



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:33 am BST

PDB ID : 5KYA  
Title : Brain penetrant liver X receptor (LXR) modulators based on a 2,4,5,6-tetrahydroindolo[3,4-c]pyrazole core  
Authors : Chen, G.; McKeever, B.M.  
Deposited on : 2016-07-21  
Resolution : 2.60 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

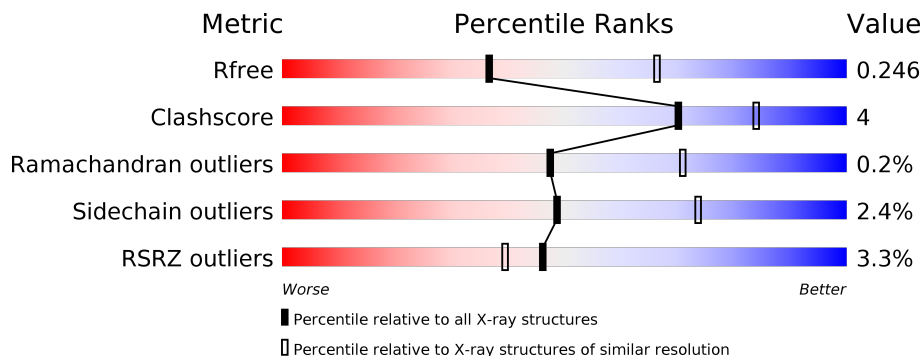
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	287	 3% 76% 8% • 15%
1	E	287	 78% 8% • 13%
2	B	256	 2% 75% 8% • 16%
2	F	256	 7% 78% 7% 15%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7550 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 Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	1986	1272	348	359	7	0	0	0
1	E	251	2028	1297	355	369	7	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	MET	-	initiating methionine	UNP P55055
A	195	GLY	-	expression tag	UNP P55055
A	196	SER	-	expression tag	UNP P55055
A	197	SER	-	expression tag	UNP P55055
A	198	HIS	-	expression tag	UNP P55055
A	199	HIS	-	expression tag	UNP P55055
A	200	HIS	-	expression tag	UNP P55055
A	201	HIS	-	expression tag	UNP P55055
A	202	HIS	-	expression tag	UNP P55055
A	203	HIS	-	expression tag	UNP P55055
A	204	SER	-	expression tag	UNP P55055
A	205	SER	-	expression tag	UNP P55055
A	206	GLY	-	expression tag	UNP P55055
A	207	LEU	-	expression tag	UNP P55055
A	208	VAL	-	expression tag	UNP P55055
A	209	PRO	-	expression tag	UNP P55055
A	210	ARG	GLN	conflict	UNP P55055
A	213	HIS	GLY	engineered mutation	UNP P55055
A	214	MET	GLU	engineered mutation	UNP P55055
A	259	ALA	GLN	engineered mutation	UNP P55055
A	261	GLY	ARG	engineered mutation	UNP P55055
A	262	SER	ASP	engineered mutation	UNP P55055
A	264	SER	ARG	engineered mutation	UNP P55055
A	462	GLY	-	expression tag	UNP P55055
A	463	SER	-	expression tag	UNP P55055

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	464	GLY	-	expression tag	UNP P55055
A	465	SER	-	expression tag	UNP P55055
A	466	GLY	-	expression tag	UNP P55055
A	467	SER	-	expression tag	UNP P55055
A	468	HIS	-	expression tag	UNP P55055
A	469	LYS	-	expression tag	UNP P55055
A	470	ILE	-	expression tag	UNP P55055
A	471	LEU	-	expression tag	UNP P55055
A	472	HIS	-	expression tag	UNP P55055
A	473	ARG	-	expression tag	UNP P55055
A	474	LEU	-	expression tag	UNP P55055
A	475	LEU	-	expression tag	UNP P55055
A	476	GLN	-	expression tag	UNP P55055
A	477	ASP	-	expression tag	UNP P55055
A	478	SER	-	expression tag	UNP P55055
A	479	SER	-	expression tag	UNP P55055
A	480	SER	-	expression tag	UNP P55055
E	194	MET	-	initiating methionine	UNP P55055
E	195	GLY	-	expression tag	UNP P55055
E	196	SER	-	expression tag	UNP P55055
E	197	SER	-	expression tag	UNP P55055
E	198	HIS	-	expression tag	UNP P55055
E	199	HIS	-	expression tag	UNP P55055
E	200	HIS	-	expression tag	UNP P55055
E	201	HIS	-	expression tag	UNP P55055
E	202	HIS	-	expression tag	UNP P55055
E	203	HIS	-	expression tag	UNP P55055
E	204	SER	-	expression tag	UNP P55055
E	205	SER	-	expression tag	UNP P55055
E	206	GLY	-	expression tag	UNP P55055
E	207	LEU	-	expression tag	UNP P55055
E	208	VAL	-	expression tag	UNP P55055
E	209	PRO	-	expression tag	UNP P55055
E	210	ARG	GLN	conflict	UNP P55055
E	213	HIS	GLY	engineered mutation	UNP P55055
E	214	MET	GLU	engineered mutation	UNP P55055
E	259	ALA	GLN	engineered mutation	UNP P55055
E	261	GLY	ARG	engineered mutation	UNP P55055
E	262	SER	ASP	engineered mutation	UNP P55055
E	264	SER	ARG	engineered mutation	UNP P55055
E	462	GLY	-	expression tag	UNP P55055
E	463	SER	-	expression tag	UNP P55055

