



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 10:21 AM EDT

PDB ID : 8UAS
Title : Rhodococcus ruber Alcohol Dehydrogenase NADH Biomimetic Complex -
Compound 1a
Authors : Wilson, L.A.; Guddat, L.W.; Schenk, G.; Scott, C.
Deposited on : 2023-09-22
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

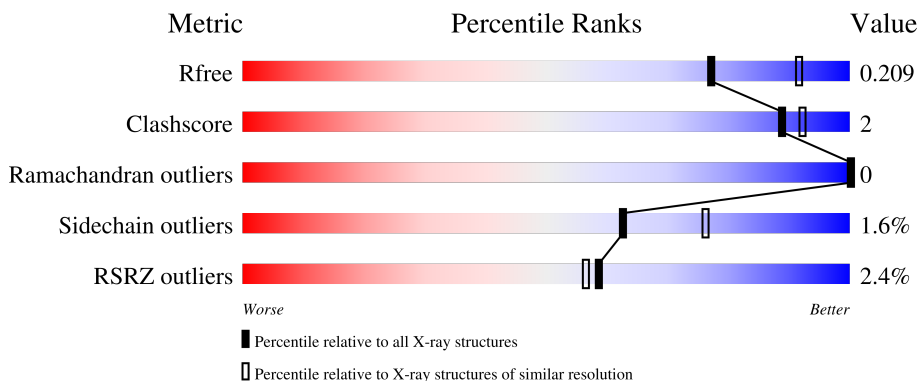
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	A	365	93%
1	B	365	93%
1	C	365	3%
1	D	365	90%
1	E	365	2%

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Mol	Chain	Length	Quality of chain
1	F	365	<p>2% 92% 6% 5%</p>
1	G	365	<p>2% 89% 6% 5%</p>
1	H	365	<p>4% 91% 5% .</p>
1	I	365	<p>4% 90% 6% .</p>
1	J	365	<p>% 91% 5% .</p>
1	K	365	<p>4% 92% 5% . . .</p>
1	L	365	<p>3% 92% 5% . .</p>

2 Entry composition [i](#)

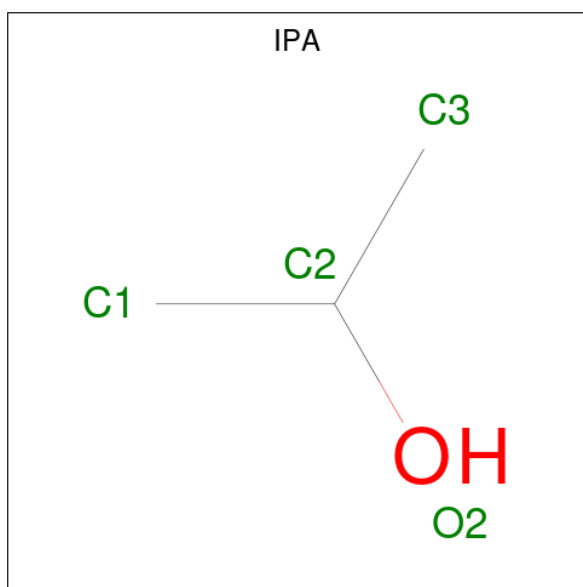
There are 7 unique types of molecules in this entry. The entry contains 62122 atoms, of which 29639 are hydrogens and 0 are deuteriums.

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 *Rhodococcus ruber* Alcohol Dehydrogenase Chain A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	352	4981	1594	2455	445	475	12	0	0	0
1	B	349	4972	1582	2464	442	472	12	0	1	0
1	C	348	4961	1576	2464	438	471	12	0	1	0
1	D	349	4972	1582	2464	442	472	12	13	1	0
1	E	348	4961	1576	2464	438	471	12	13	1	0
1	F	349	4972	1582	2464	442	472	12	0	1	0
1	G	348	4961	1576	2464	438	471	12	0	1	0
1	H	349	4973	1582	2465	442	472	12	0	1	0
1	I	349	4972	1582	2464	442	472	12	0	1	0
1	J	349	4972	1582	2464	442	472	12	0	1	0
1	K	350	4966	1583	2455	443	473	12	0	0	0
1	L	349	4972	1582	2464	442	472	12	0	1	0

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	12	3	8	1	0	0
2	C	1	12	3	8	1	0	0
2	D	1	12	3	8	1	0	0
2	D	1	12	3	8	1	0	0
2	F	1	12	3	8	1	0	0
2	G	1	12	3	8	1	0	0
2	I	1	12	3	8	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	2	3	3	0	1
3	B	2	3	3	0	1
3	C	2	2	2	0	0
3	D	2	2	2	0	0
3	E	2	2	2	0	0

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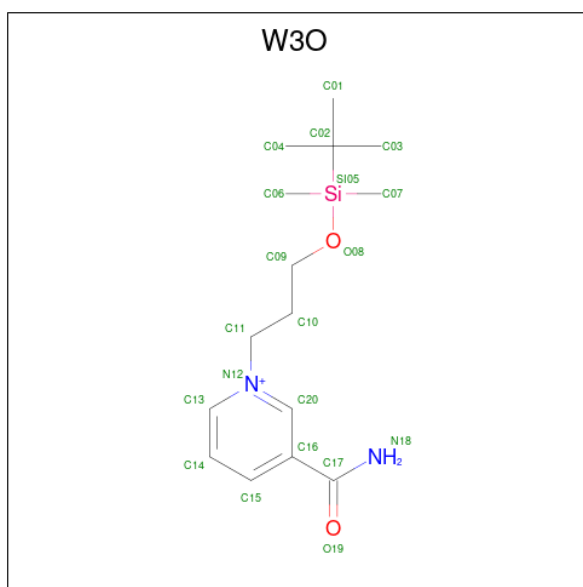
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total 2	Zn 2	0	0
3	G	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	J	2	Total 2	Zn 2	0	0
3	K	2	Total 2	Zn 2	0	0
3	L	2	Total 2	Zn 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

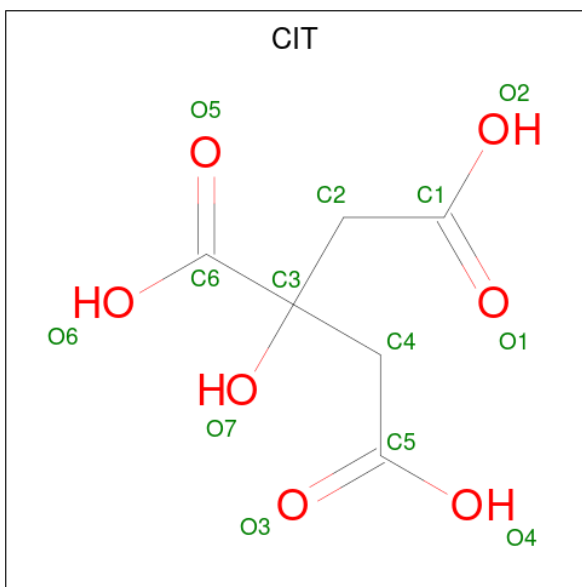
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	D	1	Total 1	Na 1	0	0
4	I	1	Total 1	Na 1	0	0
4	J	1	Total 1	Na 1	0	0

- Molecule 5 is 1-[3-[{tert}-butyl(dimethyl)silyl]oxypropyl]pyridine-3-carboxamide (three-letter code: W3O) (formula: C₁₅H₂₇N₂O₂Si) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	Si			
5	C	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	D	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	E	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	F	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	G	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	H	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	I	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	J	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	K	1	Total	C	N	O	Si	0	0	
			20	15	2	2	1			
5	L	1	Total	C	H	N	O	Si	0	0
			47	15	27	2	2	1		

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	I	1	18	6	5	7	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	262	Total	O	0	0
			262	262		
7	B	156	Total	O	0	0
			156	156		
7	C	168	Total	O	0	0
			168	168		
7	D	250	Total	O	0	0
			250	250		
7	E	241	Total	O	0	0
			241	241		
7	F	213	Total	O	0	0
			213	213		
7	G	148	Total	O	0	0
			148	148		
7	H	108	Total	O	0	0
			108	108		
7	I	148	Total	O	0	0
			148	148		
7	J	176	Total	O	0	0
			176	176		
7	K	128	Total	O	0	0
			128	128		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	130	Total 130	O 130	0	0

3 Residue-property plots

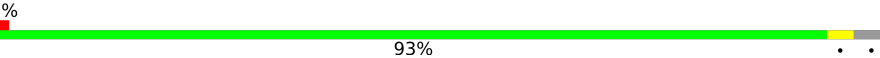
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

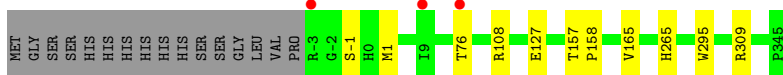
- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain A:  93%




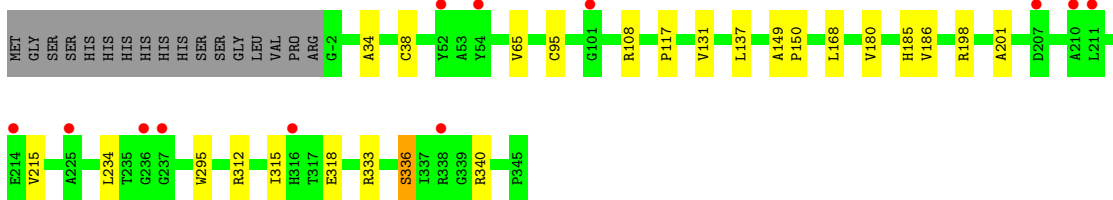
- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain B:  93%

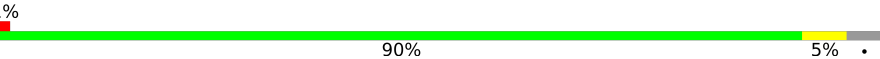


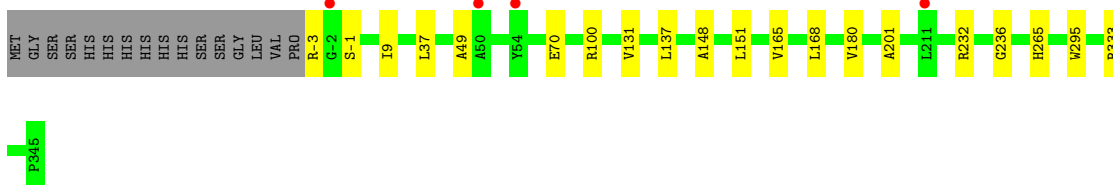
- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain C:  88% 7% 5% 3%

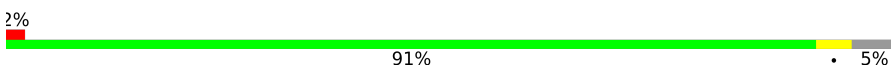


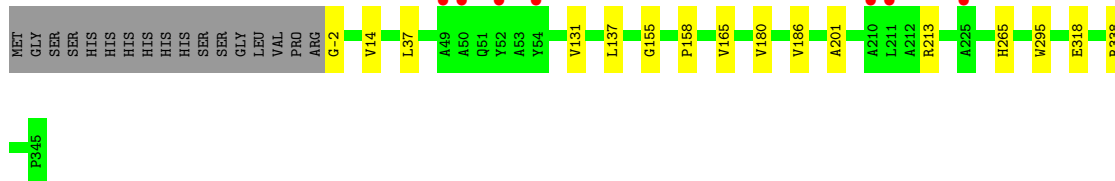
- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain D:  90% 5%

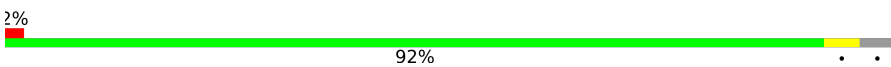


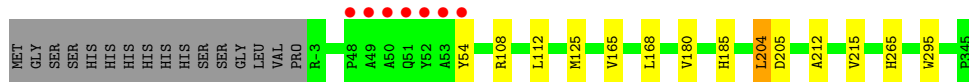
- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain E:  91% 2% 5%

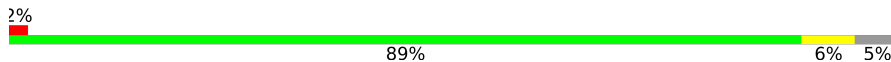


- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain F:  92% 2% 5%

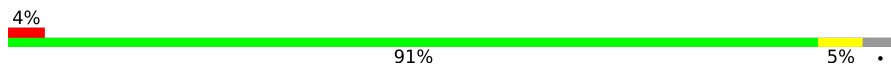


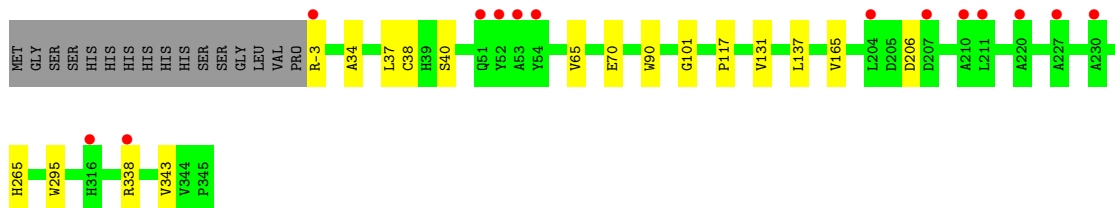
- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain G:  89% 2% 6% 5%




