



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 12:33 am BST

PDB ID : 4LEI  
Title : Spinosyn Forosaminyltransferase SpnP  
Authors : Isiorho, E.A.; Liu, H.-W.; Keatinge-Clay, A.K.  
Deposited on : 2013-06-25  
Resolution : 3.15 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

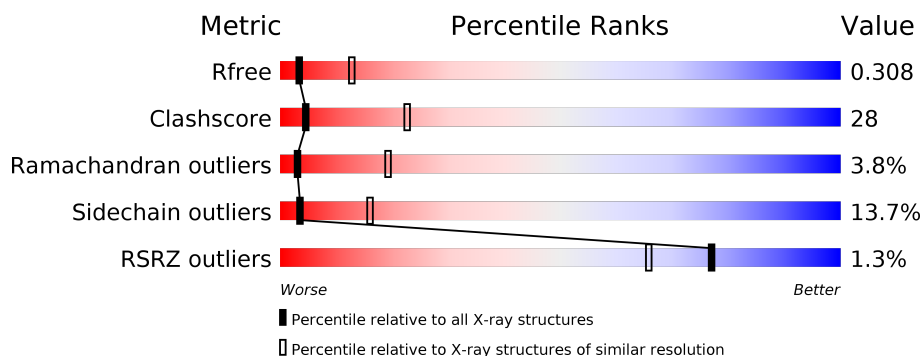
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	455	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>30%</div> <div>6%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	455	<div> <div></div> <div> <div>42%</div> <div>32%</div> <div>7%</div> <div>•</div> <div>18%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TYD	B	501	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5958 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 NDP-forosamyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2922	1852	514	543	13			
1	B	373	Total	C	N	O	S	0	0	0
			2905	1840	511	541	13			

There are 32 discrepancies between the modelled and reference sequences:

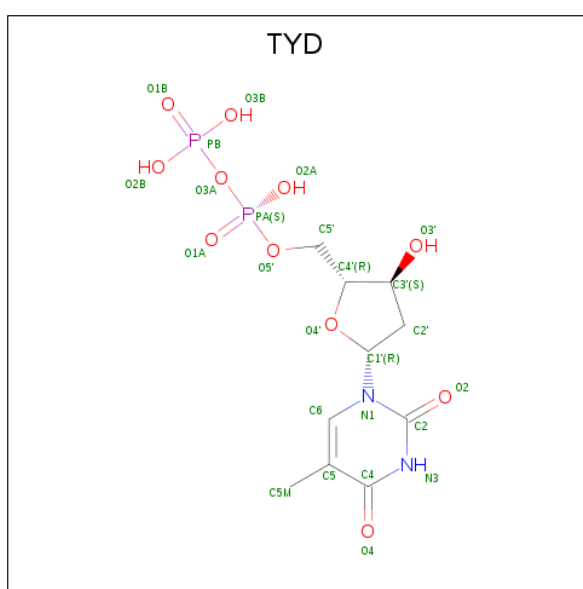
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	EXPRESSION TAG	UNP Q9ALN7
A	-14	HIS	-	EXPRESSION TAG	UNP Q9ALN7
A	-13	HIS	-	EXPRESSION TAG	UNP Q9ALN7
A	-12	HIS	-	EXPRESSION TAG	UNP Q9ALN7
A	-11	HIS	-	EXPRESSION TAG	UNP Q9ALN7
A	-10	HIS	-	EXPRESSION TAG	UNP Q9ALN7
A	-9	SER	-	EXPRESSION TAG	UNP Q9ALN7
A	-8	SER	-	EXPRESSION TAG	UNP Q9ALN7
A	-7	GLY	-	EXPRESSION TAG	UNP Q9ALN7
A	-6	LEU	-	EXPRESSION TAG	UNP Q9ALN7
A	-5	VAL	-	EXPRESSION TAG	UNP Q9ALN7
A	-4	PRO	-	EXPRESSION TAG	UNP Q9ALN7
A	-3	ARG	-	EXPRESSION TAG	UNP Q9ALN7
A	-2	GLY	-	EXPRESSION TAG	UNP Q9ALN7
A	-1	SER	-	EXPRESSION TAG	UNP Q9ALN7
A	0	HIS	-	EXPRESSION TAG	UNP Q9ALN7
B	-15	HIS	-	EXPRESSION TAG	UNP Q9ALN7
B	-14	HIS	-	EXPRESSION TAG	UNP Q9ALN7
B	-13	HIS	-	EXPRESSION TAG	UNP Q9ALN7
B	-12	HIS	-	EXPRESSION TAG	UNP Q9ALN7
B	-11	HIS	-	EXPRESSION TAG	UNP Q9ALN7
B	-10	HIS	-	EXPRESSION TAG	UNP Q9ALN7
B	-9	SER	-	EXPRESSION TAG	UNP Q9ALN7
B	-8	SER	-	EXPRESSION TAG	UNP Q9ALN7
B	-7	GLY	-	EXPRESSION TAG	UNP Q9ALN7

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	LEU	-	EXPRESSION TAG	UNP Q9ALN7
