



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:02 AM UTC

PDB ID : 4LXA / pdb_00004lxa
Title : Crystal Structure of Human Beta Secretase in Complex with Compound 11a
Authors : Rondeau, J.M.; Bourgier, E.
Deposited on : 2013-07-29
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

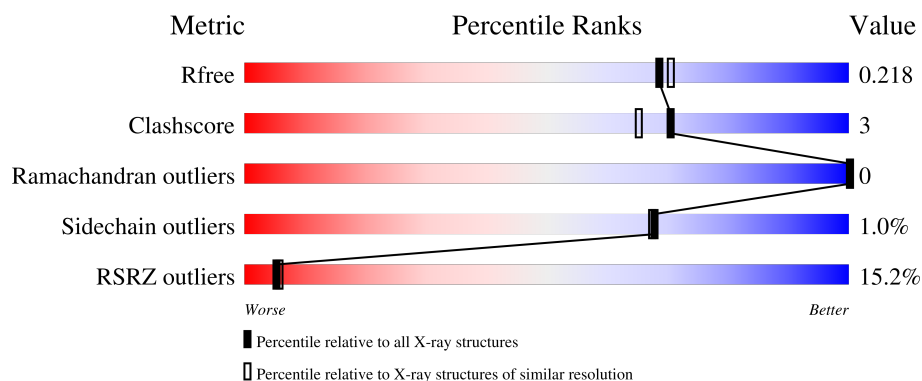
1 Overall quality at a glance

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)
Ramachandran outliers	187476	3587 (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	402	
1	B	402	
1	C	402	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9566 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.

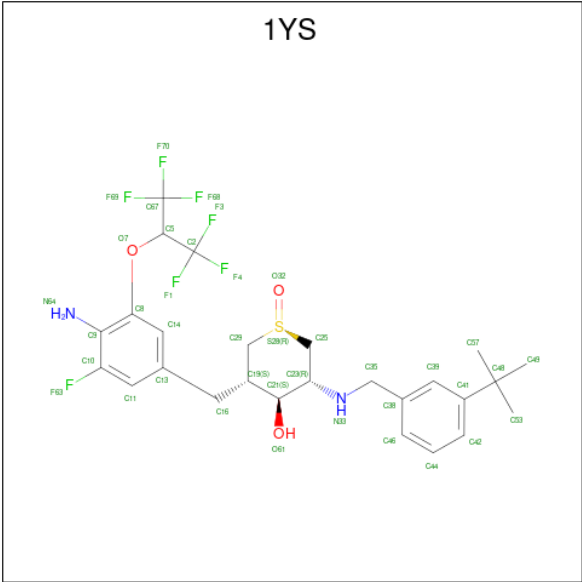
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2961	1895	492	560	14			
1	B	378	Total	C	N	O	S	0	0	0
			2971	1901	494	562	14			
1	C	381	Total	C	N	O	S	0	0	0
			2993	1917	497	565	14			

There are 6 discrepancies between the modelled and reference sequences:

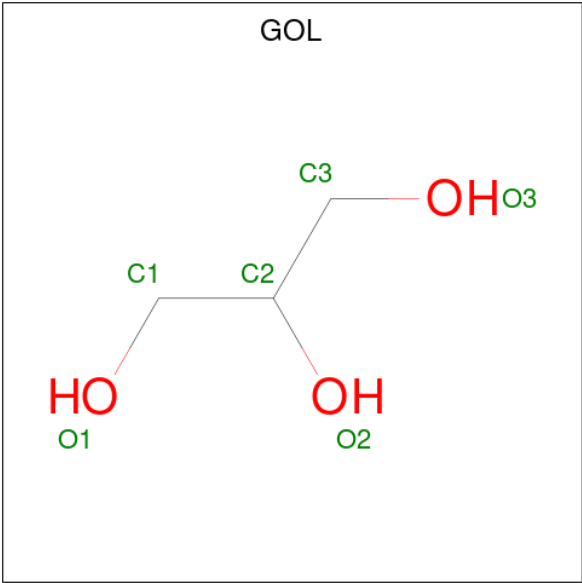
Chain	Residue	Modelled	Actual	Comment	Reference
A	33P	GLY	-	expression tag	UNP P56817
A	34P	PRO	-	expression tag	UNP P56817
B	33P	GLY	-	expression tag	UNP P56817
B	34P	PRO	-	expression tag	UNP P56817
C	33P	GLY	-	expression tag	UNP P56817
C	34P	PRO	-	expression tag	UNP P56817

- Molecule 2 is (1R,3S,4S,5R)-3-{4-amino-3-fluoro-5-[(1,1,1,3,3,3-hexafluoropropan-2-yl)oxy]benzyl}-5-[(3-tert-butylbenzyl)amino]tetrahydro-2H-thiopyran-4-ol 1-oxide (CCD ID: 1YS) (formula: C₂₆H₃₁F₇N₂O₃S).