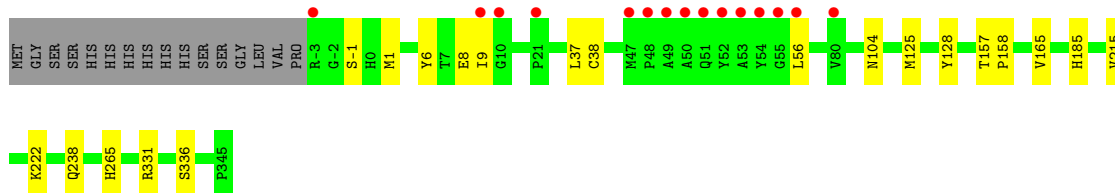
- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain H:  91% 4% 5%




- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain I:  90% 4% 6%

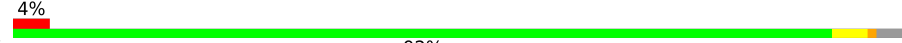


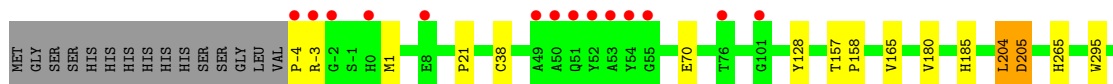
- Molecule 1: Rhodococcus ruber Alcohol Dehydrogenase Chain A

Chain J:  91% 5%




- Molecule 1: *Rhodococcus ruber* Alcohol Dehydrogenase Chain A

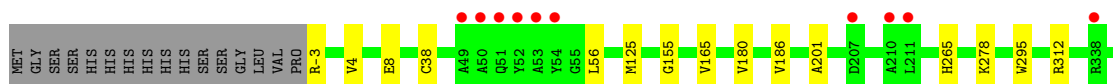
Chain K:  92% 4%



P345

- Molecule 1: *Rhodococcus ruber* Alcohol Dehydrogenase Chain A

Chain L:  92% 3%



P345

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 157.75Å 272.43Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	49.22 – 2.20 49.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.22-2.20) 98.7 (49.22-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.182 , 0.210 0.182 , 0.209	Depositor DCC
R_{free} test set	1995 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	62122	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IPA, W3O, CIT, ZN

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	A	0.25	0/2579	0.51	0/3522
1	B	0.25	0/2563	0.51	0/3499
1	C	0.25	0/2552	0.51	0/3485
1	D	0.26	0/2563	0.52	0/3499
1	E	0.26	0/2552	0.52	0/3485
1	F	0.26	0/2563	0.53	0/3499
1	G	0.25	0/2552	0.51	0/3485
1	H	0.25	0/2563	0.51	0/3499
1	I	0.25	0/2563	0.52	0/3499
1	J	0.25	0/2563	0.52	0/3499
1	K	0.25	0/2564	0.51	0/3500
1	L	0.25	0/2563	0.51	0/3499
All	All	0.25	0/30740	0.51	0/41970

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 [i](#)

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	A	2526	2455	2520	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2508	2464	2502	7	0
1	C	2497	2464	2489	14	0
1	D	2508	2464	2502	10	0
1	E	2497	2464	2489	9	0
1	F	2508	2464	2502	11	0
1	G	2497	2464	2489	11	0
1	H	2508	2465	2502	11	0
1	I	2508	2464	2502	11	0
1	J	2508	2464	2502	7	0
1	K	2511	2455	2500	8	0
1	L	2508	2464	2502	10	0
2	A	4	8	8	0	0
2	C	4	8	8	1	0
2	D	8	16	16	1	0
2	F	4	8	8	1	0
2	G	4	8	8	1	0
2	I	4	8	8	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	C	20	0	0	0	0
5	D	20	0	0	0	0
5	E	20	0	0	0	0
5	F	20	0	0	0	0
5	G	20	0	0	0	0
5	H	20	0	0	0	0
5	I	20	0	0	0	0
5	J	20	0	0	0	0
5	K	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	20	27	0	0	0
6	I	13	5	5	0	0
7	A	262	0	0	1	1
7	B	156	0	0	2	0
7	C	168	0	0	4	0
7	D	250	0	0	1	1
7	E	241	0	0	4	0
7	F	213	0	0	1	0
7	G	148	0	0	1	0
7	H	108	0	0	2	0
7	I	148	0	0	1	0
7	J	176	0	0	1	0
7	K	128	0	0	1	1
7	L	130	0	0	3	1
All	All	32483	29639	30062	113	2

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 2.

All (113) 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:C:318:GLU:OE1	7:C:501:HOH:O	1.93	0.86
1:A:238:GLN:O	7:A:501:HOH:O	1.99	0.81
1:E:-2:GLY:N	7:E:602:HOH:O	2.19	0.73
1:C:312:ARG:NH1	7:C:502:HOH:O	2.22	0.72
1:B:108:ARG:NH2	7:B:602:HOH:O	2.23	0.70
1:I:1:MET:HE1	1:I:128:TYR:HB2	1.74	0.70
1:G:34:ALA:HB3	1:G:65[B]:VAL:HG22	1.74	0.69
1:B:76:THR:O	7:B:601:HOH:O	2.11	0.68
1:C:108:ARG:NH2	7:C:504:HOH:O	2.26	0.67
1:E:318:GLU:OE1	7:E:601:HOH:O	2.10	0.67
1:I:238:GLN:O	7:I:501:HOH:O	2.14	0.66
1:H:338:ARG:N	7:H:603:HOH:O	2.28	0.66
1:F:54:TYR:OH	7:F:501:HOH:O	2.14	0.64
1:L:180:VAL:HG11	1:L:201:ALA:HB1	1.80	0.64
1:D:-3:ARG:NH2	1:D:70:GLU:OE1	2.31	0.63
1:G:34:ALA:HB3	1:G:65[B]:VAL:CG2	2.29	0.63
1:L:-3:ARG:HA	1:L:-3:ARG:HE	1.64	0.62
1:A:16:VAL:HG23	1:A:18:ILE:HG23	1.82	0.61
1:H:-3:ARG:NH2	1:H:70:GLU:OE1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:ALA:HB3	1:H:65[B]:VAL:CG2	2.31	0.60
1:F:180:VAL:O	1:F:180:VAL:HG12	2.00	0.60
1:J:338:ARG:NH2	7:J:602:HOH:O	2.36	0.59
1:F:168:LEU:HD11	2:F:401:IPA:H2	1.84	0.58
1:L:-3:ARG:HA	7:L:507:HOH:O	2.02	0.58
1:F:185:HIS:NE2	1:F:215:VAL:HG11	2.18	0.58
1:L:-3:ARG:NE	7:L:507:HOH:O	2.36	0.57
1:D:148:ALA:HA	1:D:151:LEU:HD12	1.86	0.57
1:G:186:VAL:HG22	1:G:315:ILE:HD12	1.85	0.57
1:G:168:LEU:HD11	2:G:401:IPA:H2	1.86	0.56
1:D:168:LEU:HD21	2:D:401:IPA:H13	1.87	0.56
1:J:2:LYS:NZ	1:J:323:ASP:OD1	2.34	0.55
1:K:180:VAL:HG12	1:K:180:VAL:O	2.06	0.55
1:E:213:ARG:NH1	7:E:606:HOH:O	2.39	0.55
1:C:185:HIS:CE1	1:C:215:VAL:HG11	2.42	0.54
1:F:204:LEU:HD12	1:F:205:ASP:N	2.22	0.54
1:H:38:CYS:SG	1:H:40:SER:OG	2.64	0.54
1:C:168:LEU:HD11	2:C:401:IPA:H2	1.90	0.54
1:F:108:ARG:HG2	1:F:108:ARG:HH11	1.76	0.51
1:G:180:VAL:HG11	1:G:212:ALA:HB2	1.92	0.51
1:C:336:SER:O	1:C:336:SER:OG	2.25	0.51
1:L:-3:ARG:HA	1:L:-3:ARG:NE	2.23	0.51
1:F:165:VAL:HG11	1:F:265:HIS:CG	2.47	0.50
1:K:1:MET:HE1	1:K:21:PRO:HD3	1.93	0.50
1:I:9:ILE:HD13	1:I:56:LEU:HD11	1.93	0.50
1:I:165:VAL:HG11	1:I:265:HIS:CG	2.47	0.50
1:I:9:ILE:CD1	1:I:56:LEU:HD11	2.42	0.49
1:I:8:GLU:HA	1:I:56:LEU:HD13	1.94	0.48
1:D:131:VAL:HG21	1:D:137:LEU:HD21	1.94	0.48
1:D:100:ARG:NH2	7:D:510:HOH:O	2.47	0.48
1:E:165:VAL:HG11	1:E:265:HIS:CG	2.49	0.48
1:E:180:VAL:HG11	1:E:201:ALA:HB1	1.96	0.47
1:I:185:HIS:NE2	1:I:215:VAL:HG11	2.28	0.47
1:G:131:VAL:HG21	1:G:137:LEU:HD21	1.96	0.47
1:L:312:ARG:NH2	7:L:511:HOH:O	2.47	0.47
1:F:185:HIS:CD2	1:F:215:VAL:HG11	2.50	0.47
1:B:309:ARG:HG2	1:B:309:ARG:HH11	1.80	0.47
1:H:34:ALA:HB3	1:H:65[B]:VAL:HG22	1.97	0.47
1:G:103:GLU:OE2	1:G:135:ARG:NE	2.47	0.46
1:L:165:VAL:HG11	1:L:265:HIS:CG	2.51	0.46
1:B:1:MET:HB2	1:B:127:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:VAL:HG21	1:C:137:LEU:HD21	1.97	0.46
1:H:101:GLY:O	7:H:601:HOH:O	2.20	0.46
1:K:165:VAL:HG11	1:K:265:HIS:CG	2.51	0.46
1:B:165:VAL:HG11	1:B:265:HIS:CG	2.50	0.46
1:K:-4:PRO:HD3	1:K:70:GLU:OE1	2.16	0.45
1:D:180:VAL:HG11	1:D:201:ALA:HB1	1.97	0.45
1:L:155:GLY:HA2	1:L:186:VAL:HG11	1.97	0.45
1:E:338:ARG:N	7:E:601:HOH:O	2.38	0.45
1:J:47:MET:HE1	1:J:52:TYR:HA	1.98	0.45
1:K:128:TYR:OH	7:K:601:HOH:O	2.17	0.45
1:E:14:VAL:HG11	1:I:222:LYS:HD2	1.99	0.45
1:C:186:VAL:HG22	1:C:315:ILE:HD13	1.99	0.45
1:C:180:VAL:HG11	1:C:201:ALA:HB1	1.99	0.44
1:K:1:MET:CE	1:K:21:PRO:HD3	2.46	0.44
1:E:155:GLY:HA2	1:E:186:VAL:HG11	1.99	0.44
1:C:198:ARG:NH2	1:C:234:LEU:O	2.50	0.44
1:D:9:ILE:HG21	1:D:49:ALA:CA	2.48	0.44
1:H:165:VAL:HG11	1:H:265:HIS:CG	2.52	0.44
1:G:181:GLY:O	7:G:501:HOH:O	2.21	0.44
1:G:165:VAL:HG11	1:G:265:HIS:CG	2.53	0.44
1:D:9:ILE:HG21	1:D:49:ALA:HA	1.99	0.44
1:K:157:THR:HB	1:K:158:PRO:HD3	2.00	0.44
1:B:309:ARG:HG2	1:B:309:ARG:NH1	2.32	0.43
1:I:6:TYR:O	1:I:56:LEU:HD22	2.19	0.42
1:C:149:ALA:HB3	1:C:150:PRO:HD3	2.01	0.42
1:A:165:VAL:HG11	1:A:265:HIS:CG	2.55	0.42
1:J:157:THR:HB	1:J:158:PRO:HD3	2.00	0.42
1:D:232:ARG:O	1:D:236:GLY:O	2.38	0.42
1:H:90:TRP:CZ2	1:H:117:PRO:HG3	2.54	0.42
1:B:157:THR:HB	1:B:158:PRO:HD3	2.02	0.42
1:I:104:ASN:OD1	1:I:104:ASN:N	2.52	0.42
1:F:180:VAL:HG21	1:F:212:ALA:HB2	2.00	0.41
1:L:8:GLU:HA	1:L:56:LEU:HD13	2.01	0.41
1:A:157:THR:HB	1:A:158:PRO:HD3	2.02	0.41
1:A:149:ALA:HB3	1:A:150:PRO:HD3	2.03	0.41
1:K:204:LEU:HD12	1:K:205:ASP:N	2.36	0.41
1:E:131:VAL:HG21	1:E:137:LEU:HD21	2.01	0.41
1:H:131:VAL:HG21	1:H:137:LEU:HD21	2.03	0.41
1:C:34:ALA:HB3	1:C:65[B]:VAL:CG2	2.50	0.41
1:G:149:ALA:HB3	1:G:150:PRO:HD3	2.02	0.41
1:G:180:VAL:O	1:G:185:HIS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:CYS:HB3	1:C:108:ARG:HD3	2.01	0.41
1:I:157:THR:HB	1:I:158:PRO:HD3	2.02	0.41
1:F:108:ARG:HH21	1:F:112:LEU:HD21	1.86	0.40
1:J:135:ARG:O	1:J:298:ARG:HD3	2.21	0.40
1:J:131:VAL:HG21	1:J:137:LEU:HD21	2.02	0.40
1:H:37:LEU:HD11	1:H:343:VAL:HG23	2.03	0.40
1:H:37:LEU:N	1:H:37:LEU:HD12	2.36	0.40
1:C:312:ARG:NH2	7:C:513:HOH:O	2.54	0.40
1:J:331:ARG:HH11	1:J:331:ARG:HG3	1.86	0.40
1:L:4:VAL:HB	1:L:125:MET:HG2	2.03	0.40
1:D:165:VAL:HG11	1:D:265:HIS:CG	2.57	0.40
1:F:204:LEU:HD12	1:F:204:LEU:C	2.42	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:721:HOH:O	7:L:615:HOH:O[1_455]	2.12	0.08
7:A:631:HOH:O	7:D:635:HOH:O[2_347]	2.17	0.03

