



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:21 AM UTC

PDB ID : 7LON / pdb_00007lon
Title : Ornithine Aminotransferase (OAT) cocrystallized with its inactivator - (1S,3S)-3-amino-4-(difluoromethylene)cyclohexene-1-carboxylic acid
Authors : Butrin, A.; Zhu, W.; Liu, D.; Silverman, R.
Deposited on : 2021-02-10
Resolution : 1.95 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

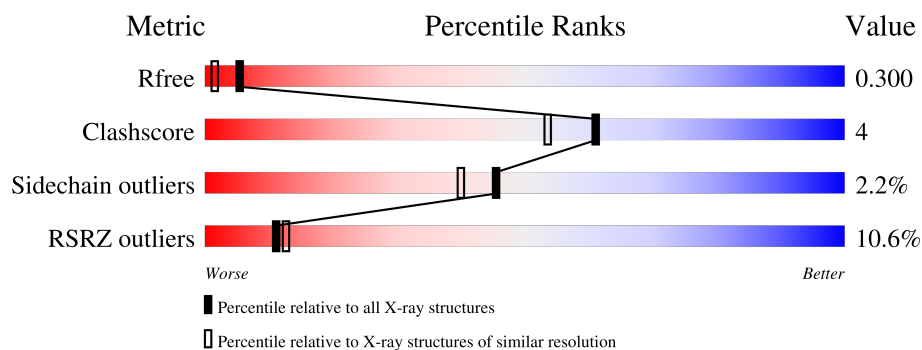
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	404	16% 86% 13%
1	B	404	2% 87% 11%
1	C	404	13% 87% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	7QP	B	502	X	-	-	-
3	7QP	C	502	X	-	-	-

2 Entry composition [i](#)

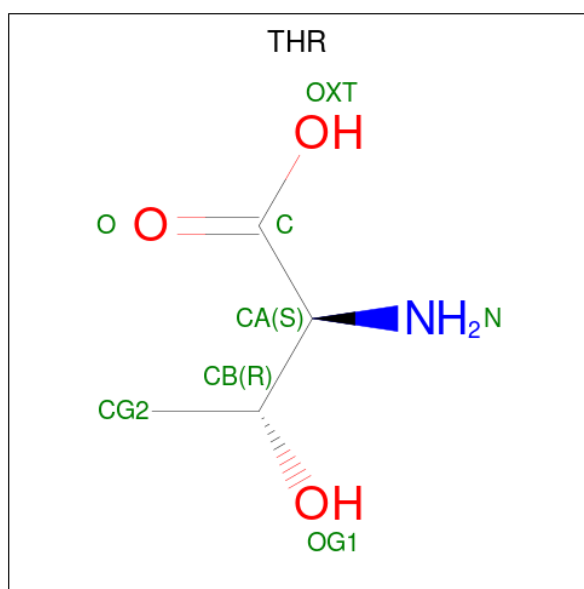
There are 4 unique types of molecules in this entry. The entry contains 10109 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ornithine aminotransferase, mitochondrial.

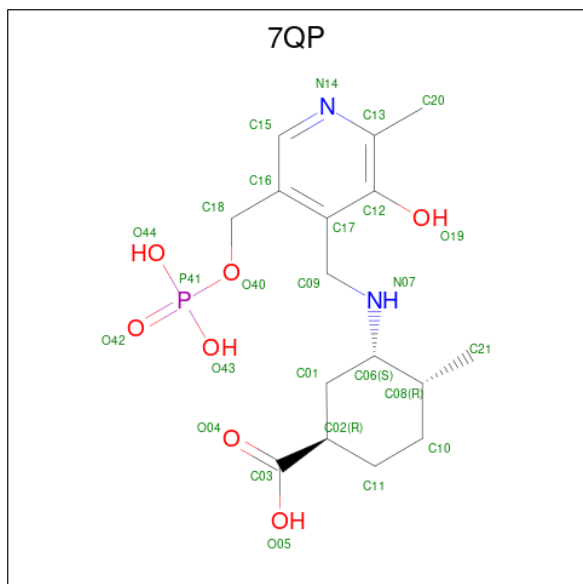
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	401	Total	C	N	O	S	0	1	0
			3148	2023	532	581	12			
1	A	401	Total	C	N	O	S	0	0	0
			3134	2015	526	581	12			
1	C	401	Total	C	N	O	S	0	2	0
			3154	2027	532	583	12			

- Molecule 2 is THREONINE (CCD ID: THR) (formula: $C_4H_9NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			7	4	1	2		
2	A	1	Total	C	N	O	0	0
			7	4	1	2		
2	C	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 3 is (1R,3S,4R)-3-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]amino]-4-methylcyclohexane-1-carboxylic acid (CCD ID: 7QP) (formula: $C_{16}H_{25}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			26	16	2	7	1		
3	A	1	Total	C	N	O	P	0	0
			26	16	2	7	1		
3	C	1	Total	C	N	O	P	0	0
			26	16	2	7	1		

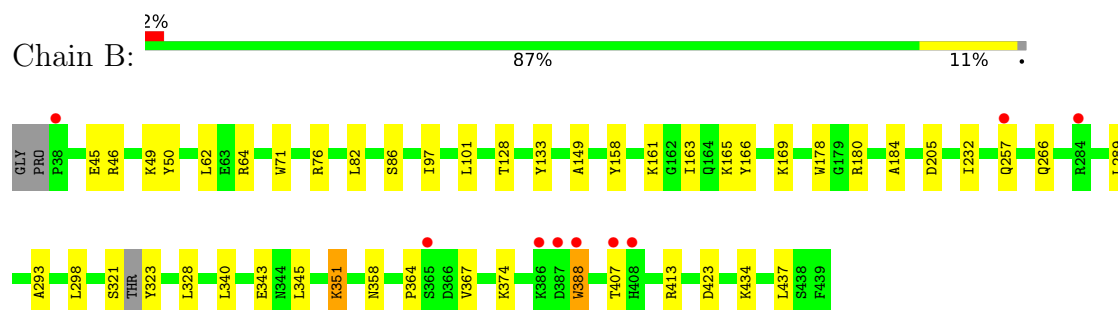
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	189	Total	O	0	0
			189	189		
4	A	190	Total	O	0	0
			190	190		
4	C	195	Total	O	0	0
			195	195		

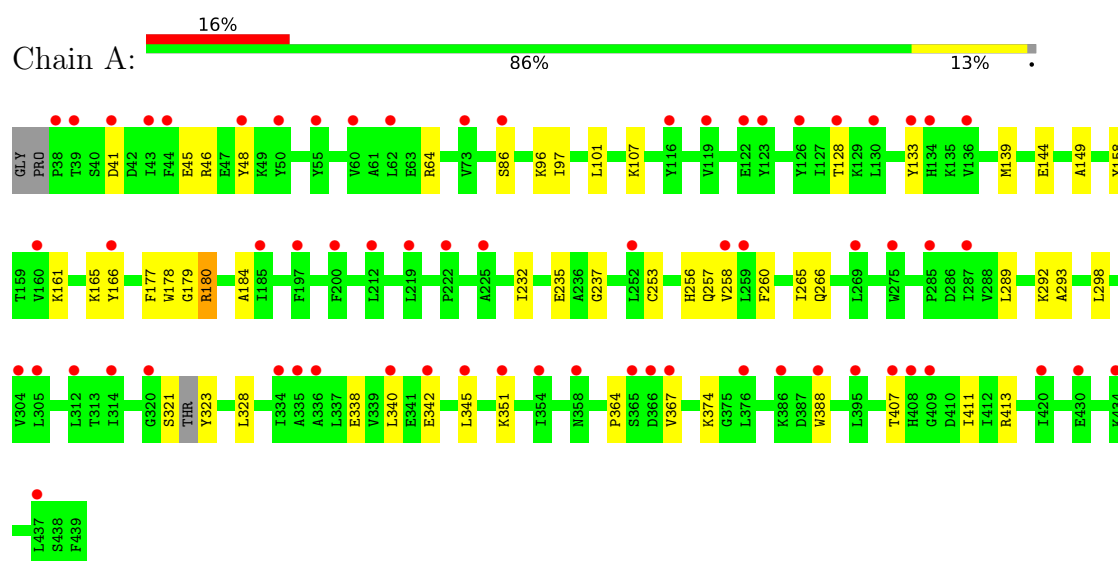
3 Residue-property plots [i](#)

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.

