Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2024 – 06:48 pm GMT

PDB ID	:	8QS0
Title	:	Acyl-ACP thioesterase from Lemna paucicostata in complex with a spirolactam
Authors	:	Freigang, J.
Deposited on	:	2023-10-10
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

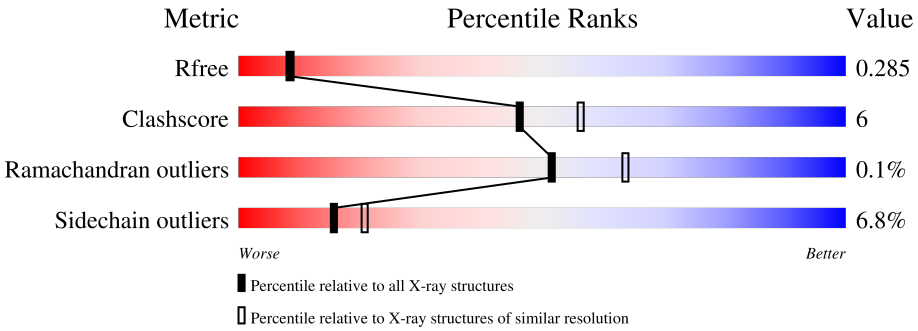
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	AAA	320	71% 12% • 15%
1	BBB	320	67% 16% • 17%
1	CCC	320	66% 16% • 17%
1	DDD	320	69% 14% • 15%

2 Entry composition

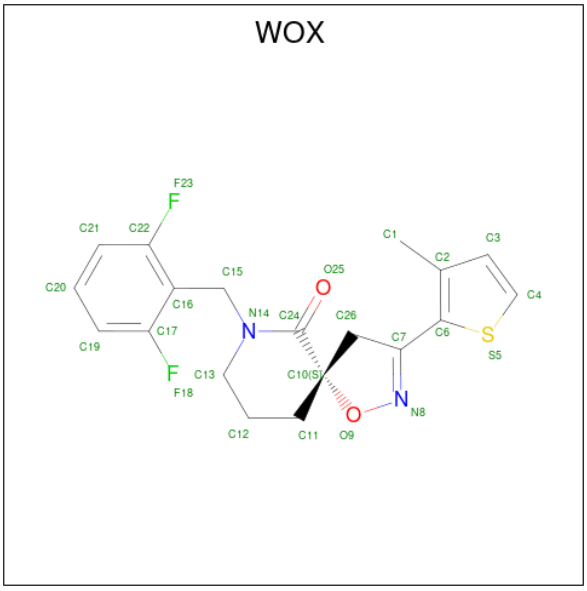
There are 3 unique types of molecules in this entry. The entry contains 9132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acyl-acp thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	271	Total	C	N	O	S	0	0	0
			2198	1380	392	416	10			
1	BBB	267	Total	C	N	O	S	0	0	0
			2170	1364	387	409	10			
1	CCC	267	Total	C	N	O	S	0	0	0
			2170	1364	387	409	10			
1	DDD	271	Total	C	N	O	S	0	0	0
			2198	1380	392	416	10			

- Molecule 2 is (5 {S})-9-[[2,6-bis(fluoranyl)phenyl]methyl]-3-(3-methylthiophen-2-yl)-1-oxa-2,9-diazaspiro[4.5]dec-2-en-10-one (three-letter code: WOX) (formula: $C_{19}H_{18}F_2N_2O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	S	0	0
			26	19	2	2	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	BBB	1	Total	C	F	N	O	S	0	0
			26	19	2	2	2	1		
2	CCC	1	Total	C	F	N	O	S	0	0
			26	19	2	2	2	1		
2	DDD	1	Total	C	F	N	O	S	0	0
			26	19	2	2	2	1		

- Molecule 3 is water.

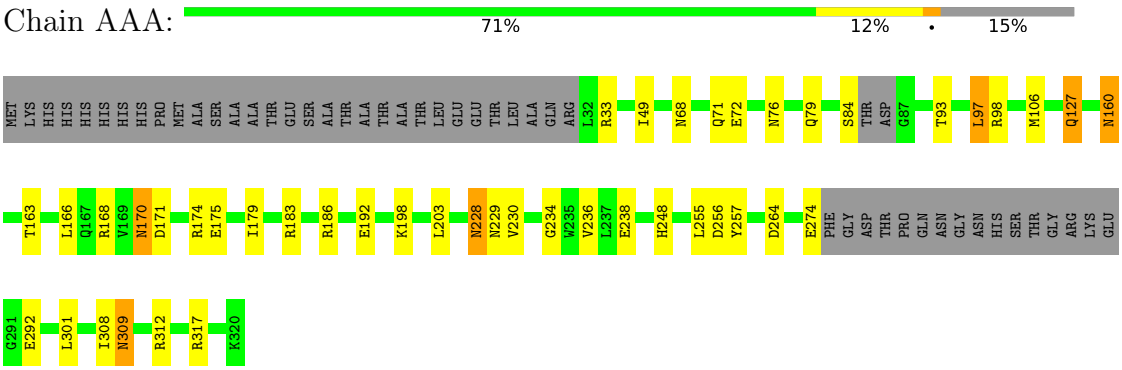
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	70	Total	O	0	0
			70	70		
3	BBB	47	Total	O	0	0
			47	47		
3	CCC	86	Total	O	0	0
			86	86		
3	DDD	89	Total	O	0	0
			89	89		

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. 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. 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.

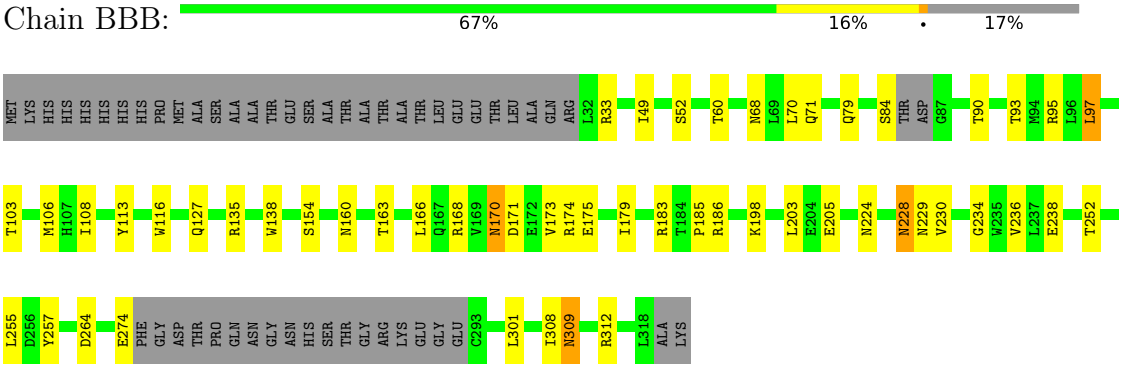
- Molecule 1: Acyl-acp thioesterase

Chain AAA:



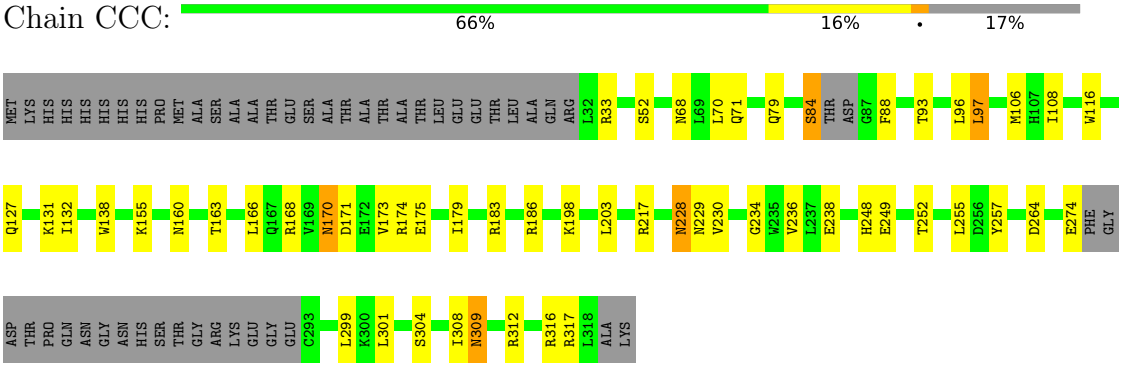
- Molecule 1: Acyl-acp thioesterase

Chain BBB:



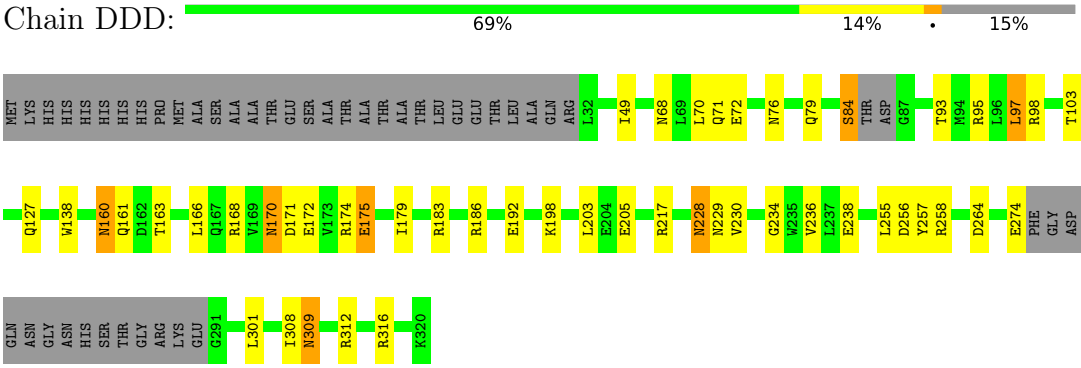
- Molecule 1: Acyl-acp thioesterase

Chain CCC:



• Molecule 1: Acyl-acp thioesterase

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.67Å 147.84Å 81.24Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.98-2.30) 99.3 (19.97-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.258 , 0.285 0.261 , 0.285	Depositor DCC
R_{free} test set	2679 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 13.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9132	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: WOX

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	0.71	0/2239	0.82	0/3026
1	BBB	0.68	0/2211	0.83	0/2991
1	CCC	0.69	0/2211	0.83	0/2991
1	DDD	0.68	0/2239	0.83	0/3026
All	All	0.69	0/8900	0.83	0/12034

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	2198	0	2179	24	0
1	BBB	2170	0	2152	31	0
1	CCC	2170	0	2152	36	0
1	DDD	2198	0	2179	30	0
2	AAA	26	0	0	0	0
2	BBB	26	0	0	0	0
2	CCC	26	0	0	0	0
2	DDD	26	0	0	0	0
3	AAA	70	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	47	0	0	1	0
3	CCC	86	0	0	5	0
3	DDD	89	0	0	6	0
All	All	9132	0	8662	110	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 6.

