



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2025 – 01:20 pm BST

PDB ID : 7P6O / pdb_00007p6o
Title : ROCK2 IN COMPLEX WITH COMPOUND 8
Authors : Maillard, M.C.
Deposited on : 2021-07-16
Resolution : 2.75 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

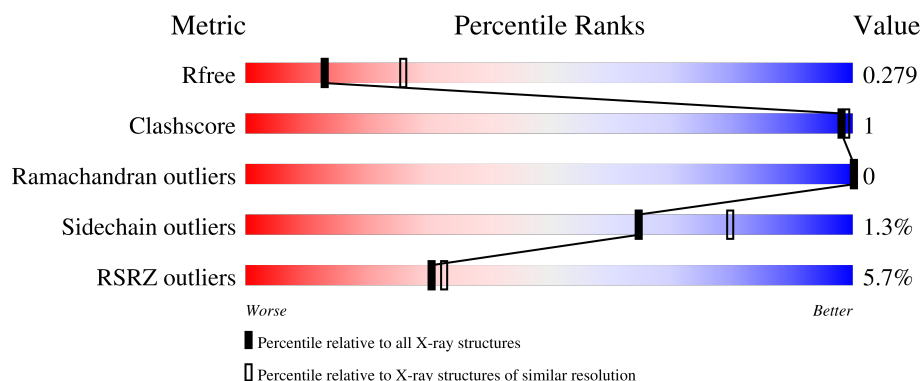
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	399	<div> <div>5%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>
1	B	399	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>.. 5%</div> </div> </div>
1	C	399	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>. 6%</div> </div> </div>
1	D	399	<div> <div>6%</div> <div> <div></div> <div>94%</div> <div>..</div> </div> </div>
1	E	399	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	399	<div> <div>5%</div> <div>93%</div> <div>• •</div> </div>
1	G	399	<div> <div>6%</div> <div>93%</div> <div>• 5%</div> </div>
1	H	399	<div> <div>7%</div> <div>90%</div> <div>• 8%</div> </div>

2 Entry composition

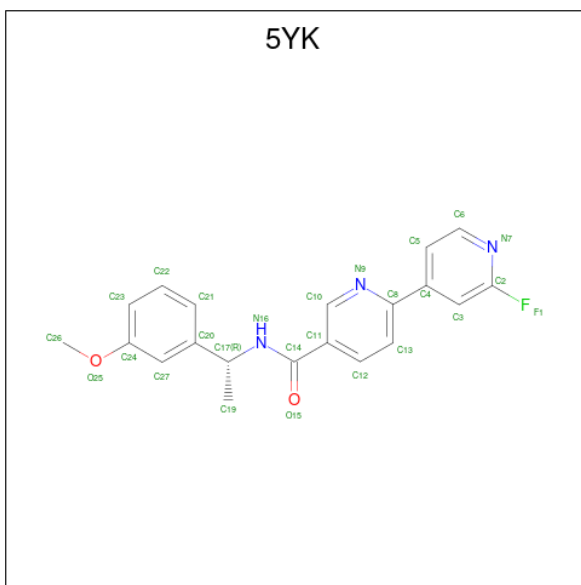
There are 4 unique types of molecules in this entry. The entry contains 25148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rho-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	93	2	0
			3168	2030	536	583	19			
1	B	379	Total	C	N	O	S	172	0	0
			3091	1986	516	570	19			
1	C	377	Total	C	N	O	S	107	1	0
			3081	1983	519	560	19			
1	D	384	Total	C	N	O	S	58	1	0
			3133	2011	526	576	20			
1	E	385	Total	C	N	O	S	136	0	0
			3132	2008	525	579	20			
1	F	383	Total	C	N	O	S	95	0	0
			3116	2002	522	572	20			
1	G	381	Total	C	N	O	S	143	0	0
			3108	1996	521	571	20			
1	H	369	Total	C	N	O	S	168	0	0
			3015	1944	506	547	18			

- Molecule 2 is 6-(2-fluoranylpyridin-4-yl)- {N}-[(1 {R})-1-(3-methoxyphenyl)ethyl]pyridine-3-carboxamide (CCD ID: 5YK) (formula: C₂₀H₁₈FN₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	B	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	C	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	D	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	E	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	F	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	G	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	H	1	Total	C	F	N	O	0	0
			26	20	1	3	2		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

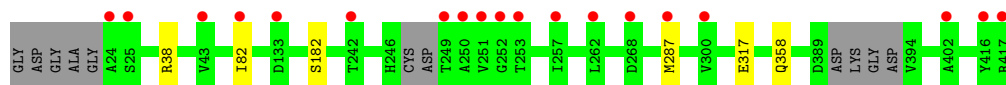
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	7	Total	O	0	0
			7	7		
4	C	11	Total	O	0	0
			11	11		
4	D	8	Total	O	0	0
			8	8		
4	E	8	Total	O	0	0
			8	8		
4	F	14	Total	O	0	0
			14	14		
4	G	9	Total	O	0	1
			10	10		
4	H	5	Total	O	0	0
			5	5		

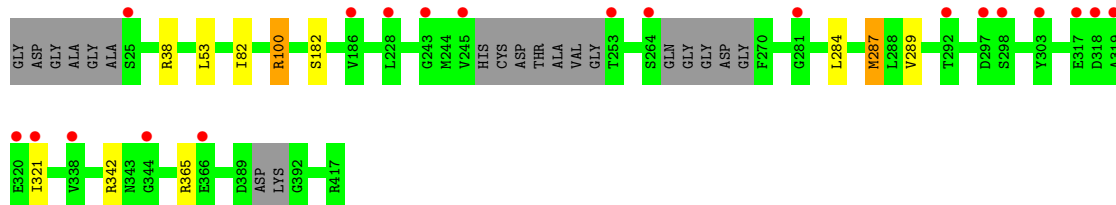
3 Residue-property plots [i](#)

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.

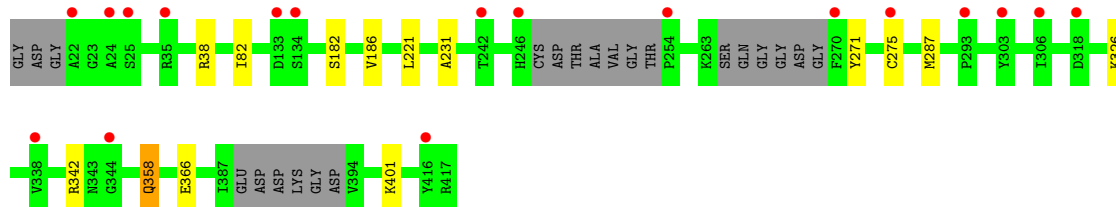
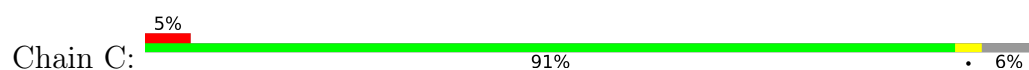
- Molecule 1: Rho-associated protein kinase 2



- Molecule 1: Rho-associated protein kinase 2

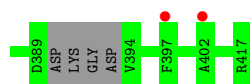


- Molecule 1: Rho-associated protein kinase 2

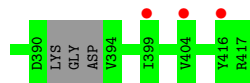
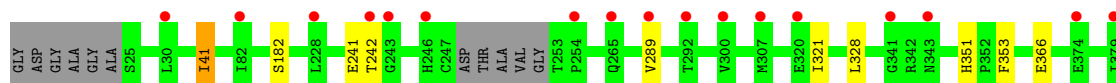
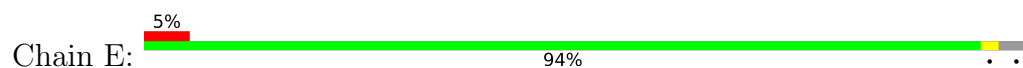