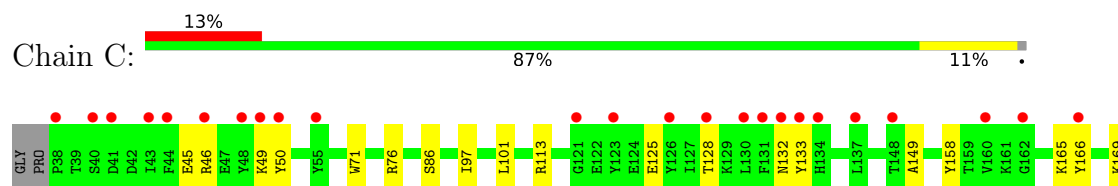
- Molecule 1: Ornithine aminotransferase, mitochondrial

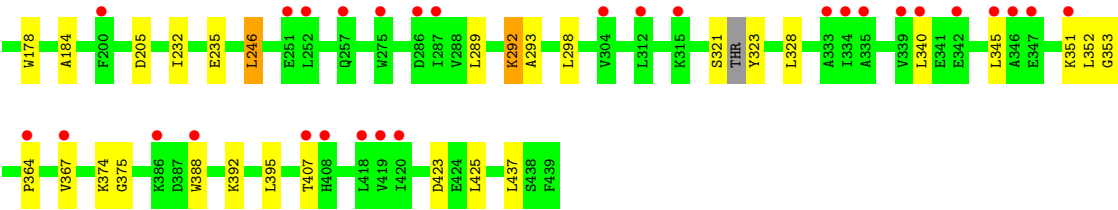


- Molecule 1: Ornithine aminotransferase, mitochondrial



- Molecule 1: Ornithine aminotransferase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	192.02Å 192.02Å 57.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.05 – 1.95 49.05 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.05-1.95) 95.3 (49.05-1.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.243 , 0.278 (Not available) , 0.300	Depositor DCC
R_{free} test set	4099 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10109	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 80.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0202e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 7QP

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	0.44	0/3206	0.60	2/4351 (0.0%)
1	B	0.52	0/3223	0.69	2/4372 (0.0%)
1	C	0.46	0/3229	0.63	2/4380 (0.0%)
All	All	0.48	0/9658	0.64	6/13103 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	LYS	CA-C-N	6.85	134.62	121.54
1	B	165	LYS	C-N-CA	6.85	134.62	121.54
1	C	165	LYS	CA-C-N	6.24	133.45	121.54
1	C	165	LYS	C-N-CA	6.24	133.45	121.54
1	A	165	LYS	CA-C-N	5.12	131.33	121.54
1	A	165	LYS	C-N-CA	5.12	131.33	121.54

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	3134	0	3130	28	2
1	B	3148	0	3154	26	3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3154	0	3160	27	3
2	A	7	0	5	0	2
2	B	7	0	5	0	3
2	C	7	0	5	0	3
3	A	26	0	0	2	0
3	B	26	0	0	1	0
3	C	26	0	0	1	0
4	A	190	0	0	3	1
4	B	189	0	0	4	0
4	C	195	0	0	6	2
All	All	10109	0	9459	79	11

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 (79) 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:128:THR:OG1	4:C:601:HOH:O	1.75	0.99
1:C:113:ARG:NH1	4:C:602:HOH:O	1.96	0.97
1:C:125:GLU:HA	4:C:601:HOH:O	1.84	0.78
1:C:46[A]:ARG:NH1	4:C:603:HOH:O	2.17	0.77
1:A:161:LYS:HE3	1:A:257:GLN:HG3	1.71	0.72
1:A:48:TYR:OH	4:A:601:HOH:O	2.09	0.69
1:C:340:LEU:HD23	1:C:345:LEU:HD12	1.78	0.66
1:C:351:LYS:HG2	1:C:352:LEU:HD23	1.77	0.65
1:A:340:LEU:HD23	1:A:345:LEU:HD12	1.77	0.65
1:B:358:ASN:OD1	4:B:601:HOH:O	2.13	0.64
1:C:86:SER:O	1:C:293:ALA:HB2	2.01	0.60
1:C:158:TYR:OH	1:C:166:TYR:HA	2.02	0.60
1:B:364:PRO:HG2	1:B:367:VAL:HG22	1.84	0.59
1:C:97:ILE:HG22	1:C:298:LEU:HD22	1.84	0.59
1:A:97:ILE:HG22	1:A:298:LEU:HD22	1.83	0.59
1:B:97:ILE:HG22	1:B:298:LEU:HD22	1.83	0.58
1:B:257:GLN:NE2	4:B:604:HOH:O	2.28	0.57
1:A:237:GLY:HA3	1:A:411:ILE:HD13	1.85	0.57
1:A:256:HIS:O	1:A:257:GLN:HG2	2.03	0.57
1:A:178:TRP:CZ2	1:A:184:ALA:HA	2.40	0.56
1:B:158:TYR:OH	1:B:166:TYR:HA	2.06	0.55
1:A:41:ASP:O	1:A:45:GLU:HG2	2.05	0.55
1:C:178:TRP:CZ2	1:C:184:ALA:HA	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.89	0.55
1:A:232:ILE:HD11	1:A:374:LYS:HD2	1.88	0.55
1:A:158:TYR:OH	1:A:166:TYR:HA	2.07	0.55
1:C:149:ALA:HB2	1:C:289:LEU:HD21	1.89	0.54
1:B:437:LEU:HD12	1:A:64:ARG:HD2	1.90	0.54
1:B:86:SER:O	1:B:293:ALA:HB2	2.08	0.54
1:C:101:LEU:HD12	1:C:328:LEU:HD11	1.90	0.54
1:C:128:THR:HB	1:C:133:TYR:O	2.08	0.53
1:A:86:SER:O	1:A:293:ALA:HB2	2.09	0.53
1:C:246:LEU:HD22	4:C:696:HOH:O	2.09	0.52
1:C:392:LYS:HD3	1:C:395:LEU:HD12	1.90	0.52
1:B:343:GLU:OE2	4:B:603:HOH:O	2.20	0.50
1:C:49[B]:LYS:HD2	1:C:50:TYR:CZ	2.46	0.49
1:B:178:TRP:CZ2	1:B:184:ALA:HA	2.46	0.49
1:A:101:LEU:HD12	1:A:328:LEU:HD11	1.95	0.49
1:B:149:ALA:HB2	1:B:289:LEU:HD21	1.94	0.48
1:B:49:LYS:HD2	1:B:50:TYR:CZ	2.48	0.48
1:C:423:ASP:OD1	1:C:423:ASP:N	2.47	0.48
1:B:169:LYS:HD3	1:B:205:ASP:OD2	2.13	0.48
1:A:178:TRP:HA	3:A:502:7QP:C15	2.44	0.47
1:C:364:PRO:HG2	1:C:367:VAL:HG22	1.96	0.47
1:A:364:PRO:HG2	1:A:367:VAL:HG22	1.96	0.47
1:C:232:ILE:HD11	1:C:374:LYS:HD2	1.95	0.47
1:A:338:GLU:O	1:A:342:GLU:HG2	2.14	0.47
1:B:46[B]:ARG:HG2	4:B:731:HOH:O	2.15	0.46
1:B:101:LEU:HD12	1:B:328:LEU:HD11	1.98	0.46
1:B:434:LYS:HB2	4:A:606:HOH:O	2.14	0.46
1:C:178:TRP:HA	3:C:502:7QP:C15	2.46	0.46
1:B:64:ARG:HD2	1:C:437:LEU:HD12	1.96	0.46
1:A:139:MET:HE3	1:A:144:GLU:HB3	1.97	0.46
1:A:265:ILE:O	1:A:292:LYS:HG3	2.16	0.46
1:B:161:LYS:HD3	1:B:163:ILE:HD11	1.98	0.46
1:A:256:HIS:C	1:A:257:GLN:HG2	2.41	0.46
1:B:266:GLN:OE1	1:B:413:ARG:NH2	2.44	0.45
1:A:46:ARG:HD3	4:A:738:HOH:O	2.16	0.45
1:A:161:LYS:CE	1:A:257:GLN:HG3	2.44	0.45
1:A:179:GLY:C	1:A:180:ARG:HD2	2.42	0.44
1:A:253:CYS:HB3	1:A:258:VAL:O	2.18	0.44
1:B:388:TRP:CD1	1:B:388:TRP:C	2.95	0.44
1:C:292:LYS:HB3	1:C:293:ALA:H	1.45	0.44
1:C:353:GLY:HA3	1:C:375:GLY:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLN:OE1	1:A:413:ARG:NH2	2.44	0.44
1:C:132:ASN:ND2	4:C:617:HOH:O	2.49	0.44
1:B:128:THR:HB	1:B:133:TYR:O	2.18	0.43
1:C:169:LYS:HD3	1:C:205:ASP:OD2	2.18	0.43
1:B:340:LEU:HD23	1:B:345:LEU:HD12	2.01	0.42
1:B:351:LYS:N	1:B:351:LYS:HD2	2.33	0.42
1:B:423:ASP:OD1	1:B:423:ASP:N	2.49	0.42
1:B:232:ILE:HD11	1:B:374:LYS:HD2	2.01	0.42
1:C:71:TRP:HA	1:C:76:ARG:O	2.19	0.42
1:C:352:LEU:HB3	1:C:425:LEU:HD22	2.02	0.42
1:A:128:THR:HB	1:A:133:TYR:O	2.20	0.41
1:A:177:PHE:CE2	3:A:502:7QP:C01	3.03	0.41
1:A:96:LYS:HE3	1:A:342:GLU:OE2	2.21	0.41
1:B:71:TRP:HA	1:B:76:ARG:O	2.21	0.41
1:B:178:TRP:HA	3:B:502:7QP:C15	2.51	0.40