B	-5	VAL	-	EXPRESSION TAG	UNP Q9ALN7
B	-4	PRO	-	EXPRESSION TAG	UNP Q9ALN7
B	-3	ARG	-	EXPRESSION TAG	UNP Q9ALN7
B	-2	GLY	-	EXPRESSION TAG	UNP Q9ALN7
B	-1	SER	-	EXPRESSION TAG	UNP Q9ALN7
B	0	HIS	-	EXPRESSION TAG	UNP Q9ALN7

- Molecule 2 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula:  $C_{10}H_{16}N_2O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
2	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

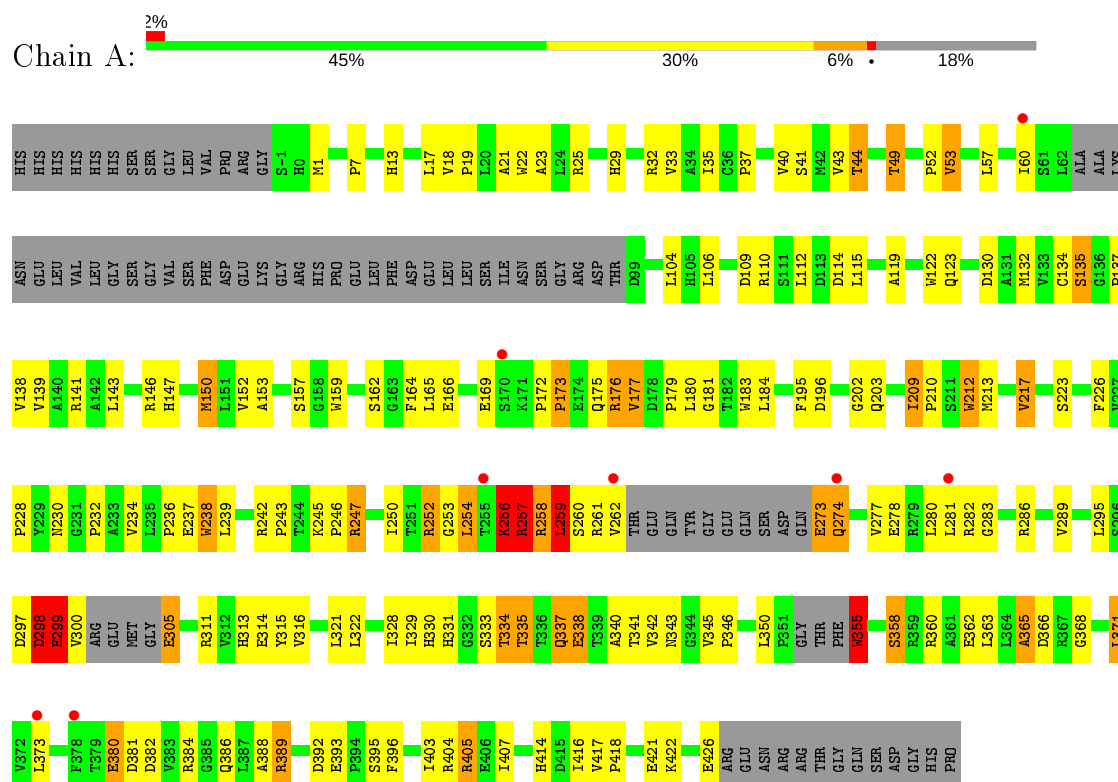
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	41	Total	O	0	0
			41	41		

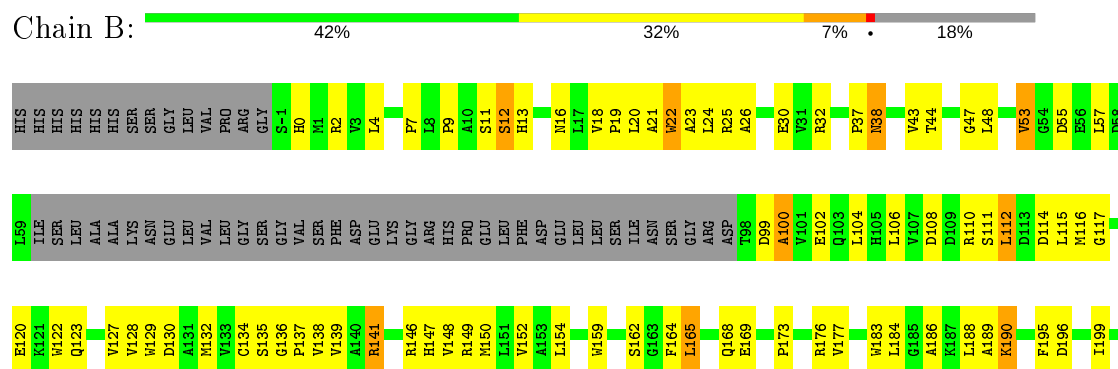
### 3 Residue-property plots

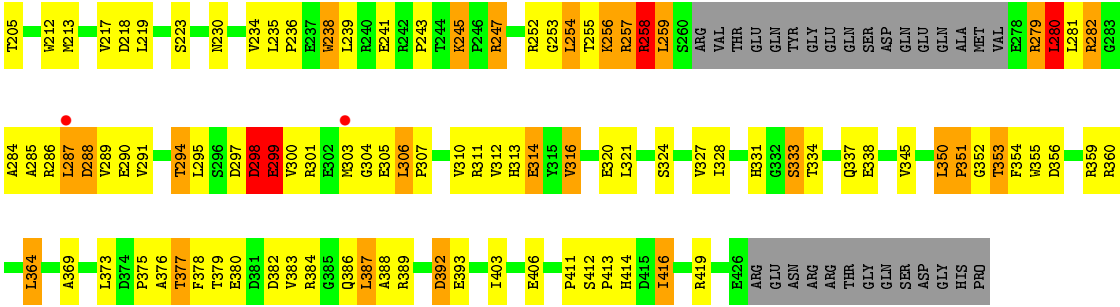
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



- Molecule 1: NDP-forosamyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.37Å 162.37Å 81.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.81 – 3.15 46.89 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (114.81-3.15) 99.1 (46.89-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.209 , 0.314 0.209 , 0.308	Depositor DCC
$R_{free}$ test set	985 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TYD

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	0.73	5/2983 (0.2%)	0.87	1/4065 (0.0%)
1	B	0.72	7/2969 (0.2%)	0.88	1/4048 (0.0%)
All	All	0.72	12/5952 (0.2%)	0.88	2/8113 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	TRP	CD2-CE2	7.51	1.50	1.41
1	B	159	TRP	CD2-CE2	6.79	1.49	1.41
1	B	22	TRP	CD2-CE2	5.92	1.48	1.41
1	B	238	TRP	CD2-CE2	5.83	1.48	1.41
1	A	355	TRP	CD2-CE2	5.75	1.48	1.41
1	A	22	TRP	CD2-CE2	5.74	1.48	1.41
1	B	355	TRP	CD2-CE2	5.53	1.48	1.41
1	B	212	TRP	CD2-CE2	5.34	1.47	1.41
1	A	183	TRP	CD2-CE2	5.18	1.47	1.41
1	A	238	TRP	CD2-CE2	5.15	1.47	1.41
1	B	183	TRP	CD2-CE2	5.12	1.47	1.41
1	B	122	TRP	CD2-CE2	5.09	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	LEU	CA-CB-CG	6.69	130.69	115.30
1	A	245	LYS	C-N-CD	5.61	140.18	128.40

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	2922	0	2933	154	0
1	B	2905	0	2906	184	0
2	A	25	0	13	5	0
2	B	25	0	13	10	0
3	A	40	0	0	6	0
3	B	41	0	0	4	0