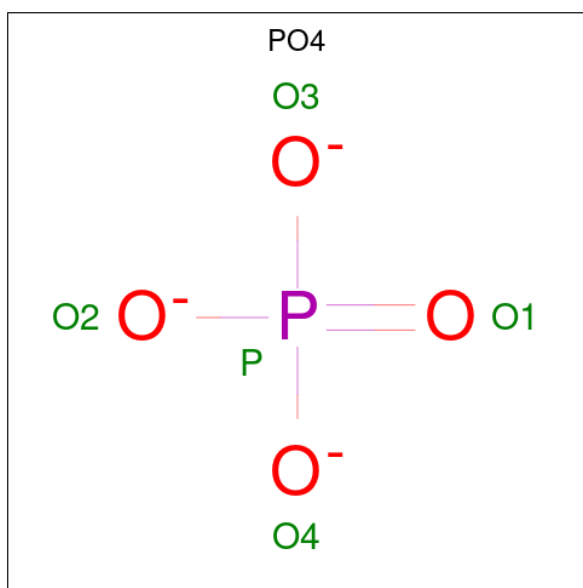
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			39	26	7	2	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			39	26	7	2	3	1		
2	C	1	Total	C	F	N	O	S	0	0
			39	26	7	2	3	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



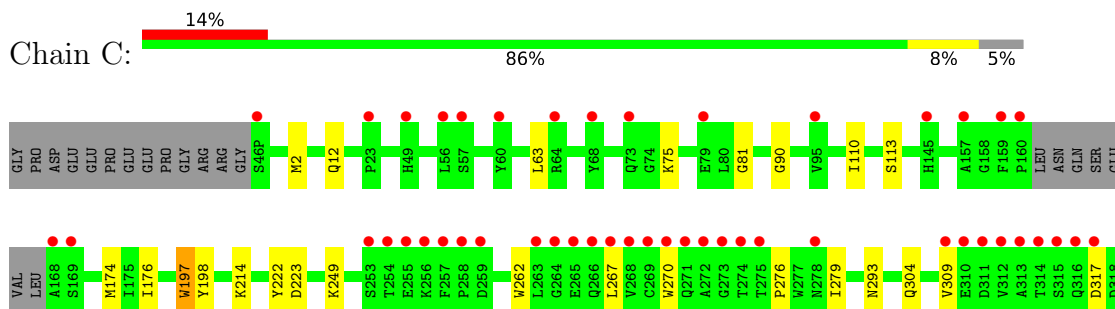
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

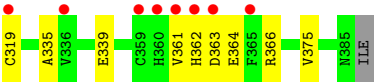
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	0
			172	172		
5	B	168	Total	O	0	0
			168	168		
5	C	173	Total	O	0	0
			173	173		

i

- Molecule 1: Beta-secretase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.93Å 103.07Å 100.23Å 90.00° 104.33° 90.00°	Depositor
Resolution (Å)	37.65 – 1.95 37.65 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.65-1.95) 99.5 (37.65-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.95Å)	Xtriage
Refinement program	CNS, CNX	Depositor
R, R_{free}	0.199 , 0.222 0.194 , 0.218	Depositor DCC
R_{free} test set	5880 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9566	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: PO4, GOL, 1YS

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	0.31	0/3036	0.67	0/4126
1	B	0.32	0/3046	0.67	0/4140
1	C	0.31	0/3070	0.66	0/4173
All	All	0.31	0/9152	0.67	0/12439