- Molecule 1: Rho-associated protein kinase 2

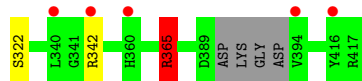
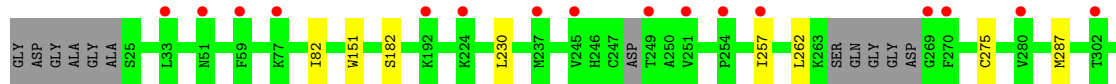
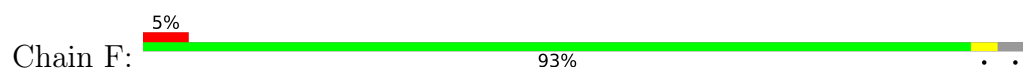




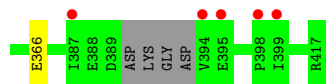
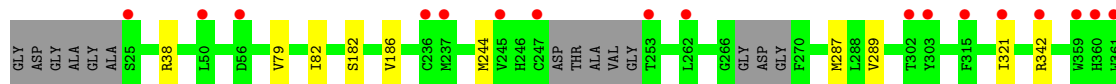
- Molecule 1: Rho-associated protein kinase 2



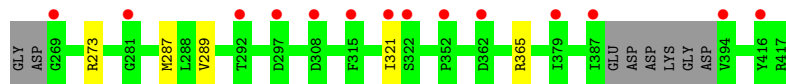
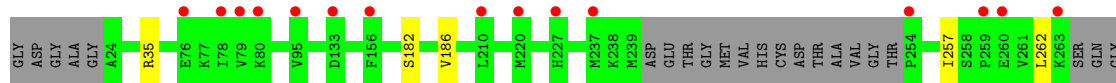
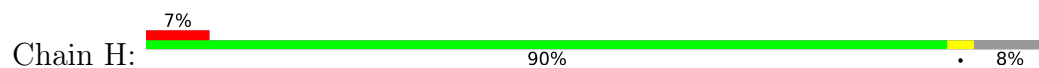
- Molecule 1: Rho-associated protein kinase 2



- Molecule 1: Rho-associated protein kinase 2



- Molecule 1: Rho-associated protein kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.55Å 101.23Å 102.48Å 83.52° 73.63° 77.83°	Depositor
Resolution (Å)	98.79 – 2.75 98.79 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.5 (98.79-2.75) 95.5 (98.79-2.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.241 , 0.286 0.241 , 0.279	Depositor DCC
R_{free} test set	700 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.7	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	0.92	EDS
Total number of atoms	25148	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: 5YK, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.78	0/3245	1.01	0/4381
1	B	0.78	0/3166	1.03	3/4274 (0.1%)
1	C	0.78	0/3160	1.04	2/4264 (0.0%)
1	D	0.79	0/3212	1.01	0/4336
1	E	0.80	1/3209 (0.0%)	1.02	1/4333 (0.0%)
1	F	0.80	0/3192	1.07	4/4310 (0.1%)
1	G	0.79	1/3184 (0.0%)	1.02	1/4298 (0.0%)
1	H	0.81	2/3090 (0.1%)	1.02	0/4170
All	All	0.79	4/25458 (0.0%)	1.03	11/34366 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	242	THR	CB-OG1	-6.80	1.32	1.43
1	G	342	ARG	CG-CD	6.25	1.71	1.52
1	H	273	ARG	CD-NE	-6.16	1.37	1.46
1	H	35	ARG	CD-NE	5.80	1.54	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	365	ARG	CG-CD-NE	12.19	138.83	112.00
1	F	342	ARG	CG-CD-NE	-9.93	90.16	112.00
1	C	358	GLN	CB-CG-CD	9.25	128.32	112.60
1	F	365	ARG	CB-CG-CD	9.05	132.12	111.30
1	F	365	ARG	NH1-CZ-NH2	-6.05	111.43	119.30
1	B	100	ARG	CB-CG-CD	6.00	125.11	111.30
1	G	342	ARG	CB-CG-CD	-5.97	97.58	111.30
1	B	342	ARG	CA-CB-CG	5.96	126.02	114.10
1	B	287	MET	CG-SD-CE	5.62	113.27	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	41	ILE	CG1-CB-CG2	-5.50	94.22	110.70
1	C	342	ARG	CA-CB-CG	5.31	124.73	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3168	0	3097	8	0
1	B	3091	0	3022	2	0
1	C	3081	0	3027	3	0
1	D	3133	0	3066	2	0
1	E	3132	0	3053	5	0
1	F	3116	0	3049	4	0
1	G	3108	0	3038	4	0
1	H	3015	0	2964	3	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	0	0
2	D	26	0	0	0	0
2	E	26	0	0	0	0
2	F	26	0	0	0	0
2	G	26	0	0	0	0
2	H	26	0	0	0	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
3	H	6	0	8	0	0
4	A	15	0	0	0	0
4	B	7	0	0	0	0
4	C	11	0	0	0	0
4	D	8	0	0	0	0
4	E	8	0	0	0	0
4	F	14	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	25148	0	24340	29	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 1.

All (29) 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:A:38[B]:ARG:HH11	1:A:38[B]:ARG:CG	1.65	1.08
1:A:38[B]:ARG:HH11	1:A:38[B]:ARG:HG3	1.11	1.08
1:A:38[B]:ARG:CG	1:A:38[B]:ARG:NH1	2.23	0.93
1:A:38[B]:ARG:NH1	1:A:38[B]:ARG:HG2	1.90	0.85
1:E:351:HIS:CD2	1:E:353:PHE:HB3	2.27	0.70
1:A:38[B]:ARG:HG3	1:A:38[B]:ARG:NH1	1.93	0.62
1:B:284:LEU:HA	1:B:287:MET:HE2	1.81	0.62
1:C:271:TYR:HB2	1:C:275:CYS:SG	2.41	0.61
1:E:351:HIS:HD2	1:E:353:PHE:HB3	1.64	0.61
1:F:151:TRP:CH2	1:F:365:ARG:HG2	2.39	0.58
1:E:328:LEU:HB2	1:E:351:HIS:NE2	2.21	0.56
1:H:289:VAL:HG22	1:H:321:ILE:HD11	1.90	0.54
1:G:289:VAL:HG22	1:G:321:ILE:HD11	1.91	0.53
1:B:289:VAL:HG22	1:B:321:ILE:HD11	1.91	0.53
1:E:289:VAL:HG22	1:E:321:ILE:HD11	1.91	0.52
1:F:151:TRP:CH2	1:F:365:ARG:CG	2.95	0.50
1:A:38[A]:ARG:HG3	1:A:38[A]:ARG:HH11	1.78	0.49
1:A:317:GLU:O	1:F:322:SER:HB2	2.12	0.48
1:E:241:GLU:O	1:G:244:MET:HG3	2.15	0.47
1:C:221:LEU:HD13	1:C:231:ALA:HB3	1.97	0.45
1:G:79:VAL:HA	1:G:82:ILE:CG1	2.48	0.43
1:G:186:VAL:HG11	1:G:287:MET:HE2	2.02	0.42
1:H:186:VAL:HG11	1:H:287:MET:HE2	2.02	0.42
1:C:186:VAL:HG11	1:C:287:MET:HE2	2.02	0.42
1:A:38[A]:ARG:HG3	1:A:38[A]:ARG:NH1	2.36	0.41
1:D:186:VAL:HG11	1:D:287:MET:HE2	2.02	0.41
1:H:257:ILE:HG21	1:H:262:LEU:HD21	2.03	0.41
1:F:257:ILE:HG21	1:F:262:LEU:HD21	2.03	0.40
1:D:257:ILE:HG21	1:D:262:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	384/399 (96%)	365 (95%)	19 (5%)	0	100	100
1	B	371/399 (93%)	354 (95%)	17 (5%)	0	100	100
1	C	370/399 (93%)	355 (96%)	15 (4%)	0	100	100
1	D	377/399 (94%)	360 (96%)	17 (4%)	0	100	100
1	E	379/399 (95%)	362 (96%)	17 (4%)	0	100	100
1	F	375/399 (94%)	359 (96%)	16 (4%)	0	100	100
1	G	373/399 (94%)	357 (96%)	16 (4%)	0	100	100
1	H	361/399 (90%)	347 (96%)	14 (4%)	0	100	100
All	All	2990/3192 (94%)	2859 (96%)	131 (4%)	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	343/347 (99%)	339 (99%)	4 (1%)	67	81
1	B	337/347 (97%)	331 (98%)	6 (2%)	54	72
1	C	334/347 (96%)	327 (98%)	7 (2%)	48	69
1	D	342/347 (99%)	339 (99%)	3 (1%)	75	86
1	E	341/347 (98%)	338 (99%)	3 (1%)	75	86
1	F	339/347 (98%)	333 (98%)	6 (2%)	54	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	339/347 (98%)	336 (99%)	3 (1%)	75	86
1	H	327/347 (94%)	325 (99%)	2 (1%)	84	90
All	All	2702/2776 (97%)	2668 (99%)	34 (1%)	65	80