All	All	5958	0	5865	334	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 28.

All (334) 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:273:GLU:HA	1:A:274:GLN:HB3	1.23	1.18
1:B:287:LEU:HD23	1:B:384:ARG:HB2	1.28	1.09
1:A:316:VAL:HG21	1:A:321:LEU:HD22	1.38	1.06
1:B:287:LEU:CD2	1:B:384:ARG:HB2	1.87	1.05
1:A:273:GLU:CA	1:A:274:GLN:HB3	1.89	1.03
1:B:419:ARG:NH2	3:B:632:HOH:O	1.93	1.01
1:B:297:ASP:OD1	1:B:312:VAL:HA	1.63	0.98
1:A:299:GLU:HB2	1:A:300:VAL:CB	1.94	0.97
1:A:299:GLU:HB2	1:A:300:VAL:HB	1.46	0.97
1:B:287:LEU:HD13	1:B:380:GLU:HB3	1.50	0.92
1:A:152:VAL:O	1:A:334:THR:HG21	1.69	0.92
1:B:254:LEU:HB3	1:B:255:THR:HA	1.53	0.87
1:A:389:ARG:HH11	1:A:389:ARG:HG2	1.40	0.87
1:A:153:ALA:HB1	1:A:355:TRP:N	1.89	0.87
1:A:257:ARG:NH2	1:A:260:SER:HB2	1.89	0.87
1:B:253:GLY:O	1:B:331:HIS:CE1	2.28	0.86
1:A:300:VAL:HG22	1:A:305:GLU:N	1.90	0.85
1:B:253:GLY:H	1:B:254:LEU:HD22	1.42	0.85
1:B:173:PRO:HA	1:B:176:ARG:HD2	1.58	0.85
1:B:254:LEU:HD11	1:B:257:ARG:HG3	1.59	0.85
1:B:301:ARG:NE	1:B:301:ARG:HA	1.92	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ARG:HH11	1:A:247:ARG:CG	1.87	0.83
1:B:297:ASP:OD2	1:B:312:VAL:HG13	1.77	0.83
1:B:301:ARG:HA	1:B:301:ARG:HE	1.43	0.82
1:A:257:ARG:HH21	1:A:260:SER:HB2	1.42	0.81
1:A:60:ILE:CG2	1:A:259:LEU:HD22	2.12	0.80
1:B:134:CYS:O	1:B:138:VAL:HG23	1.82	0.80
1:B:254:LEU:CD1	1:B:255:THR:HA	2.12	0.78
1:A:252:ARG:NE	1:A:331:HIS:HB2	1.98	0.78
1:B:12:SER:CB	2:B:501:TYD:O1A	2.31	0.78
1:A:242:ARG:HD2	1:A:243:PRO:HD2	1.66	0.77
1:A:299:GLU:HB2	1:A:300:VAL:CA	2.14	0.77
1:B:254:LEU:HB3	1:B:255:THR:CA	2.14	0.77
1:B:116:MET:HE1	1:B:139:VAL:HA	1.66	0.77
1:B:12:SER:HB3	2:B:501:TYD:O1A	1.83	0.77
1:B:287:LEU:CD1	1:B:380:GLU:HB3	2.15	0.76
1:A:252:ARG:HB2	1:A:331:HIS:HD2	1.50	0.76
1:B:254:LEU:CB	1:B:255:THR:HA	2.15	0.75
1:B:306:LEU:HD22	1:B:306:LEU:H	1.51	0.74
1:A:338:GLU:O	1:A:342:VAL:N	2.16	0.74
1:B:115:LEU:HG	1:B:139:VAL:HG21	1.70	0.74
1:A:273:GLU:CA	1:A:274:GLN:CB	2.65	0.73
1:A:230:ASN:O	1:A:315:TYR:OH	2.06	0.72
1:B:234:VAL:O	1:B:236:PRO:HD3	1.90	0.72
1:A:147:HIS:CD2	1:A:202:GLY:HA2	2.25	0.71
1:B:287:LEU:HB2	1:B:380:GLU:HG2	1.74	0.69
1:B:257:ARG:HH11	1:B:257:ARG:HG3	1.58	0.69