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	2961	0	2870	19	0
1	B	2971	0	2880	22	0
1	C	2993	0	2899	19	0
2	A	39	0	31	0	0
2	B	39	0	31	0	0
2	C	39	0	31	0	0
3	B	6	0	8	0	0
4	C	5	0	0	0	0
5	A	172	0	0	2	0
5	B	168	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	173	0	0	1	0
All	All	9566	0	8750	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (60) 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:B:267:LEU:HD13	1:B:319:CYS:HB3	1.71	0.71
1:A:267:LEU:HD13	1:A:319:CYS:HB3	1.75	0.67
1:A:254:THR:HG23	1:A:255:GLU:HG3	1.81	0.62
1:B:267:LEU:HD22	1:B:309:VAL:HG21	1.82	0.62
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.83	0.61
1:B:357:SER:O	1:B:360:HIS:HB3	2.01	0.60
1:C:335:ALA:O	1:C:339:GLU:HG3	2.02	0.60
1:B:264:GLY:O	1:B:321:LYS:HE3	2.03	0.58
1:B:64:ARG:HH11	1:B:64:ARG:HB3	1.69	0.58
1:B:232:THR:O	1:B:336:VAL:HG13	2.03	0.58
1:A:278:ASN:HD22	1:A:278:ASN:H	1.52	0.57
1:A:125:GLU:HG3	5:A:744:HOH:O	2.05	0.56
1:B:276:PRO:O	1:B:279:ILE:HG12	2.06	0.56
1:C:249:LYS:HE2	1:C:262:TRP:CD1	2.41	0.55
1:C:267:LEU:HD13	1:C:319:CYS:HB3	1.88	0.55
1:C:363:ASP:HB3	1:C:366:ARG:O	2.05	0.55
1:A:335:ALA:O	1:A:339:GLU:HG3	2.08	0.54
1:C:267:LEU:HD22	1:C:309:VAL:HG21	1.89	0.54
1:B:63:LEU:HG	1:B:81:GLY:HA2	1.92	0.52
1:A:365:PHE:HB2	5:A:768:HOH:O	2.08	0.52
1:C:63:LEU:HG	1:C:81:GLY:HA2	1.93	0.50
1:B:9:LYS:HZ1	1:B:168:ALA:N	2.10	0.49
1:A:267:LEU:HD22	1:A:309:VAL:HG21	1.94	0.49
1:B:205:ARG:NH2	1:B:212:ASP:HB2	2.28	0.49
1:C:110:ILE:HB	1:C:113:SER:HB3	1.94	0.49
1:B:174:MET:HE3	1:B:176:ILE:HD11	1.95	0.49
1:B:267:LEU:HD21	1:B:312:VAL:HG13	1.94	0.49
1:C:304:GLN:HG3	1:C:361:VAL:HG21	1.94	0.49
1:B:197:TRP:CG	1:B:198:TYR:H	2.31	0.48
1:B:267:LEU:HD22	1:B:309:VAL:CG2	2.42	0.48
1:C:174:MET:HE3	1:C:176:ILE:HD11	1.95	0.48
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASP:HB3	1:A:366:ARG:O	2.14	0.48
1:B:110:ILE:HB	1:B:113:SER:HB3	1.96	0.47
1:A:197:TRP:CG	1:A:198:TYR:H	2.32	0.47
1:C:12:GLN:OE1	1:C:113:SER:HA	2.15	0.47
1:C:267:LEU:HD22	1:C:309:VAL:CG2	2.44	0.47
1:C:197:TRP:CG	1:C:198:TYR:H	2.33	0.46
1:A:205:ARG:HB3	1:A:286:TYR:HB2	1.98	0.46
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.98	0.45
1:B:222:TYR:HA	1:B:223:ASP:HA	1.62	0.45
1:C:276:PRO:O	1:C:279:ILE:HG12	2.17	0.45
1:A:282:VAL:HG12	1:A:301:LEU:HD23	1.99	0.44
1:A:244:ALA:O	1:A:248:ILE:HG13	2.17	0.44
1:C:293:ASN:HA	1:C:375:VAL:HA	1.99	0.43
1:A:110:ILE:HB	1:A:113:SER:HB3	2.01	0.43
1:A:211:GLN:HE21	1:A:211:GLN:HB2	1.62	0.43
1:C:2:MET:HG2	1:C:90:GLY:HA2	2.00	0.43
1:C:222:TYR:HA	1:C:223:ASP:HA	1.65	0.43
1:C:75:LYS:NZ	5:C:728:HOH:O	2.51	0.43
1:A:222:TYR:HA	1:A:223:ASP:HA	1.70	0.43
1:A:9:LYS:HE2	1:A:9:LYS:HB3	1.83	0.42
1:B:249:LYS:HE2	1:B:262:TRP:CD1	2.54	0.42
1:B:364:GLU:HG3	1:B:365:PHE:CD2	2.55	0.42
1:B:314:THR:O	1:B:314:THR:HG23	2.20	0.41
1:C:304:GLN:CG	1:C:361:VAL:HG21	2.50	0.41
1:B:288:MET:HE2	1:B:379:MET:HB3	2.02	0.41
1:C:270:TRP:O	1:C:317:ASP:HB3	2.21	0.41
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.93	0.40
1:B:125:GLU:O	1:B:125:GLU:HG3	2.21	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	A	372/402 (92%)	366 (98%)	6 (2%)	0	100	100
1	B	374/402 (93%)	366 (98%)	8 (2%)	0	100	100
1	C	377/402 (94%)	368 (98%)	9 (2%)	0	100	100
All	All	1123/1206 (93%)	1100 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	322/342 (94%)	318 (99%)	4 (1%)	63	61
1	B	322/342 (94%)	320 (99%)	2 (1%)	78	79
1	C	324/342 (95%)	320 (99%)	4 (1%)	63	61
All	All	968/1026 (94%)	958 (99%)	10 (1%)	68	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	197	TRP
1	A	211	GLN
1	A	278	ASN
1	B	125	GLU
1	B	197	TRP
1	C	197	TRP
1	C	214	LYS
1	C	362	HIS
1	C	364	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	114	ASN
1	A	278	ASN
1	A	316	GLN
1	A	326	GLN
1	A	385	ASN
1	B	89	HIS
1	B	114	ASN
1	B	278	ASN
1	B	293	ASN
1	B	326	GLN
1	C	89	HIS
1	C	114	ASN
1	C	326	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	1YS	C	501	-	38,41,41	1.62	5 (13%)	52,63,63	1.19	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	501	-	5,5,5	0.76	0	5,5,5	0.46	0
2	1YS	B	502	-	38,41,41	1.64	5 (13%)	52,63,63	1.23	6 (11%)
4	PO4	C	502	-	4,4,4	1.68	0	6,6,6	0.46	0
2	1YS	A	501	-	38,41,41	1.63	5 (13%)	52,63,63	1.25	5 (9%)