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	A	350/365 (96%)	343 (98%)	7 (2%)	0	100	100
1	B	348/365 (95%)	341 (98%)	7 (2%)	0	100	100
1	C	347/365 (95%)	335 (96%)	12 (4%)	0	100	100
1	D	348/365 (95%)	340 (98%)	8 (2%)	0	100	100
1	E	347/365 (95%)	341 (98%)	6 (2%)	0	100	100
1	F	348/365 (95%)	339 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	347/365 (95%)	339 (98%)	8 (2%)	0	100	100
1	H	348/365 (95%)	340 (98%)	8 (2%)	0	100	100
1	I	348/365 (95%)	339 (97%)	9 (3%)	0	100	100
1	J	348/365 (95%)	337 (97%)	11 (3%)	0	100	100
1	K	348/365 (95%)	337 (97%)	11 (3%)	0	100	100
1	L	348/365 (95%)	341 (98%)	7 (2%)	0	100	100
All	All	4175/4380 (95%)	4072 (98%)	103 (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	A	254/265 (96%)	252 (99%)	2 (1%)	81	90
1	B	252/265 (95%)	250 (99%)	2 (1%)	81	90
1	C	251/265 (95%)	245 (98%)	6 (2%)	49	62
1	D	252/265 (95%)	248 (98%)	4 (2%)	62	76
1	E	251/265 (95%)	248 (99%)	3 (1%)	71	83
1	F	252/265 (95%)	249 (99%)	3 (1%)	71	83
1	G	251/265 (95%)	245 (98%)	6 (2%)	49	62
1	H	252/265 (95%)	250 (99%)	2 (1%)	81	90
1	I	252/265 (95%)	246 (98%)	6 (2%)	49	62
1	J	252/265 (95%)	246 (98%)	6 (2%)	49	62
1	K	252/265 (95%)	246 (98%)	6 (2%)	49	62
1	L	252/265 (95%)	249 (99%)	3 (1%)	71	83
All	All	3023/3180 (95%)	2974 (98%)	49 (2%)	62	76

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
1	A	295	TRP
1	B	-1	SER
1	B	295	TRP
1	C	38	CYS
1	C	117	PRO
1	C	295	TRP
1	C	333	ARG
1	C	336	SER
1	C	340	ARG
1	D	-1	SER
1	D	37	LEU
1	D	295	TRP
1	D	333	ARG
1	E	37	LEU
1	E	158	PRO
1	E	295	TRP
1	F	125	MET
1	F	204	LEU
1	F	295	TRP
1	G	11	SER
1	G	38	CYS
1	G	223	SER
1	G	295	TRP
1	G	314	ASP
1	G	338	ARG
1	H	206	ASP
1	H	295	TRP
1	I	-1	SER
1	I	37	LEU
1	I	38	CYS
1	I	125	MET
1	I	331	ARG
1	I	336	SER
1	J	-1	SER
1	J	37	LEU
1	J	38	CYS
1	J	185	HIS
1	J	238	GLN
1	J	295	TRP
1	K	-3	ARG
1	K	38	CYS
1	K	185	HIS

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Mol	Chain	Res	Type
1	K	204	LEU
1	K	205	ASP
1	K	295	TRP
1	L	38	CYS
1	L	278	LYS
1	L	295	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	HIS
1	D	265	HIS
1	E	238	GLN
1	E	316	HIS
1	F	276	HIS
1	G	96	HIS
1	I	0	HIS
1	I	51	GLN

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 48 ligands modelled in this entry, 30 are monoatomic - leaving 18 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	W3O	C	404	-	20,20,20	2.23	4 (20%)	29,29,29	0.83	2 (6%)
5	W3O	F	404	-	20,20,20	2.23	4 (20%)	29,29,29	0.80	1 (3%)
5	W3O	L	401	-	20,20,20	2.24	4 (20%)	29,29,29	0.81	2 (6%)
5	W3O	K	503	-	20,20,20	2.24	4 (20%)	29,29,29	0.82	2 (6%)
5	W3O	H	503	-	20,20,20	2.25	4 (20%)	29,29,29	0.78	2 (6%)
2	IPA	D	402	-	3,3,3	0.56	0	3,3,3	0.28	0
2	IPA	A	401	-	3,3,3	0.54	0	3,3,3	0.32	0
2	IPA	I	401	-	3,3,3	0.58	0	3,3,3	0.30	0
2	IPA	F	401	-	3,3,3	0.56	0	3,3,3	0.31	0
2	IPA	C	401	-	3,3,3	0.58	0	3,3,3	0.31	0
5	W3O	D	405	-	20,20,20	2.22	4 (20%)	29,29,29	0.88	2 (6%)
5	W3O	E	503	-	20,20,20	2.22	4 (20%)	29,29,29	0.79	1 (3%)
2	IPA	D	401	-	3,3,3	0.55	0	3,3,3	0.30	0
5	W3O	J	503	-	20,20,20	2.22	4 (20%)	29,29,29	0.81	1 (3%)
6	CIT	I	402	-	12,12,12	1.05	0	17,17,17	1.48	1 (5%)
2	IPA	G	401	-	3,3,3	0.56	0	3,3,3	0.30	0
5	W3O	G	404	-	20,20,20	2.25	4 (20%)	29,29,29	0.79	2 (6%)
5	W3O	I	405	-	20,20,20	2.23	4 (20%)	29,29,29	0.85	2 (6%)

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	W3O	F	404	-	-	11/21/21/21	0/1/1/1
5	W3O	C	404	-	-	7/21/21/21	0/1/1/1
5	W3O	L	401	-	-	13/21/21/21	0/1/1/1
5	W3O	K	503	-	-	12/21/21/21	0/1/1/1
5	W3O	H	503	-	-	14/21/21/21	0/1/1/1
5	W3O	D	405	-	-	4/21/21/21	0/1/1/1
5	W3O	E	503	-	-	2/21/21/21	0/1/1/1
5	W3O	J	503	-	-	5/21/21/21	0/1/1/1
6	CIT	I	402	-	-	0/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	W3O	G	404	-	-	12/21/21/21	0/1/1/1
5	W3O	I	405	-	-	11/21/21/21	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	405	W3O	C17-N18	7.20	1.46	1.33
5	L	401	W3O	C17-N18	7.17	1.46	1.33
5	H	503	W3O	C17-N18	7.16	1.46	1.33
5	J	503	W3O	C17-N18	7.16	1.46	1.33
5	C	404	W3O	C17-N18	7.15	1.46	1.33
5	G	404	W3O	C17-N18	7.15	1.46	1.33
5	I	405	W3O	C17-N18	7.11	1.46	1.33
5	K	503	W3O	C17-N18	7.10	1.46	1.33
5	F	404	W3O	C17-N18	7.10	1.46	1.33
5	E	503	W3O	C17-N18	7.09	1.46	1.33
5	H	503	W3O	C16-C17	4.93	1.58	1.50
5	G	404	W3O	C16-C17	4.91	1.58	1.50
5	K	503	W3O	C16-C17	4.89	1.57	1.50
5	F	404	W3O	C16-C17	4.88	1.57	1.50
5	L	401	W3O	C16-C17	4.80	1.57	1.50
5	I	405	W3O	C16-C17	4.77	1.57	1.50
5	E	503	W3O	C16-C17	4.76	1.57	1.50
5	C	404	W3O	C16-C17	4.70	1.57	1.50
5	D	405	W3O	C16-C17	4.64	1.57	1.50
5	J	503	W3O	C16-C17	4.61	1.57	1.50
5	D	405	W3O	O19-C17	-2.77	1.18	1.24
5	G	404	W3O	O19-C17	-2.72	1.18	1.24
5	K	503	W3O	O19-C17	-2.72	1.18	1.24
5	L	401	W3O	O19-C17	-2.72	1.18	1.24
5	I	405	W3O	O19-C17	-2.71	1.19	1.24
5	E	503	W3O	O19-C17	-2.69	1.19	1.24
5	H	503	W3O	O19-C17	-2.69	1.19	1.24
5	J	503	W3O	O19-C17	-2.68	1.19	1.24
5	F	404	W3O	O19-C17	-2.68	1.19	1.24
5	C	404	W3O	O19-C17	-2.67	1.19	1.24
5	C	404	W3O	SI05-O08	2.40	1.71	1.65
5	J	503	W3O	SI05-O08	2.36	1.70	1.65
5	L	401	W3O	SI05-O08	2.32	1.70	1.65
5	I	405	W3O	SI05-O08	2.26	1.70	1.65
5	G	404	W3O	SI05-O08	2.26	1.70	1.65
5	H	503	W3O	SI05-O08	2.26	1.70	1.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	503	W3O	SI05-O08	2.25	1.70	1.65
5	E	503	W3O	SI05-O08	2.24	1.70	1.65
5	F	404	W3O	SI05-O08	2.24	1.70	1.65
5	D	405	W3O	SI05-O08	2.22	1.70	1.65

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	402	CIT	O6-C6-C3	3.93	119.87	113.05
5	D	405	W3O	C16-C17-N18	2.64	120.92	117.75
5	I	405	W3O	C16-C17-N18	2.42	120.66	117.75
5	D	405	W3O	C14-C15-C16	-2.38	117.52	120.34
5	J	503	W3O	C14-C15-C16	-2.37	117.53	120.34
5	I	405	W3O	C14-C15-C16	-2.32	117.60	120.34
5	C	404	W3O	C14-C15-C16	-2.31	117.61	120.34
5	E	503	W3O	C14-C15-C16	-2.26	117.67	120.34
5	L	401	W3O	C14-C15-C16	-2.19	117.75	120.34
5	F	404	W3O	C14-C15-C16	-2.18	117.76	120.34
5	G	404	W3O	C14-C15-C16	-2.18	117.77	120.34
5	H	503	W3O	C14-C15-C16	-2.17	117.78	120.34
5	K	503	W3O	C14-C15-C16	-2.16	117.78	120.34
5	K	503	W3O	C16-C17-N18	2.14	120.32	117.75
5	L	401	W3O	C16-C17-N18	2.13	120.30	117.75
5	G	404	W3O	C16-C17-N18	2.11	120.28	117.75
5	H	503	W3O	C16-C17-N18	2.05	120.22	117.75
5	C	404	W3O	C16-C17-N18	2.03	120.19	117.75

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	404	W3O	C09-C10-C11-N12
5	C	404	W3O	O08-C09-C10-C11
5	C	404	W3O	C09-O08-SI05-C02
5	J	503	W3O	C09-O08-SI05-C02
5	K	503	W3O	C01-C02-SI05-O08
5	K	503	W3O	C03-C02-SI05-O08
5	K	503	W3O	C01-C02-SI05-C06
5	K	503	W3O	C03-C02-SI05-C07
5	K	503	W3O	C04-C02-SI05-C06
5	K	503	W3O	C04-C02-SI05-C07
5	K	503	W3O	C04-C02-SI05-O08

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Mol	Chain	Res	Type	Atoms
5	K	503	W3O	C01-C02-SI05-C07
5	K	503	W3O	C03-C02-SI05-C06
5	F	404	W3O	C03-C02-SI05-O08
5	F	404	W3O	C01-C02-SI05-C06
5	F	404	W3O	C04-C02-SI05-O08
5	F	404	W3O	C01-C02-SI05-C07
5	F	404	W3O	C03-C02-SI05-C06
5	F	404	W3O	C04-C02-SI05-C06
5	F	404	W3O	C04-C02-SI05-C07
5	F	404	W3O	C03-C02-SI05-C07
5	I	405	W3O	C01-C02-SI05-O08
5	F	404	W3O	C01-C02-SI05-O08
5	G	404	W3O	C04-C02-SI05-O08
5	I	405	W3O	C03-C02-SI05-C07
5	I	405	W3O	C04-C02-SI05-C06
5	I	405	W3O	C01-C02-SI05-C07
5	I	405	W3O	C04-C02-SI05-C07
5	I	405	W3O	C03-C02-SI05-C06
5	I	405	W3O	C01-C02-SI05-C06
5	G	404	W3O	C04-C02-SI05-C07
5	I	405	W3O	C04-C02-SI05-O08
5	G	404	W3O	C01-C02-SI05-C07
5	G	404	W3O	C01-C02-SI05-C06
5	G	404	W3O	C04-C02-SI05-C06
5	G	404	W3O	C03-C02-SI05-C06
5	G	404	W3O	C03-C02-SI05-C07
5	C	404	W3O	C10-C11-N12-C20
5	I	405	W3O	C03-C02-SI05-O08
5	C	404	W3O	C10-C11-N12-C13
5	G	404	W3O	C03-C02-SI05-O08
5	G	404	W3O	C01-C02-SI05-O08
5	L	401	W3O	C03-C02-SI05-C06
5	H	503	W3O	C04-C02-SI05-C07
5	H	503	W3O	C01-C02-SI05-C07
5	L	401	W3O	C03-C02-SI05-C07
5	L	401	W3O	C04-C02-SI05-C07
5	H	503	W3O	C04-C02-SI05-O08
5	H	503	W3O	C03-C02-SI05-C07
5	L	401	W3O	C01-C02-SI05-C07
5	L	401	W3O	C01-C02-SI05-C06
5	H	503	W3O	C03-C02-SI05-C06
5	L	401	W3O	C04-C02-SI05-C06