1:B:287:LEU:CD2	1:B:384:ARG:CB	2.69	0.69
1:A:257:ARG:HD3	3:A:636:HOH:O	1.92	0.69
1:B:53:VAL:HG22	1:B:114:ASP:HB3	1.75	0.69
1:A:389:ARG:HG2	1:A:393:GLU:OE2	1.92	0.68
1:A:371:LEU:HD13	1:A:386:GLN:OE1	1.94	0.68
1:B:141:ARG:CG	1:B:199:ILE:HD11	2.23	0.68
1:B:295:LEU:HD12	1:B:310:VAL:HG22	1.74	0.68
1:B:253:GLY:HA2	1:B:331:HIS:CD2	2.29	0.68
1:A:252:ARG:HA	1:A:252:ARG:NE	2.10	0.67
1:B:2:ARG:NH2	1:B:123:GLN:O	2.25	0.67
1:A:256:LYS:O	1:A:257:ARG:C	2.32	0.67
1:B:285:ALA:O	1:B:289:VAL:HG13	1.94	0.67
1:A:252:ARG:HE	1:A:331:HIS:HB2	1.59	0.67
1:A:209:ILE:HG22	1:A:210:PRO:HD2	1.77	0.67
1:B:186:ALA:O	1:B:189:ALA:HB3	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HG3	1:B:199:ILE:HD11	1.77	0.66
1:B:7:PRO:HA	1:B:130:ASP:HB2	1.77	0.66
1:B:43:VAL:HG12	1:B:48:LEU:O	1.95	0.66
1:B:389:ARG:HG2	1:B:393:GLU:OE2	1.95	0.66
1:B:9:PRO:HD3	1:B:106:LEU:HD11	1.76	0.66
1:A:7:PRO:HA	1:A:130:ASP:HB2	1.78	0.65
1:B:254:LEU:HD13	1:B:256:LYS:H	1.60	0.65
1:A:247:ARG:HH11	1:A:247:ARG:HG3	1.60	0.65
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.62	0.64
1:B:254:LEU:HD11	1:B:257:ARG:CG	2.28	0.64
1:B:254:LEU:HD12	1:B:255:THR:HA	1.79	0.64
1:A:60:ILE:HG23	1:A:259:LEU:HD22	1.81	0.63
1:A:373:LEU:CD2	1:A:386:GLN:HG3	2.28	0.63
1:B:353:THR:HB	1:B:354:PHE:HD2	1.62	0.63
1:B:297:ASP:CG	1:B:312:VAL:HA	2.18	0.62
1:B:99:ASP:OD2	1:B:102:GLU:HB2	2.00	0.62
1:A:247:ARG:NH1	1:A:247:ARG:HG3	2.13	0.62
1:A:273:GLU:N	1:A:274:GLN:HB3	2.15	0.61
1:B:12:SER:HB2	2:B:501:TYD:O1A	2.00	0.61
1:B:30:GLU:HA	3:B:633:HOH:O	2.00	0.61
1:B:253:GLY:HA2	1:B:331:HIS:CE1	2.34	0.61
1:A:316:VAL:HG21	1:A:321:LEU:CD2	2.23	0.61
1:B:106:LEU:HB3	1:B:135:SER:HB3	1.81	0.61
1:B:149:ARG:NH1	1:B:205:THR:OG1	2.34	0.61
1:B:230:ASN:HB3	2:B:501:TYD:O2	2.01	0.61
1:B:38:ASN:H	1:B:38:ASN:HD22	1.47	0.61
1:A:403:ILE:O	1:A:407:ILE:HG12	2.02	0.60
1:B:334:THR:O	1:B:338:GLU:HG2	2.01	0.60
1:B:255:THR:O	1:B:256:LYS:HB2	2.01	0.60
1:B:257:ARG:CG	1:B:257:ARG:HH11	2.14	0.60
1:B:279:ARG:HA	1:B:281:LEU:HG	1.84	0.60
1:A:404:ARG:NH1	1:A:405:ARG:NH2	2.50	0.59
1:B:353:THR:HB	1:B:354:PHE:CD2	2.37	0.59
1:A:254:LEU:H	1:A:254:LEU:HD22	1.67	0.59