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	464	GLY	-	expression tag	UNP P55055
E	465	SER	-	expression tag	UNP P55055
E	466	GLY	-	expression tag	UNP P55055
E	467	SER	-	expression tag	UNP P55055
E	468	HIS	-	expression tag	UNP P55055
E	469	LYS	-	expression tag	UNP P55055
E	470	ILE	-	expression tag	UNP P55055
E	471	LEU	-	expression tag	UNP P55055
E	472	HIS	-	expression tag	UNP P55055
E	473	ARG	-	expression tag	UNP P55055
E	474	LEU	-	expression tag	UNP P55055
E	475	LEU	-	expression tag	UNP P55055
E	476	GLN	-	expression tag	UNP P55055
E	477	ASP	-	expression tag	UNP P55055
E	478	SER	-	expression tag	UNP P55055
E	479	SER	-	expression tag	UNP P55055
E	480	SER	-	expression tag	UNP P55055

- Molecule 2 is a protein called Retinoic acid receptor RXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	216	Total 1726	C 1106	N 303	O 307	S 10	0	0	0
2	F	217	Total 1730	C 1108	N 304	O 308	S 10	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

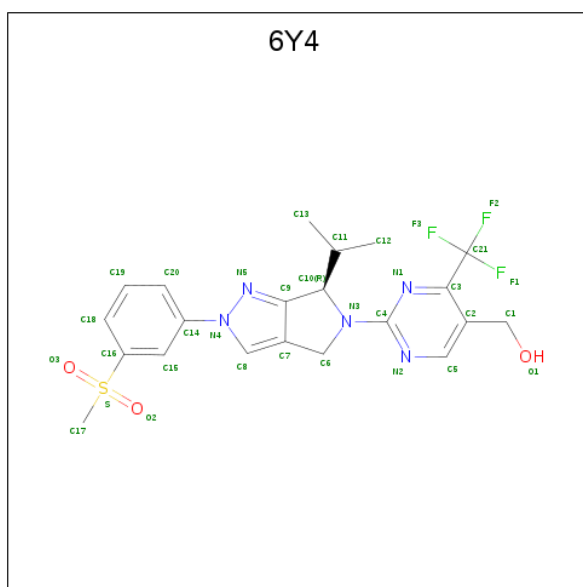
Chain	Residue	Modelled	Actual	Comment	Reference
B	292	HIS	-	expression tag	UNP P28702
B	293	MET	GLY	engineered mutation	UNP P28702
B	529	GLY	-	expression tag	UNP P28702
B	530	SER	-	expression tag	UNP P28702
B	531	GLY	-	expression tag	UNP P28702
B	532	SER	-	expression tag	UNP P28702
B	533	GLY	-	expression tag	UNP P28702
B	534	SER	-	expression tag	UNP P28702
B	535	HIS	-	expression tag	UNP P28702
B	536	LYS	-	expression tag	UNP P28702
B	537	ILE	-	expression tag	UNP P28702
B	538	LEU	-	expression tag	UNP P28702
B	539	HIS	-	expression tag	UNP P28702