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	1YS	B	502	-	-	2/31/47/47	0/3/3/3
3	GOL	B	501	-	-	2/4/4/4	-
2	1YS	A	501	-	-	2/31/47/47	0/3/3/3
2	1YS	C	501	-	-	1/31/47/47	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	1YS	C25-C23	4.08	1.56	1.52
2	B	502	1YS	C25-C23	3.93	1.56	1.52
2	C	501	1YS	C25-C23	3.81	1.56	1.52
2	A	501	1YS	C16-C19	3.32	1.57	1.53
2	C	501	1YS	C16-C19	3.07	1.57	1.53
2	B	502	1YS	C16-C19	3.03	1.57	1.53
2	B	502	1YS	C11-C10	2.61	1.42	1.37
2	C	501	1YS	C11-C10	2.57	1.42	1.37
2	A	501	1YS	C39-C41	2.56	1.43	1.39
2	B	502	1YS	C39-C41	2.54	1.43	1.39
2	C	501	1YS	C39-C41	2.53	1.43	1.39
2	C	501	1YS	C42-C41	2.37	1.43	1.39
2	A	501	1YS	C42-C41	2.36	1.43	1.39
2	B	502	1YS	C42-C41	2.35	1.43	1.39
2	A	501	1YS	C11-C10	2.24	1.41	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	1YS	C35-N33-C23	3.59	122.27	114.84
2	A	501	1YS	C35-N33-C23	3.50	122.10	114.84
2	A	501	1YS	C29-C19-C16	3.31	114.69	109.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	1YS	C13-C16-C19	-3.22	108.58	113.61
2	C	501	1YS	C29-C19-C16	3.21	114.55	109.65
2	B	502	1YS	C29-C19-C16	3.15	114.45	109.65
2	C	501	1YS	C35-N33-C23	3.13	121.32	114.84
2	B	502	1YS	C13-C16-C19	-2.78	109.27	113.61
2	C	501	1YS	C13-C16-C19	-2.65	109.47	113.61
2	A	501	1YS	C53-C48-C41	2.50	116.25	110.35
2	B	502	1YS	C25-C23-N33	2.24	113.16	109.23
2	C	501	1YS	C53-C48-C41	2.22	115.58	110.35
2	B	502	1YS	C8-C9-C10	2.17	119.46	116.08
2	C	501	1YS	C8-C9-C10	2.14	119.42	116.08
2	B	502	1YS	C53-C48-C41	2.12	115.36	110.35
2	C	501	1YS	C11-C10-C9	-2.05	120.34	123.36
2	A	501	1YS	C8-C9-C10	2.02	119.24	116.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

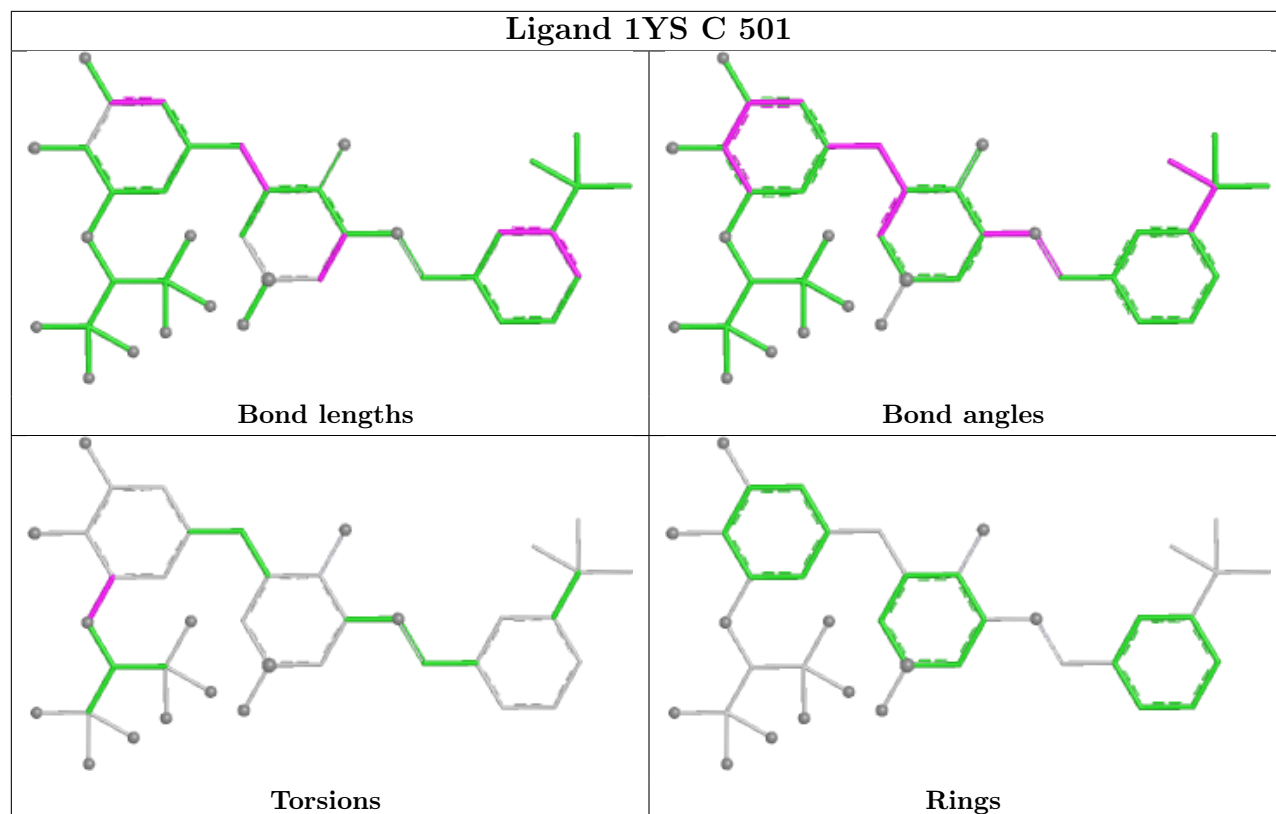
Mol	Chain	Res	Type	Atoms
3	B	501	GOL	O1-C1-C2-C3
3	B	501	GOL	O1-C1-C2-O2
2	A	501	1YS	C9-C8-O7-C5
2	B	502	1YS	C9-C8-O7-C5
2	A	501	1YS	C14-C8-O7-C5
2	B	502	1YS	C14-C8-O7-C5
2	C	501	1YS	C14-C8-O7-C5