All (110) 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:CCC:127:GLN:HE22	1:CCC:186:ARG:H	1.37	0.72
1:DDD:84:SER:HA	3:DDD:566:HOH:O	1.89	0.72
1:CCC:132:ILE:HG22	3:CCC:531:HOH:O	1.90	0.71
1:AAA:274:GLU:OE1	1:AAA:312:ARG:HD3	1.90	0.71
1:BBB:127:GLN:HE22	1:BBB:186:ARG:H	1.38	0.71
1:CCC:274:GLU:OE1	1:CCC:312:ARG:HD3	1.90	0.71
1:CCC:71:GLN:HE22	1:CCC:228:ASN:HD21	1.37	0.70
1:BBB:274:GLU:OE1	1:BBB:312:ARG:HD3	1.91	0.69
1:DDD:274:GLU:OE1	1:DDD:312:ARG:HD3	1.93	0.69
1:AAA:49:ILE:HD13	1:BBB:33:ARG:HA	1.77	0.66
1:AAA:301:LEU:HG	1:AAA:308:ILE:HD11	1.78	0.66
1:DDD:127:GLN:HE22	1:DDD:186:ARG:H	1.44	0.64
1:DDD:301:LEU:HG	1:DDD:308:ILE:HD11	1.81	0.62
1:CCC:301:LEU:HG	1:CCC:308:ILE:HD11	1.81	0.62
1:BBB:175:GLU:O	1:BBB:179:ILE:HG13	2.01	0.61
1:DDD:161:GLN:HB2	3:DDD:554:HOH:O	2.00	0.61
1:CCC:175:GLU:O	1:CCC:179:ILE:HG13	2.01	0.60
1:DDD:175:GLU:O	1:DDD:179:ILE:HG13	2.02	0.60
1:AAA:175:GLU:O	1:AAA:179:ILE:HG13	2.02	0.59
1:CCC:88:PHE:HD1	3:CCC:502:HOH:O	1.85	0.59
1:AAA:186:ARG:HD3	3:AAA:564:HOH:O	2.02	0.59
1:DDD:172:GLU:HB3	3:DDD:559:HOH:O	2.03	0.58
1:BBB:224:ASN:HD22	1:CCC:304:SER:HB3	1.66	0.58
1:AAA:236:VAL:HG21	1:AAA:255:LEU:HD21	1.86	0.57
1:BBB:170:ASN:C	1:BBB:170:ASN:HD22	2.08	0.57
1:CCC:84:SER:HA	3:CCC:536:HOH:O	2.04	0.56
1:CCC:170:ASN:HD22	1:CCC:170:ASN:C	2.08	0.56
1:BBB:236:VAL:HG21	1:BBB:255:LEU:HD21	1.87	0.56
1:DDD:236:VAL:HG21	1:DDD:255:LEU:HD21	1.87	0.56
1:CCC:160:ASN:HD22	1:CCC:163:THR:H	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:301:LEU:HG	1:BBB:308:ILE:HD11	1.88	0.55
1:BBB:160:ASN:HD22	1:BBB:163:THR:H	1.55	0.55
1:AAA:170:ASN:C	1:AAA:170:ASN:HD22	2.09	0.55
1:DDD:170:ASN:C	1:DDD:170:ASN:HD22	2.09	0.55
1:CCC:33:ARG:HA	1:DDD:49:ILE:HD13	1.89	0.55
1:CCC:236:VAL:HG21	1:CCC:255:LEU:HD21	1.88	0.54
1:AAA:234:GLY:O	1:AAA:238:GLU:HG2	2.08	0.54
1:DDD:174:ARG:NH1	3:DDD:504:HOH:O	2.42	0.53
1:BBB:93:THR:HG22	1:BBB:97:LEU:CD2	2.38	0.52
1:DDD:229:ASN:ND2	1:DDD:257:TYR:OH	2.42	0.52
1:DDD:234:GLY:O	1:DDD:238:GLU:HG2	2.10	0.52
1:AAA:229:ASN:ND2	1:AAA:257:TYR:OH	2.43	0.52
1:BBB:229:ASN:ND2	1:BBB:257:TYR:OH	2.44	0.50
1:CCC:234:GLY:O	1:CCC:238:GLU:HG2	2.11	0.50
1:CCC:171:ASP:OD1	1:CCC:174:ARG:NH2	2.45	0.50
1:AAA:33:ARG:HA	1:BBB:49:ILE:HD13	1.93	0.49
1:BBB:171:ASP:OD1	1:BBB:174:ARG:NH2	2.45	0.49
1:DDD:171:ASP:OD1	1:DDD:174:ARG:NH2	2.46	0.49
1:BBB:234:GLY:O	1:BBB:238:GLU:HG2	2.11	0.49
1:CCC:229:ASN:ND2	1:CCC:257:TYR:OH	2.45	0.49
1:AAA:68:ASN:OD1	1:AAA:230:VAL:HG21	2.13	0.49
1:DDD:160:ASN:HD22	1:DDD:163:THR:H	1.61	0.49
1:CCC:228:ASN:HD22	1:CCC:229:ASN:N	2.12	0.48
1:DDD:127:GLN:HE22	1:DDD:186:ARG:N	2.11	0.48
1:BBB:68:ASN:OD1	1:BBB:230:VAL:HG21	2.13	0.48
1:CCC:93:THR:HG22	1:CCC:97:LEU:CD2	2.43	0.48
1:CCC:127:GLN:HE22	1:CCC:186:ARG:N	2.08	0.48
1:DDD:68:ASN:OD1	1:DDD:230:VAL:HG21	2.14	0.48
1:CCC:68:ASN:OD1	1:CCC:230:VAL:HG21	2.14	0.48
1:DDD:203:LEU:HD12	1:DDD:203:LEU:C	2.34	0.48
1:AAA:171:ASP:OD1	1:AAA:174:ARG:NH2	2.46	0.47
1:BBB:203:LEU:C	1:BBB:203:LEU:HD12	2.35	0.47
1:BBB:127:GLN:HE22	1:BBB:186:ARG:N	2.08	0.47
1:BBB:228:ASN:HD22	1:BBB:229:ASN:N	2.13	0.47
1:CCC:249:GLU:OE1	1:CCC:316:ARG:NH2	2.47	0.47
1:AAA:160:ASN:HD22	1:AAA:163:THR:H	1.63	0.46
1:AAA:203:LEU:HD12	1:AAA:203:LEU:C	2.35	0.46
1:CCC:203:LEU:C	1:CCC:203:LEU:HD12	2.36	0.46
1:AAA:93:THR:HG22	1:AAA:97:LEU:CD2	2.46	0.46
1:CCC:155:LYS:HE2	3:CCC:552:HOH:O	2.16	0.46
1:DDD:228:ASN:HD22	1:DDD:229:ASN:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:258:ARG:NE	3:DDD:502:HOH:O	2.39	0.45
1:BBB:90:THR:O	1:BBB:95:ARG:NH1	2.50	0.45
1:AAA:49:ILE:CD1	1:BBB:33:ARG:HA	2.46	0.45
1:CCC:248:HIS:CE1	1:CCC:317:ARG:HG3	2.53	0.44
1:AAA:228:ASN:HD22	1:AAA:229:ASN:N	2.15	0.44
1:CCC:52:SER:OG	1:DDD:72:GLU:OE1	2.25	0.44
1:CCC:217:ARG:CZ	1:DDD:217:ARG:NH2	2.81	0.43
1:DDD:228:ASN:HD22	1:DDD:229:ASN:H	1.66	0.43
1:CCC:88:PHE:HB3	3:CCC:502:HOH:O	2.18	0.43
1:BBB:93:THR:HG21	1:BBB:173:VAL:HG22	2.01	0.43
1:DDD:95:ARG:HA	3:DDD:534:HOH:O	2.18	0.43
1:BBB:93:THR:HG22	1:BBB:97:LEU:HD22	2.01	0.42
1:CCC:228:ASN:HD22	1:CCC:229:ASN:H	1.64	0.42
1:BBB:60:THR:HB	1:BBB:113:TYR:HB3	2.01	0.42
1:BBB:257:TYR:HD2	3:BBB:520:HOH:O	2.02	0.42
1:DDD:93:THR:HG22	1:DDD:97:LEU:CD2	2.50	0.42
1:AAA:228:ASN:HD22	1:AAA:229:ASN:H	1.67	0.42
1:DDD:70:LEU:HD22	1:DDD:138:TRP:CG	2.55	0.42
1:CCC:131:LYS:HA	1:CCC:131:LYS:HE2	2.01	0.42
1:AAA:76:ASN:ND2	1:BBB:116:TRP:CZ2	2.88	0.41
1:CCC:52:SER:N	1:DDD:72:GLU:OE1	2.52	0.41
1:BBB:108:ILE:O	1:BBB:252:THR:HA	2.19	0.41
1:DDD:256:ASP:O	1:DDD:309:ASN:HB2	2.20	0.41
1:CCC:93:THR:HG21	1:CCC:173:VAL:HG22	2.03	0.41
1:CCC:116:TRP:HE1	1:DDD:76:ASN:HD21	1.67	0.41
1:DDD:309:ASN:C	1:DDD:309:ASN:HD22	2.24	0.41
1:AAA:256:ASP:O	1:AAA:309:ASN:HB2	2.21	0.41
1:BBB:135:ARG:HA	1:BBB:154:SER:O	2.21	0.41
1:CCC:108:ILE:O	1:CCC:252:THR:HA	2.20	0.41
1:AAA:309:ASN:C	1:AAA:309:ASN:HD22	2.24	0.41
1:BBB:228:ASN:HD22	1:BBB:229:ASN:H	1.66	0.41
1:BBB:309:ASN:C	1:BBB:309:ASN:HD22	2.24	0.41
1:CCC:70:LEU:HD22	1:CCC:138:TRP:CG	2.56	0.41
1:AAA:127:GLN:HE22	1:AAA:186:ARG:H	1.69	0.41
1:BBB:70:LEU:HD22	1:BBB:138:TRP:CG	2.56	0.41
1:CCC:309:ASN:C	1:CCC:309:ASN:HD22	2.25	0.40
1:AAA:72:GLU:OE1	1:BBB:52:SER:N	2.50	0.40
1:CCC:299:LEU:HD13	1:CCC:309:ASN:HD21	1.86	0.40
1:AAA:248:HIS:CE1	1:AAA:317:ARG:HG3	2.56	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	265/320 (83%)	259 (98%)	6 (2%)	0	100	100
1	BBB	261/320 (82%)	254 (97%)	6 (2%)	1 (0%)	34	42
1	CCC	261/320 (82%)	252 (97%)	9 (3%)	0	100	100
1	DDD	265/320 (83%)	259 (98%)	6 (2%)	0	100	100
All	All	1052/1280 (82%)	1024 (97%)	27 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	185	PRO