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ILE
1	A	182	SER
1	A	287	MET
1	A	358	GLN
1	B	38	ARG
1	B	53	LEU
1	B	82	ILE
1	B	100	ARG
1	B	182	SER
1	B	365	ARG
1	C	38	ARG
1	C	82	ILE
1	C	182	SER
1	C	326	LYS
1	C	358	GLN
1	C	366	GLU
1	C	401	LYS
1	D	38	ARG
1	D	50	LEU
1	D	182	SER
1	E	41	ILE
1	E	182	SER
1	E	366	GLU
1	F	82	ILE
1	F	182	SER
1	F	230	LEU
1	F	275	CYS
1	F	287	MET
1	F	365	ARG
1	G	38	ARG
1	G	182	SER
1	G	366	GLU
1	H	182	SER
1	H	365	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	358	GLN
1	B	154	GLN
1	C	70	ASN
1	D	51	ASN
1	D	70	ASN
1	D	154	GLN
1	E	70	ASN
1	E	86	GLN
1	E	154	GLN
1	E	225	HIS
1	F	70	ASN
1	F	154	GLN
1	F	358	GLN
1	G	86	GLN
1	H	70	ASN
1	H	358	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](#)

11 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	5YK	C	501	-	28,28,28	0.93	1 (3%)	35,38,38	1.94	4 (11%)
2	5YK	F	501	-	28,28,28	0.98	2 (7%)	35,38,38	1.99	7 (20%)
3	GOL	D	502	-	5,5,5	0.35	0	5,5,5	0.31	0
3	GOL	H	502	-	5,5,5	0.40	0	5,5,5	0.45	0
2	5YK	H	501	-	28,28,28	0.98	1 (3%)	35,38,38	1.90	5 (14%)
2	5YK	D	501	-	28,28,28	0.96	2 (7%)	35,38,38	1.90	7 (20%)
2	5YK	B	501	-	28,28,28	0.99	2 (7%)	35,38,38	1.89	6 (17%)
2	5YK	G	501	-	28,28,28	0.96	1 (3%)	35,38,38	2.00	5 (14%)
3	GOL	A	502	-	5,5,5	0.60	0	5,5,5	0.50	0
2	5YK	E	501	-	28,28,28	0.98	2 (7%)	35,38,38	1.88	7 (20%)
2	5YK	A	501	-	28,28,28	0.98	2 (7%)	35,38,38	1.84	7 (20%)

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	5YK	C	501	-	-	4/18/18/18	0/3/3/3
2	5YK	F	501	-	-	2/18/18/18	0/3/3/3
3	GOL	D	502	-	-	1/4/4/4	-
3	GOL	H	502	-	-	1/4/4/4	-
2	5YK	H	501	-	-	6/18/18/18	0/3/3/3
2	5YK	D	501	-	-	2/18/18/18	0/3/3/3
2	5YK	B	501	-	-	2/18/18/18	0/3/3/3
2	5YK	G	501	-	-	2/18/18/18	0/3/3/3
3	GOL	A	502	-	-	3/4/4/4	-
2	5YK	E	501	-	-	0/18/18/18	0/3/3/3
2	5YK	A	501	-	-	0/18/18/18	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	5YK	C2-N7	2.79	1.33	1.30
2	E	501	5YK	C2-N7	2.75	1.33	1.30
2	G	501	5YK	C2-N7	2.71	1.33	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	5YK	C2-N7	2.66	1.33	1.30
2	F	501	5YK	C2-N7	2.63	1.33	1.30
2	B	501	5YK	C2-N7	2.55	1.33	1.30
2	A	501	5YK	C2-N7	2.46	1.33	1.30
2	D	501	5YK	C2-N7	2.44	1.33	1.30
2	E	501	5YK	C10-C11	2.17	1.42	1.39
2	A	501	5YK	C10-C11	2.16	1.42	1.39
2	D	501	5YK	C10-C11	2.12	1.42	1.39
2	F	501	5YK	C10-C11	2.09	1.42	1.39
2	B	501	5YK	C10-C11	2.05	1.42	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	5YK	F1-C2-N7	7.36	119.73	114.95
2	F	501	5YK	F1-C2-N7	6.90	119.43	114.95
2	C	501	5YK	F1-C2-N7	6.76	119.34	114.95
2	H	501	5YK	C6-N7-C2	6.50	121.89	115.55
2	G	501	5YK	C6-N7-C2	6.47	121.87	115.55
2	F	501	5YK	C6-N7-C2	6.33	121.73	115.55
2	C	501	5YK	C6-N7-C2	6.24	121.65	115.55
2	H	501	5YK	F1-C2-N7	6.19	118.97	114.95
2	D	501	5YK	C6-N7-C2	6.11	121.51	115.55
2	B	501	5YK	C6-N7-C2	6.07	121.48	115.55
2	E	501	5YK	C6-N7-C2	6.04	121.45	115.55
2	A	501	5YK	C6-N7-C2	6.01	121.41	115.55
2	D	501	5YK	F1-C2-N7	5.52	118.54	114.95
2	B	501	5YK	F1-C2-N7	5.36	118.44	114.95
2	E	501	5YK	F1-C2-N7	5.34	118.42	114.95
2	A	501	5YK	F1-C2-N7	4.50	117.88	114.95
2	F	501	5YK	C10-N9-C8	3.61	122.65	117.90
2	G	501	5YK	C10-N9-C8	3.57	122.60	117.90
2	C	501	5YK	C10-N9-C8	3.56	122.60	117.90
2	B	501	5YK	C10-N9-C8	3.50	122.51	117.90
2	A	501	5YK	C10-N9-C8	3.47	122.47	117.90
2	E	501	5YK	C10-N9-C8	3.42	122.40	117.90
2	D	501	5YK	C10-N9-C8	3.32	122.28	117.90
2	H	501	5YK	C10-N9-C8	3.30	122.25	117.90
2	A	501	5YK	C13-C8-N9	-2.58	118.41	122.26
2	B	501	5YK	C13-C8-N9	-2.56	118.44	122.26
2	D	501	5YK	C4-C8-N9	2.53	121.78	116.84
2	E	501	5YK	C4-C8-N9	2.50	121.73	116.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	5YK	C4-C8-N9	2.49	121.71	116.84
2	E	501	5YK	C13-C8-N9	-2.48	118.57	122.26
2	E	501	5YK	C26-O25-C24	2.46	122.85	117.51
2	A	501	5YK	C4-C8-N9	2.45	121.63	116.84
2	H	501	5YK	C5-C6-N7	-2.32	121.08	123.96
2	F	501	5YK	C4-C8-N9	2.29	121.31	116.84
2	F	501	5YK	C13-C8-N9	-2.27	118.87	122.26
2	C	501	5YK	C11-C10-N9	-2.25	120.53	123.67
2	D	501	5YK	C13-C8-N9	-2.23	118.94	122.26
2	D	501	5YK	C5-C6-N7	-2.16	121.27	123.96
2	A	501	5YK	C5-C6-N7	-2.15	121.28	123.96
2	E	501	5YK	C5-C6-N7	-2.15	121.28	123.96
2	H	501	5YK	C11-C10-N9	-2.12	120.71	123.67
2	G	501	5YK	C11-C10-N9	-2.12	120.72	123.67
2	A	501	5YK	C26-O25-C24	2.09	122.04	117.51
2	B	501	5YK	C5-C6-N7	-2.07	121.39	123.96
2	F	501	5YK	C5-C6-N7	-2.06	121.40	123.96
2	D	501	5YK	C11-C10-N9	-2.06	120.80	123.67
2	G	501	5YK	C5-C6-N7	-2.05	121.41	123.96
2	F	501	5YK	C11-C10-N9	-2.02	120.84	123.67