1:A:335:THR:OG1	2:A:501:TYD:O1A	2.20	0.59
1:B:282:ARG:HH22	1:B:286:ARG:HH11	1.51	0.59
1:B:327:VAL:HG12	1:B:328:ILE:N	2.18	0.59
1:B:168:GLN:NE2	1:B:177:VAL:O	2.36	0.59
1:A:298:ASP:C	1:A:299:GLU:HG3	2.23	0.58
1:B:280:LEU:HB2	1:B:378:PHE:HZ	1.69	0.58
1:A:146:ARG:NH2	1:A:426:GLU:HB2	2.18	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PRO:HA	1:A:176:ARG:HD2	1.84	0.58
1:A:259:LEU:HA	1:A:260:SER:C	2.24	0.58
1:B:256:LYS:H	1:B:257:ARG:HB2	1.68	0.58
1:B:247:ARG:HG2	1:B:294:THR:HG23	1.85	0.58
1:A:1:MET:H	1:A:29:HIS:HD2	1.51	0.58
1:A:259:LEU:HG	1:A:259:LEU:O	2.03	0.58
1:A:32:ARG:NH1	3:A:622:HOH:O	2.29	0.58
1:B:331:HIS:NE2	1:B:333:SER:HB2	2.19	0.58
1:B:282:ARG:HH22	1:B:286:ARG:NH1	2.02	0.57
1:B:331:HIS:O	1:B:351:PRO:HA	2.04	0.57
1:A:355:TRP:N	1:A:355:TRP:CD1	2.73	0.57
1:B:169:GLU:OE2	1:B:176:ARG:NH2	2.37	0.57
1:B:213:MET:SD	1:B:360:ARG:HG2	2.45	0.57
1:B:243:PRO:HG3	1:B:324:SER:HB2	1.87	0.57
1:B:257:ARG:NH1	1:B:299:GLU:OE1	2.37	0.57
1:B:306:LEU:N	1:B:306:LEU:HD22	2.18	0.57
1:A:13:HIS:HB3	1:A:130:ASP:OD2	2.05	0.57
1:A:226:PHE:CE2	1:A:228:PRO:HG3	2.40	0.57
1:B:279:ARG:HH21	1:B:301:ARG:HB3	1.70	0.57
1:A:106:LEU:HB2	1:A:135:SER:HB2	1.86	0.56
1:A:259:LEU:H	1:A:260:SER:HB3	1.70	0.56
1:B:254:LEU:HB2	2:B:501:TYD:H51	1.87	0.56
1:A:258:ARG:O	1:A:259:LEU:HB3	2.05	0.56
1:A:316:VAL:CG2	1:A:321:LEU:HD22	2.26	0.56
1:B:285:ALA:HA	1:B:288:ASP:OD1	2.05	0.56
1:B:16:ASN:HD22	1:B:152:VAL:HG22	1.70	0.56
1:A:257:ARG:O	1:A:259:LEU:N	2.39	0.56
1:A:247:ARG:HH11	1:A:247:ARG:HG2	1.67	0.56
1:B:280:LEU:HB2	1:B:378:PHE:CZ	2.41	0.55
1:B:253:GLY:HA2	1:B:331:HIS:NE2	2.21	0.55
1:B:99:ASP:O	1:B:100:ALA:CB	2.54	0.55
1:A:273:GLU:N	1:A:274:GLN:CB	2.70	0.55
1:A:252:ARG:HH12	1:A:333:SER:HB3	1.71	0.55
1:A:297:ASP:O	1:A:298:ASP:HB3	2.07	0.55
1:B:141:ARG:HG2	1:B:199:ILE:HD11	1.89	0.55
1:B:301:ARG:NE	1:B:301:ARG:CA	2.67	0.55
1:A:252:ARG:HB2	1:A:331:HIS:CD2	2.38	0.54
1:B:152:VAL:O	1:B:334:THR:HG21	2.06	0.54
1:A:134:CYS:O	1:A:137:PRO:HD2	2.06	0.54
1:A:226:PHE:HE2	1:A:228:PRO:HG3	1.73	0.54
1:A:246:PRO:O	1:A:289:VAL:HB	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LYS:N	1:B:257:ARG:HB2	2.23	0.54