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	540	ARG	-	expression tag	UNP P28702
B	541	LEU	-	expression tag	UNP P28702
B	542	LEU	-	expression tag	UNP P28702
B	543	GLN	-	expression tag	UNP P28702
B	544	ASP	-	expression tag	UNP P28702
B	545	SER	-	expression tag	UNP P28702
B	546	SER	-	expression tag	UNP P28702
B	547	SER	-	expression tag	UNP P28702
F	292	HIS	-	expression tag	UNP P28702
F	293	MET	GLY	engineered mutation	UNP P28702
F	529	GLY	-	expression tag	UNP P28702
F	530	SER	-	expression tag	UNP P28702
F	531	GLY	-	expression tag	UNP P28702
F	532	SER	-	expression tag	UNP P28702
F	533	GLY	-	expression tag	UNP P28702
F	534	SER	-	expression tag	UNP P28702
F	535	HIS	-	expression tag	UNP P28702
F	536	LYS	-	expression tag	UNP P28702
F	537	ILE	-	expression tag	UNP P28702
F	538	LEU	-	expression tag	UNP P28702
F	539	HIS	-	expression tag	UNP P28702
F	540	ARG	-	expression tag	UNP P28702
F	541	LEU	-	expression tag	UNP P28702
F	542	LEU	-	expression tag	UNP P28702
F	543	GLN	-	expression tag	UNP P28702
F	544	ASP	-	expression tag	UNP P28702
F	545	SER	-	expression tag	UNP P28702
F	546	SER	-	expression tag	UNP P28702
F	547	SER	-	expression tag	UNP P28702

- Molecule 3 is [2-[(6 {R})-2-(3-methylsulfonylphenyl)-6-propan-2-yl-4,6-dihydropyrrolo[3,4-c]pyrazol-5-yl]-4-(trifluoromethyl)pyrimidin-5-yl]methanol (three-letter code: 6Y4) (formula: C<sub>21</sub>H<sub>22</sub>F<sub>3</sub>N<sub>5</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
3	A	1	33	21	3	5	3	1	0	0
3	E	1	33	21	3	5	3	1	0	0

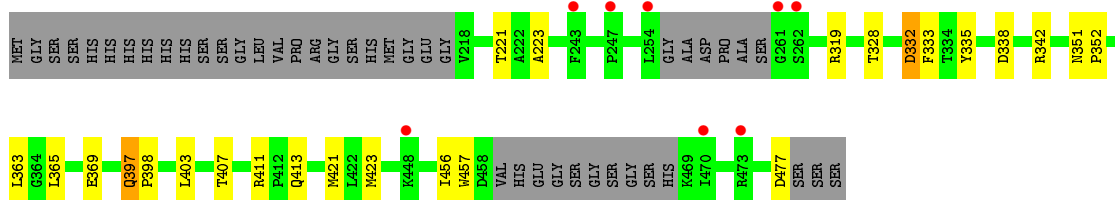
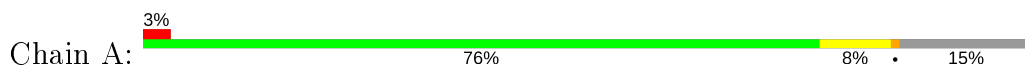
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total 7 7	0	0
4	B	2	Total 2 2	0	0
4	E	4	Total 4 4	0	0
4	F	1	Total 1 1	0	0

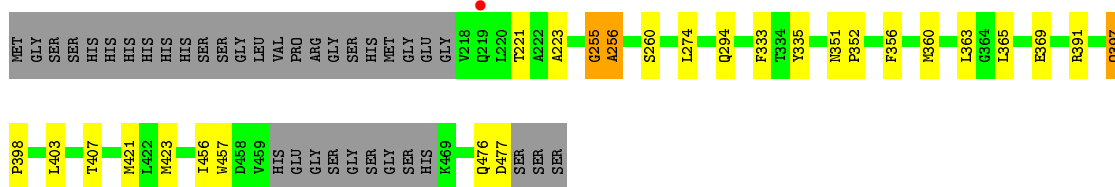
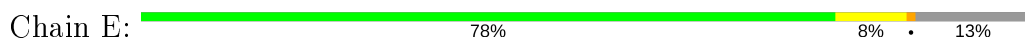
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

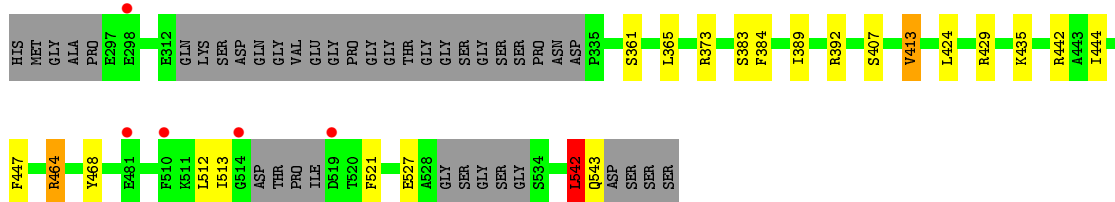
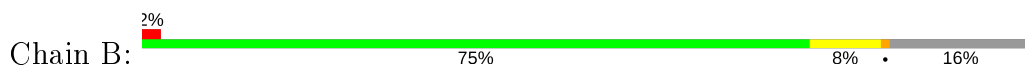
- Molecule 1: Oxysterols receptor LXR-beta