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	243/282 (86%)	225 (93%)	18 (7%)	13	17
1	BBB	241/282 (86%)	226 (94%)	15 (6%)	18	25
1	CCC	241/282 (86%)	228 (95%)	13 (5%)	22	30
1	DDD	243/282 (86%)	223 (92%)	20 (8%)	11	14
All	All	968/1128 (86%)	902 (93%)	66 (7%)	16	21

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	71	GLN
1	AAA	79	GLN
1	AAA	84	SER
1	AAA	97	LEU
1	AAA	98	ARG
1	AAA	106	MET
1	AAA	127	GLN
1	AAA	160	ASN
1	AAA	166	LEU
1	AAA	168	ARG
1	AAA	170	ASN
1	AAA	183	ARG
1	AAA	192	GLU
1	AAA	198	LYS
1	AAA	228	ASN
1	AAA	264	ASP
1	AAA	292	GLU
1	AAA	309	ASN
1	BBB	71	GLN
1	BBB	79	GLN
1	BBB	84	SER
1	BBB	97	LEU
1	BBB	103	THR
1	BBB	106	MET
1	BBB	166	LEU
1	BBB	168	ARG
1	BBB	170	ASN
1	BBB	183	ARG
1	BBB	198	LYS
1	BBB	205	GLU
1	BBB	228	ASN
1	BBB	264	ASP
1	BBB	309	ASN
1	CCC	79	GLN
1	CCC	84	SER
1	CCC	96	LEU
1	CCC	97	LEU
1	CCC	106	MET
1	CCC	166	LEU
1	CCC	168	ARG
1	CCC	170	ASN
1	CCC	183	ARG
1	CCC	198	LYS

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Mol	Chain	Res	Type
1	CCC	228	ASN
1	CCC	264	ASP
1	CCC	309	ASN
1	DDD	71	GLN
1	DDD	79	GLN
1	DDD	84	SER
1	DDD	97	LEU
1	DDD	98	ARG
1	DDD	103	THR
1	DDD	106	MET
1	DDD	160	ASN
1	DDD	166	LEU
1	DDD	168	ARG
1	DDD	170	ASN
1	DDD	175	GLU
1	DDD	183	ARG
1	DDD	192	GLU
1	DDD	198	LYS
1	DDD	205	GLU
1	DDD	228	ASN
1	DDD	264	ASP
1	DDD	309	ASN
1	DDD	316	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)

4 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	WOX	AAA	401	-	24,29,29	0.95	0	29,43,43	3.28	14 (48%)
2	WOX	DDD	401	-	24,29,29	0.88	2 (8%)	29,43,43	3.12	13 (44%)
2	WOX	BBB	401	-	24,29,29	0.92	1 (4%)	29,43,43	3.28	13 (44%)
2	WOX	CCC	401	-	24,29,29	1.42	4 (16%)	29,43,43	3.34	11 (37%)