1:A:1:MET:H	1:A:29:HIS:CD2	2.26	0.54
1:B:108:ASP:O	1:B:112:LEU:HB2	2.08	0.54
1:B:328:ILE:HG22	1:B:345:VAL:HG12	1.89	0.54
1:A:147:HIS:HD2	1:A:202:GLY:HA2	1.71	0.53
1:B:281:LEU:HD12	1:B:282:ARG:N	2.24	0.53
1:A:146:ARG:HD2	1:A:203:GLN:OE1	2.09	0.53
1:B:255:THR:O	1:B:256:LYS:CB	2.55	0.53
1:B:364:LEU:CD1	1:B:369:ALA:HB3	2.39	0.53
1:B:298:ASP:O	1:B:299:GLU:HB2	2.09	0.53
1:B:38:ASN:ND2	1:B:38:ASN:H	2.07	0.53
1:A:389:ARG:NH1	1:A:389:ARG:HG2	2.15	0.52
1:A:414:HIS:CD2	1:B:414:HIS:CD2	2.98	0.52
1:A:7:PRO:HB3	1:A:17:LEU:HD12	1.91	0.52
1:A:209:ILE:HG22	1:A:210:PRO:CD	2.39	0.52
1:A:112:LEU:HD21	1:A:138:VAL:HG11	1.91	0.52
1:B:297:ASP:CG	1:B:298:ASP:N	2.62	0.52
1:B:294:THR:OG1	3:B:630:HOH:O	1.98	0.52
1:A:146:ARG:HH22	1:A:426:GLU:HB2	1.73	0.52
1:B:55:ASP:OD1	1:B:110:ARG:NH1	2.41	0.51
1:A:226:PHE:CD2	1:A:338:GLU:HB2	2.46	0.51
1:B:386:GLN:O	1:B:387:LEU:C	2.48	0.51
1:B:254:LEU:HD13	1:B:255:THR:HA	1.91	0.51
1:B:306:LEU:CD2	1:B:306:LEU:H	2.21	0.51
1:B:352:GLY:HA3	1:B:353:THR:HG23	1.92	0.51
1:B:141:ARG:HG3	1:B:199:ILE:CD1	2.41	0.51
1:A:286:ARG:NH1	1:A:286:ARG:HG2	2.21	0.51
1:A:404:ARG:HH11	1:A:405:ARG:NH2	2.09	0.51
1:B:154:LEU:HD12	1:B:356:ASP:HB2	1.92	0.51
1:A:256:LYS:HD3	1:A:257:ARG:N	2.26	0.50
1:B:300:VAL:O	1:B:301:ARG:NH2	2.45	0.50
1:A:106:LEU:N	1:A:106:LEU:HD23	2.27	0.50
1:A:250:ILE:HG12	1:A:329:ILE:HB	1.93	0.50
1:A:342:VAL:HG22	1:A:407:ILE:HG21	1.94	0.50
1:A:337:GLN:O	1:A:340:ALA:HB3	2.11	0.50
1:B:256:LYS:CA	1:B:257:ARG:HB2	2.42	0.50
1:A:166:GLU:O	1:A:169:GLU:HB3	2.12	0.49
1:B:196:ASP:O	1:B:199:ILE:HG12	2.11	0.49
1:B:287:LEU:HD12	1:B:380:GLU:OE1	2.12	0.49
1:B:350:LEU:HD11	1:B:378:PHE:CE1	2.48	0.49
1:A:115:LEU:HD23	1:A:139:VAL:HG21	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLY:HA2	1:B:331:HIS:CG	2.47	0.49
1:A:135:SER:O	1:A:139:VAL:HG23	2.13	0.49
1:B:253:GLY:O	1:B:331:HIS:HE1	1.90	0.49
1:A:41:SER:HA	1:A:44:THR:HG22	1.95	0.49
1:B:253:GLY:C	1:B:331:HIS:CE1	2.85	0.49
1:A:368:GLY:O	1:A:396:PHE:HA	2.13	0.49
1:B:327:VAL:CG1	1:B:328:ILE:N	2.75	0.48
1:B:254:LEU:HD23	1:B:298:ASP:OD2	2.13	0.48
1:A:18:VAL:O	1:A:21:ALA:HB3	2.12	0.48
1:A:278:GLU:O	1:A:282:ARG:HG2	2.13	0.48