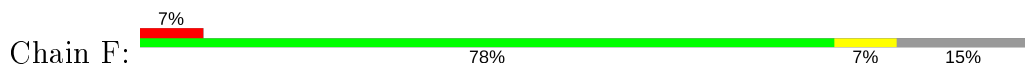
- Molecule 1: Oxysterols receptor LXR-beta



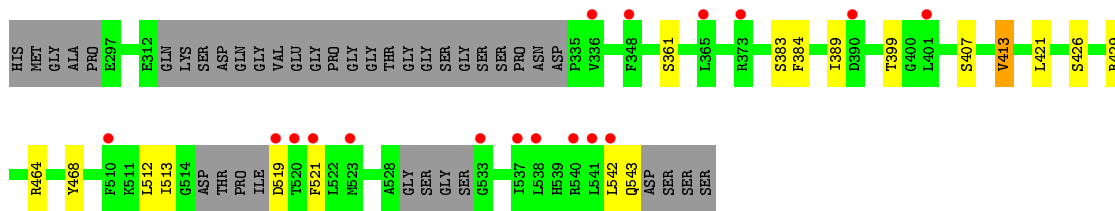
- Molecule 2: Retinoic acid receptor RXR-beta



- Molecule 2: Retinoic acid receptor RXR-beta







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.44Å 101.09Å 143.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.48 – 2.60 44.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.48-2.60) 99.9 (44.48-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.197 , 0.249 0.200 , 0.246	Depositor DCC
$R_{free}$ test set	1581 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 6Y4

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	0.63	0/2023	0.74	0/2733
1	E	0.64	0/2067	0.76	1/2796 (0.0%)
2	B	0.59	0/1755	0.77	4/2362 (0.2%)
2	F	0.54	0/1759	0.73	1/2367 (0.0%)
All	All	0.60	0/7604	0.75	6/10258 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	464	ARG	CG-CD-NE	6.74	125.96	111.80
1	E	255	GLY	N-CA-C	6.25	128.72	113.10
2	B	542	LEU	CB-CG-CD1	-5.99	100.81	111.00
2	F	464	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	B	392	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	442	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	1986	0	2023	15	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2028	0	2062	21	0
2	B	1726	0	1777	13	0
2	F	1730	0	1780	8	0
3	A	33	0	0	0	0
3	E	33	0	0	1	0
4	A	7	0	0	0	0
4	B	2	0	0	0	0
4	E	4	0	0	0	0
4	F	1	0	0	0	0
All	All	7550	0	7642	54	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 4.

All (54) 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)
2:B:444:ILE:O	2:B:464:ARG:NH1	2.06	0.88
1:E:356:PHE:CE1	1:E:360:MET:HE1	2.20	0.76
1:A:221:THR:HG22	1:A:223:ALA:H	1.55	0.72
1:E:294:GLN:O	1:E:391:ARG:NH2	2.23	0.71
1:E:221:THR:HG22	1:E:223:ALA:H	1.55	0.71
1:E:423:MET:HG3	2:F:468:TYR:OH	1.92	0.69
1:E:255:GLY:O	1:E:256:ALA:HB3	1.94	0.67
1:E:255:GLY:O	1:E:256:ALA:CB	2.46	0.61
1:E:356:PHE:CZ	1:E:360:MET:HE1	2.36	0.61
1:E:477:ASP:C	1:E:477:ASP:OD1	2.40	0.58
1:E:356:PHE:CZ	1:E:360:MET:CE	2.87	0.57
2:B:447:PHE:O	2:B:464:ARG:NH1	2.37	0.57
1:E:363:LEU:HB3	1:E:365:LEU:HD13	1.89	0.55
1:E:221:THR:HG22	1:E:223:ALA:N	2.23	0.54
1:A:221:THR:HG22	1:A:223:ALA:N	2.24	0.53
1:A:332:ASP:N	1:A:332:ASP:OD1	2.41	0.52
1:A:369:GLU:OE2	1:A:407:THR:HG22	2.09	0.52
1:A:477:ASP:OD1	1:A:477:ASP:C	2.48	0.52
2:B:365:LEU:HD11	2:B:542:LEU:CD1	2.40	0.51
1:A:363:LEU:HB3	1:A:365:LEU:HD13	1.92	0.51
2:B:542:LEU:O	2:B:543:GLN:HG3	2.10	0.51
1:E:369:GLU:OE2	1:E:407:THR:HG22	2.11	0.50
2:F:389:ILE:O	2:F:429:ARG:NH1	2.37	0.49
2:F:542:LEU:O	2:F:543:GLN:HG3	2.11	0.49