All (11) 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)
1:B:321:SER:C	2:B:501:THR:N[5_554]	1.43	0.77
1:B:323:TYR:N	2:B:501:THR:C[5_554]	1.43	0.77
1:A:321:SER:C	2:A:501:THR:N[4_554]	1.43	0.77
1:A:323:TYR:N	2:A:501:THR:C[4_554]	1.43	0.77
1:C:321:SER:C	2:C:501:THR:N[6_544]	1.43	0.77
1:C:323:TYR:N	2:C:501:THR:C[6_544]	1.43	0.77
1:B:321:SER:O	2:B:501:THR:N[5_554]	2.05	0.15
1:C:321:SER:O	2:C:501:THR:N[6_544]	2.06	0.14
4:A:779:HOH:O	4:A:782:HOH:O[4_554]	2.09	0.11
4:C:610:HOH:O	4:C:654:HOH:O[6_544]	2.17	0.03
4:C:760:HOH:O	4:C:762:HOH:O[1_554]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

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	333/337 (99%)	326 (98%)	7 (2%)	47	41
1	B	335/337 (99%)	328 (98%)	7 (2%)	47	41
1	C	336/337 (100%)	330 (98%)	6 (2%)	51	47
All	All	1004/1011 (99%)	984 (98%)	20 (2%)	45	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	GLU
1	B	62	LEU
1	B	82	LEU
1	B	180	ARG
1	B	351	LYS
1	B	388	TRP
1	B	407	THR
1	A	107	LYS
1	A	180	ARG
1	A	235	GLU
1	A	260	PHE
1	A	351	LYS
1	A	388	TRP
1	A	407	THR
1	C	45	GLU
1	C	235	GLU
1	C	246	LEU
1	C	292	LYS
1	C	388	TRP
1	C	407	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	256	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	THR	B	501	3	5,6,7	1.02	0	5,7,9	4.24	2 (40%)
2	THR	C	501	3	5,6,7	0.69	0	5,7,9	1.62	1 (20%)
2	THR	A	501	3	5,6,7	0.70	0	5,7,9	1.11	0
3	7QP	B	502	1,2	27,27,27	2.07	7 (25%)	34,39,39	3.30	10 (29%)
3	7QP	A	502	1,2	27,27,27	1.93	3 (11%)	34,39,39	2.83	11 (32%)
3	7QP	C	502	1,2	27,27,27	2.05	5 (18%)	34,39,39	2.47	9 (26%)

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	THR	C	501	3	-	5/5/6/8	-
2	THR	B	501	3	-	1/5/6/8	-
2	THR	A	501	3	-	3/5/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7QP	B	502	1,2	2/2/5/6	4/15/28/28	0/2/2/2
3	7QP	A	502	1,2	-	5/15/28/28	0/2/2/2
3	7QP	C	502	1,2	1/1/5/6	6/15/28/28	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	7QP	C06-N07	-7.51	1.32	1.47
3	C	502	7QP	C06-N07	-7.50	1.32	1.47
3	B	502	7QP	C06-N07	-6.50	1.34	1.47
3	B	502	7QP	C09-C17	4.31	1.58	1.52
3	C	502	7QP	C09-C17	4.26	1.58	1.52
3	A	502	7QP	C09-C17	3.58	1.57	1.52
3	C	502	7QP	C02-C03	3.07	1.56	1.51
3	B	502	7QP	C09-N07	2.93	1.55	1.46
3	B	502	7QP	P41-O40	2.34	1.67	1.60
3	B	502	7QP	C01-C06	2.29	1.56	1.53
3	A	502	7QP	P41-O40	2.28	1.67	1.60
3	B	502	7QP	O04-C03	2.20	1.28	1.22
3	C	502	7QP	P41-O40	2.18	1.67	1.60
3	B	502	7QP	C02-C03	2.08	1.55	1.51
3	C	502	7QP	O04-C03	2.05	1.28	1.22

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	7QP	C10-C11-C02	-11.01	91.80	111.18
3	B	502	7QP	C01-C02-C03	8.69	129.34	110.92
2	B	501	THR	OG1-CB-CA	-8.30	91.47	109.01
3	C	502	7QP	C10-C11-C02	-8.10	96.93	111.18
3	B	502	7QP	C01-C06-N07	7.93	129.55	112.04
3	A	502	7QP	C09-C17-C12	7.20	129.54	119.98
3	A	502	7QP	C09-C17-C16	-6.78	112.37	119.75
3	C	502	7QP	C01-C02-C03	5.77	123.16	110.92
3	A	502	7QP	C01-C06-C08	-5.51	105.55	112.14
3	B	502	7QP	C21-C08-C06	5.13	120.67	113.07
3	A	502	7QP	C01-C02-C11	4.88	118.90	109.96
3	A	502	7QP	C11-C10-C08	-4.77	104.48	112.23
2	B	501	THR	O-C-CA	-4.28	113.75	124.77
3	B	502	7QP	C21-C08-C10	-4.19	103.25	111.06
3	C	502	7QP	C21-C08-C06	4.18	119.28	113.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	7QP	C21-C08-C06	-4.07	107.03	113.07
3	B	502	7QP	C11-C02-C03	-3.97	103.10	111.28
3	C	502	7QP	C01-C06-N07	3.97	120.81	112.04
3	A	502	7QP	C21-C08-C10	3.89	118.32	111.06
3	C	502	7QP	C11-C02-C03	-3.79	103.47	111.28
3	A	502	7QP	C11-C02-C03	3.68	118.86	111.28
3	A	502	7QP	C01-C06-N07	3.52	119.82	112.04
3	A	502	7QP	C09-N07-C06	-3.43	107.74	114.84
3	B	502	7QP	C11-C10-C08	-3.36	106.77	112.23
3	C	502	7QP	O05-C03-C02	3.18	122.41	114.16
3	C	502	7QP	C09-C17-C12	3.12	124.13	119.98
2	C	501	THR	O-C-CA	-3.01	117.03	124.77
3	C	502	7QP	C16-C15-N14	-2.28	120.13	123.83
3	B	502	7QP	C01-C02-C11	2.20	113.99	109.96
3	B	502	7QP	O44-P41-O40	2.17	112.34	106.67
3	A	502	7QP	C16-C15-N14	-2.07	120.47	123.83
3	C	502	7QP	C15-C16-C17	2.05	119.61	118.06
3	B	502	7QP	C01-C06-C08	-2.05	109.69	112.14

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	502	7QP	C02
3	B	502	7QP	C06
3	C	502	7QP	C06

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	THR	O-C-CA-CB
2	C	501	THR	O-C-CA-CB
2	C	501	THR	N-CA-CB-OG1
2	C	501	THR	C-CA-CB-OG1
3	B	502	7QP	N07-C09-C17-C16
3	B	502	7QP	N07-C09-C17-C12
3	B	502	7QP	C08-C06-N07-C09
3	A	502	7QP	N07-C09-C17-C16
3	C	502	7QP	N07-C09-C17-C16
3	C	502	7QP	C08-C06-N07-C09
3	B	502	7QP	C01-C06-N07-C09
3	C	502	7QP	C01-C06-N07-C09
3	A	502	7QP	C08-C06-N07-C09

Continued on next page...

Continued from previous page...