There are no ring outliers.

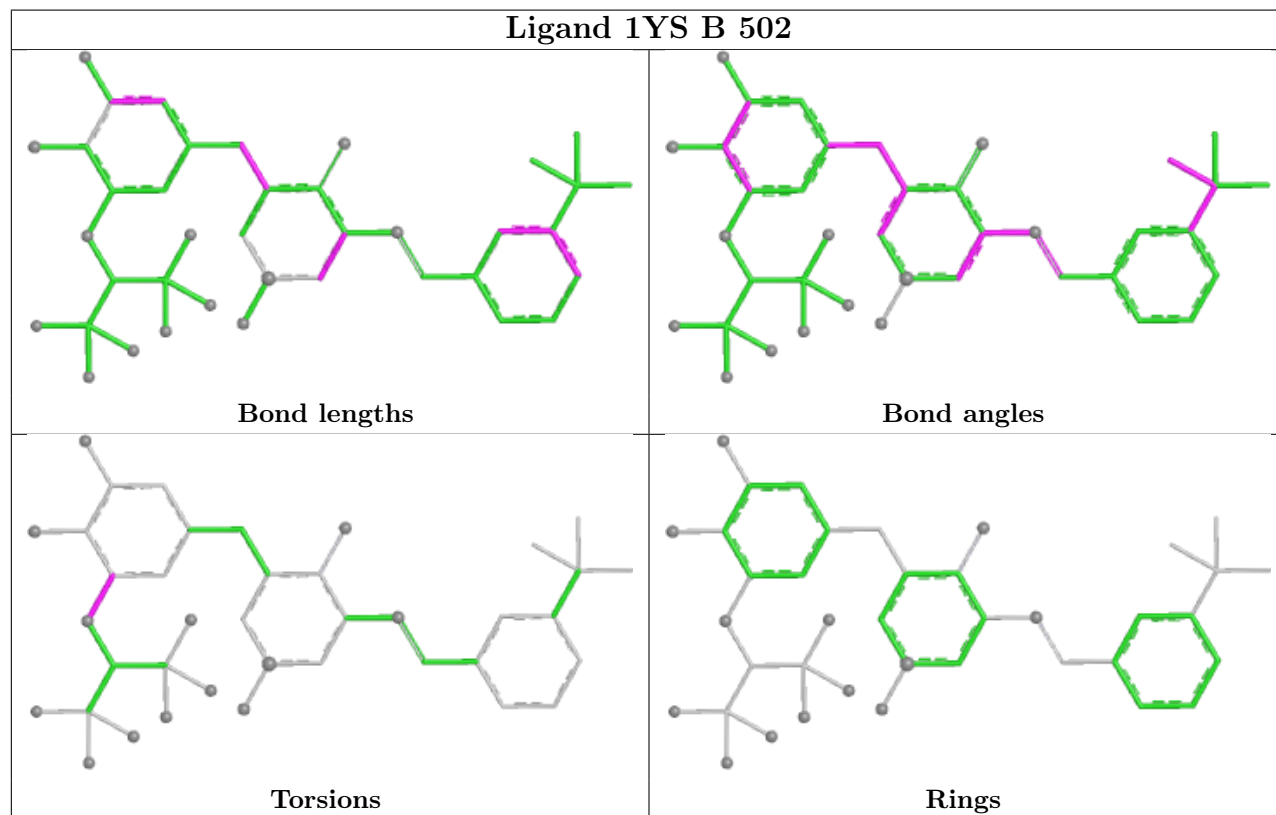
No monomer is involved in short contacts.