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	WOX	AAA	401	-	-	0/4/36/36	0/4/4/4
2	WOX	DDD	401	-	-	0/4/36/36	0/4/4/4
2	WOX	BBB	401	-	-	1/4/36/36	0/4/4/4
2	WOX	CCC	401	-	-	1/4/36/36	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	401	WOX	C26-C7	3.92	1.53	1.50
2	CCC	401	WOX	C11-C10	-3.39	1.48	1.53
2	CCC	401	WOX	O9-N8	2.64	1.46	1.42
2	DDD	401	WOX	O9-N8	2.55	1.46	1.42
2	CCC	401	WOX	C6-C7	2.46	1.50	1.47
2	BBB	401	WOX	O9-N8	2.29	1.46	1.42
2	DDD	401	WOX	C26-C7	2.14	1.52	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CCC	401	WOX	C26-C7-N8	-12.59	105.23	113.96
2	AAA	401	WOX	C26-C7-N8	-10.19	106.90	113.96
2	BBB	401	WOX	C26-C7-N8	-9.95	107.06	113.96
2	DDD	401	WOX	C26-C7-N8	-8.36	108.17	113.96
2	DDD	401	WOX	C6-C7-N8	7.92	132.52	120.46
2	AAA	401	WOX	O9-N8-C7	7.39	113.71	109.29
2	BBB	401	WOX	C6-C7-N8	7.37	131.69	120.46
2	CCC	401	WOX	C6-C7-N8	6.95	131.04	120.46
2	DDD	401	WOX	C11-C10-C26	-5.95	104.82	113.30
2	AAA	401	WOX	C6-C7-N8	5.88	129.42	120.46
2	BBB	401	WOX	C13-N14-C24	-5.50	119.25	125.20
2	AAA	401	WOX	C11-C10-C26	-5.39	105.62	113.30
2	BBB	401	WOX	C15-N14-C24	5.08	123.85	119.70
2	BBB	401	WOX	C11-C10-C26	-4.64	106.69	113.30
2	DDD	401	WOX	O9-N8-C7	4.61	112.05	109.29
2	CCC	401	WOX	O9-N8-C7	4.60	112.04	109.29
2	CCC	401	WOX	C1-C2-C3	-4.60	118.43	125.59
2	CCC	401	WOX	C12-C11-C10	-4.26	106.71	111.78
2	DDD	401	WOX	C22-C16-C17	4.07	120.17	114.51
2	AAA	401	WOX	C22-C16-C17	3.97	120.04	114.51
2	BBB	401	WOX	F23-C22-C16	3.70	122.04	117.63
2	AAA	401	WOX	C10-C26-C7	3.63	104.90	101.21
2	BBB	401	WOX	C22-C16-C17	3.41	119.25	114.51
2	DDD	401	WOX	C13-N14-C24	-3.40	121.52	125.20
2	DDD	401	WOX	C11-C12-C13	-3.29	105.13	110.69
2	CCC	401	WOX	C22-C16-C17	3.19	118.95	114.51
2	DDD	401	WOX	C26-C7-C6	-3.17	119.31	125.07
2	AAA	401	WOX	O25-C24-N14	-3.03	117.60	122.34
2	BBB	401	WOX	F18-C17-C16	3.00	121.21	117.63
2	BBB	401	WOX	O9-N8-C7	2.89	111.02	109.29
2	AAA	401	WOX	C19-C17-C16	-2.84	118.88	124.02
2	DDD	401	WOX	C15-N14-C24	2.83	122.01	119.70
2	AAA	401	WOX	F18-C17-C16	2.81	120.98	117.63
2	BBB	401	WOX	C10-C26-C7	2.72	103.97	101.21
2	DDD	401	WOX	C19-C17-C16	-2.68	119.15	124.02
2	CCC	401	WOX	C13-N14-C24	-2.53	122.47	125.20
2	AAA	401	WOX	C1-C2-C3	-2.50	121.70	125.59
2	CCC	401	WOX	C15-N14-C24	2.46	121.71	119.70
2	CCC	401	WOX	O25-C24-N14	-2.46	118.49	122.34
2	DDD	401	WOX	F18-C17-C16	2.39	120.48	117.63
2	BBB	401	WOX	C21-C22-C16	-2.38	119.70	124.02
2	DDD	401	WOX	C1-C2-C3	-2.36	121.91	125.59
2	AAA	401	WOX	C15-N14-C24	2.24	121.53	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	401	WOX	C26-C7-C6	-2.22	121.04	125.07
2	DDD	401	WOX	C15-C16-C22	-2.20	117.35	122.50
2	BBB	401	WOX	C19-C17-C16	-2.18	120.07	124.02
2	AAA	401	WOX	C11-C12-C13	-2.18	107.01	110.69
2	AAA	401	WOX	C13-N14-C24	-2.13	122.90	125.20
2	CCC	401	WOX	C21-C22-C16	-2.11	120.20	124.02
2	AAA	401	WOX	C15-C16-C22	-2.06	117.68	122.50
2	CCC	401	WOX	C3-C2-C6	2.06	115.47	108.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

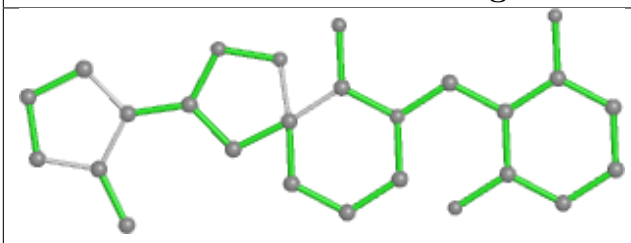
Mol	Chain	Res	Type	Atoms
2	BBB	401	WOX	C16-C15-N14-C24
2	CCC	401	WOX	C16-C15-N14-C24

There are no ring outliers.

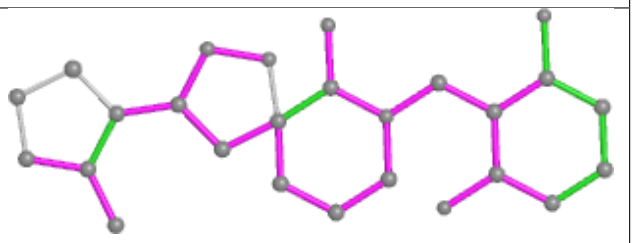
No monomer is involved in short contacts.

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.