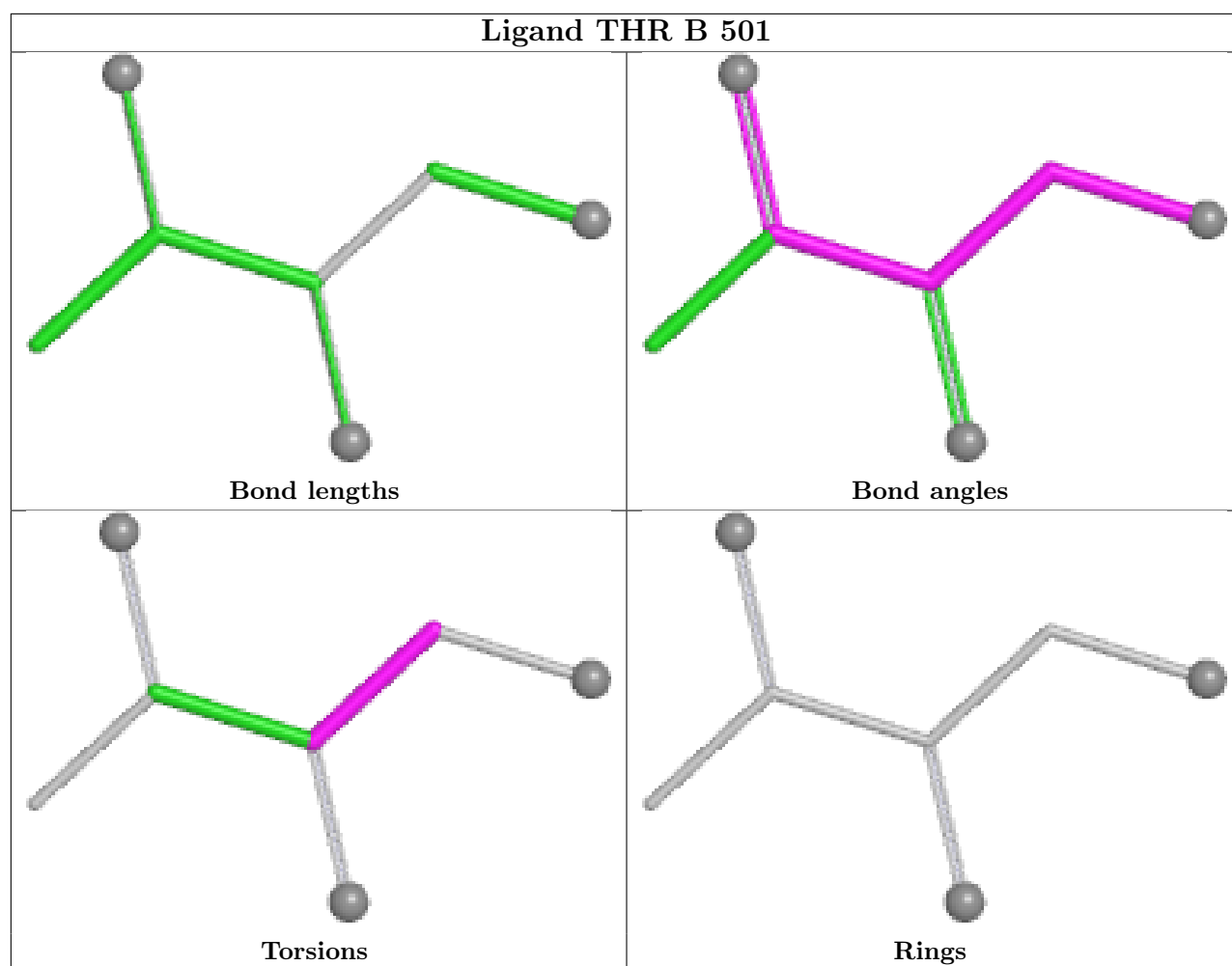
Mol	Chain	Res	Type	Atoms
3	A	502	7QP	C01-C06-N07-C09
3	A	502	7QP	N07-C09-C17-C12
3	C	502	7QP	N07-C09-C17-C12
2	A	501	THR	C-CA-CB-OG1
3	A	502	7QP	C18-O40-P41-O42
2	C	501	THR	C-CA-CB-CG2
3	C	502	7QP	C01-C02-C03-O05
2	B	501	THR	O-C-CA-CB
3	C	502	7QP	C01-C02-C03-O04
2	A	501	THR	N-CA-CB-CG2
2	C	501	THR	N-CA-CB-CG2

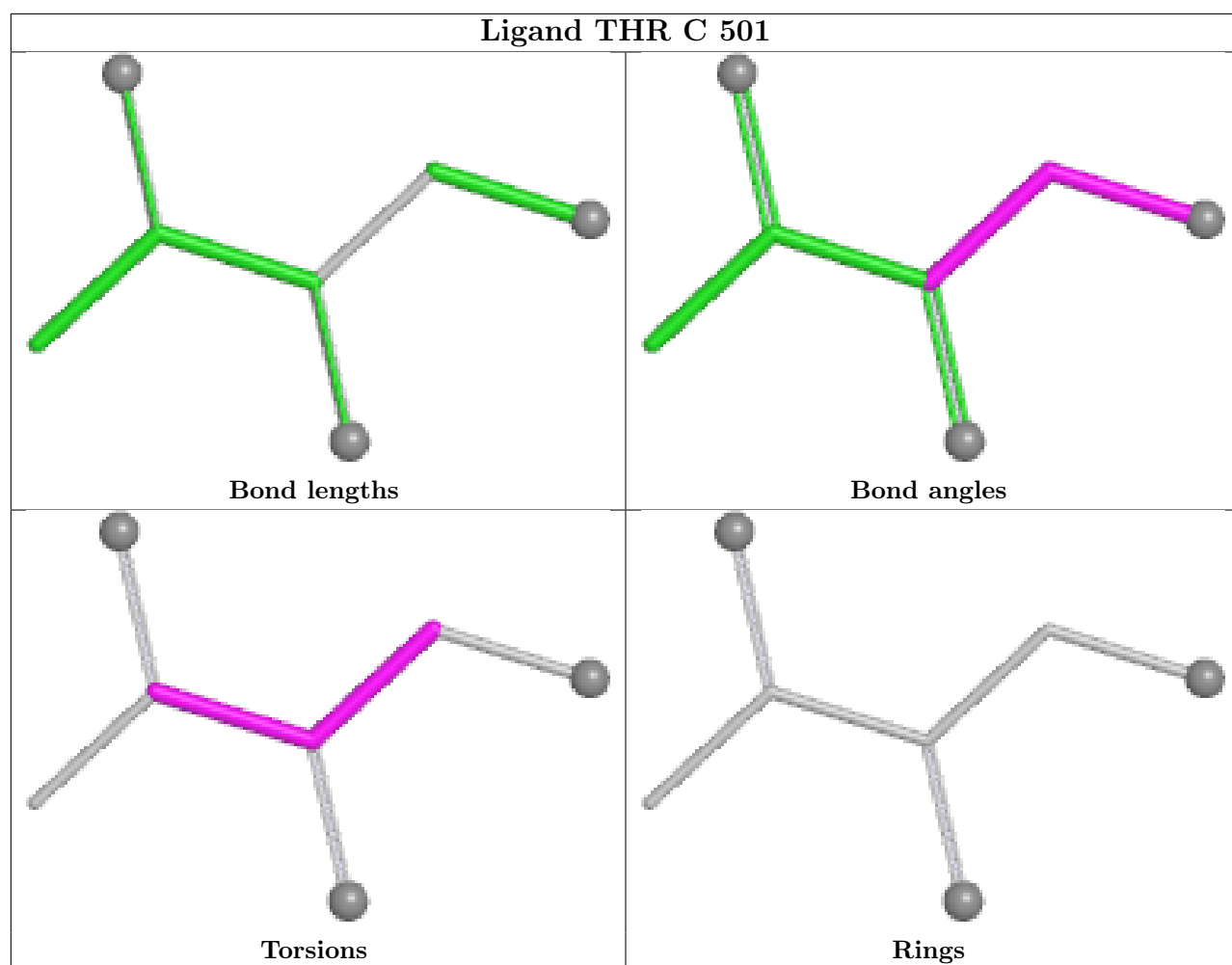
There are no ring outliers.

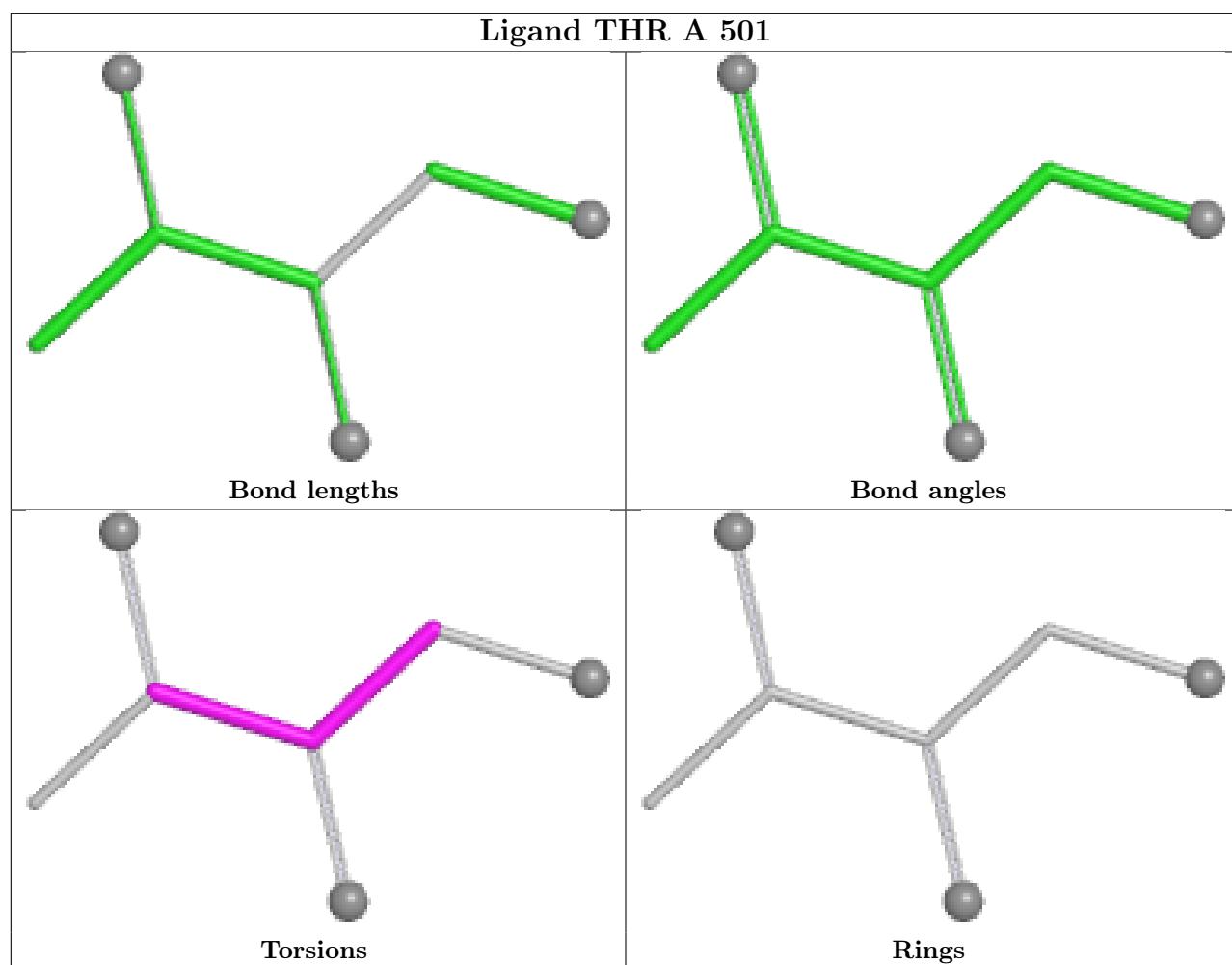
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	THR	0	3
2	C	501	THR	0	3
2	A	501	THR	0	2
3	B	502	7QP	1	0
3	A	502	7QP	2	0
3	C	502	7QP	1	0