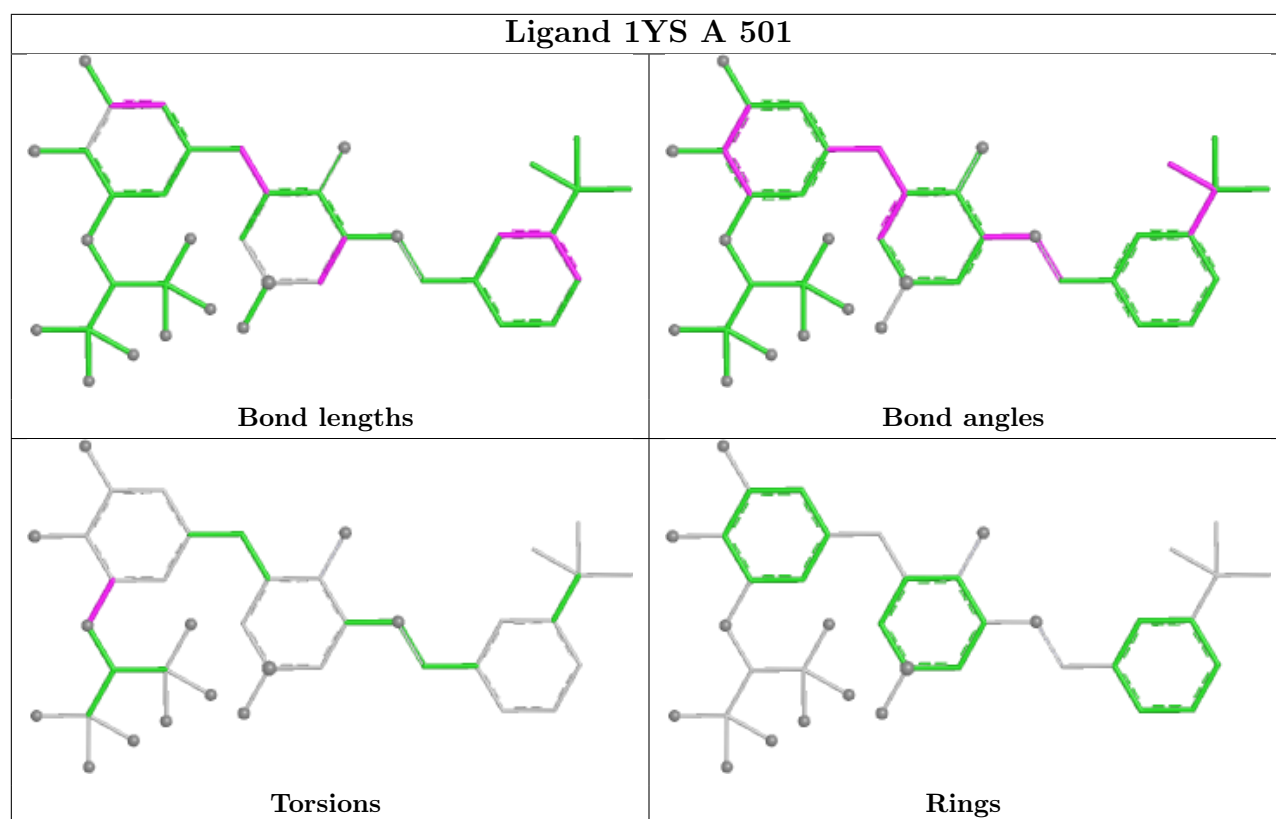
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 1YS C 501