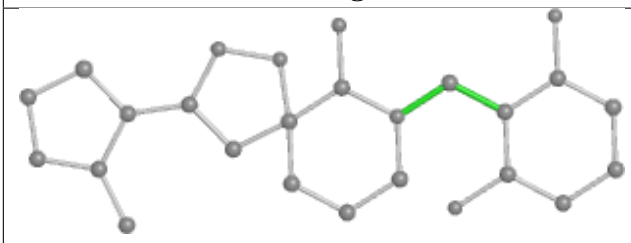
Ligand WOX AAA 401



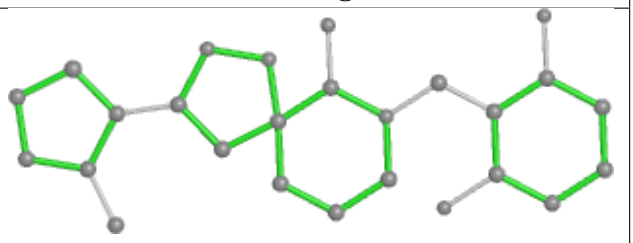
Bond lengths



Bond angles

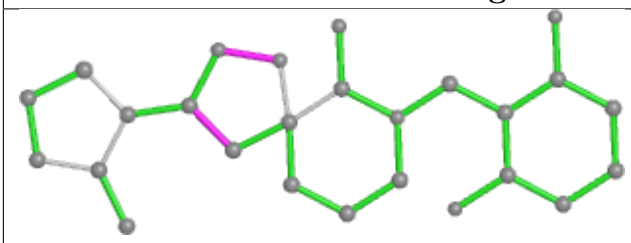


Torsions

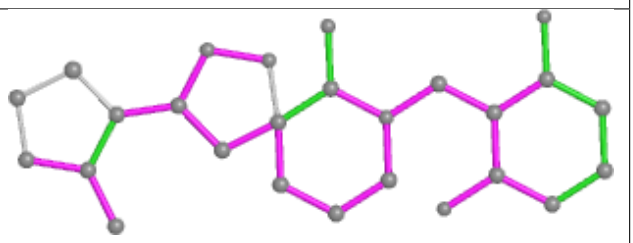


Rings

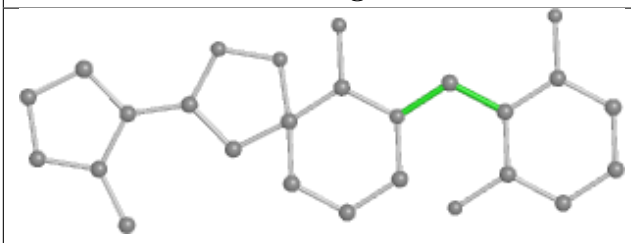
Ligand WOX DDD 401



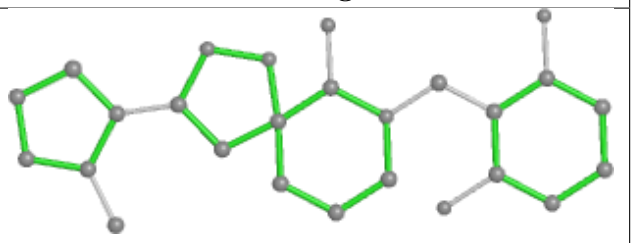
Bond lengths



Bond angles