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:ILE:O	2:B:429:ARG:NH1	2.38	0.49
1:A:456:ILE:HG23	1:A:457:TRP:CD1	2.48	0.48
2:B:413:VAL:O	2:B:413:VAL:HG13	2.13	0.48
2:F:413:VAL:HG13	2:F:413:VAL:O	2.15	0.47
2:B:365:LEU:CD1	2:B:542:LEU:HD13	2.45	0.47
2:F:413:VAL:CG1	2:F:413:VAL:O	2.63	0.47
1:E:356:PHE:CE1	1:E:360:MET:CE	2.95	0.46
2:B:413:VAL:O	2:B:413:VAL:CG1	2.63	0.46
2:B:373:ARG:NH1	2:B:527:GLU:O	2.45	0.45
1:E:333:PHE:HB3	1:E:335:TYR:CE2	2.51	0.45
1:A:351:ASN:HB2	1:A:352:PRO:HD3	1.99	0.44
1:A:411:ARG:HD2	1:A:413:GLN:HE22	1.82	0.44
1:E:274:LEU:HD22	3:E:501:6Y4:C17	2.48	0.44
1:E:456:ILE:HG23	1:E:457:TRP:CD1	2.53	0.43
1:E:403:LEU:HD11	1:E:421:MET:HE1	1.99	0.43
2:B:365:LEU:CD1	2:B:542:LEU:CD1	2.97	0.43
1:E:351:ASN:HB2	1:E:352:PRO:HD3	2.01	0.43
1:A:319:ARG:HD3	1:A:328:THR:O	2.19	0.42
1:E:356:PHE:CZ	1:E:360:MET:HE3	2.55	0.42
1:E:423:MET:HG3	2:F:468:TYR:CZ	2.54	0.42
2:F:512:LEU:C	2:F:513:ILE:HG13	2.40	0.42
2:B:512:LEU:C	2:B:513:ILE:HG13	2.39	0.41
1:A:423:MET:HG3	2:B:468:TYR:OH	2.20	0.41
1:A:397:GLN:HB3	1:A:398:PRO:HD3	2.02	0.41
1:A:333:PHE:HB3	1:A:335:TYR:CE2	2.56	0.41
1:A:403:LEU:HD11	1:A:421:MET:HE1	2.02	0.41
2:F:421:LEU:O	2:F:426:SER:HB2	2.19	0.41
1:A:338:ASP:HB3	1:A:342:ARG:NH1	2.36	0.40
1:E:397:GLN:HB3	1:E:398:PRO:HD3	2.03	0.40
2:B:424:LEU:HA	2:B:424:LEU:HD23	1.94	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	238/287 (83%)	237 (100%)	1 (0%)	0	100	100
1	E	247/287 (86%)	242 (98%)	3 (1%)	2 (1%)	19	39
2	B	208/256 (81%)	199 (96%)	9 (4%)	0	100	100
2	F	209/256 (82%)	201 (96%)	8 (4%)	0	100	100
All	All	902/1086 (83%)	879 (98%)	21 (2%)	2 (0%)	47	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	256	ALA
1	E	260	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/250 (87%)	216 (99%)	2 (1%)	78	91
1	E	222/250 (89%)	220 (99%)	2 (1%)	78	91
2	B	189/217 (87%)	181 (96%)	8 (4%)	30	55
2	F	189/217 (87%)	181 (96%)	8 (4%)	30	55
All	All	818/934 (88%)	798 (98%)	20 (2%)	49	74

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

Mol	Chain	Res	Type
1	A	332	ASP
1	A	397	GLN
2	B	361	SER
2	B	383	SER
2	B	384	PHE
2	B	407	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	413	VAL
2	B	435	LYS
2	B	521	PHE
2	B	542	LEU
1	E	397	GLN
1	E	476	GLN
2	F	361	SER
2	F	383	SER
2	F	384	PHE
2	F	399	THR
2	F	407	SER
2	F	413	VAL
2	F	519	ASP
2	F	521	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	294	GLN
2	B	338	ASN
1	E	239	ASN
1	E	294	GLN
2	F	338	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

2 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
3	6Y4	A	501	-	29,36,36	3.36	5 (17%)	38,56,56	3.59	20 (52%)
3	6Y4	E	501	-	29,36,36	2.96	5 (17%)	38,56,56	4.27	20 (52%)

