3
4	BBB	303	TAR	O1-C1-C2-O2
4	BBB	303	TAR	O11-C1-C2-O2
5	BBB	305	GOL	C1-C2-C3-O3
4	AAA	304	TAR	C1-C2-C3-O3
4	AAA	304	TAR	O2-C2-C3-C4
4	AAA	303	TAR	O2-C2-C3-O3
4	AAA	303	TAR	C1-C2-C3-C4
4	AAA	303	TAR	O2-C2-C3-C4
4	AAA	304	TAR	O1-C1-C2-O2
4	AAA	304	TAR	O11-C1-C2-O2
4	BBB	303	TAR	O3-C3-C4-O4
4	BBB	303	TAR	O3-C3-C4-O41
4	BBB	304	TAR	O1-C1-C2-O2
4	BBB	304	TAR	O11-C1-C2-O2
4	AAA	303	TAR	O11-C1-C2-C3
4	AAA	304	TAR	O1-C1-C2-C3
4	AAA	304	TAR	O11-C1-C2-C3
4	BBB	304	TAR	O11-C1-C2-C3
4	BBB	304	TAR	O2-C2-C3-C4
4	BBB	304	TAR	O2-C2-C3-O3
4	AAA	303	TAR	C1-C2-C3-O3
4	AAA	303	TAR	O1-C1-C2-C3
4	BBB	304	TAR	O1-C1-C2-C3
4	BBB	304	TAR	C1-C2-C3-O3
4	AAA	304	TAR	C2-C3-C4-O41
4	AAA	304	TAR	C2-C3-C4-O4
4	BBB	304	TAR	C1-C2-C3-C4
5	BBB	305	GOL	O2-C2-C3-O3
4	AAA	304	TAR	O3-C3-C4-O4
4	AAA	304	TAR	O3-C3-C4-O41

There are no ring outliers.

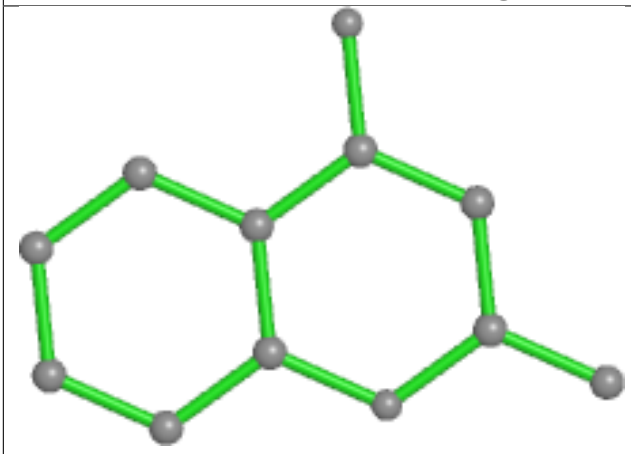
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	304	TAR	2	0
4	AAA	303	TAR	1	0
4	AAA	304	TAR	2	0
3	BBB	302	OXY	1	0

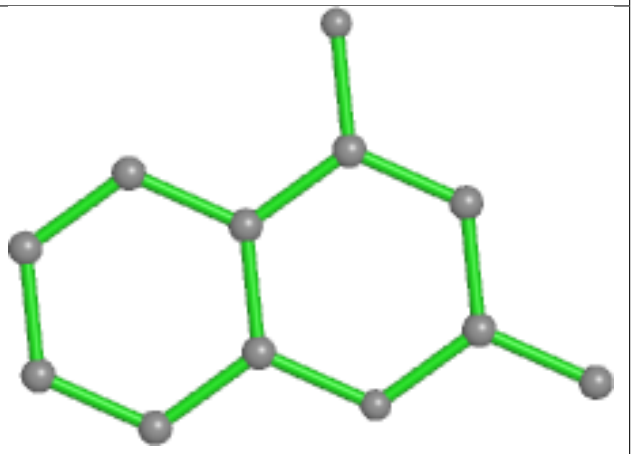
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