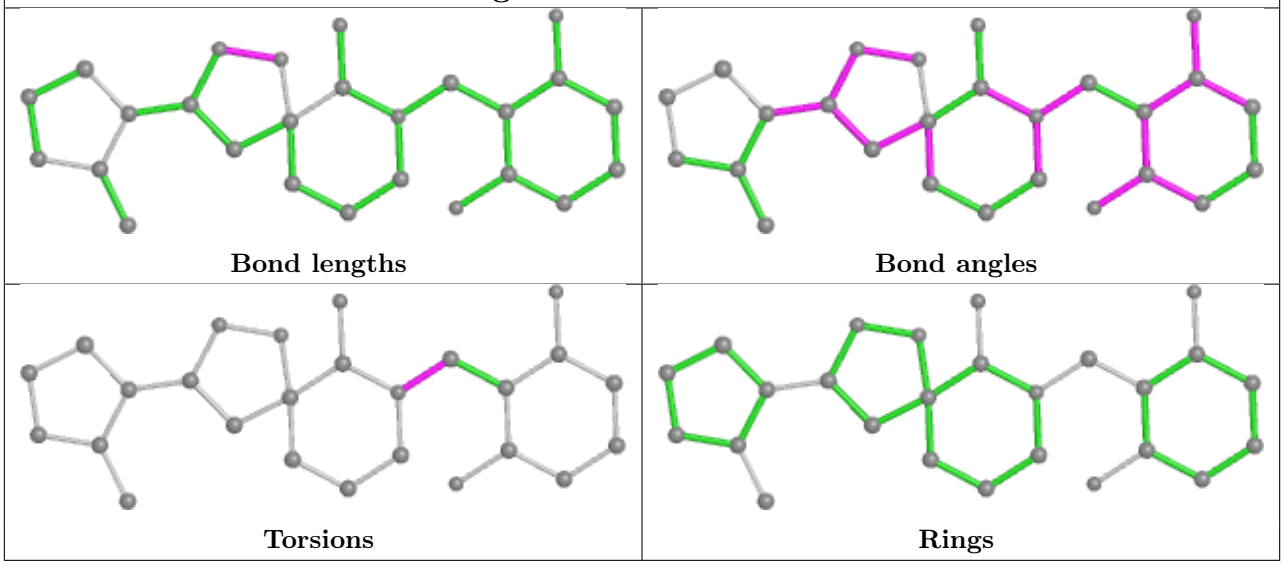


Torsions

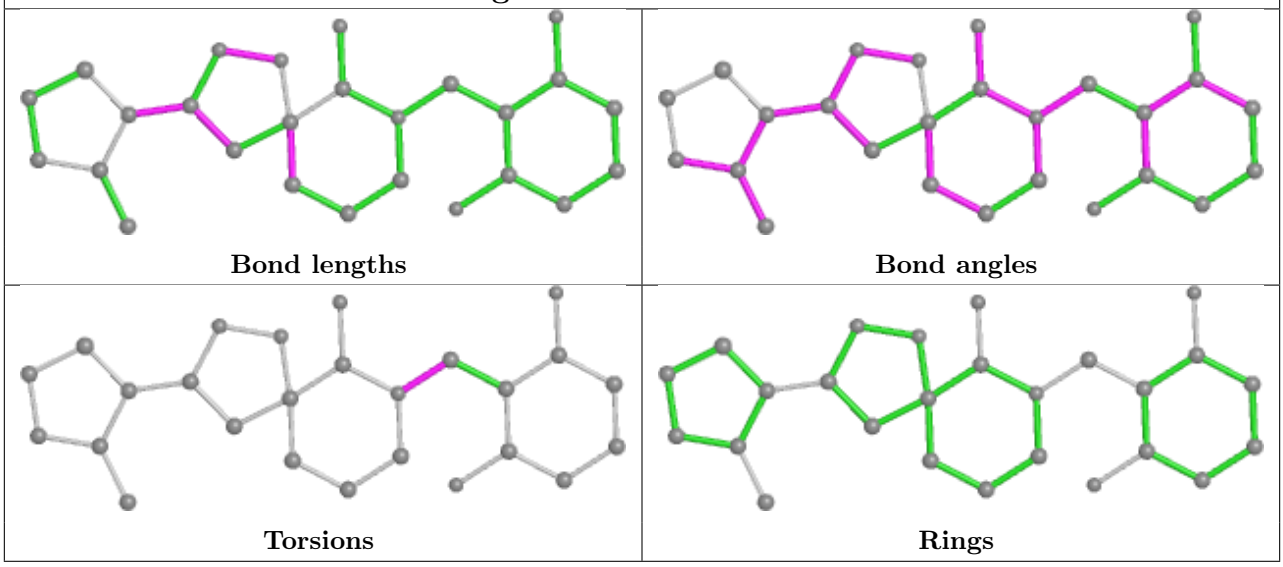


Rings

Ligand WOX BBB 401



Ligand WOX CCC 401



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

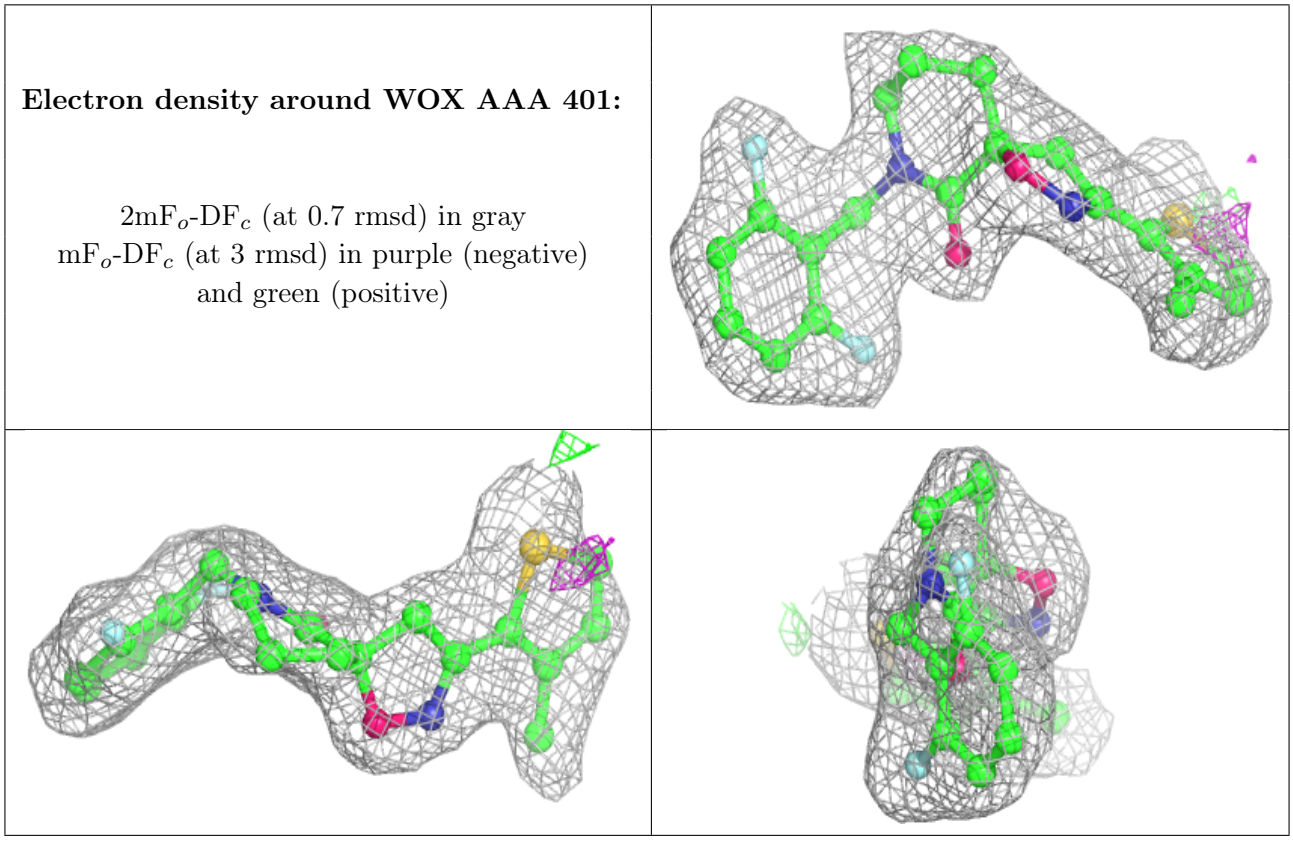
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

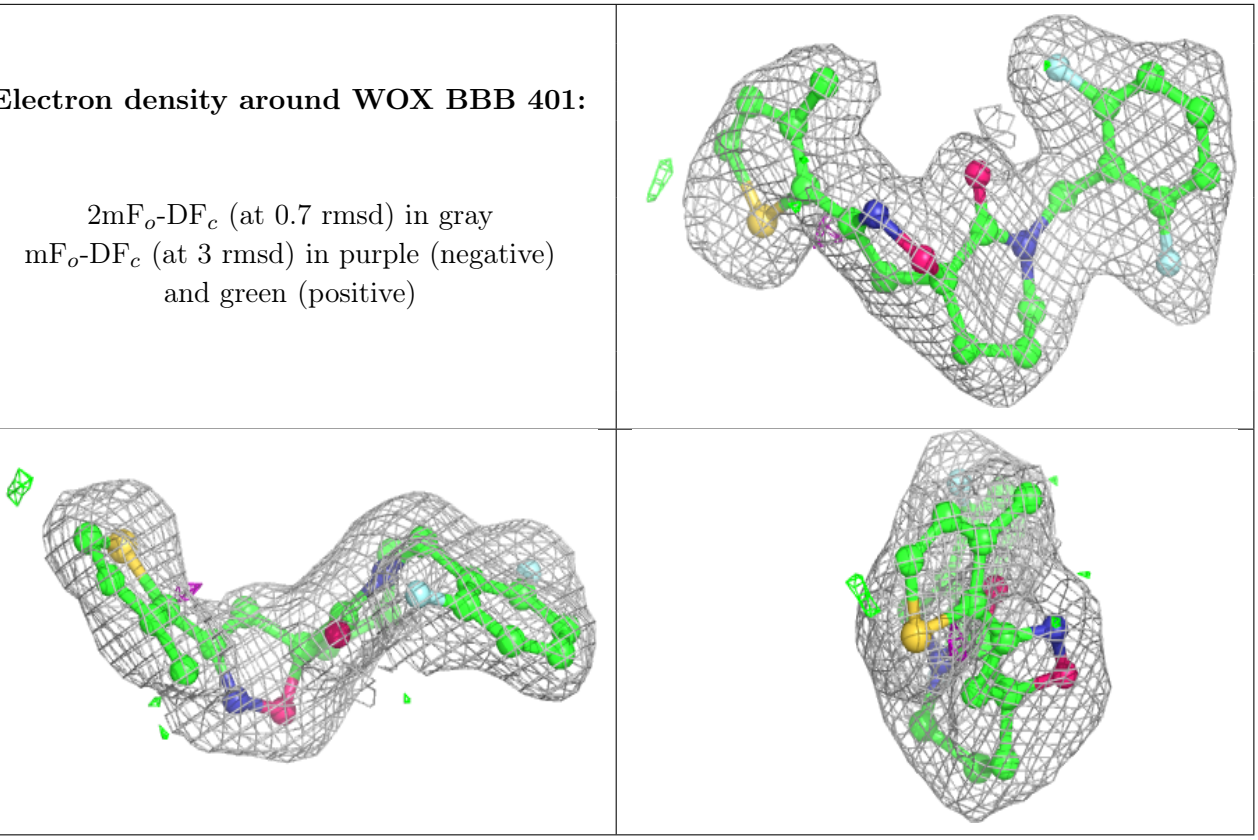
Electron density around WOX AAA 401:

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



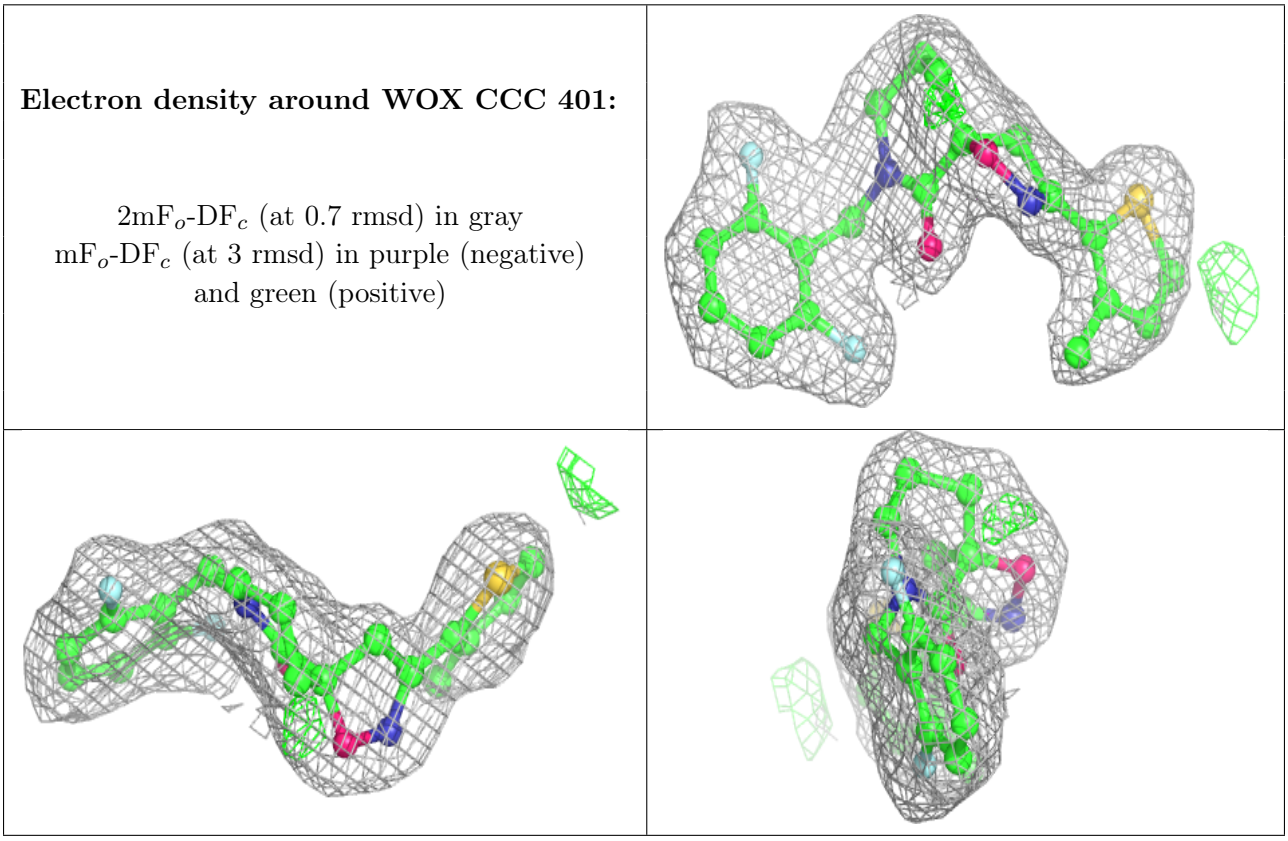
Electron density around WOX BBB 401:

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



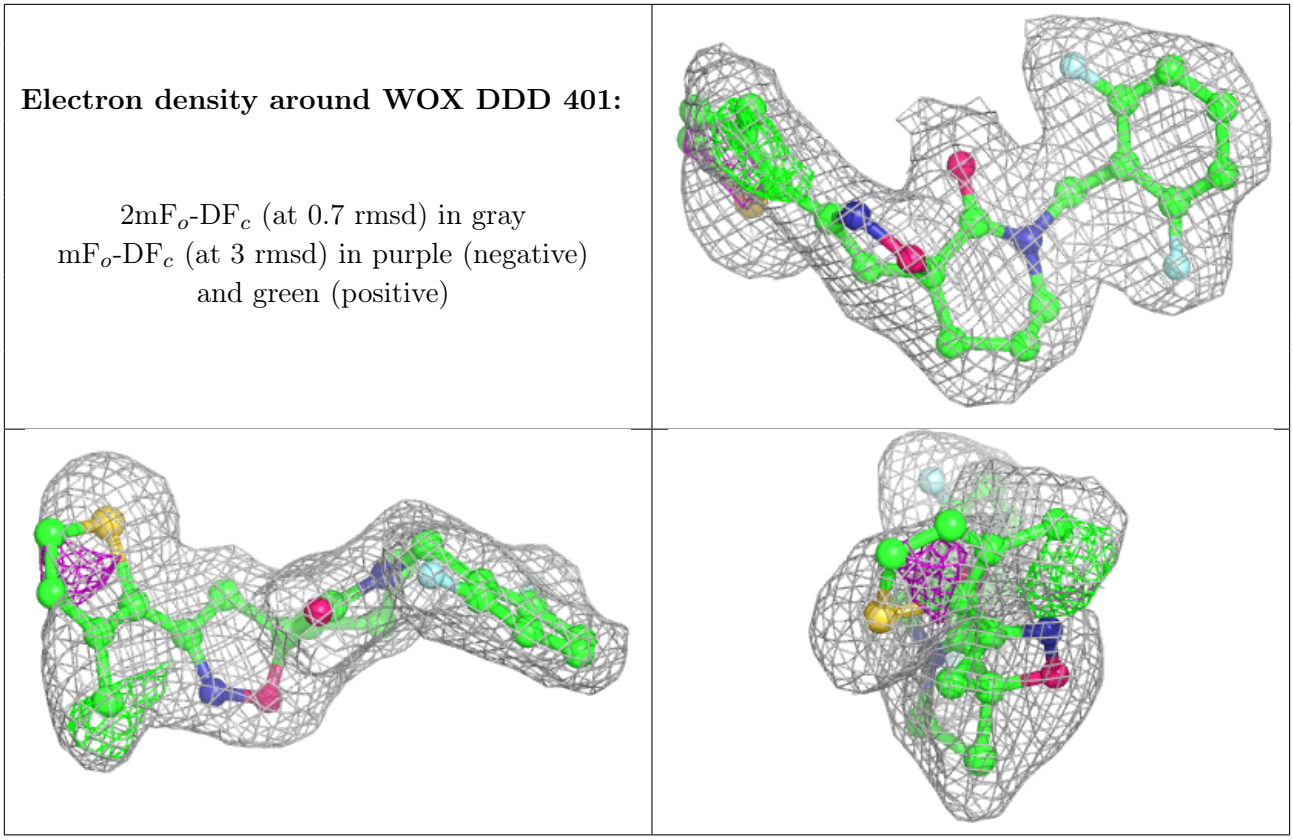
Electron density around WOX CCC 401:

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



Electron density around WOX DDD 401:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.