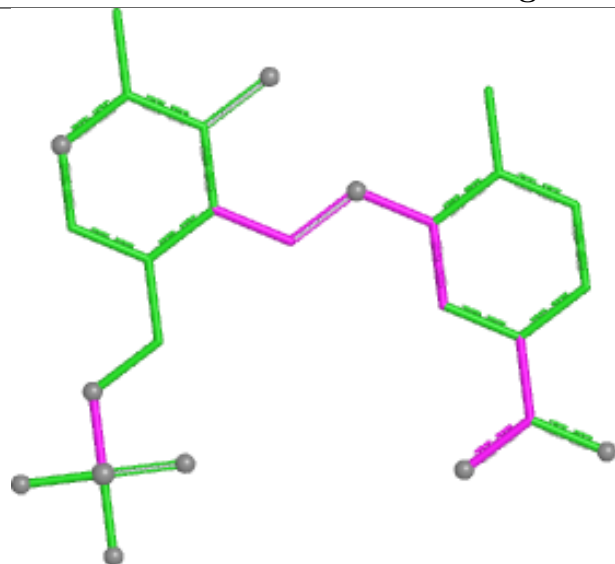
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



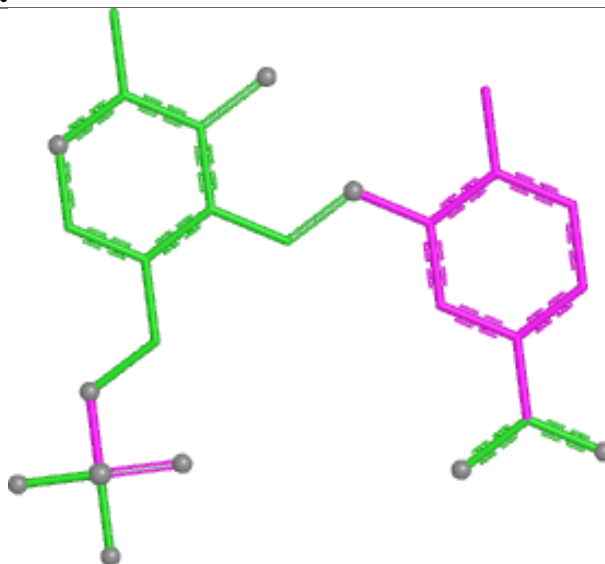




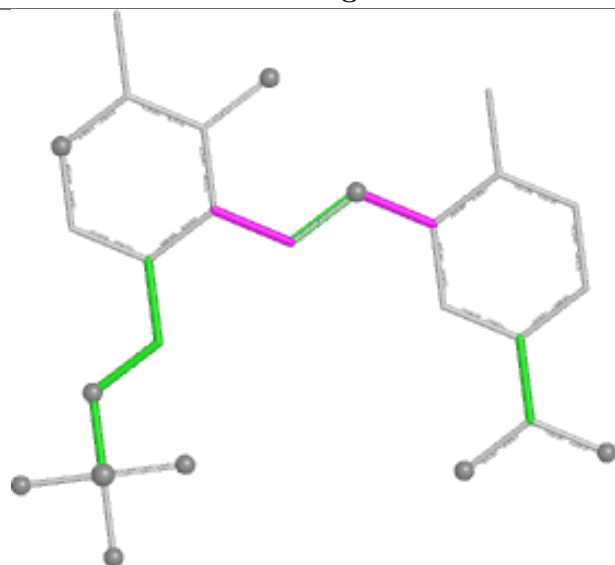
Ligand 7QP B 502



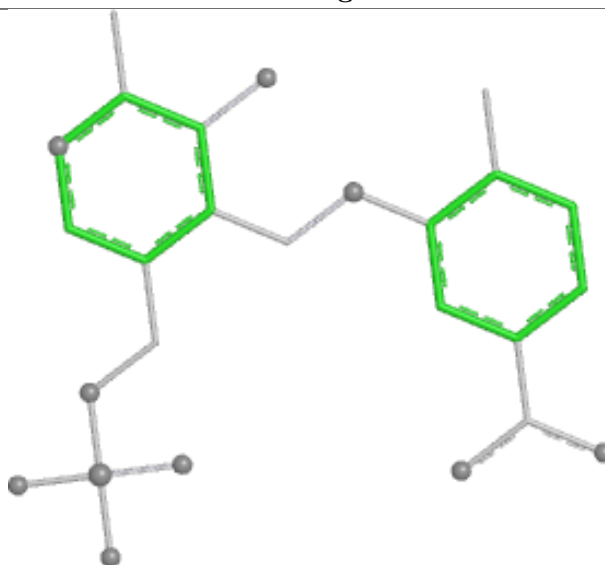
Bond lengths



Bond angles

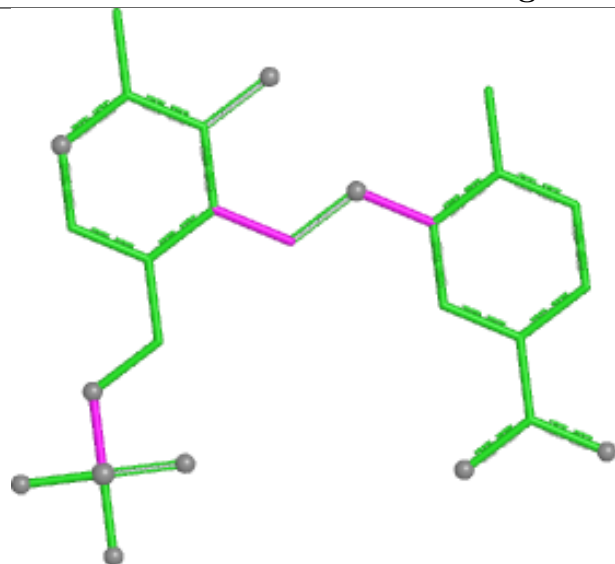


Torsions

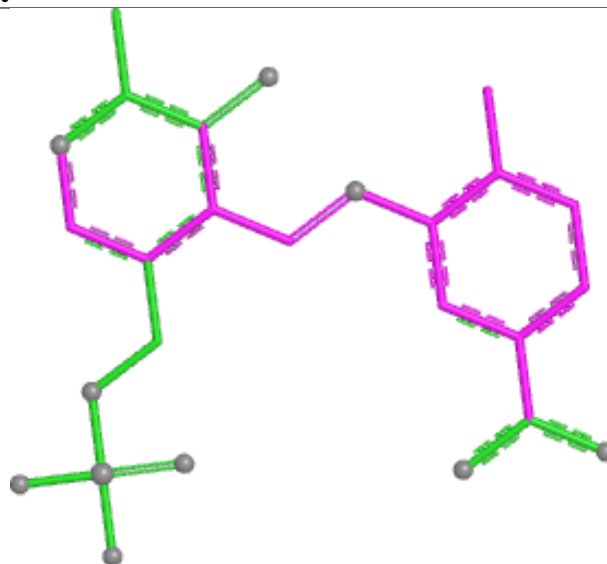


Rings

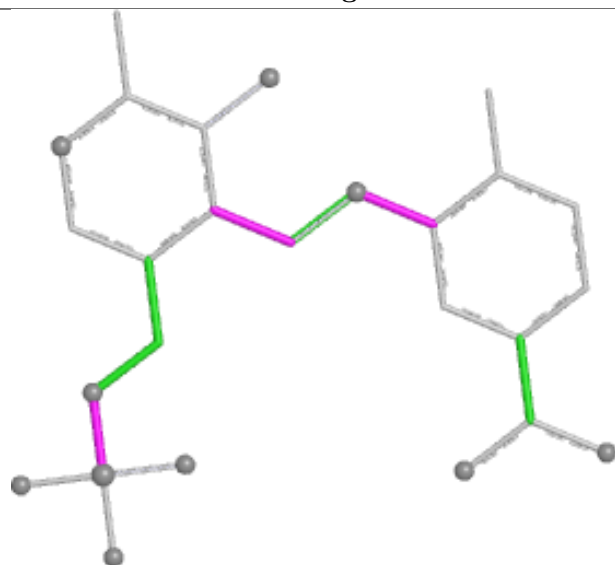
Ligand 7QP A 502



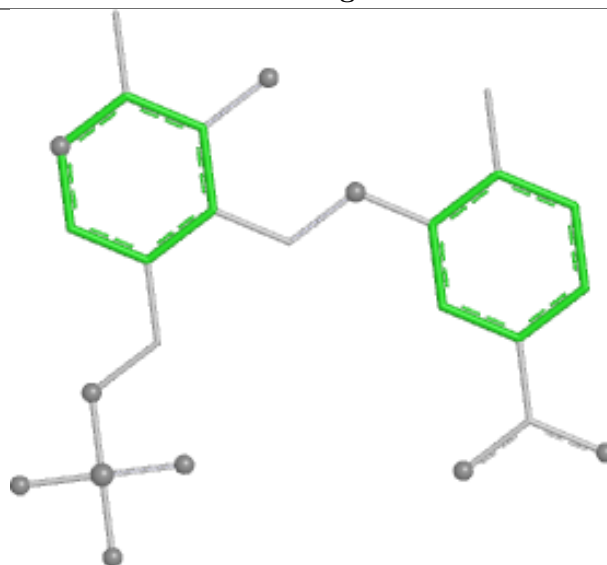
Bond lengths



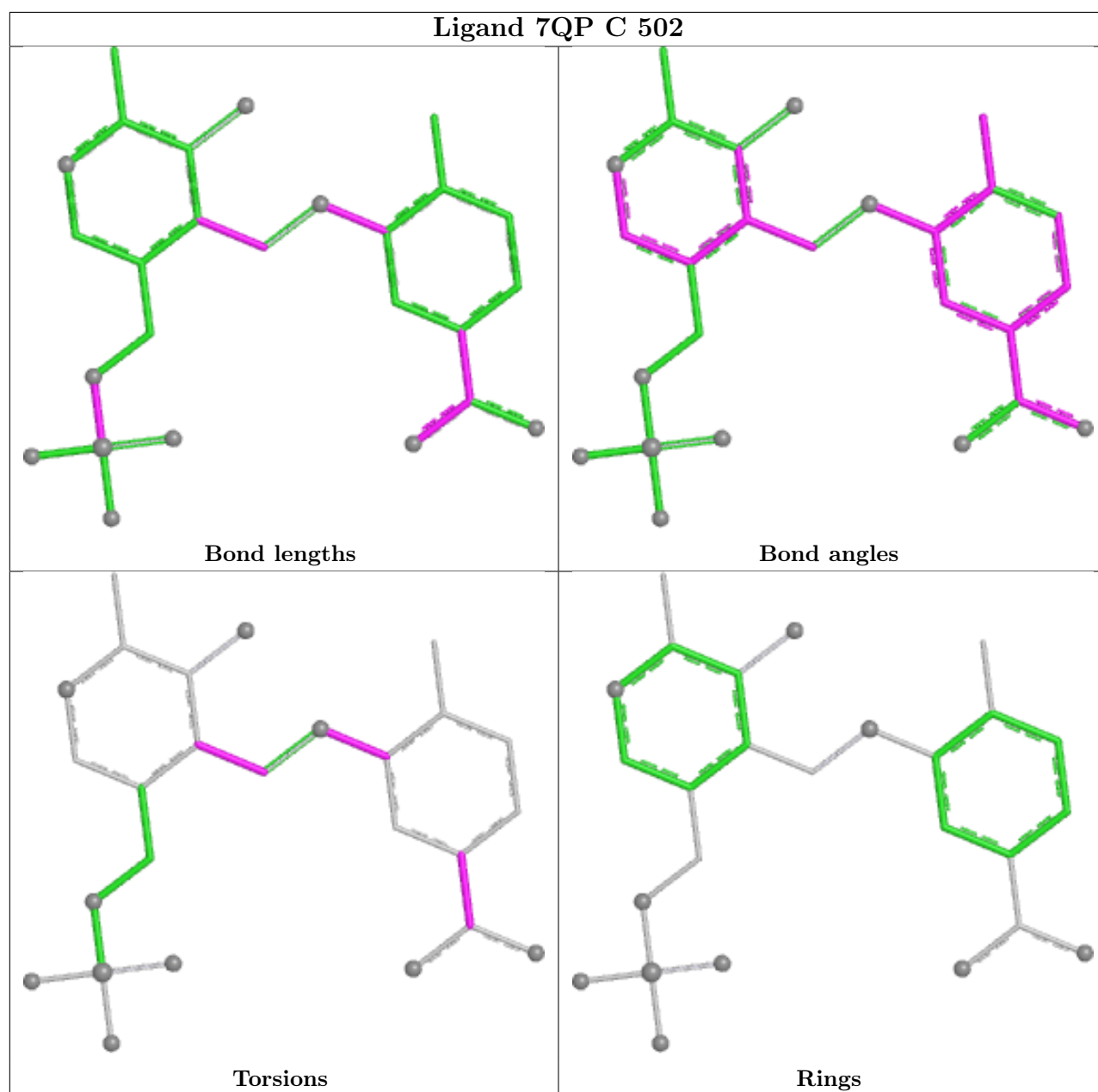
Bond angles



Torsions



Rings



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, 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	401/404 (99%)	1.16	66 (16%) 4 4	29, 43, 67, 125	0
1	B	401/404 (99%)	-0.06	9 (2%) 62 69	17, 28, 45, 97	1 (0%)
1	C	401/404 (99%)	1.08	53 (13%) 7 8	20, 42, 61, 117	2 (0%)
All	All	1203/1212 (99%)	0.73	128 (10%) 11 13	17, 38, 62, 125	3 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ASP	4.8
1	C	41	ASP	4.3
1	C	275	TRP	4.3
1	C	407	THR	4.2
1	B	388	TRP	4.2
1	C	130	LEU	4.2
1	C	38	PRO	4.2
1	C	388	TRP	4.0
1	A	48	TYR	3.9
1	C	345	LEU	3.8
1	C	126	TYR	3.7
1	A	388	TRP	3.6
1	B	408	HIS	3.6
1	A	275	TRP	3.5
1	C	334	ILE	3.5
1	A	133	TYR	3.4
1	C	287	ILE	3.4
1	C	40	SER	3.4
1	C	386	LYS	3.3
1	A	166	TYR	3.3
1	B	407	THR	3.3
1	C	340	LEU	3.3
1	A	38	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	386	LYS	3.3
1	A	407	THR	3.2
1	A	55	TYR	3.1
1	C	43	ILE	3.1
1	A	160	VAL	3.1
1	C	48	TYR	3.0
1	A	320	GLY	3.0
1	A	314	ILE	2.9
1	C	367	VAL	2.9
1	A	50	TYR	2.9
1	A	126	TYR	2.9
1	A	408	HIS	2.9
1	B	365	SER	2.9
1	A	212	LEU	2.8
1	B	38	PRO	2.8
1	C	166	TYR	2.8
1	C	346	ALA	2.8