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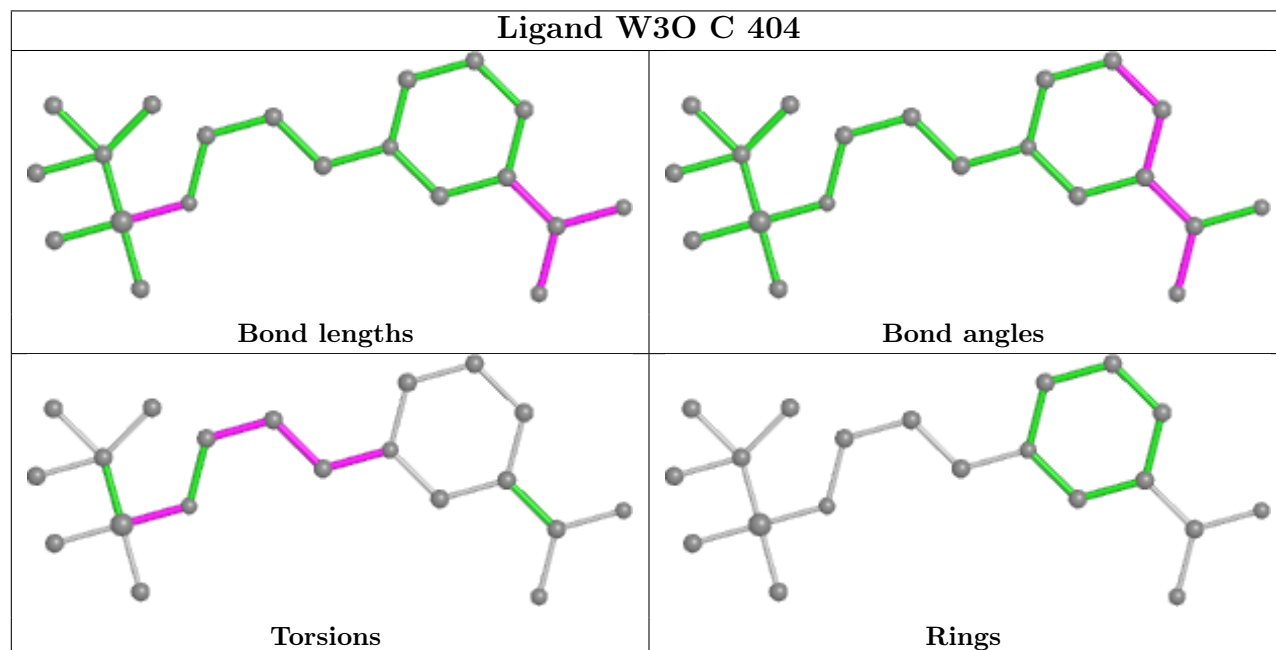
Mol	Chain	Res	Type	Atoms
5	H	503	W3O	C04-C02-SI05-C06
5	L	401	W3O	C04-C02-SI05-O08
5	H	503	W3O	C01-C02-SI05-C06
5	J	503	W3O	C10-C11-N12-C20
5	I	405	W3O	C10-C11-N12-C13
5	L	401	W3O	C03-C02-SI05-O08
5	J	503	W3O	C10-C11-N12-C13
5	G	404	W3O	C10-C11-N12-C13
5	H	503	W3O	C03-C02-SI05-O08
5	H	503	W3O	C01-C02-SI05-O08
5	G	404	W3O	C10-C11-N12-C20
5	L	401	W3O	C01-C02-SI05-O08
5	E	503	W3O	C10-C11-N12-C20
5	I	405	W3O	C10-C11-N12-C20
5	E	503	W3O	C10-C11-N12-C13
5	F	404	W3O	C10-C09-O08-SI05
5	H	503	W3O	C10-C11-N12-C20
5	J	503	W3O	C09-O08-SI05-C07
5	C	404	W3O	C09-O08-SI05-C06
5	D	405	W3O	C09-O08-SI05-C06
5	H	503	W3O	C10-C11-N12-C13
5	K	503	W3O	C10-C11-N12-C20
5	C	404	W3O	C09-O08-SI05-C07
5	K	503	W3O	C10-C11-N12-C13
5	L	401	W3O	C10-C11-N12-C13
5	D	405	W3O	C09-O08-SI05-C07
5	L	401	W3O	C10-C11-N12-C20
5	L	401	W3O	C09-O08-SI05-C02
5	H	503	W3O	C09-O08-SI05-C07
5	J	503	W3O	C09-O08-SI05-C06
5	D	405	W3O	O08-C09-C10-C11
5	D	405	W3O	C09-O08-SI05-C02
5	F	404	W3O	C09-O08-SI05-C06
5	L	401	W3O	C09-O08-SI05-C06
5	G	404	W3O	C09-O08-SI05-C07
5	K	503	W3O	C09-O08-SI05-C07
5	H	503	W3O	C09-O08-SI05-C06
5	H	503	W3O	C09-O08-SI05-C02

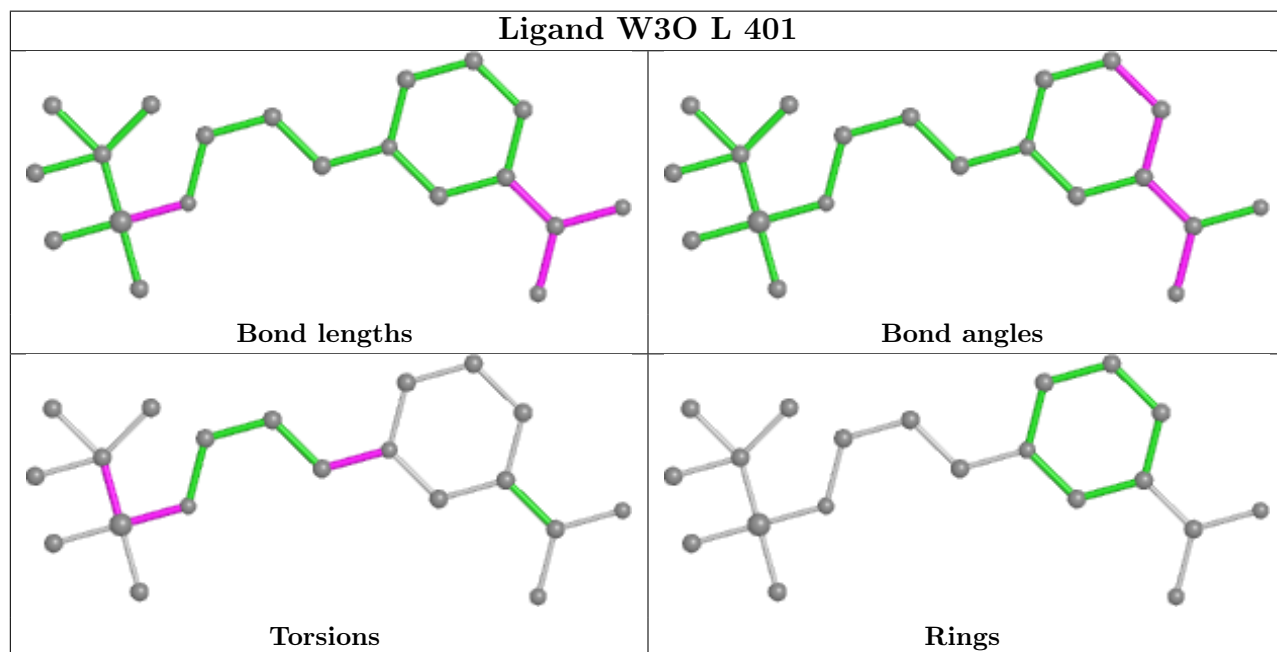
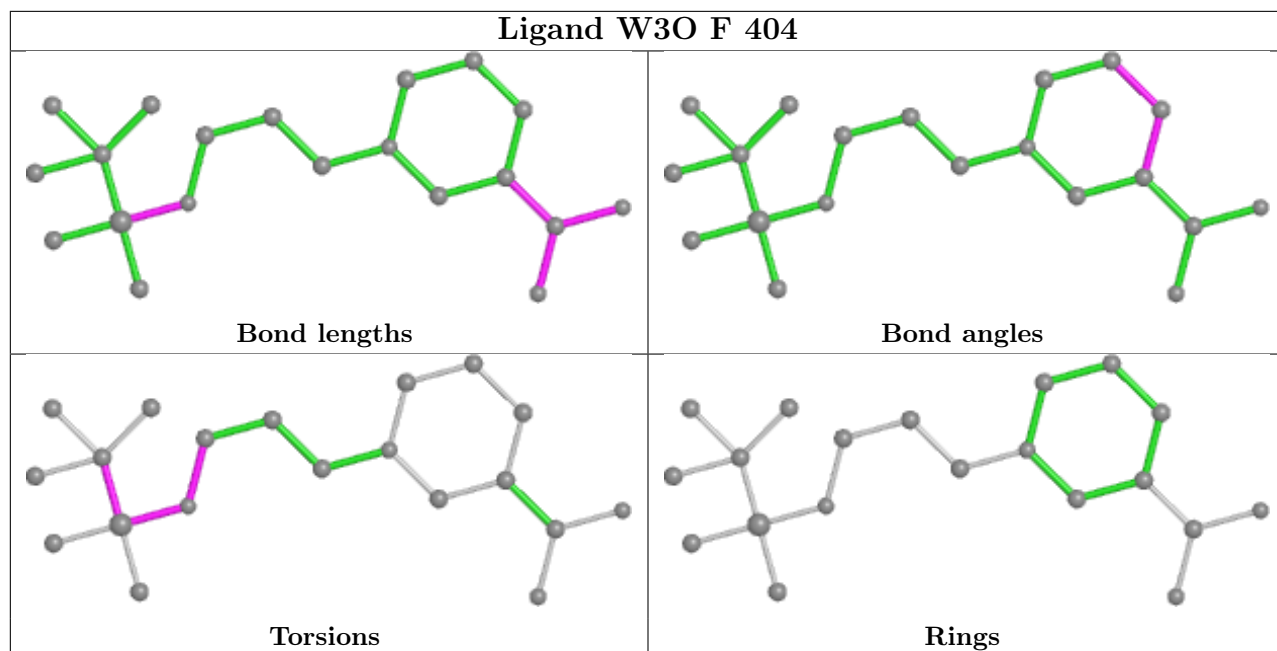
There are no ring outliers.