1:B:257:ARG:NH1	1:B:257:ARG:HG3	2.25	0.48
1:A:139:VAL:HG12	1:A:143:LEU:HD12	1.96	0.48
1:B:350:LEU:HD12	1:B:373:LEU:HB2	1.96	0.48
1:A:322:LEU:HD21	1:A:328:ILE:HD12	1.95	0.48
1:A:37:PRO:HA	1:A:40:VAL:HG23	1.94	0.48
1:A:18:VAL:HB	1:A:19:PRO:HD3	1.96	0.47
1:A:315:TYR:CE1	2:A:501:TYD:C2	2.98	0.47
1:A:23:ALA:HB2	1:B:26:ALA:HB1	1.95	0.47
1:A:35:ILE:O	1:A:52:PRO:HA	2.15	0.47
1:A:7:PRO:HB3	1:A:17:LEU:CD1	2.44	0.47
1:B:22:TRP:O	1:B:23:ALA:C	2.52	0.47
1:B:375:PRO:O	1:B:377:THR:N	2.40	0.47
1:A:247:ARG:HB2	3:A:605:HOH:O	2.14	0.47
1:B:316:VAL:HG21	1:B:321:LEU:HD22	1.96	0.47
1:A:17:LEU:HD23	1:A:150:MET:CE	2.44	0.47
1:A:234:VAL:O	1:A:236:PRO:HD3	2.15	0.47
1:A:299:GLU:HB2	1:A:300:VAL:CG2	2.44	0.47
1:A:253:GLY:HA3	2:A:501:TYD:H5'1	1.96	0.47
1:B:287:LEU:HD13	1:B:380:GLU:CB	2.35	0.47
1:B:287:LEU:HD13	1:B:380:GLU:C	2.35	0.47
1:B:186:ALA:O	1:B:189:ALA:CB	2.63	0.46
1:A:238:TRP:CZ3	1:A:239:LEU:HD13	2.49	0.46
1:A:257:ARG:HE	1:A:257:ARG:CA	2.29	0.46
1:A:260:SER:O	1:A:262:VAL:N	2.49	0.46
1:B:253:GLY:CA	1:B:331:HIS:CE1	2.98	0.46
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.79	0.46
1:B:189:ALA:O	1:B:190:LYS:C	2.54	0.46
1:A:164:PHE:O	1:A:165:LEU:C	2.53	0.46
1:A:232:PRO:HB3	1:B:44:THR:HB	1.97	0.46
1:A:373:LEU:HD21	1:A:386:GLN:HG3	1.97	0.46
1:B:281:LEU:O	1:B:284:ALA:HB3	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:HB2	1:A:300:VAL:HA	1.93	0.45
1:A:286:ARG:NH2	1:A:380:GLU:OE1	2.49	0.45
1:B:18:VAL:O	1:B:21:ALA:HB3	2.16	0.45
1:A:159:TRP:O	1:A:162:SER:HB3	2.16	0.45
1:A:33:VAL:HB	1:A:43:VAL:HG11	1.97	0.45
1:B:130:ASP:O	1:B:132:MET:N	2.50	0.45
1:B:383:VAL:O	1:B:387:LEU:HB2	2.17	0.45
1:A:355:TRP:N	1:A:355:TRP:HD1	2.13	0.45
1:A:333:SER:CB	2:A:501:TYD:O2B	2.64	0.45
1:A:175:GLN:O	1:A:177:VAL:N	2.45	0.45
1:A:252:ARG:NH1	1:A:333:SER:HB3	2.30	0.45
1:B:135:SER:OG	1:B:136:GLY:N	2.50	0.45
1:B:24:LEU:O	1:B:25:ARG:C	2.55	0.45
1:B:403:ILE:O	1:B:406:GLU:HB2	2.16	0.45
1:B:190:LYS:HB3	1:B:190:LYS:HE2	1.70	0.45
1:A:418:PRO:HA	1:A:421:GLU:HG3	1.99	0.44
1:A:226:PHE:CE2	1:A:338:GLU:HB2	2.52	0.44
1:A:213:MET:HE3	1:A:360:ARG:HB3	1.98	0.44
1:A:286:ARG:HB2	1:A:384:ARG:HD3	1.99	0.44
1:B:282:ARG:NH1	1:B:286:ARG:HG3	2.32	0.44