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
2	G	501	5YK	C23-C24-O25-C26
2	F	501	5YK	C23-C24-O25-C26
2	F	501	5YK	C27-C24-O25-C26
2	G	501	5YK	C27-C24-O25-C26
2	C	501	5YK	C23-C24-O25-C26
2	H	501	5YK	C23-C24-O25-C26
2	C	501	5YK	C27-C24-O25-C26
2	H	501	5YK	C27-C24-O25-C26
2	D	501	5YK	C23-C24-O25-C26
2	D	501	5YK	C27-C24-O25-C26
3	A	502	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
3	D	502	GOL	O1-C1-C2-C3
2	H	501	5YK	C5-C4-C8-C13
2	H	501	5YK	C5-C4-C8-N9
2	H	501	5YK	C3-C4-C8-C13

Continued on next page...

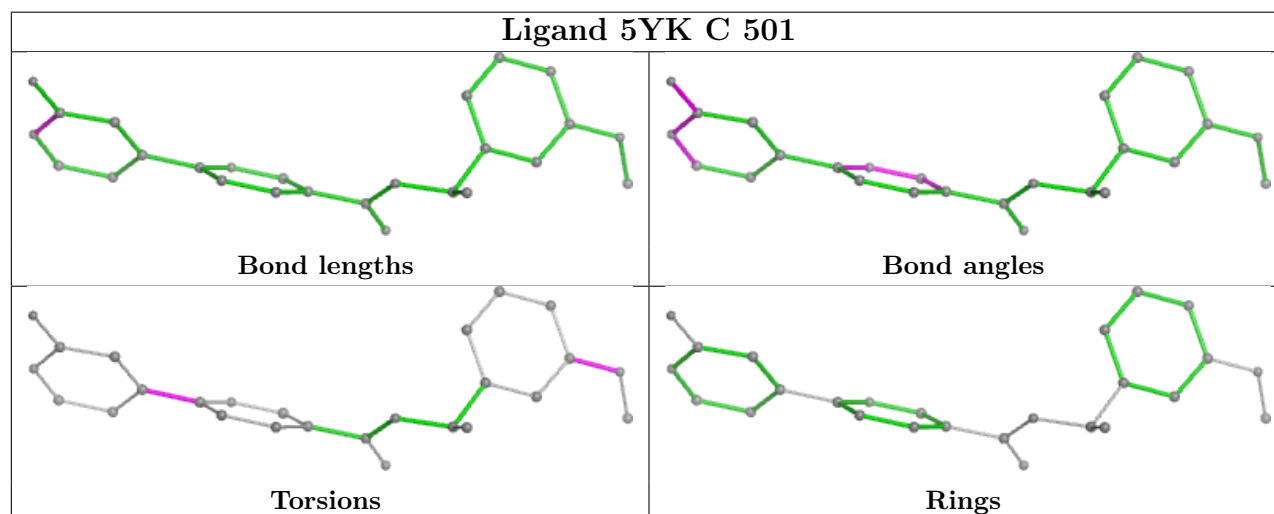
Continued from previous page...

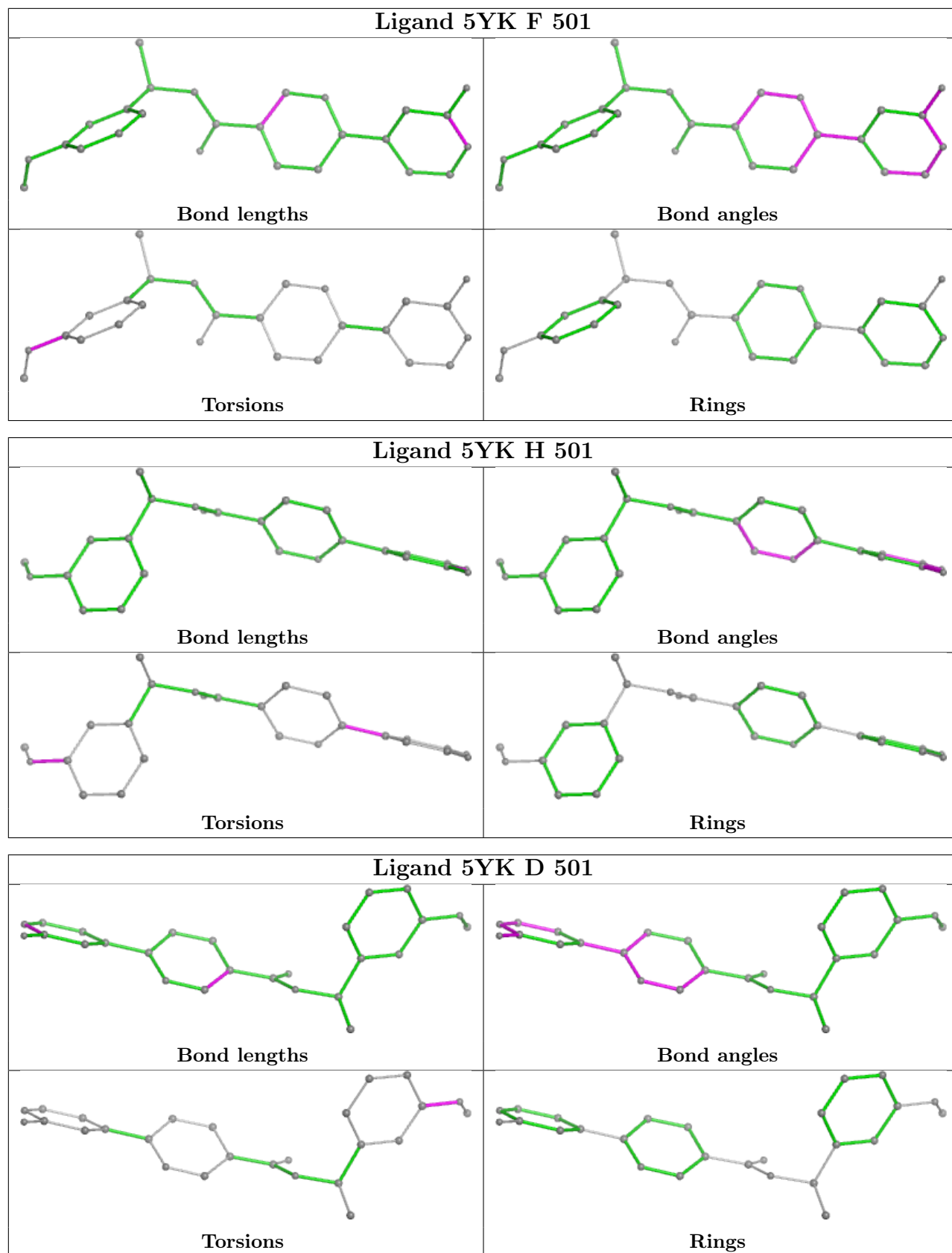
Mol	Chain	Res	Type	Atoms
2	H	501	5YK	C3-C4-C8-N9
3	H	502	GOL	C1-C2-C3-O3
2	C	501	5YK	C5-C4-C8-N9
2	C	501	5YK	C5-C4-C8-C13
2	B	501	5YK	C23-C24-O25-C26
2	B	501	5YK	C27-C24-O25-C26

There are no ring outliers.