Ligand 1YS B 502





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	376/402 (93%)	0.65	49 (13%) 7 8	24, 38, 71, 106	0
1	B	378/402 (94%)	0.85	68 (17%) 3 3	23, 39, 76, 110	0
1	C	381/402 (94%)	0.76	55 (14%) 6 6	26, 40, 73, 105	0
All	All	1135/1206 (94%)	0.75	172 (15%) 5 6	23, 39, 74, 110	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	THR	8.8
1	C	312	VAL	7.4
1	A	365	PHE	6.6
1	B	312	VAL	6.3
1	C	168	ALA	6.3
1	B	267	LEU	6.2
1	B	313	ALA	6.2
1	C	160	PRO	5.8
1	A	315	SER	5.7
1	A	272	ALA	5.6
1	B	361	VAL	5.4
1	A	312	VAL	5.4
1	B	258	PRO	5.3
1	B	272	ALA	5.2
1	C	313	ALA	5.2
1	A	314	THR	5.0
1	A	313	ALA	5.0
1	B	273	GLY	4.9
1	C	267	LEU	4.9
1	C	159	PHE	4.8
1	C	362	HIS	4.8
1	B	256	LYS	4.7
1	B	268	VAL	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	361	VAL	4.6
1	A	267	LEU	4.6
1	C	254	THR	4.6
1	C	314	THR	4.5
1	B	270	TRP	4.5
1	B	365	PHE	4.4
1	A	258	PRO	4.4
1	B	257	PHE	4.4
1	A	309	VAL	4.4
1	B	316	GLN	4.2
1	C	365	PHE	4.2
1	B	309	VAL	4.2
1	B	46(P)	SER	4.2
1	B	362	HIS	4.2
1	C	315	SER	4.2
1	A	169	SER	4.1
1	A	361	VAL	4.1
1	C	311	ASP	4.1
1	C	317	ASP	4.0
1	C	258	PRO	4.0
1	B	254	THR	4.0
1	B	317	ASP	3.9
1	C	273	GLY	3.9
1	C	46(P)	SER	3.9
1	B	250	ALA	3.9
1	B	263	LEU	3.7
1	B	251	ALA	3.7
1	A	264	GLY	3.7
1	A	319	CYS	3.7
1	C	269	CYS	3.6
1	A	156	GLY	3.6
1	A	317	ASP	3.6
1	A	268	VAL	3.4
1	A	318	ASP	3.4
1	B	56	LEU	3.4
1	B	269	CYS	3.4
1	C	310	GLU	3.3
1	A	316	GLN	3.3
1	B	168	ALA	3.3
1	C	309	VAL	3.3
1	B	315	SER	3.3
1	B	262	TRP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	362	HIS	3.2
1	C	68	TYR	3.2
1	B	359	CYS	3.2
1	B	211	GLN	3.2
1	A	253	SER	3.1
1	C	49	HIS	3.1
1	B	340	GLY	3.1
1	C	272	ALA	3.1
1	C	169	SER	3.0
1	A	254	THR	3.0
1	A	256	LYS	3.0
1	A	360	HIS	3.0
1	A	311	ASP	3.0
1	C	264	GLY	2.9
1	B	51	TYR	2.9
1	C	270	TRP	2.9
1	C	360	HIS	2.9
1	A	257	PHE	2.9
1	A	263	LEU	2.9
1	B	213	LEU	2.9
1	C	56	LEU	2.9
1	B	363	ASP	2.8
1	C	359	CYS	2.8
1	A	270	TRP	2.8
1	A	266	GLN	2.8
1	B	360	HIS	2.8
1	B	308	PRO	2.8
1	B	274	THR	2.8
1	B	252	SER	2.8
1	C	316	GLN	2.8
1	C	268	VAL	2.8
1	B	266	GLN	2.7
1	A	269	CYS	2.7
1	A	56	LEU	2.7
1	C	64	ARG	2.7
1	A	259	ASP	2.7
1	B	276	PRO	2.7
1	A	364	GLU	2.7
1	C	257	PHE	2.7
1	B	253	SER	2.6
1	B	61	ARG	2.6
1	B	210	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	363	ASP	2.6
1	A	336	VAL	2.6
1	B	255	GLU	2.6
1	B	261	PHE	2.6
1	C	263	LEU	2.6
1	C	271	GLN	2.6
1	B	364	GLU	2.6
1	C	274	THR	2.6
1	A	271	GLN	2.5
1	A	261	PHE	2.5
1	B	279	ILE	2.5
1	B	318	ASP	2.5
1	C	255	GLU	2.5
1	A	273	GLY	2.4
1	B	264	GLY	2.4
1	A	278	ASN	2.4
1	B	22	SER	2.4
1	B	157	ALA	2.4
1	A	310	GLU	2.4
1	B	310	GLU	2.4
1	B	319	CYS	2.4
1	B	42	ALA	2.4
1	C	73	GLN	2.4
1	C	253	SER	2.4
1	B	275	THR	2.4
1	C	60	TYR	2.3
1	A	274	THR	2.3
1	B	265	GLU	2.3
1	A	73	GLN	2.3
1	A	46(P)	SER	2.3
1	A	86	SER	2.3
1	A	363	ASP	2.3
1	C	265	GLU	2.3
1	B	59	THR	2.3
1	C	57	SER	2.3
1	C	259	ASP	2.3
1	C	145	HIS	2.3
1	C	256	LYS	2.3
1	A	260	GLY	2.2
1	B	60	TYR	2.2
1	C	157	ALA	2.2
1	B	49	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	79	GLU	2.2
1	B	57	SER	2.2
1	B	311	ASP	2.2
1	C	23	PRO	2.2
1	B	320	TYR	2.2
1	A	359	CYS	2.2
1	A	60	TYR	2.2
1	B	280	PHE	2.2
1	B	336	VAL	2.2
1	A	58	SER	2.2
1	C	319	CYS	2.2
1	B	92	ASN	2.1
1	C	336	VAL	2.1
1	B	238	LYS	2.1
1	C	278	ASN	2.1
1	B	243	ALA	2.1
1	C	266	GLN	2.1
1	A	68	TYR	2.1
1	B	50	ARG	2.1
1	C	95	VAL	2.0
1	A	367	THR	2.0
1	C	275	THR	2.0
1	B	385	ASN	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.

Continued on next page...