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
3	6Y4	A	501	-	-	11/26/38/38	0/4/4/4
3	6Y4	E	501	-	-	7/26/38/38	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	6Y4	C16-S	-16.69	1.59	1.77
3	E	501	6Y4	C16-S	-14.19	1.61	1.77
3	E	501	6Y4	C21-C3	-3.86	1.45	1.51
3	A	501	6Y4	C14-N4	-3.82	1.33	1.44
3	E	501	6Y4	C14-N4	-3.75	1.33	1.44
3	A	501	6Y4	C6-N3	3.09	1.49	1.46
3	E	501	6Y4	C17-S	-3.03	1.63	1.75
3	A	501	6Y4	C21-C3	-2.85	1.47	1.51
3	A	501	6Y4	C17-S	-2.60	1.64	1.75
3	E	501	6Y4	C6-N3	2.40	1.48	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	6Y4	C7-C6-N3	-12.71	96.64	102.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	6Y4	C7-C6-N3	-12.57	96.70	102.25
3	E	501	6Y4	C5-N2-C4	10.72	125.14	115.64
3	A	501	6Y4	C5-N2-C4	9.30	123.89	115.64
3	E	501	6Y4	C17-S-C16	7.72	113.70	104.58
3	E	501	6Y4	O3-S-C16	-6.62	102.85	108.25
3	E	501	6Y4	C14-C15-C16	6.49	124.40	119.26
3	E	501	6Y4	O2-S-C16	6.31	113.39	108.25
3	E	501	6Y4	F2-C21-C3	-6.10	102.77	112.32
3	E	501	6Y4	C20-C14-C15	-5.19	115.60	121.74
3	A	501	6Y4	F1-C21-C3	-5.04	104.42	112.32
3	E	501	6Y4	F3-C21-C3	-4.58	105.15	112.32
3	A	501	6Y4	C17-S-C16	4.58	109.98	104.58
3	E	501	6Y4	C20-C14-N4	4.35	122.95	119.15
3	A	501	6Y4	C8-N4-N5	4.32	117.13	112.72
3	A	501	6Y4	O2-S-O3	-4.10	110.85	117.92
3	A	501	6Y4	F2-C21-C3	-4.07	105.94	112.32
3	A	501	6Y4	N2-C4-N1	-4.06	121.94	126.00
3	A	501	6Y4	C20-C14-C15	-4.04	116.96	121.74
3	E	501	6Y4	F1-C21-C3	-3.85	106.30	112.32
3	E	501	6Y4	O3-S-C17	-3.76	103.09	108.49
3	A	501	6Y4	O2-S-C17	3.74	113.86	108.49
3	E	501	6Y4	C2-C5-N2	-3.61	117.80	123.82
3	A	501	6Y4	C7-C8-N4	-3.58	103.35	107.58
3	A	501	6Y4	C6-N3-C4	3.53	129.10	123.34
3	E	501	6Y4	C13-C11-C10	3.27	115.12	110.72
3	A	501	6Y4	C13-C11-C10	3.09	114.89	110.72
3	A	501	6Y4	C14-C15-C16	2.98	121.62	119.26
3	E	501	6Y4	C7-C8-N4	-2.89	104.16	107.58
3	E	501	6Y4	N2-C4-N1	-2.80	123.20	126.00
3	A	501	6Y4	F3-C21-C3	-2.77	107.99	112.32
3	A	501	6Y4	C2-C5-N2	-2.68	119.35	123.82
3	A	501	6Y4	C20-C14-N4	2.58	121.41	119.15
3	E	501	6Y4	F2-C21-F1	2.47	114.77	105.72
3	A	501	6Y4	C19-C20-C14	2.44	121.80	118.63
3	E	501	6Y4	C12-C11-C10	-2.41	107.48	110.72
3	E	501	6Y4	C19-C20-C14	2.28	121.60	118.63
3	E	501	6Y4	F1-C21-F3	2.26	114.03	105.72
3	A	501	6Y4	F2-C21-F1	2.18	113.72	105.72
3	A	501	6Y4	O2-S-C16	-2.06	106.57	108.25

There are no chirality outliers.