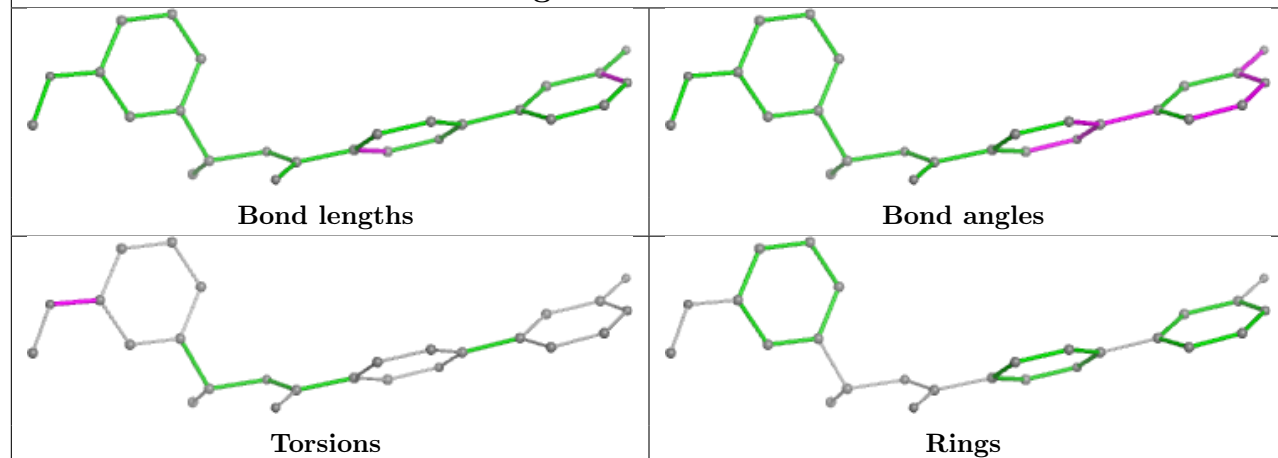
No monomer is involved in short contacts.

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.