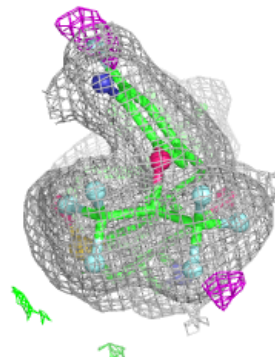
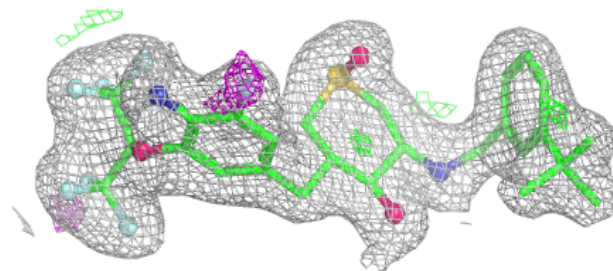
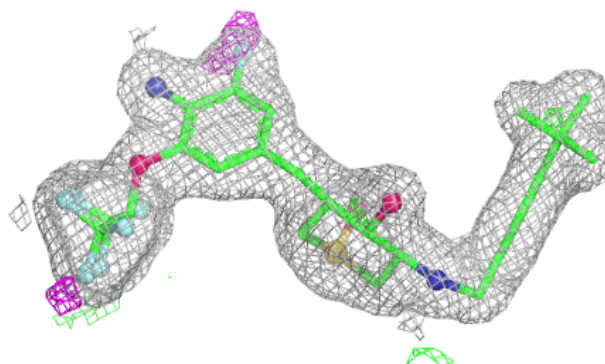
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1YS	A	501	39/39	0.95	0.08	27,33,41,44	0
2	1YS	B	502	39/39	0.96	0.07	26,32,44,46	0
2	1YS	C	501	39/39	0.96	0.08	28,34,44,46	0
3	GOL	B	501	6/6	0.96	0.08	40,43,44,46	0
4	PO4	C	502	5/5	0.96	0.14	45,46,47,49	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.

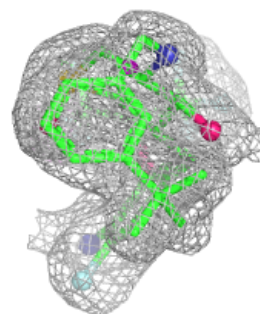
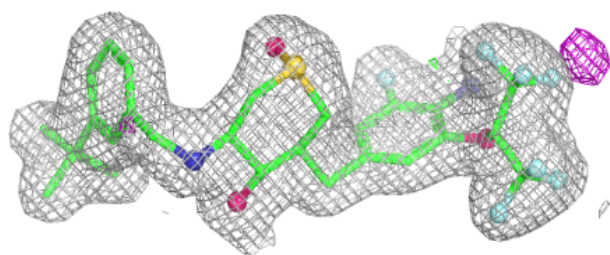
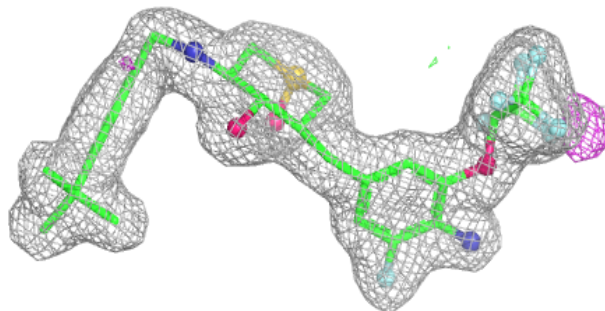
Electron density around 1YS A 501:

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

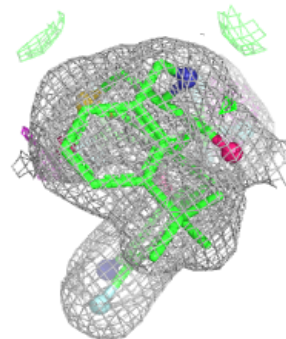
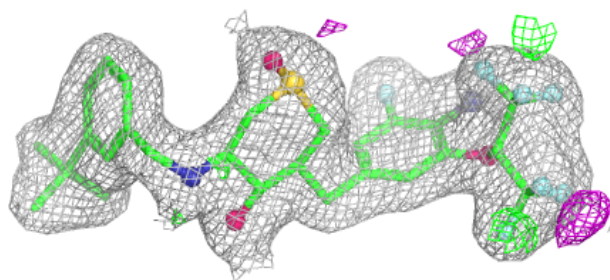
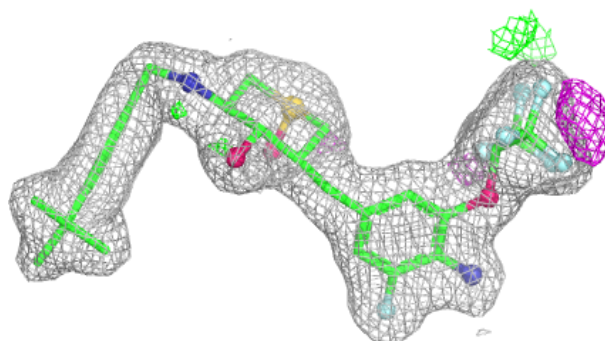


Electron density around 1YS B 502:

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

**Electron density around 1YS 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.