1	A	128	THR	2.8
1	C	123	TYR	2.7
1	C	408	HIS	2.7
1	A	409	GLY	2.7
1	C	419	VAL	2.7
1	C	418	LEU	2.7
1	C	128	THR	2.6
1	C	351	LYS	2.6
1	A	287	ILE	2.6
1	A	334	ILE	2.6
1	C	160	VAL	2.6
1	C	46[A]	ARG	2.6
1	C	312	LEU	2.6
1	A	354	ILE	2.6
1	A	304	VAL	2.6
1	C	333	ALA	2.6
1	C	49[A]	LYS	2.6
1	A	376	LEU	2.5
1	A	420	ILE	2.5
1	C	50	TYR	2.5
1	A	269	LEU	2.5
1	C	420	ILE	2.5
1	A	365	SER	2.5
1	A	367	VAL	2.5
1	C	339	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	437	LEU	2.4
1	C	133	TYR	2.4
1	B	257	GLN	2.4
1	A	39	THR	2.4
1	A	342	GLU	2.4
1	A	43	ILE	2.3
1	C	335	ALA	2.3
1	B	387	ASP	2.3
1	A	430	GLU	2.3
1	A	305	LEU	2.3
1	A	225	ALA	2.3
1	A	60	VAL	2.3
1	A	119	VAL	2.3
1	C	342	GLU	2.3
1	A	351	LYS	2.3
1	C	162	GLY	2.3
1	C	347	GLU	2.3
1	A	130	LEU	2.3
1	A	200	PHE	2.2
1	A	86	SER	2.2
1	C	134	HIS	2.2
1	A	219	LEU	2.2
1	A	123	TYR	2.2
1	A	197	PHE	2.2
1	C	55	TYR	2.2
1	A	434	LYS	2.2
1	C	132	ASN	2.2
1	A	122	GLU	2.2
1	A	62	LEU	2.2
1	C	257	GLN	2.2
1	C	44	PHE	2.2
1	C	251	GLU	2.2
1	C	121	GLY	2.2
1	C	286	ASP	2.1
1	A	136	VAL	2.1
1	A	312	LEU	2.1
1	C	137	LEU	2.1
1	A	116	TYR	2.1
1	C	148	THR	2.1
1	A	258	VAL	2.1
1	C	304	VAL	2.1
1	A	134	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	345	LEU	2.1
1	A	358	ASN	2.1
1	A	336	ALA	2.1
1	A	366	ASP	2.1
1	B	386	LYS	2.1
1	A	73	VAL	2.1
1	A	222	PRO	2.1
1	A	252	LEU	2.1
1	A	259	LEU	2.1
1	A	340	LEU	2.1
1	B	284	ARG	2.1
1	A	44	PHE	2.0
1	A	185	ILE	2.0
1	C	131	PHE	2.0
1	A	285	PRO	2.0
1	A	395	LEU	2.0
1	C	252	LEU	2.0
1	A	335	ALA	2.0
1	C	315	LYS	2.0
1	C	200	PHE	2.0
1	C	364	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	7QP	A	502	26/26	0.80	0.17	47,56,65,65	0
3	7QP	C	502	26/26	0.80	0.17	49,58,67,69	0