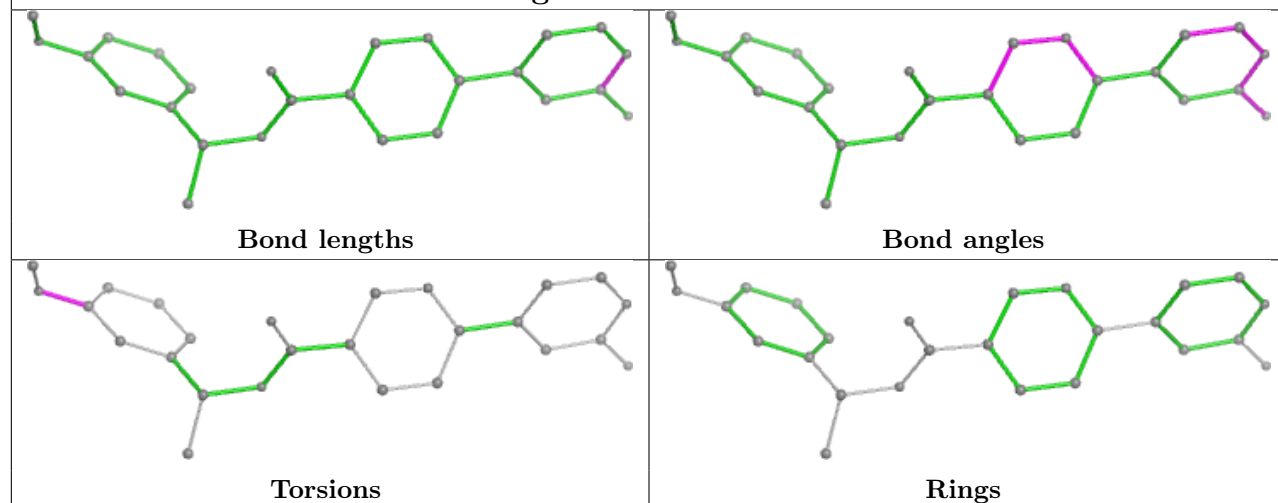




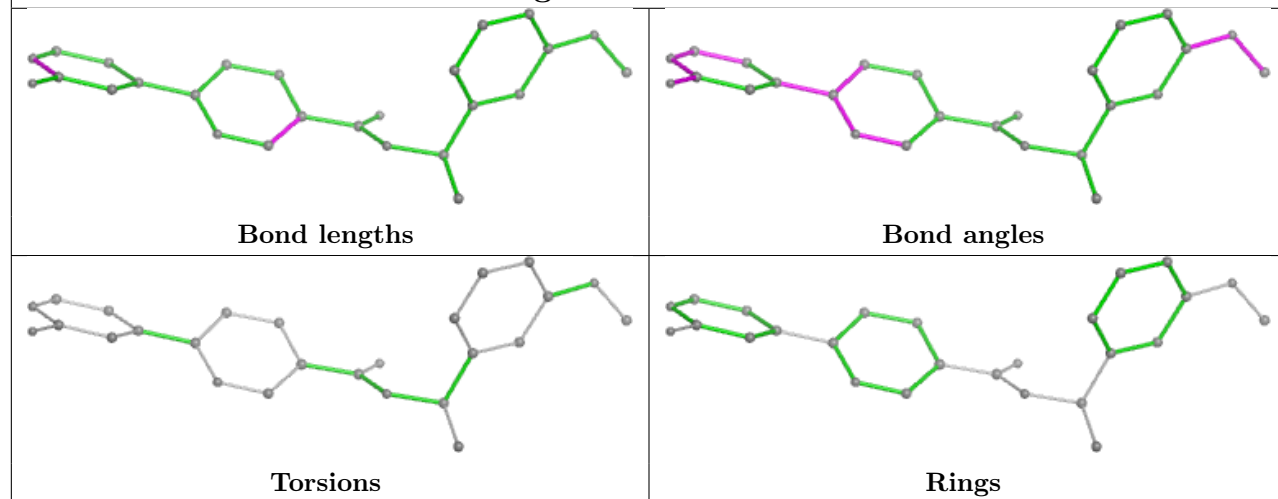
Ligand 5YK B 501

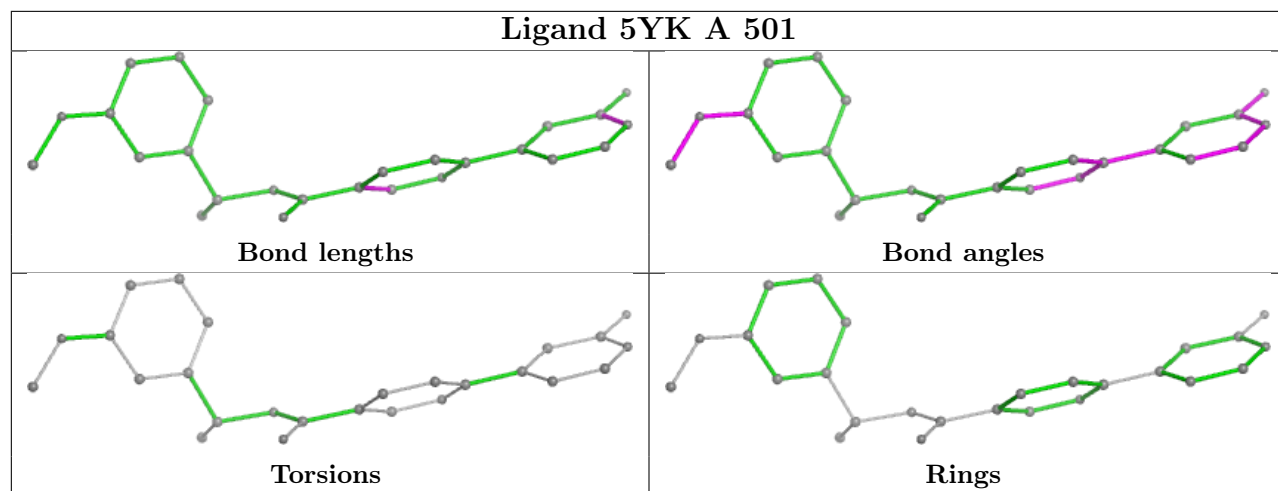


Ligand 5YK G 501



Ligand 5YK E 501





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	388/399 (97%)	0.45	19 (4%)	36	38	25, 57, 97, 157	26 (6%)
1	B	379/399 (94%)	0.54	20 (5%)	33	35	29, 65, 101, 137	47 (12%)
1	C	377/399 (94%)	0.55	18 (4%)	36	38	32, 64, 102, 129	34 (9%)
1	D	384/399 (96%)	0.51	24 (6%)	27	30	28, 62, 102, 150	15 (3%)
1	E	385/399 (96%)	0.59	20 (5%)	34	35	33, 67, 105, 136	40 (10%)
1	F	383/399 (95%)	0.62	21 (5%)	32	34	27, 65, 107, 150	25 (6%)
1	G	381/399 (95%)	0.65	22 (5%)	30	32	30, 67, 102, 141	35 (9%)
1	H	369/399 (92%)	0.68	29 (7%)	20	23	30, 70, 116, 141	43 (11%)
All	All	3046/3192 (95%)	0.57	173 (5%)	30	33	25, 65, 105, 157	265 (8%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	242	THR	4.7
1	D	269	GLY	4.6
1	A	251	VAL	4.5
1	E	300	VAL	4.5
1	A	133	ASP	4.3
1	G	262	LEU	4.2
1	C	246	HIS	4.2
1	C	254	PRO	4.1
1	F	270	PHE	4.1
1	H	156	PHE	4.0
1	G	25	SER	4.0
1	F	269	GLY	3.9
1	H	416	TYR	3.8
1	B	281	GLY	3.8
1	A	24	ALA	3.8
1	B	264	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	302	THR	3.6
1	C	275	CYS	3.6
1	C	306	ILE	3.6
1	H	321	ILE	3.5
1	C	303	TYR	3.5
1	A	253	THR	3.5
1	H	263	LYS	3.3
1	E	374	GLU	3.3
1	D	299	LEU	3.3
1	B	318	ASP	3.2
1	B	319	ALA	3.2
1	C	270	PHE	3.2
1	B	245	VAL	3.2
1	A	300	VAL	3.1
1	G	359	TRP	3.1
1	C	318	ASP	3.1
1	B	321	ILE	3.0
1	F	360	HIS	3.0
1	C	22	ALA	3.0
1	B	320	GLU	3.0
1	B	338	VAL	3.0
1	E	246	HIS	3.0
1	H	292	THR	3.0
1	D	251	VAL	3.0
1	G	360	HIS	2.9
1	D	292	THR	2.9
1	F	280	VAL	2.9
1	H	79	VAL	2.9
1	A	287	MET	2.9
1	G	394	VAL	2.9
1	H	76	GLU	2.9
1	D	264	SER	2.9
1	H	254	PRO	2.9
1	A	25	SER	2.8
1	A	257	ILE	2.8
1	E	82	ILE	2.8
1	E	265	GLN	2.8
1	E	254	PRO	2.8
1	B	317	GLU	2.8
1	D	156	PHE	2.8
1	A	268	ASP	2.8
1	A	250	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	416	TYR	2.7
1	F	257	ILE	2.7
1	H	362	ASP	2.7
1	F	302	THR	2.7
1	F	237	MET	2.7
1	A	82	ILE	2.7
1	A	252	GLY	2.6
1	G	237	MET	2.6
1	F	342	ARG	2.6
1	B	243	GLY	2.6
1	D	255	ASP	2.6
1	G	342	ARG	2.6
1	F	249	THR	2.6
1	C	344	GLY	2.6
1	G	387	ILE	2.6
1	F	251	VAL	2.6
1	A	242	THR	2.6
1	B	344	GLY	2.6
1	G	303	TYR	2.5
1	D	287	MET	2.5
1	F	77	LYS	2.5
1	B	366	GLU	2.5
1	D	254	PRO	2.5
1	G	315	PHE	2.5
1	A	402	ALA	2.5
1	D	402	ALA	2.5
1	G	399	ILE	2.5
1	H	78	ILE	2.5
1	B	298	SER	2.5
1	C	293	PRO	2.5
1	D	257	ILE	2.5
1	G	395	GLU	2.5
1	H	210	LEU	2.5
1	C	24	ALA	2.5
1	E	243	GLY	2.5
1	E	320	GLU	2.4
1	G	321	ILE	2.4
1	A	249	THR	2.4
1	H	394	VAL	2.4
1	G	247	CYS	2.4
1	D	253	THR	2.4
1	C	338	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	224	LYS	2.4
1	F	254	PRO	2.4
1	H	80	LYS	2.4
1	H	95	VAL	2.4
1	C	25	SER	2.4
1	F	59	PHE	2.4
1	E	343	ASN	2.4
1	A	262	LEU	2.3
1	G	50	LEU	2.3
1	D	86	GLN	2.3
1	D	249	THR	2.3
1	G	253	THR	2.3
1	H	220	MET	2.3
1	H	352	PRO	2.3
1	H	227	HIS	2.3
1	F	245	VAL	2.3
1	G	245	VAL	2.3
1	E	399	ILE	2.3
1	H	281	GLY	2.3
1	B	228	LEU	2.3
1	B	297	ASP	2.3
1	C	35	ARG	2.3
1	D	203	ASP	2.3
1	E	289	VAL	2.3
1	F	394	VAL	2.3
1	E	379	ILE	2.3
1	D	237	MET	2.2
1	E	307	MET	2.2
1	C	242	THR	2.2
1	F	51	ASN	2.2
1	H	297	ASP	2.2
1	H	387	ILE	2.2
1	B	292	THR	2.2
1	D	240	ASP	2.2
1	G	236	CYS	2.2
1	F	416	TYR	2.2
1	D	248	ASP	2.2
1	D	78	ILE	2.2
1	E	30	LEU	2.2
1	H	269	GLY	2.2
1	H	259	PRO	2.2
1	H	308	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	416	TYR	2.1
1	B	303	TYR	2.1
1	C	133	ASP	2.1
1	E	416	TYR	2.1
1	D	397	PHE	2.1
1	F	33	LEU	2.1
1	A	417	ARG	2.1
1	H	260	GLU	2.1
1	B	253	THR	2.1
1	B	186	VAL	2.1
1	D	82	ILE	2.1
1	H	133	ASP	2.1
1	H	379	ILE	2.1
1	E	341	GLY	2.1
1	B	25	SER	2.1
1	D	224	LYS	2.1
1	H	237	MET	2.1
1	H	315	PHE	2.1
1	D	247	CYS	2.1
1	F	192	LYS	2.1
1	A	43	VAL	2.1
1	G	398	PRO	2.0
1	G	361	TRP	2.0
1	E	292	THR	2.0
1	C	134	SER	2.0
1	E	228	LEU	2.0
1	G	56	ASP	2.0
1	E	404	VAL	2.0
1	F	340	LEU	2.0
1	D	207	SER	2.0
1	H	322	SER	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](#)