All (18) torsion outliers are listed below:

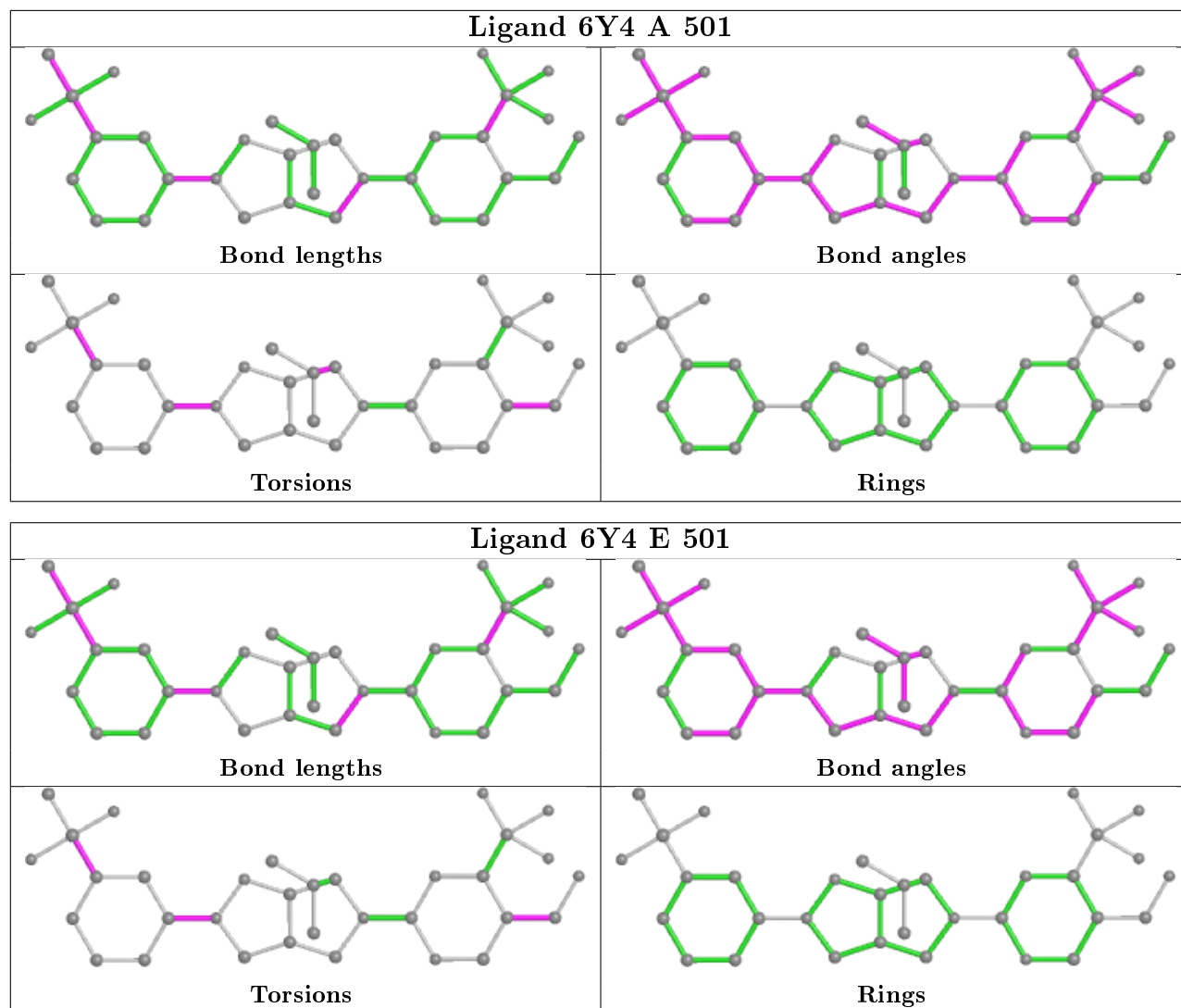
Mol	Chain	Res	Type	Atoms
3	A	501	6Y4	N3-C10-C11-C13
3	A	501	6Y4	N3-C10-C11-C12
3	A	501	6Y4	C9-C10-C11-C12
3	E	501	6Y4	C15-C16-S-C17
3	E	501	6Y4	C18-C16-S-C17
3	E	501	6Y4	O1-C1-C2-C5
3	A	501	6Y4	C15-C16-S-C17
3	A	501	6Y4	C18-C16-S-C17
3	A	501	6Y4	C20-C14-N4-C8
3	A	501	6Y4	C15-C16-S-O3
3	A	501	6Y4	C18-C16-S-O3
3	E	501	6Y4	C15-C16-S-O3
3	E	501	6Y4	C18-C16-S-O3
3	A	501	6Y4	O1-C1-C2-C5
3	A	501	6Y4	C15-C14-N4-C8
3	E	501	6Y4	C20-C14-N4-C8
3	E	501	6Y4	C15-C14-N4-C8
3	A	501	6Y4	C9-C10-C11-C13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	6Y4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	244/287 (85%)	-0.10	8 (3%) 46 39	30, 43, 81, 112	0
1	E	251/287 (87%)	-0.21	1 (0%) 92 91	28, 43, 74, 97	0
2	B	216/256 (84%)	-0.06	5 (2%) 60 54	29, 51, 85, 113	0
2	F	217/256 (84%)	0.18	17 (7%) 13 9	35, 59, 89, 119	0
All	All	928/1086 (85%)	-0.06	31 (3%) 46 39	28, 48, 83, 119	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	LEU	5.8
2	F	533	GLY	5.3
2	F	348	PHE	3.9
2	F	538	LEU	3.6
1	A	261	GLY	3.5
2	B	510	PHE	3.4
2	F	540	ARG	3.2
2	F	521	PHE	3.1
1	A	262	SER	3.0
2	B	481	GLU	3.0
2	F	542	LEU	2.9
2	F	537	ILE	2.8
2	F	519	ASP	2.8
2	F	390	ASP	2.8
2	B	519	ASP	2.6
1	A	243	PHE	2.5
2	F	401	LEU	2.5
2	F	541	LEU	2.4
2	F	520	THR	2.3
2	B	298	GLU	2.3
1	A	247	PRO	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	510	PHE	2.2
1	A	473	ARG	2.2
1	E	219	GLN	2.1
2	F	336	VAL	2.1
1	A	448	LYS	2.1
2	F	365	LEU	2.1
2	F	373	ARG	2.1
1	A	470	ILE	2.1
2	B	514	GLY	2.1
2	F	523	MET	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