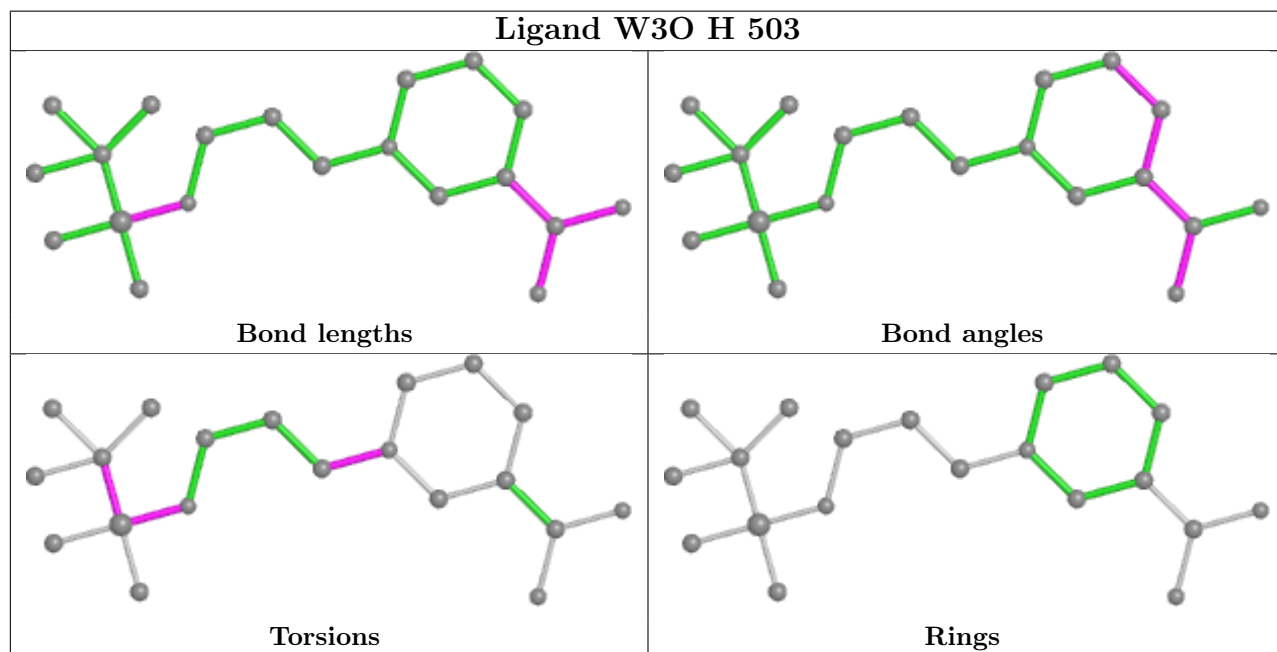
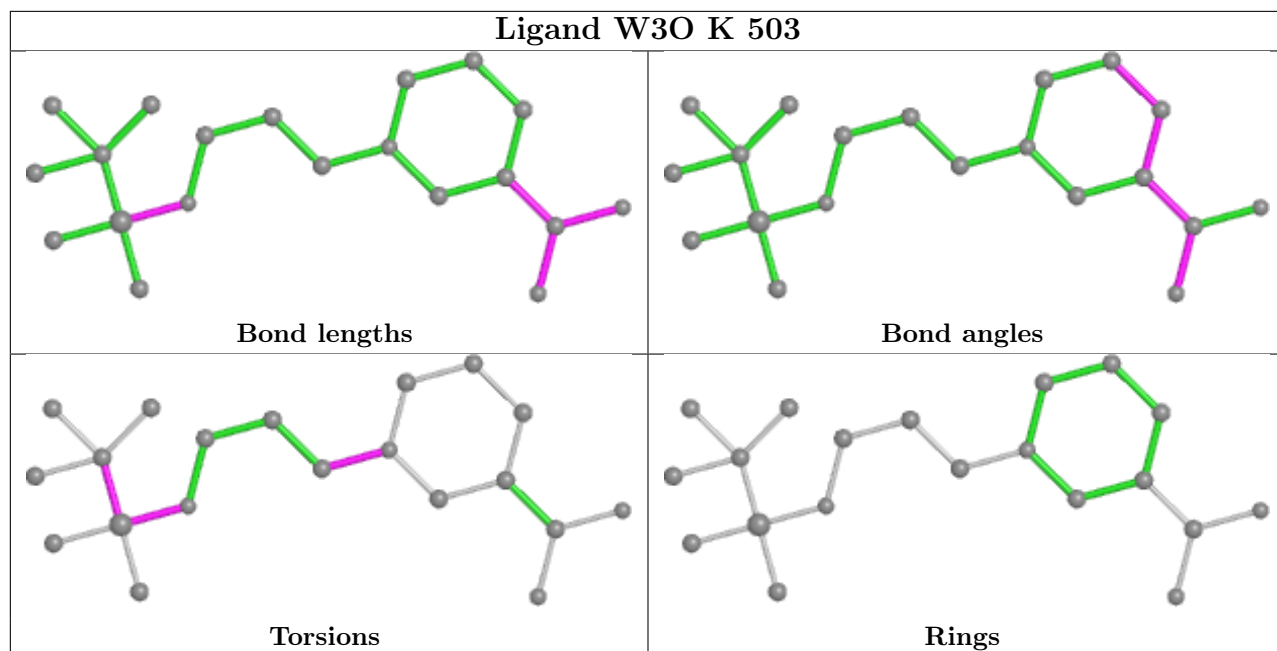
4 monomers are involved in 4 short contacts:

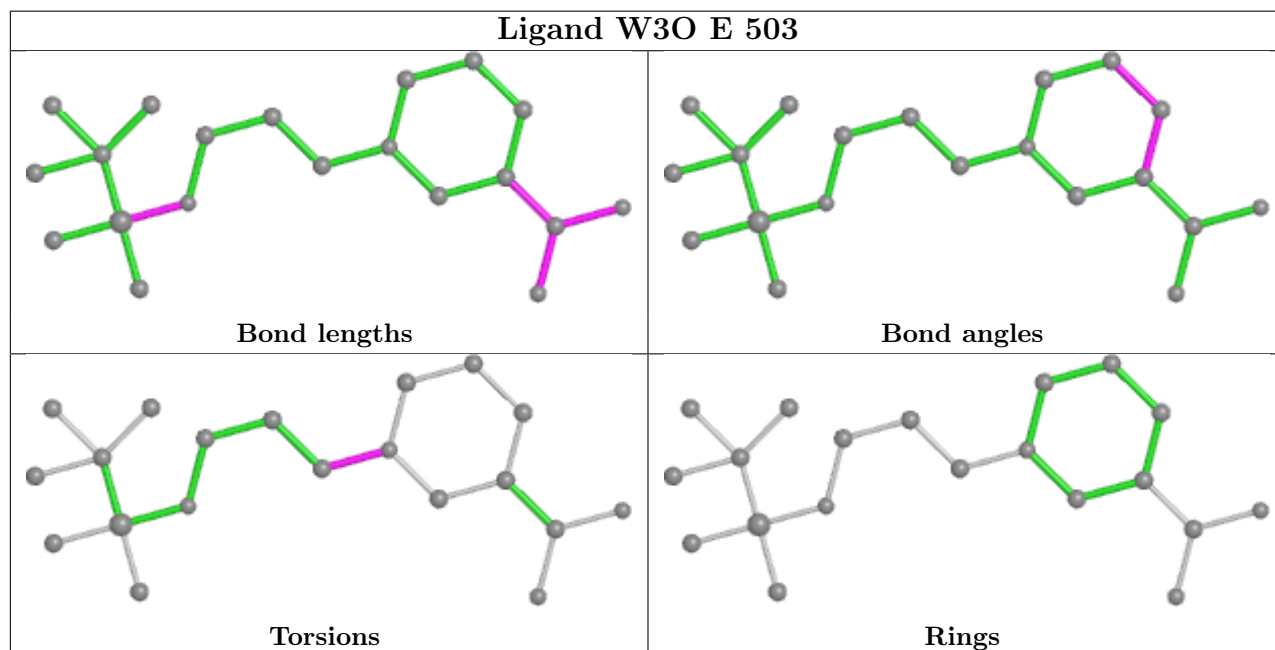
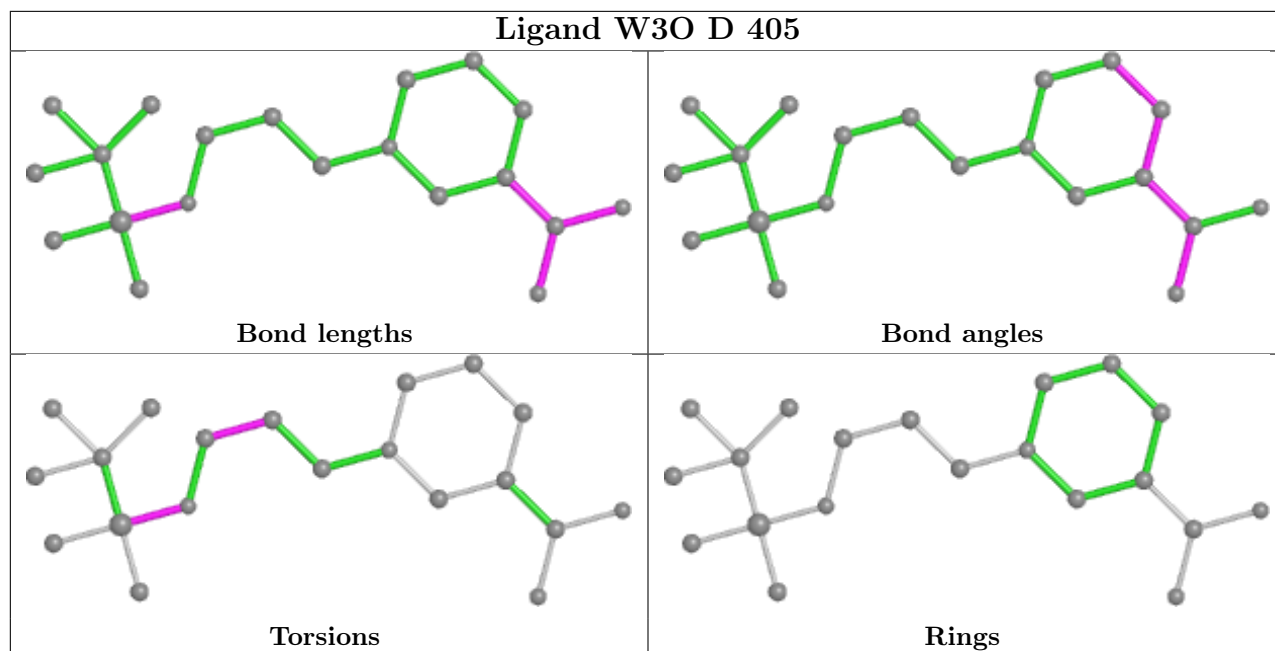
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	IPA	1	0
2	C	401	IPA	1	0
2	D	401	IPA	1	0
2	G	401	IPA	1	0

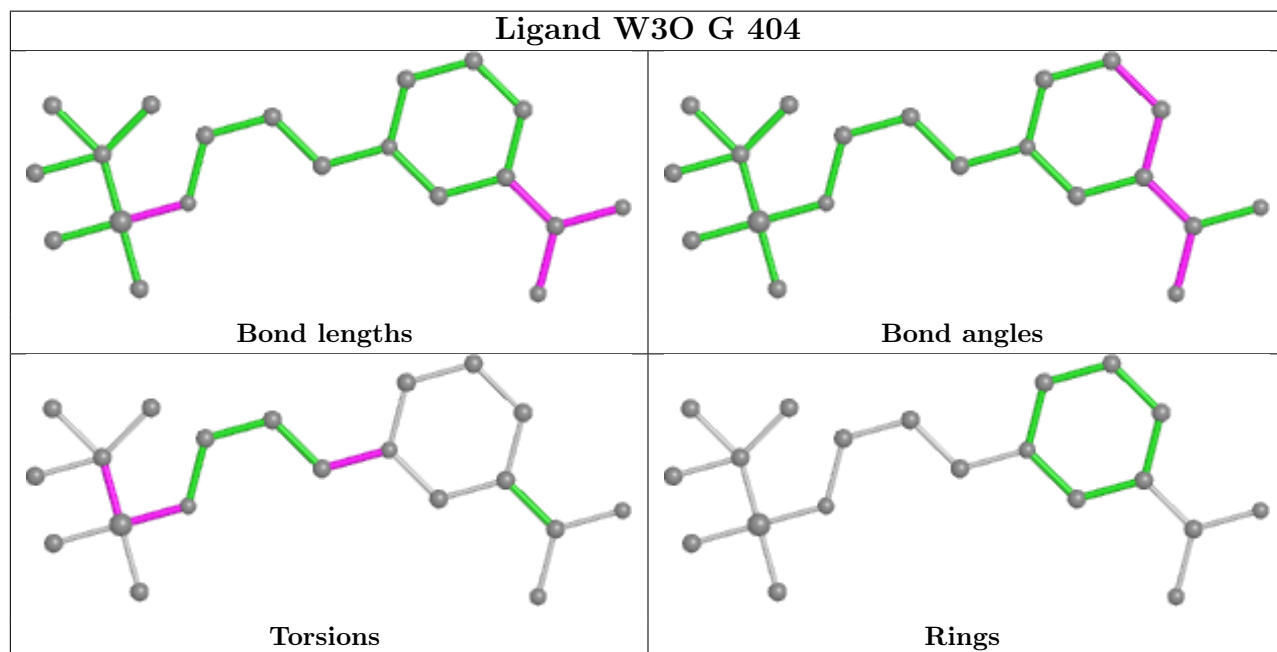
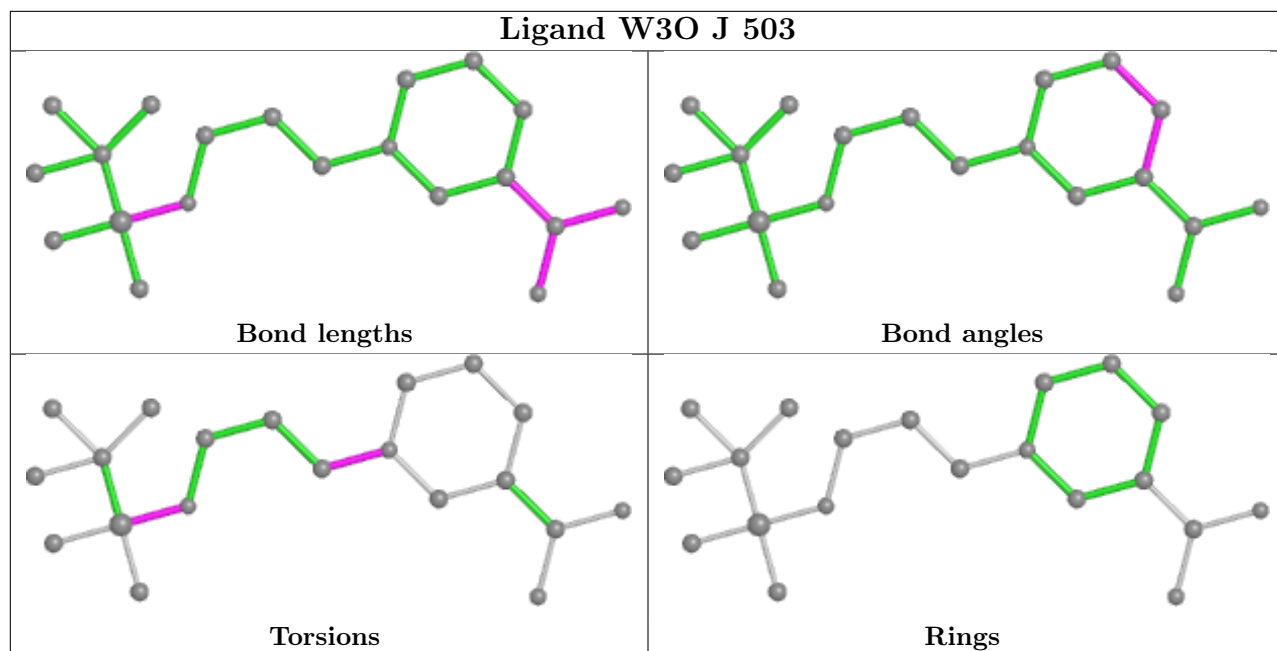
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