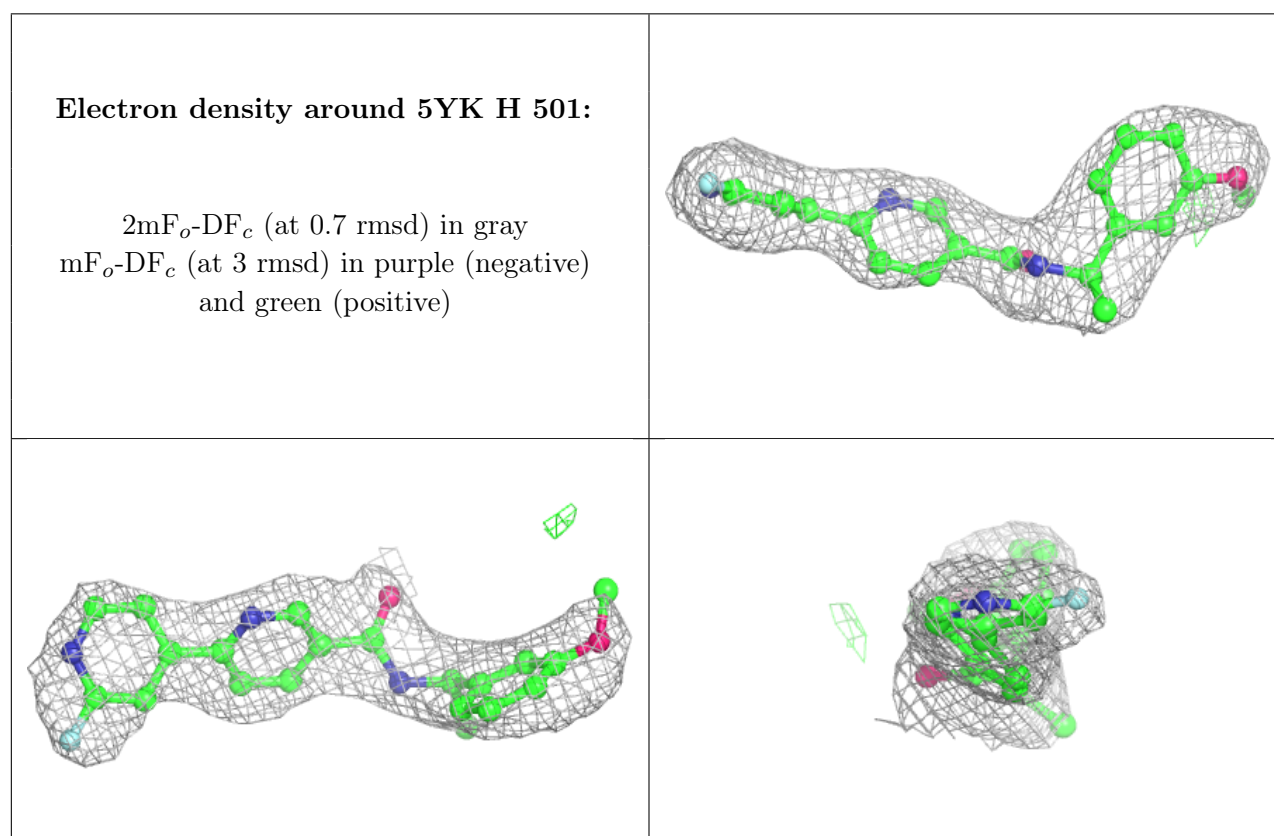
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

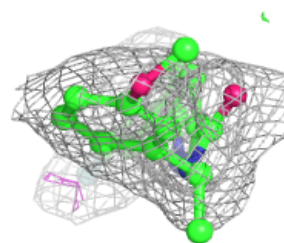
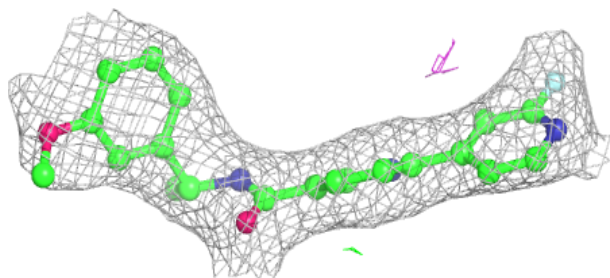
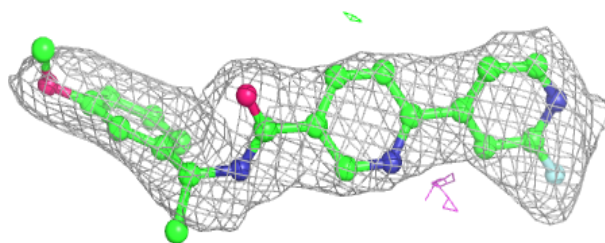
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	H	502	6/6	0.44	0.25	76,82,95,96	0
3	GOL	A	502	6/6	0.63	0.19	65,75,84,85	0
3	GOL	D	502	6/6	0.78	0.15	53,56,65,70	0
2	5YK	H	501	26/26	0.89	0.11	51,66,73,74	0
2	5YK	F	501	26/26	0.90	0.11	53,61,69,76	0
2	5YK	C	501	26/26	0.92	0.09	44,50,55,66	0
2	5YK	D	501	26/26	0.92	0.09	44,51,56,63	0
2	5YK	B	501	26/26	0.92	0.10	42,50,53,57	0
2	5YK	G	501	26/26	0.92	0.09	40,45,49,65	0
2	5YK	E	501	26/26	0.94	0.08	40,47,57,66	0
2	5YK	A	501	26/26	0.95	0.07	37,39,45,52	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.

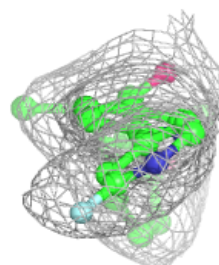
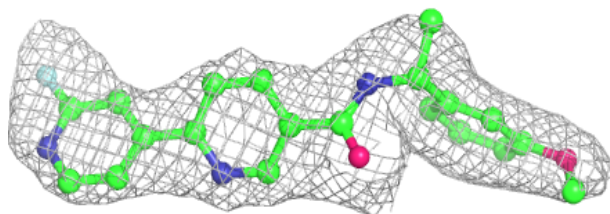
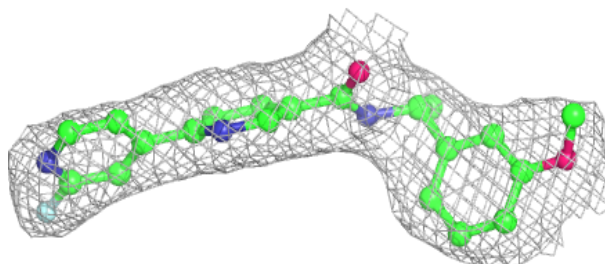


Electron density around 5YK F 501:

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

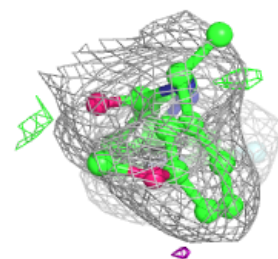
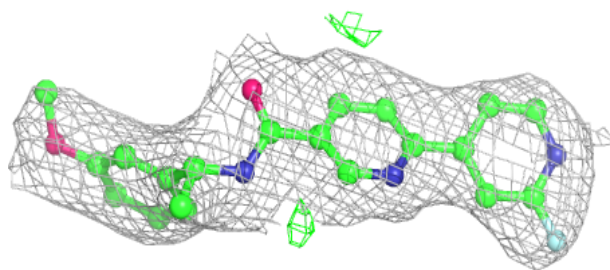
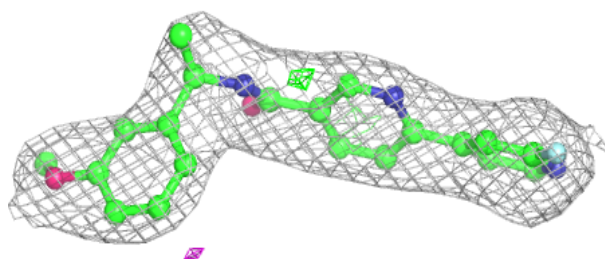
**Electron density around 5YK C 501:**