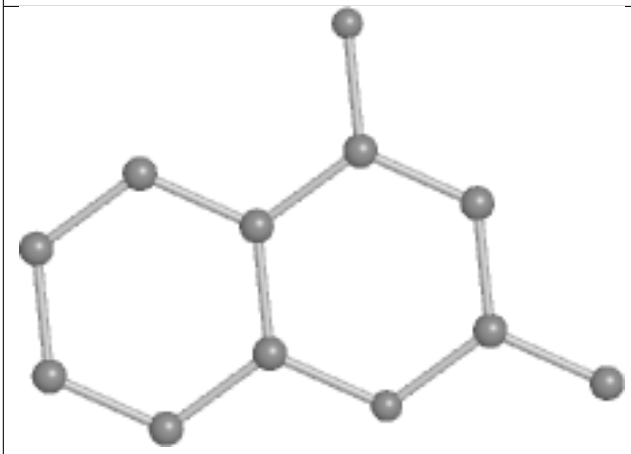
Ligand VFH AAA 301



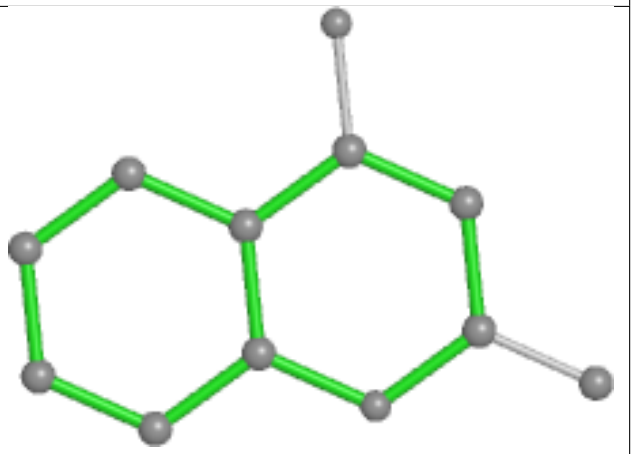
Bond lengths



Bond angles

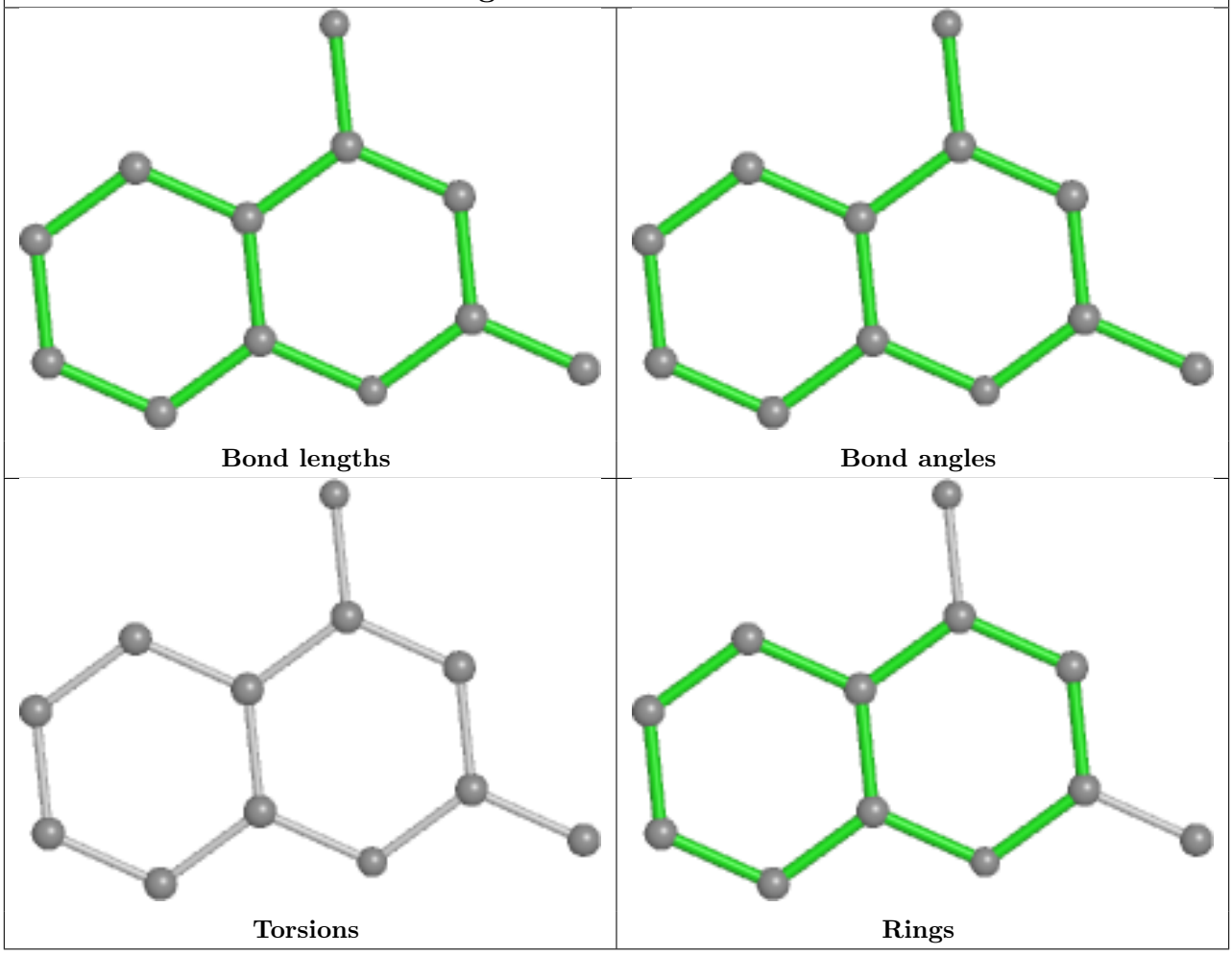


Torsions

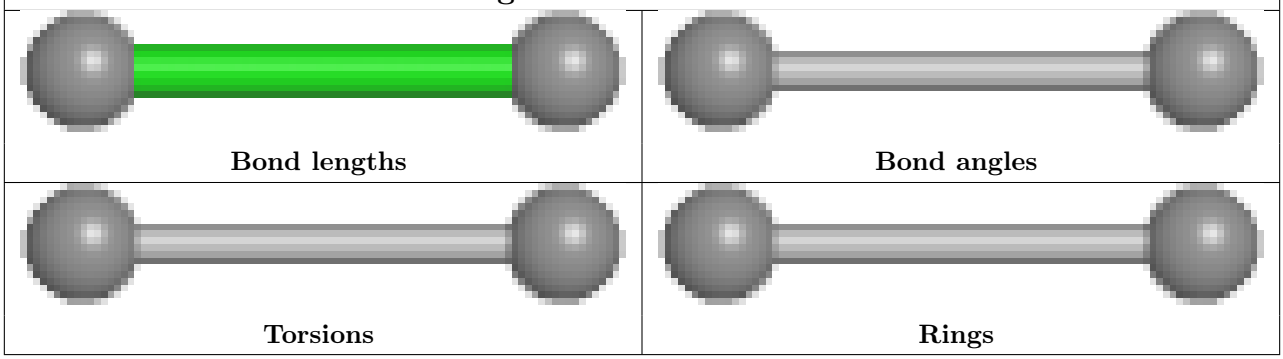


Rings

Ligand VFH BBB 301



Ligand OXY BBB 302



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%)	0.20	9 (3%) 46 45	17, 30, 42, 57	0
1	BBB	273/288 (94%)	0.16	2 (0%) 87 87	18, 29, 44, 57	0
All	All	546/576 (94%)	0.18	11 (2%) 65 63	17, 29, 43, 57	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	204	GLN	3.6
1	AAA	52	ALA	2.8
1	AAA	24	ASP	2.7
1	AAA	22	GLN	2.5
1	AAA	27	GLY	2.5
1	BBB	230	ILE	2.2
1	BBB	275	GLY	2.1
1	AAA	8	GLU	2.1
1	AAA	3[A]	ASP	2.1
1	AAA	13	ASP	2.0
1	AAA	185	TRP	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)