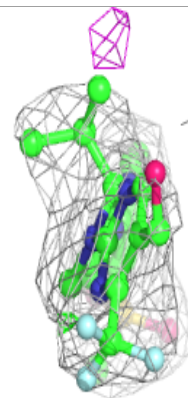
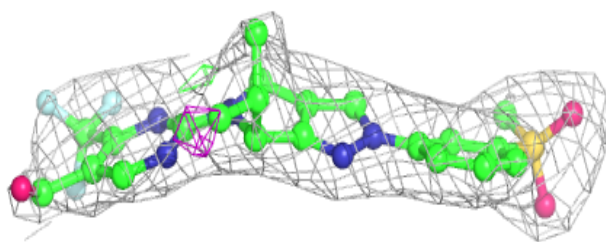
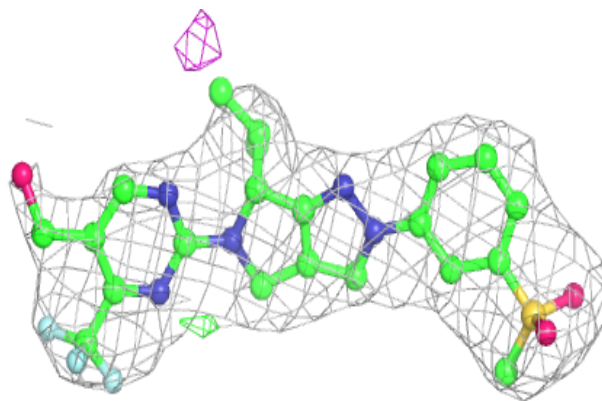
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	6Y4	A	501	33/33	0.96	0.16	37,45,85,95	0
3	6Y4	E	501	33/33	0.97	0.15	31,38,68,72	0

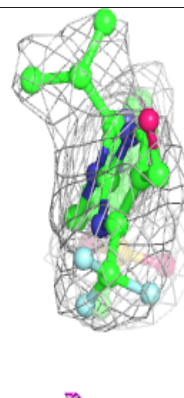
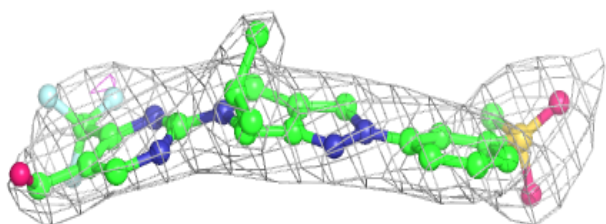
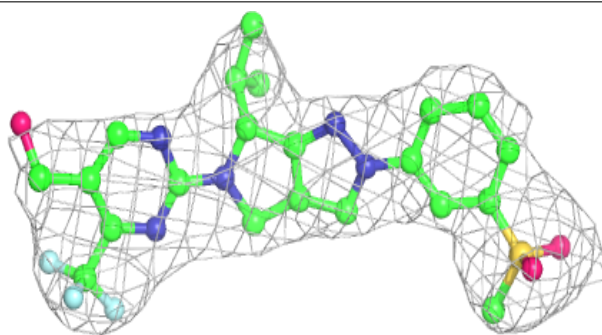
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 6Y4 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 6Y4 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

There are no such residues in this entry.