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

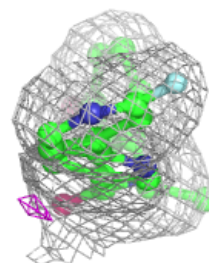
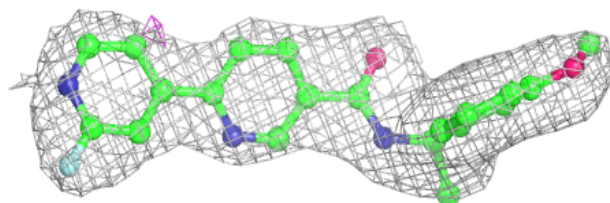
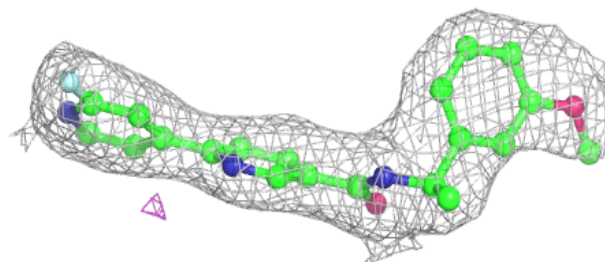


Electron density around 5YK D 501:

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

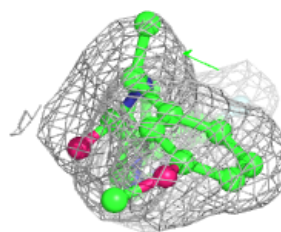
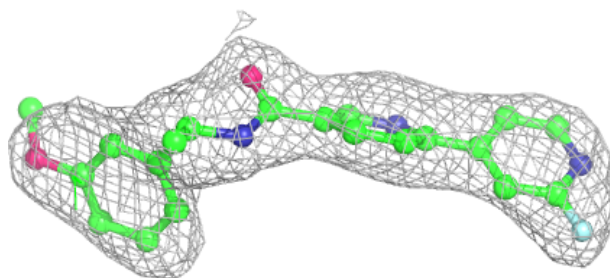
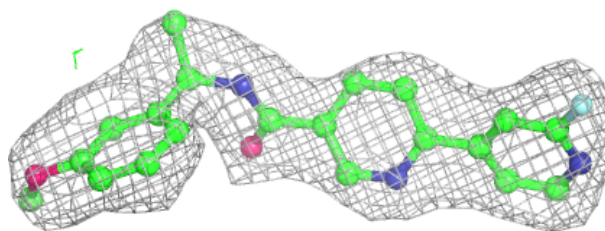
**Electron density around 5YK B 501:**

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

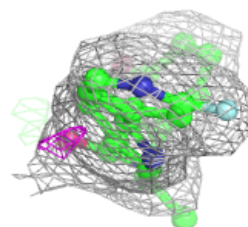
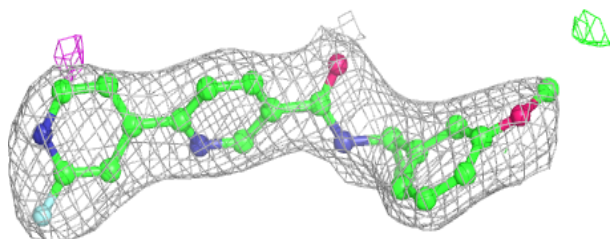
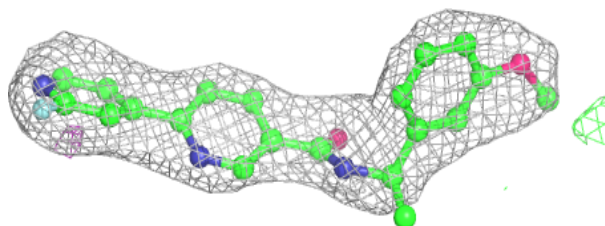


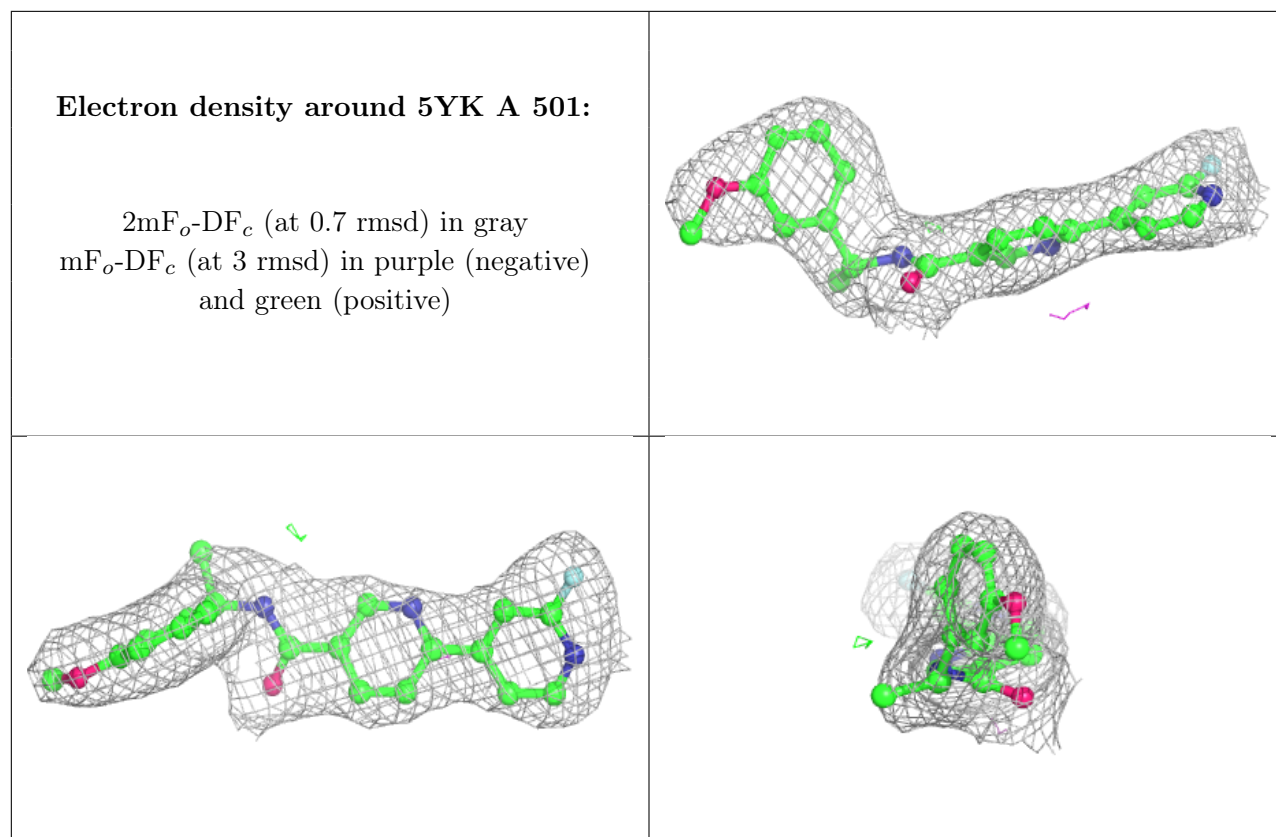
Electron density around 5YK G 501:

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

**Electron density around 5YK E 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.