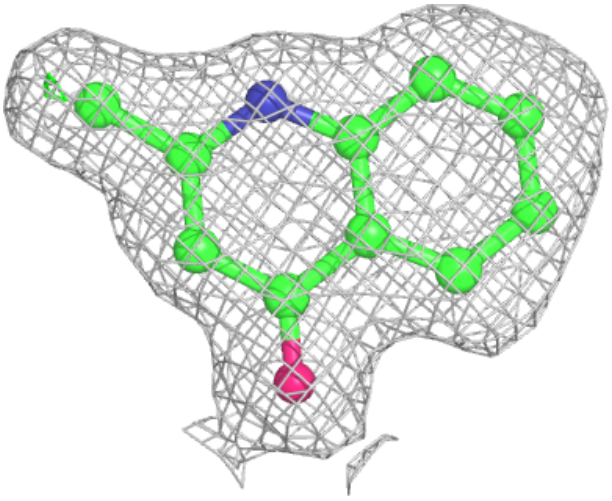
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

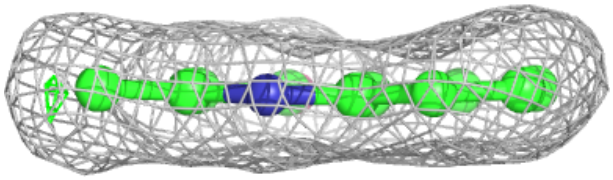
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	BBB	305	6/6	0.76	0.23	42,45,45,47	0
4	TAR	BBB	303	10/10	0.81	0.25	27,30,32,35	0
4	TAR	AAA	304	10/10	0.84	0.17	22,27,30,35	0
4	TAR	BBB	304	10/10	0.87	0.16	25,30,30,32	0
4	TAR	AAA	303	10/10	0.87	0.15	27,31,34,35	0
2	VFH	BBB	301	12/12	0.88	0.12	20,21,22,23	0
2	VFH	AAA	301	12/12	0.92	0.09	19,21,21,22	0
3	OXY	BBB	302	2/2	0.97	0.27	30,30,30,30	2
3	OXY	AAA	302	2/2	0.97	0.10	19,19,19,20	0
6	NA	BBB	306	1/1	0.99	0.13	16,16,16,16	0

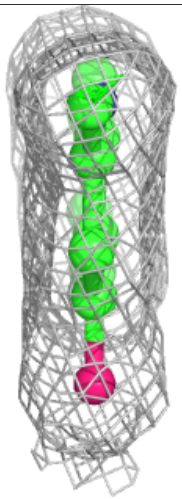
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

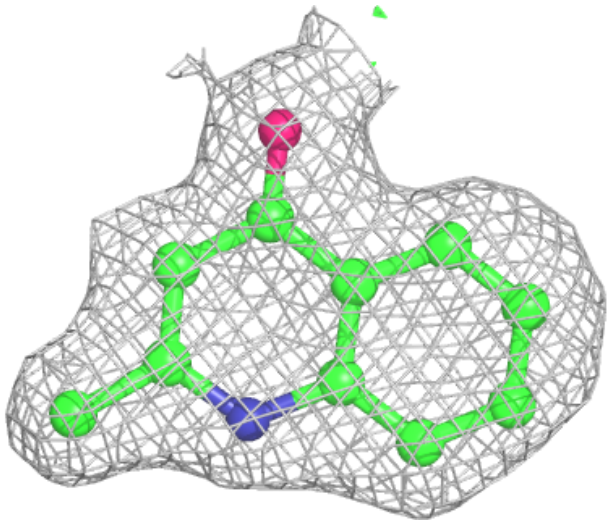


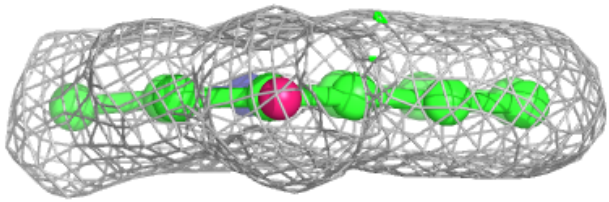


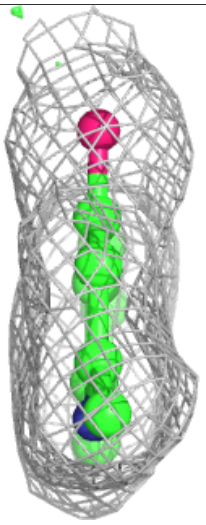


Electron density around VFH AAA 301:

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

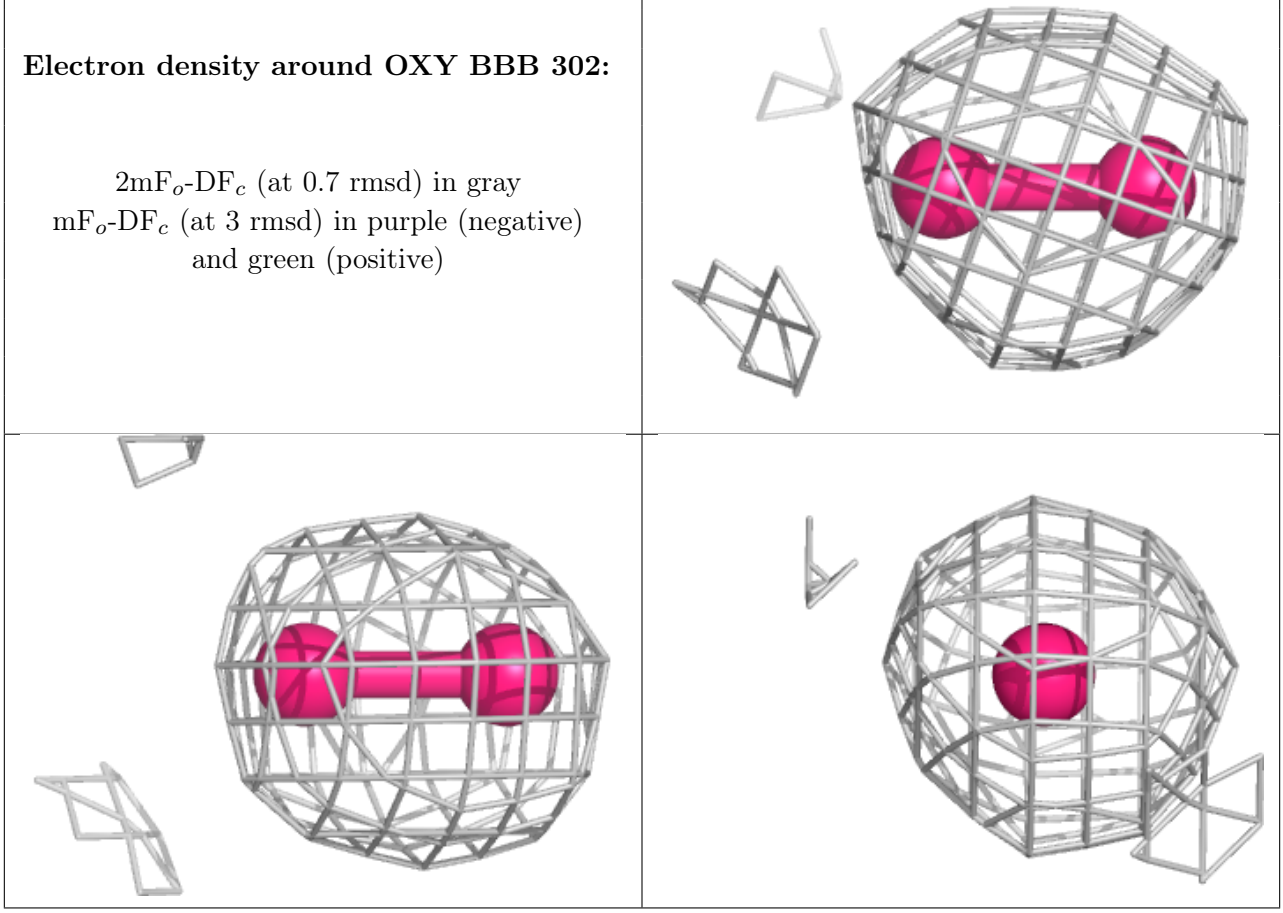






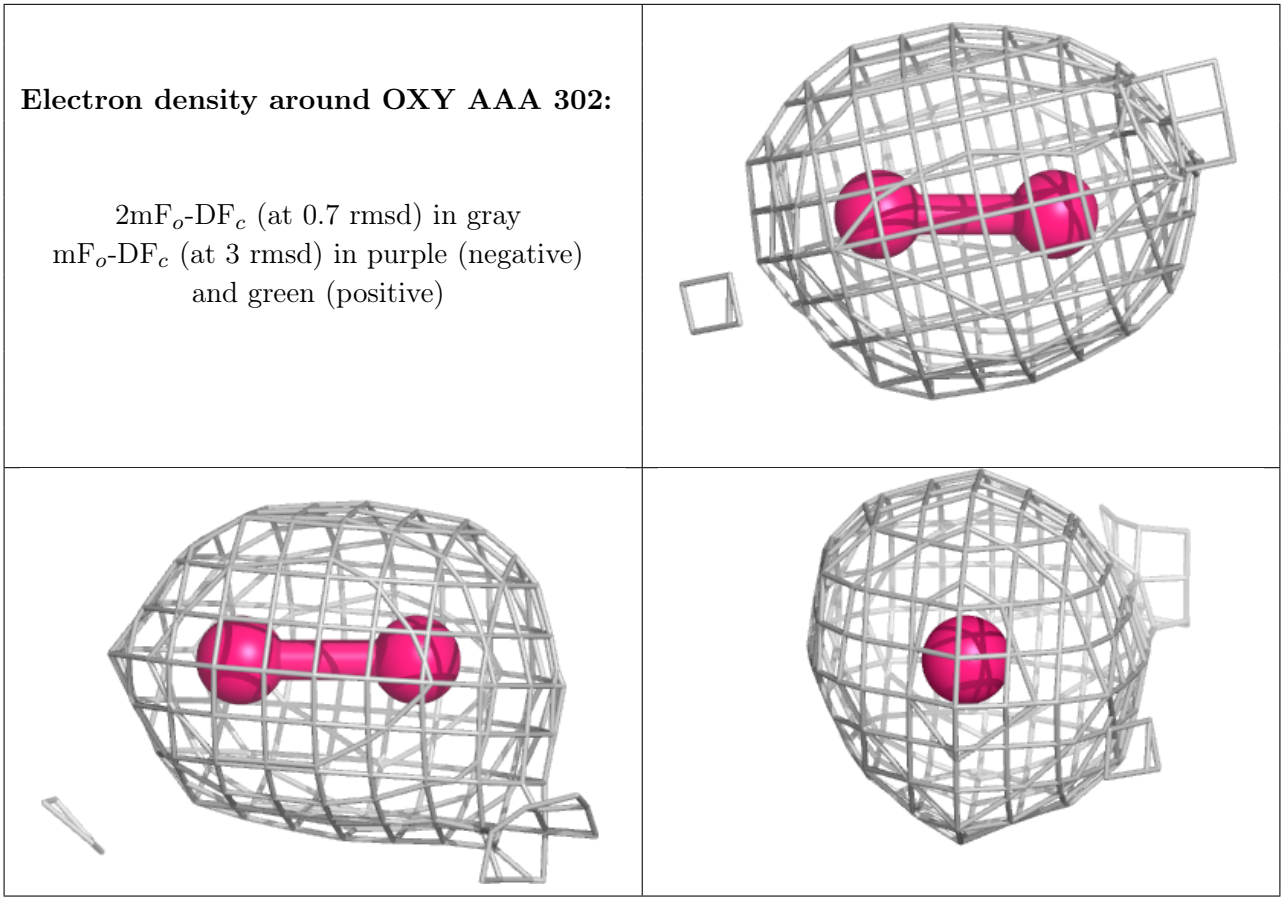
Electron density around OXY BBB 302:

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



Electron density around OXY AAA 302:

$2mF_o$-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.