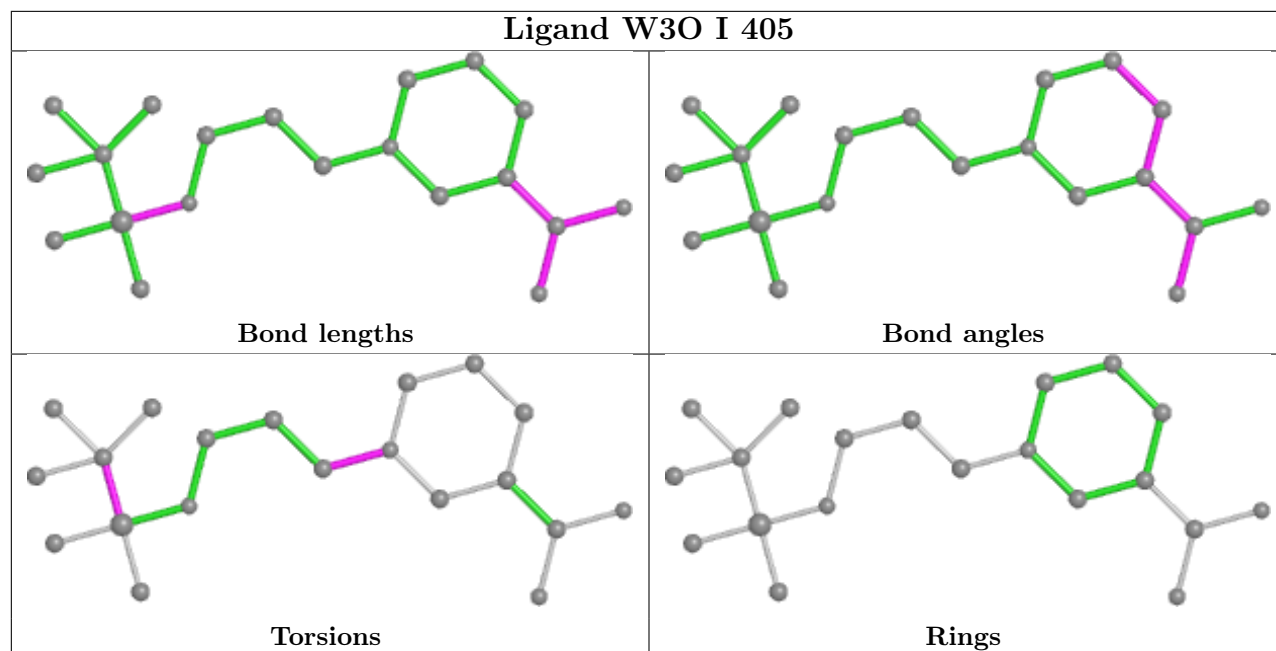












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	A	352/365 (96%)	-0.38	1 (0%) 94 93	24, 32, 55, 79	0
1	B	349/365 (95%)	-0.29	3 (0%) 84 83	31, 44, 67, 80	0
1	C	348/365 (95%)	-0.15	12 (3%) 45 43	28, 41, 72, 93	0
1	D	349/365 (95%)	-0.30	4 (1%) 80 79	25, 33, 56, 82	0
1	E	348/365 (95%)	-0.26	7 (2%) 65 63	25, 34, 60, 91	0
1	F	349/365 (95%)	-0.26	7 (2%) 65 63	24, 37, 66, 118	0
1	G	348/365 (95%)	-0.10	9 (2%) 56 53	31, 43, 76, 114	0
1	H	349/365 (95%)	-0.03	14 (4%) 38 36	33, 46, 80, 113	0
1	I	349/365 (95%)	-0.06	15 (4%) 35 33	25, 43, 89, 120	0
1	J	349/365 (95%)	-0.30	5 (1%) 75 73	27, 41, 67, 109	0
1	K	350/365 (95%)	-0.16	14 (4%) 38 36	31, 47, 77, 138	0
1	L	349/365 (95%)	-0.10	10 (2%) 51 49	33, 45, 73, 114	0
All	All	4189/4380 (95%)	-0.20	101 (2%) 59 56	24, 41, 73, 138	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	54	TYR	7.3
1	K	52	TYR	7.1
1	I	50	ALA	6.4
1	K	51	GLN	6.3
1	I	49	ALA	6.2
1	I	52	TYR	5.8
1	L	52	TYR	5.6
1	K	53	ALA	5.3
1	L	50	ALA	5.1
1	J	54	TYR	5.1
1	F	52	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
1	L	54	TYR	5.0
1	L	53	ALA	5.0
1	I	48	PRO	4.6
1	I	54	TYR	4.3
1	C	211	LEU	4.3
1	F	54	TYR	4.3
1	H	52	TYR	4.2
1	F	51	GLN	4.1
1	G	54	TYR	4.1
1	G	338	ARG	4.1
1	I	53	ALA	3.9
1	H	211	LEU	3.9
1	H	54	TYR	3.9
1	J	50	ALA	3.8
1	G	-2	GLY	3.7
1	D	50	ALA	3.7
1	J	53	ALA	3.6
1	I	47	MET	3.5
1	E	54	TYR	3.5
1	E	50	ALA	3.5
1	F	49	ALA	3.5
1	G	51	GLN	3.4
1	J	52	TYR	3.4
1	L	49	ALA	3.4
1	H	338	ARG	3.4
1	G	211	LEU	3.4
1	H	204	LEU	3.4
1	D	54	TYR	3.3
1	I	51	GLN	3.3
1	F	53	ALA	3.2
1	I	55	GLY	3.1
1	L	211	LEU	3.1
1	C	52	TYR	3.0
1	L	51	GLN	3.0
1	H	53	ALA	3.0
1	C	338	ARG	2.9
1	K	-4	PRO	2.9
1	C	207	ASP	2.9
1	K	55	GLY	2.9
1	C	54	TYR	2.9
1	K	-3	ARG	2.8
1	H	51	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	-3	ARG	2.8
1	C	236	GLY	2.7
1	K	50	ALA	2.7
1	I	56	LEU	2.7
1	K	0	HIS	2.7
1	I	10	GLY	2.7
1	I	9	ILE	2.6
1	F	48	PRO	2.6
1	H	210	ALA	2.6
1	E	211	LEU	2.6
1	H	220	ALA	2.6
1	A	-2	GLY	2.6
1	C	210	ALA	2.6
1	K	49	ALA	2.5
1	I	21	PRO	2.5
1	K	-2	GLY	2.5
1	K	76	THR	2.5
1	E	52	TYR	2.4
1	D	-2	GLY	2.4
1	B	9	ILE	2.4
1	D	211	LEU	2.4
1	L	207	ASP	2.4
1	E	49	ALA	2.3
1	H	227	ALA	2.3
1	G	237	GLY	2.3
1	E	210	ALA	2.3
1	H	207	ASP	2.2
1	K	8	GLU	2.2
1	L	338	ARG	2.2
1	F	50	ALA	2.2
1	H	230	ALA	2.2
1	I	-3	ARG	2.2
1	C	225	ALA	2.2
1	C	214	GLU	2.2
1	C	316	HIS	2.1
1	L	210	ALA	2.1
1	K	101	GLY	2.1
1	E	225	ALA	2.1
1	G	209	LEU	2.1
1	G	55	GLY	2.1
1	H	316	HIS	2.1
1	B	76	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	237	GLY	2.1
1	I	80	VAL	2.1
1	H	-3	ARG	2.0
1	G	214	GLU	2.0
1	C	101	GLY	2.0
1	J	49	ALA	2.0

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, 95th 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	W3O	C	404	20/20	0.79	0.25	44,49,72,73	0
5	W3O	F	404	20/20	0.85	0.22	39,49,64,71	5
5	W3O	H	503	20/20	0.88	0.22	50,55,69,72	0
5	W3O	K	503	20/20	0.89	0.18	46,56,71,76	0
5	W3O	I	405	20/20	0.90	0.19	36,47,66,66	0
5	W3O	L	401	20/20	0.90	0.20	54,68,84,85	0
5	W3O	J	503	20/20	0.92	0.17	40,49,64,70	0
5	W3O	E	503	20/20	0.92	0.19	37,41,59,61	0
2	IPA	G	401	4/4	0.92	0.33	36,44,49,54	0
5	W3O	G	404	20/20	0.93	0.17	43,49,62,62	0
2	IPA	D	401	4/4	0.93	0.31	36,44,48,50	0
6	CIT	I	402	13/13	0.93	0.14	48,65,80,80	0
2	IPA	F	401	4/4	0.94	0.29	33,40,43,43	0
2	IPA	C	401	4/4	0.94	0.30	35,43,46,49	0
2	IPA	A	401	4/4	0.94	0.26	29,39,47,47	0
2	IPA	D	402	4/4	0.94	0.29	34,45,46,48	0
5	W3O	D	405	20/20	0.95	0.18	31,36,48,53	0

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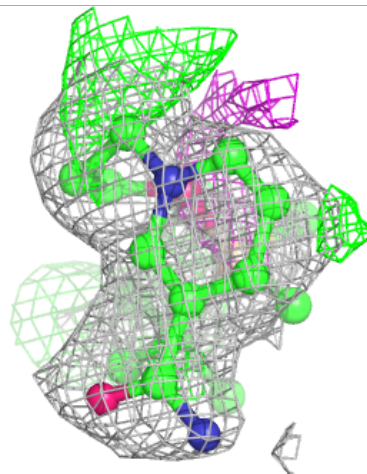
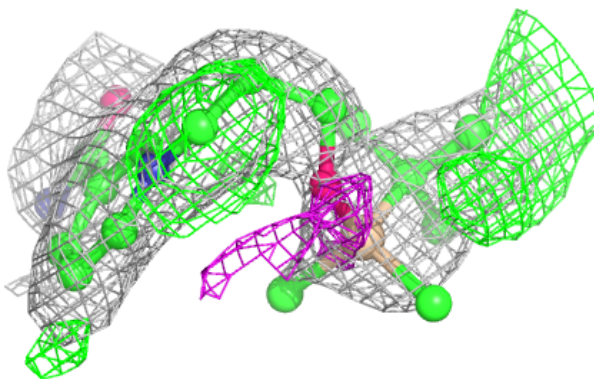
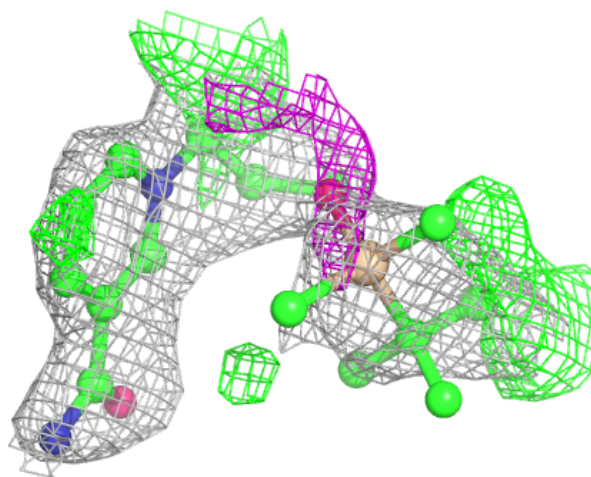
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	K	502	1/1	0.96	0.06	59,59,59,59	0
2	IPA	I	401	4/4	0.96	0.28	35,42,45,46	0
4	NA	D	406	1/1	0.97	0.26	19,19,19,19	0
3	ZN	H	502	1/1	0.97	0.08	57,57,57,57	0
3	ZN	C	403	1/1	0.97	0.05	60,60,60,60	0
3	ZN	G	403	1/1	0.98	0.08	45,45,45,45	0
3	ZN	F	403	1/1	0.98	0.05	56,56,56,56	0
3	ZN	I	404	1/1	0.98	0.10	47,47,47,47	0
3	ZN	G	402	1/1	0.98	0.14	35,35,35,35	0
3	ZN	A	402	1/1	0.99	0.17	31,31,31,31	0
3	ZN	L	403	1/1	0.99	0.06	51,51,51,51	0
4	NA	A	404	1/1	0.99	0.27	17,17,17,17	0
3	ZN	D	403	1/1	0.99	0.12	28,28,28,28	0
4	NA	I	406	1/1	0.99	0.22	20,20,20,20	0
4	NA	J	504	1/1	0.99	0.29	23,23,23,23	0
3	ZN	D	404	1/1	0.99	0.10	32,32,32,32	0
3	ZN	A	403[A]	1/1	0.99	0.10	28,28,28,28	1
3	ZN	A	403[B]	1/1	0.99	0.10	35,35,35,35	1
3	ZN	B	502[A]	1/1	0.99	0.15	38,38,38,38	1
3	ZN	H	501	1/1	0.99	0.12	37,37,37,37	0
3	ZN	B	502[B]	1/1	0.99	0.15	62,62,62,62	1
3	ZN	I	403	1/1	0.99	0.13	36,36,36,36	0
3	ZN	C	402	1/1	0.99	0.13	33,33,33,33	0
3	ZN	J	501	1/1	0.99	0.11	28,28,28,28	0
3	ZN	J	502	1/1	0.99	0.10	44,44,44,44	0
3	ZN	K	501	1/1	0.99	0.12	35,35,35,35	0
3	ZN	B	501	1/1	1.00	0.12	35,35,35,35	0
3	ZN	E	501	1/1	1.00	0.12	26,26,26,26	0
3	ZN	E	502	1/1	1.00	0.12	35,35,35,35	0
3	ZN	L	402	1/1	1.00	0.11	36,36,36,36	0
3	ZN	F	402	1/1	1.00	0.12	27,27,27,27	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.