Continued on next page...

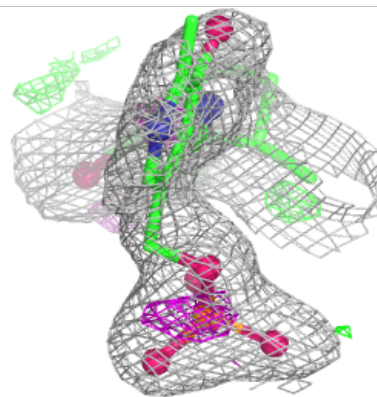
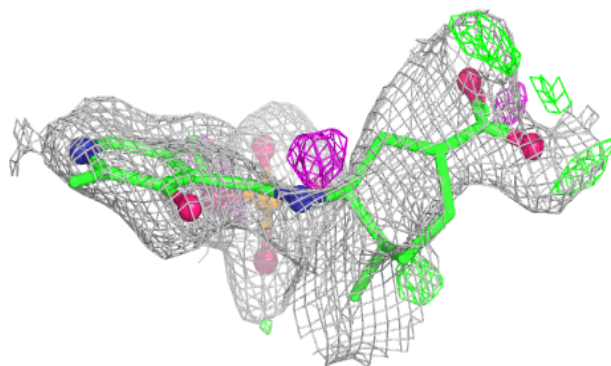
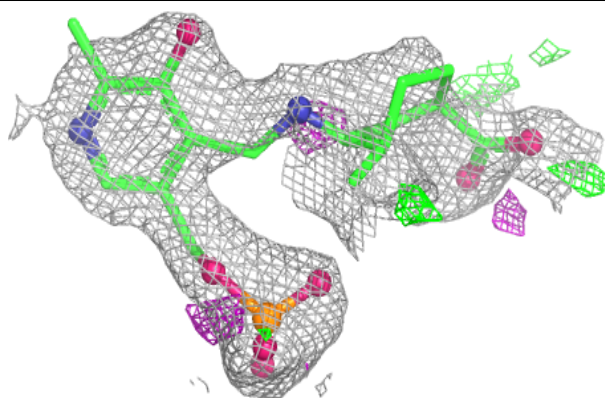
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	7QP	B	502	26/26	0.86	0.12	26,35,46,48	0
2	THR	C	501	7/8	0.90	0.15	46,49,54,58	0
2	THR	A	501	7/8	0.93	0.11	45,46,55,59	0
2	THR	B	501	7/8	0.95	0.07	22,25,31,32	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.

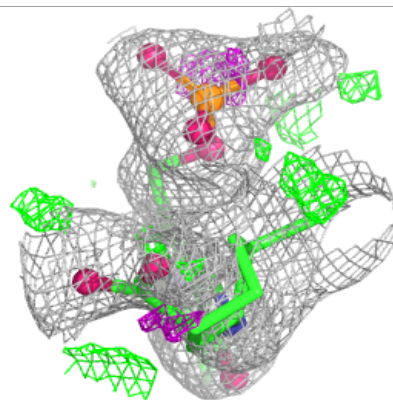
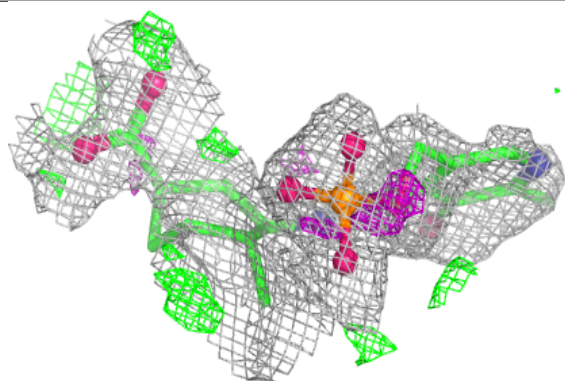
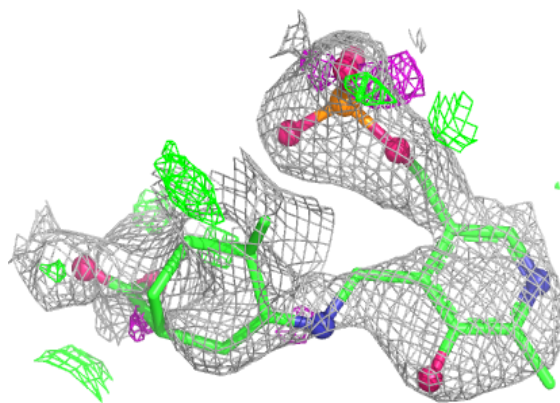
Electron density around 7QP A 502:

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



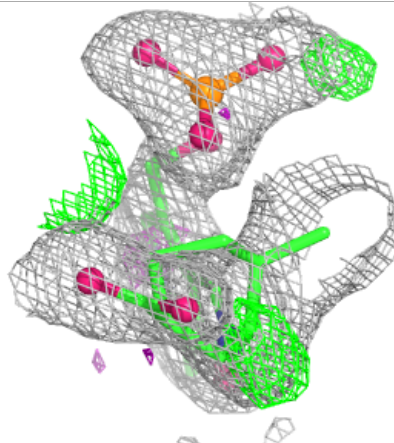
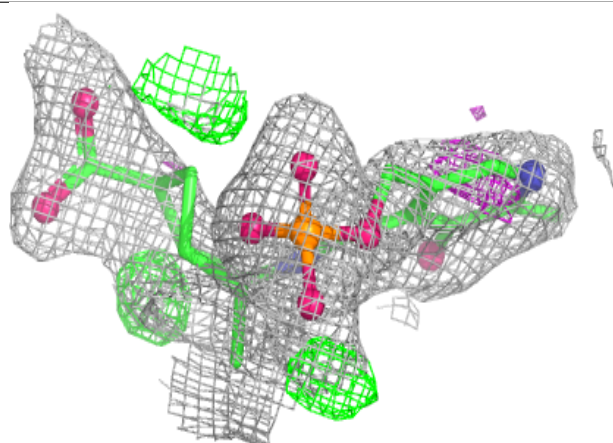
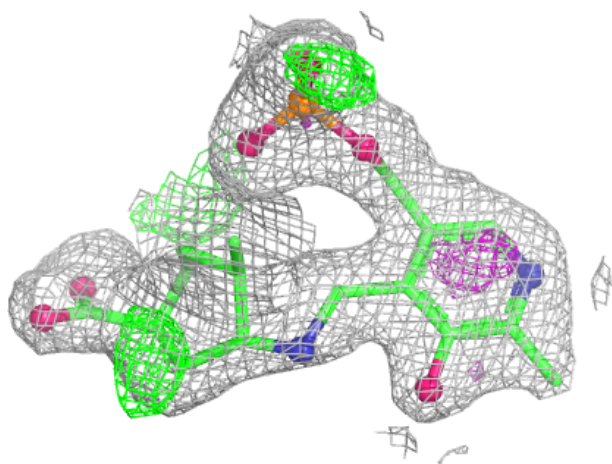
Electron density around 7QP C 502:

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



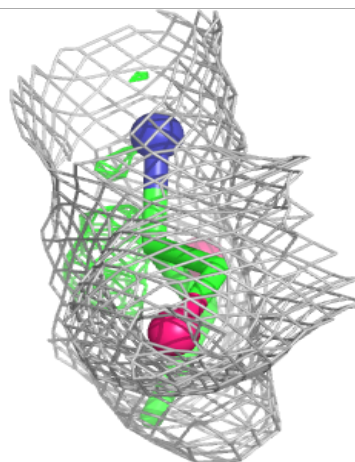
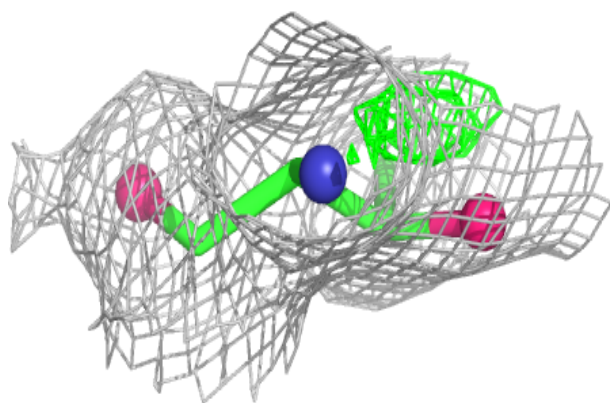
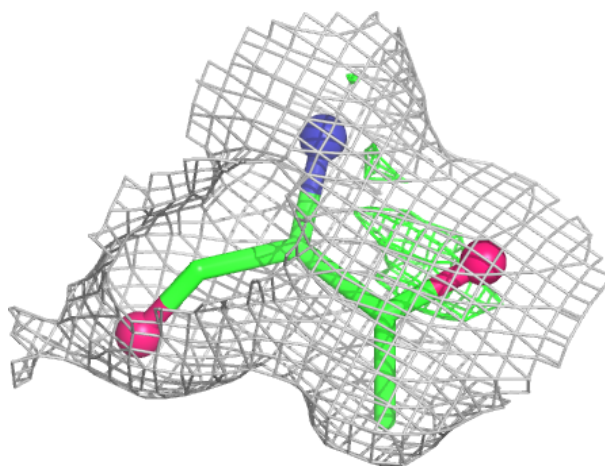
Electron density around 7QP B 502:

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



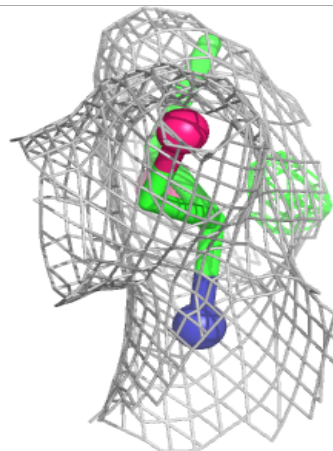
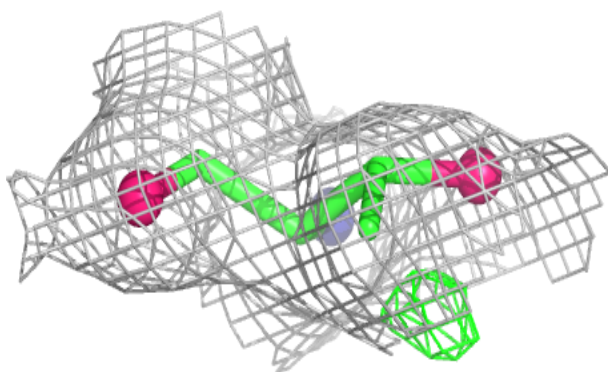
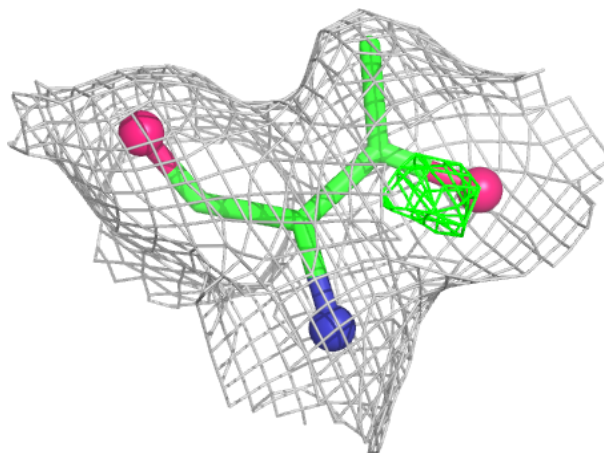
Electron density around THR C 501:

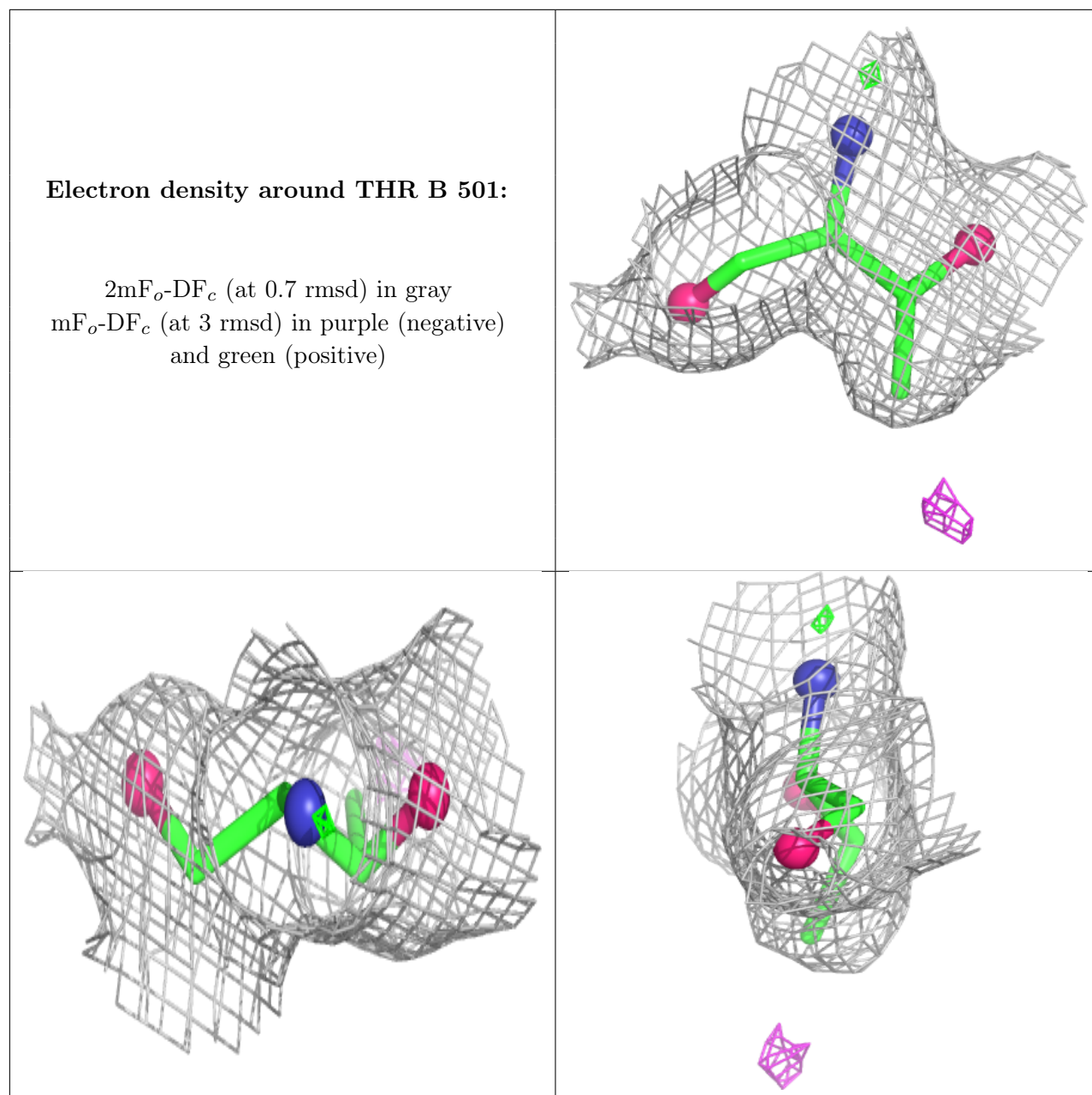
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around THR A 501:

$2mF_o-DF_c$ (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.