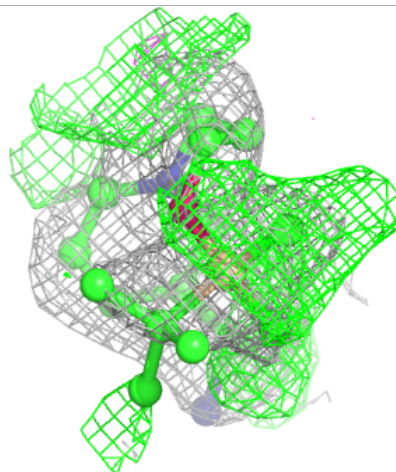
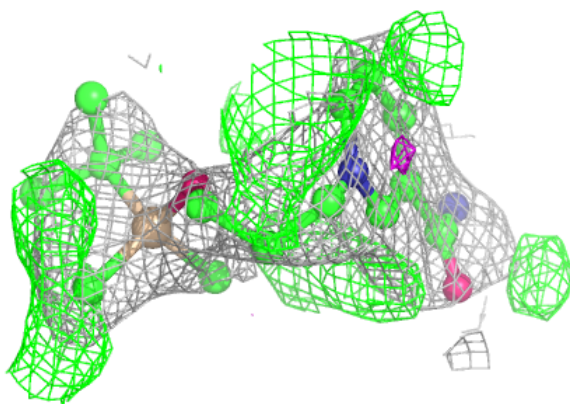
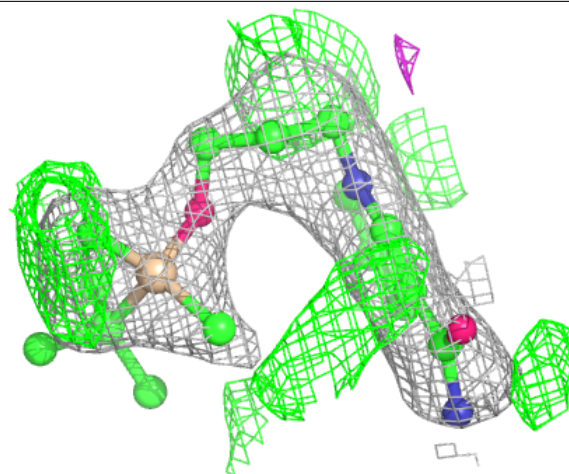
Electron density around W3O C 404:

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



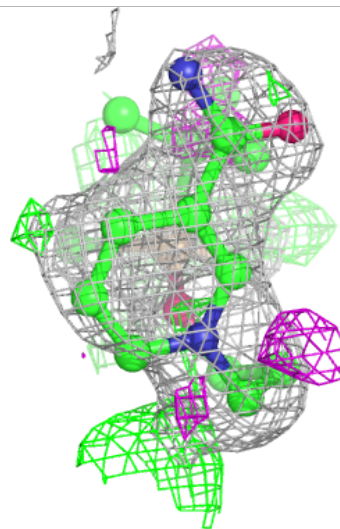
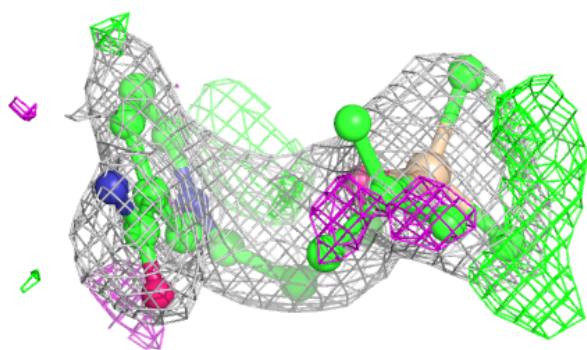
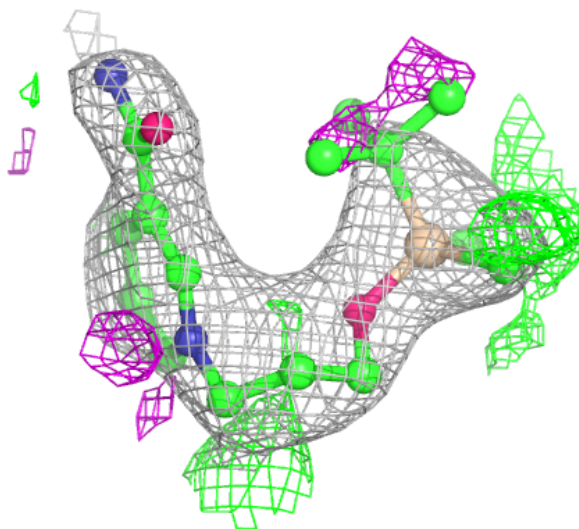
Electron density around W3O F 404:

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



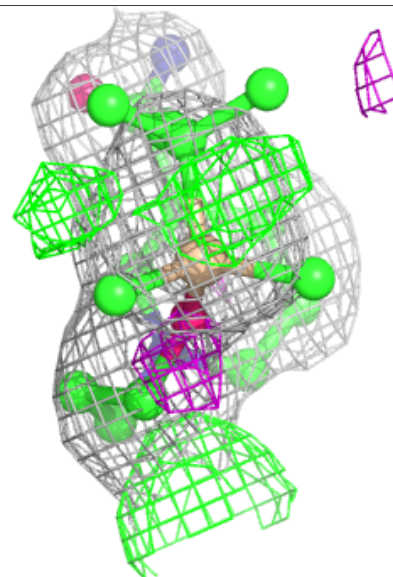
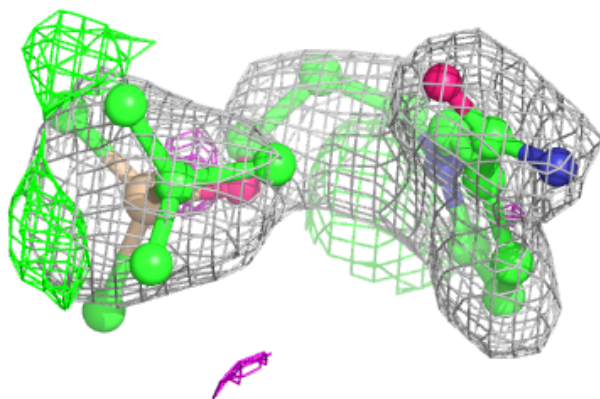
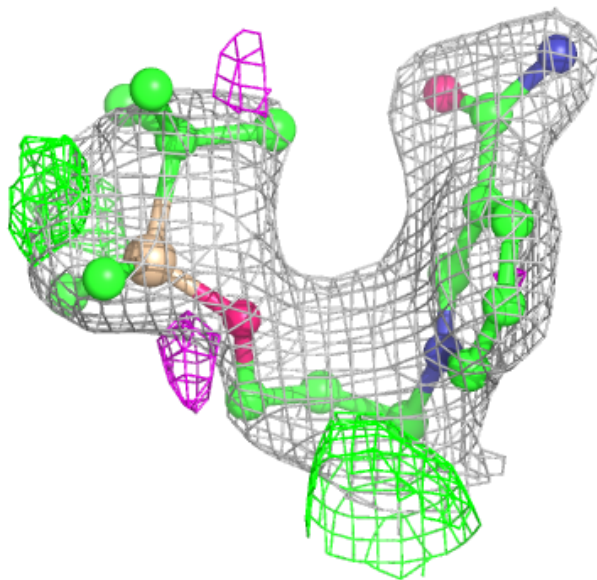
Electron density around W3O H 503:

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



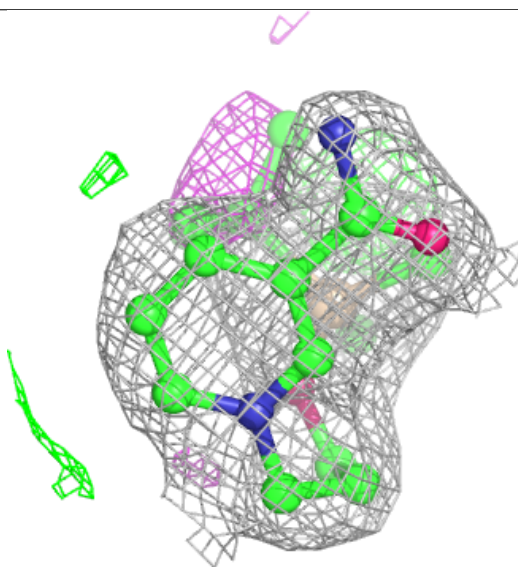
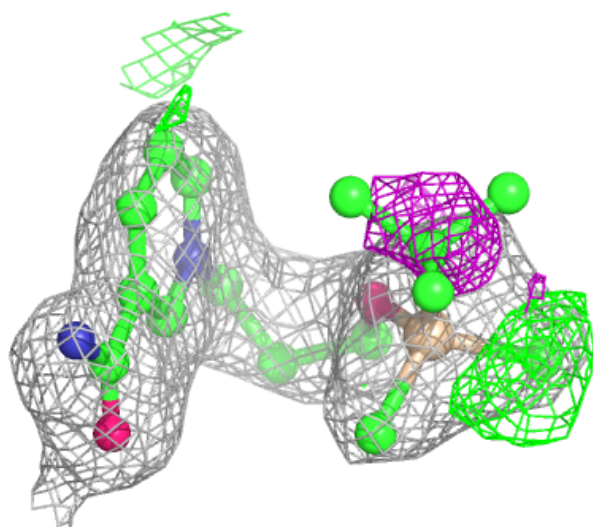
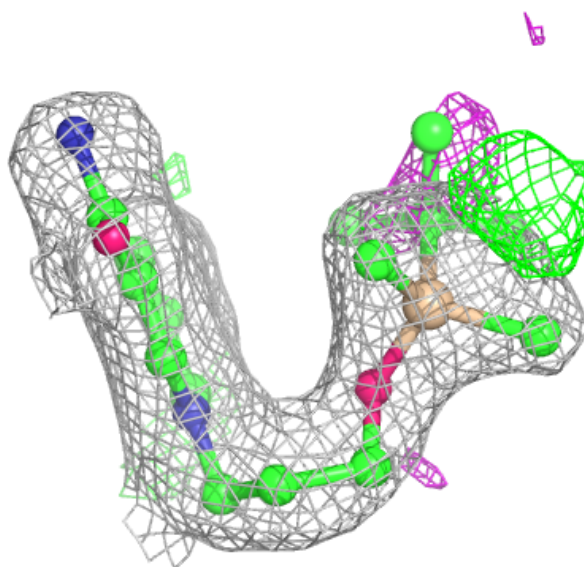
Electron density around W30 K 503:

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



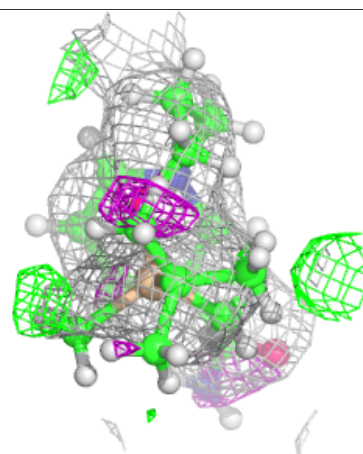
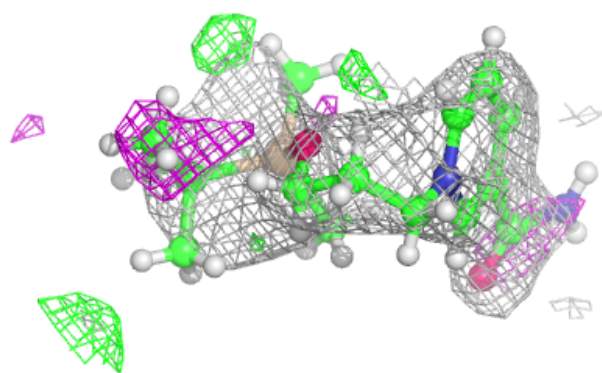
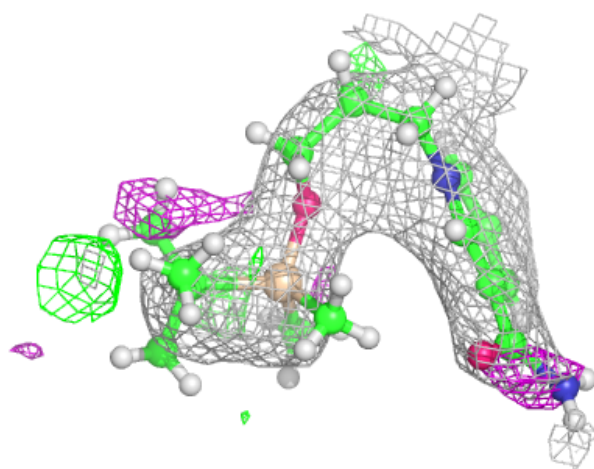
Electron density around W3O I 405:

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



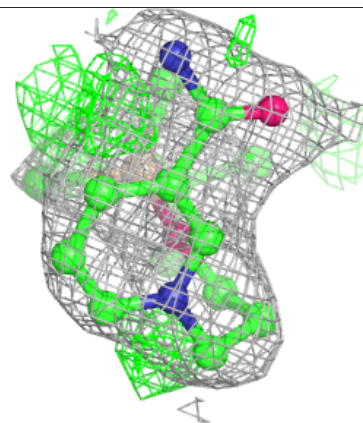
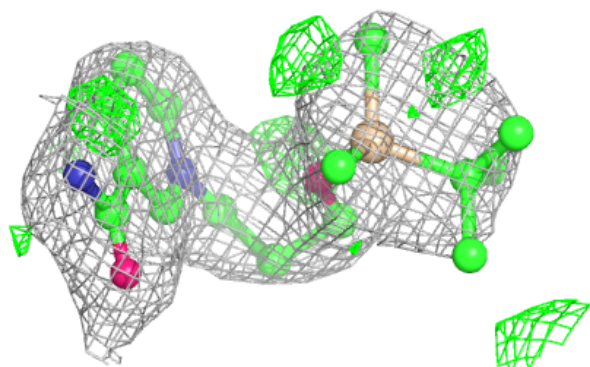
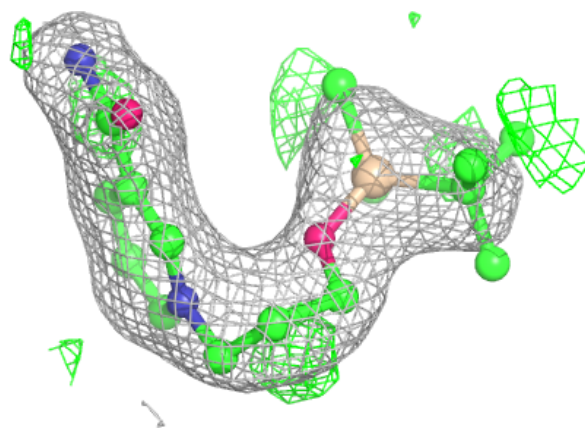
Electron density around W3O L 401:

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



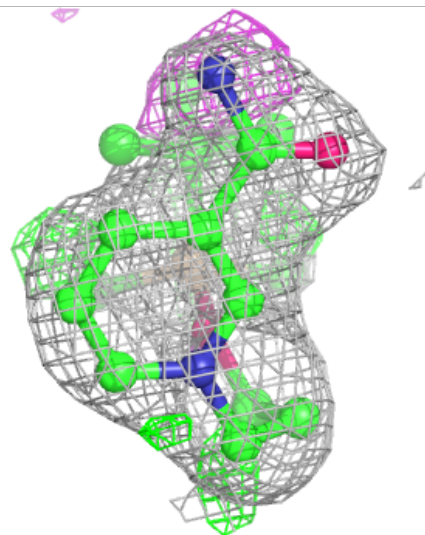
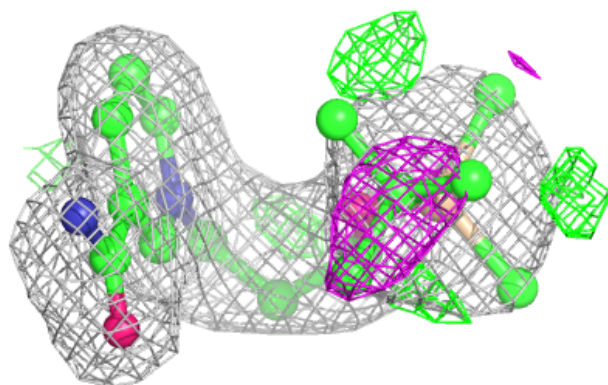
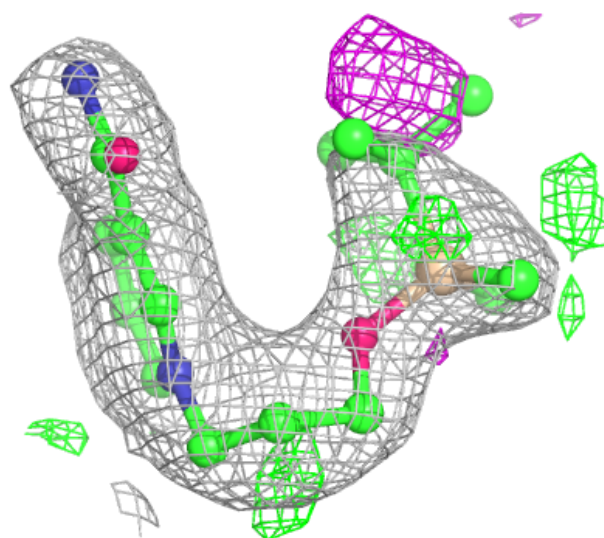
Electron density around W30 J 503:

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



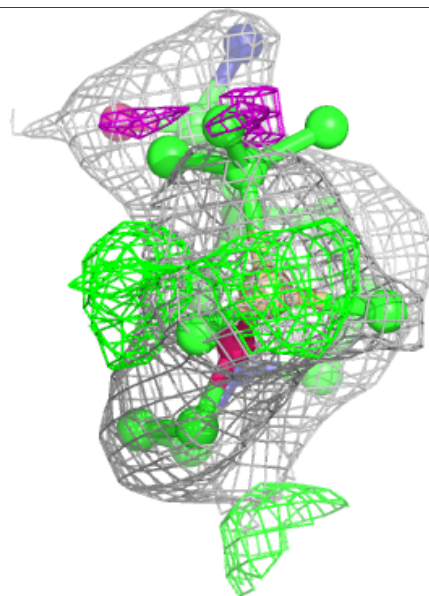
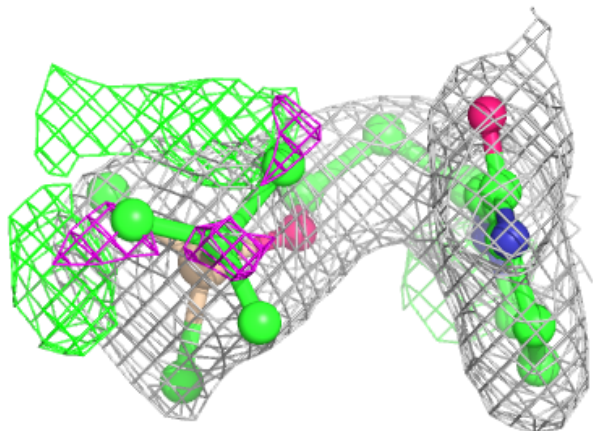
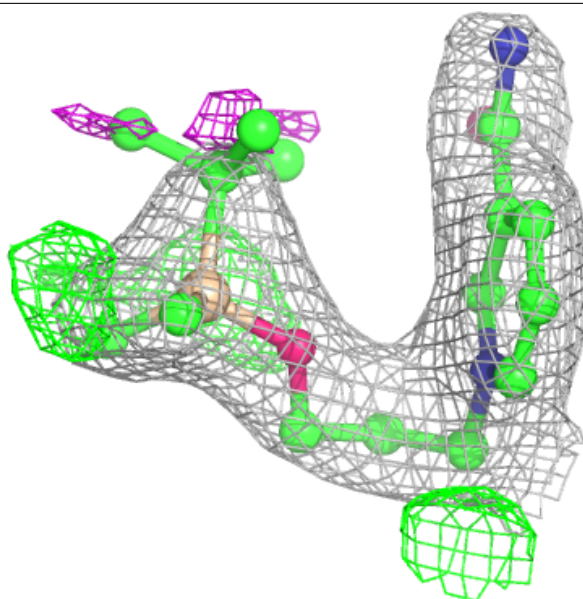
Electron density around W3O E 503:

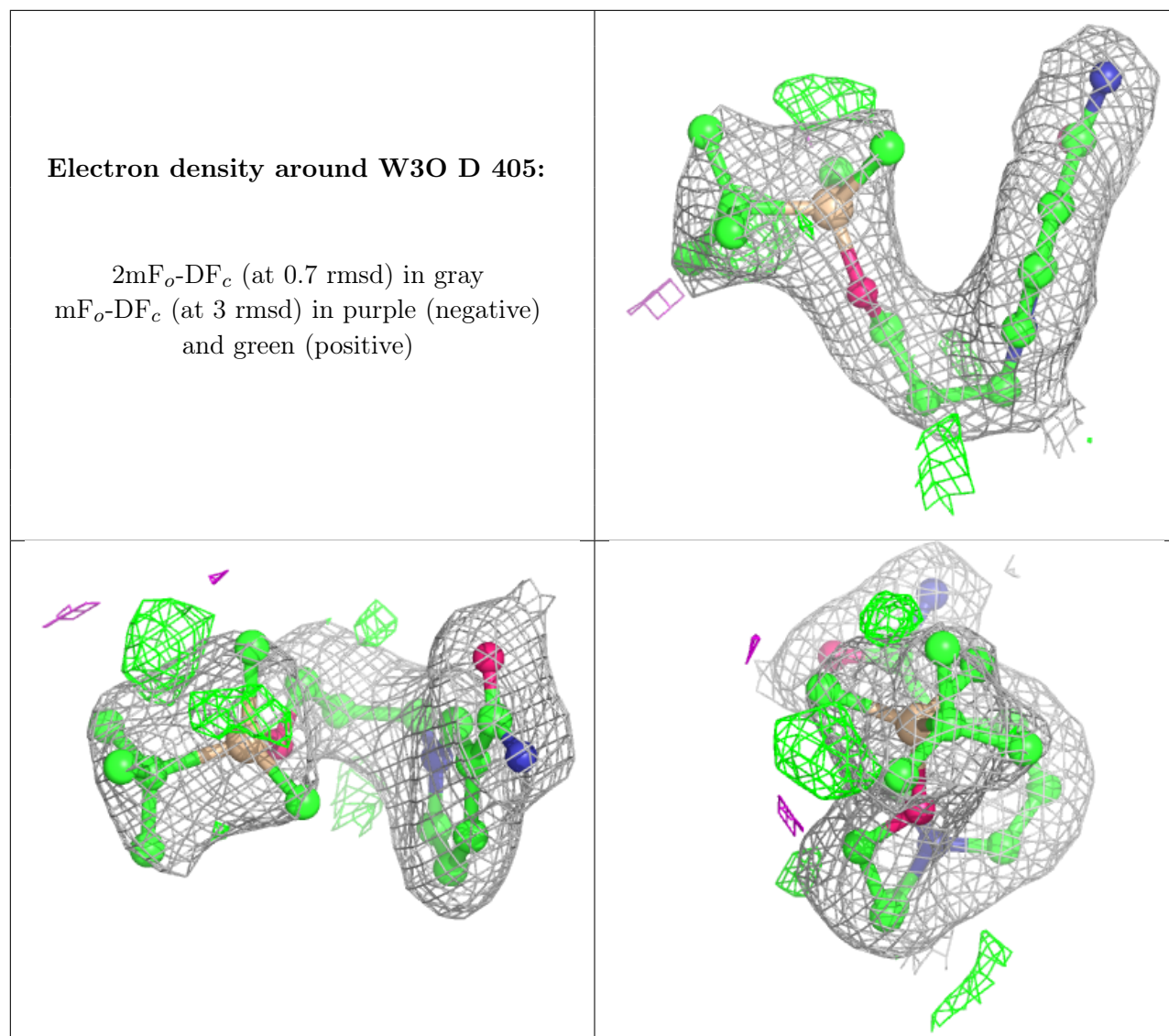
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around W3O G 404:

$2mF_o-DF_c$ (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.