1:A:49:THR:HG22	3:A:610:HOH:O	2.17	0.44
1:B:117:GLY:HA2	1:B:120:GLU:OE1	2.18	0.44
1:B:11:SER:O	1:B:12:SER:C	2.55	0.44
1:B:218:ASP:O	1:B:219:LEU:HD23	2.16	0.44
1:B:241:GLU:OE1	1:B:241:GLU:HA	2.16	0.44
1:B:388:ALA:O	1:B:392:ASP:HB2	2.17	0.44
1:A:141:ARG:NH1	1:A:196:ASP:HB2	2.31	0.44
1:B:282:ARG:NH2	1:B:286:ARG:HH11	2.15	0.44
1:A:388:ALA:O	1:A:392:ASP:HB2	2.18	0.44
1:A:300:VAL:O	1:A:305:GLU:N	2.51	0.44
1:A:280:LEU:HD11	1:A:350:LEU:HD22	2.00	0.44
1:B:18:VAL:HB	1:B:19:PRO:HD3	1.99	0.43
1:A:322:LEU:HD11	1:A:328:ILE:HD12	2.00	0.43
1:B:254:LEU:CB	1:B:255:THR:CA	2.85	0.43
1:B:4:LEU:HD23	1:B:127:VAL:HG22	2.00	0.43
1:B:188:LEU:HD13	1:B:195:PHE:HA	2.00	0.43
1:B:289:VAL:CG2	1:B:290:GLU:N	2.80	0.43
1:A:1:MET:HG3	1:A:29:HIS:CD2	2.54	0.43
1:B:254:LEU:O	2:B:501:TYD:O3A	2.37	0.43
1:B:254:LEU:HB2	2:B:501:TYD:H6	2.01	0.43
1:B:37:PRO:HD2	1:B:55:ASP:O	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:HIS:HB3	1:B:130:ASP:OD2	2.19	0.43
1:B:230:ASN:HD22	2:B:501:TYD:H2'1	1.84	0.43
1:B:298:ASP:OD2	2:B:501:TYD:H53	2.18	0.43
1:A:330:HIS:CE1	1:A:337:GLN:HG2	2.54	0.43
1:B:258:ARG:H	1:B:258:ARG:HG3	1.48	0.43
1:B:297:ASP:OD2	1:B:298:ASP:N	2.52	0.43
1:B:387:LEU:C	1:B:387:LEU:CD1	2.87	0.43
1:A:213:MET:CE	1:A:360:ARG:HB3	2.49	0.43
1:A:283:GLY:O	1:A:286:ARG:HG3	2.19	0.43
1:B:314:GLU:CD	1:B:314:GLU:H	2.18	0.43
1:B:230:ASN:HD22	2:B:501:TYD:C2'	2.31	0.43
1:A:172:PRO:HA	1:A:173:PRO:HD2	1.89	0.43
1:A:338:GLU:O	1:A:342:VAL:HB	2.19	0.42
1:B:129:TRP:CD2	1:B:137:PRO:HD3	2.53	0.42
3:A:602:HOH:O	1:B:47:GLY:HA2	2.18	0.42
1:A:181:GLY:O	1:A:184:LEU:HB2	2.19	0.42
1:B:164:PHE:CZ	1:B:168:GLN:HG3	2.54	0.42
1:B:199:ILE:HD13	1:B:199:ILE:N	2.34	0.42
1:A:416:ILE:O	1:A:417:VAL:C	2.58	0.42
1:B:55:ASP:CG	1:B:110:ARG:HD3	2.40	0.42
1:B:116:MET:O	1:B:120:GLU:HG3	2.19	0.42
1:A:299:GLU:CB	1:A:300:VAL:CA	2.92	0.42
1:B:297:ASP:OD1	1:B:313:HIS:N	2.53	0.42
1:B:411:PRO:HB2	1:B:416:ILE:HD13	2.01	0.42
1:B:162:SER:HA	1:B:165:LEU:HB2	2.02	0.42
1:A:295:LEU:O	1:A:314:GLU:HA	2.19	0.42
1:B:129:TRP:HE1	1:B:147:HIS:HD2	1.66	0.42
1:B:258:ARG:HB2	1:B:259:LEU:H	1.49	0.42
1:A:122:TRP:O	1:A:123:GLN:HB2	2.20	0.42
1:A:259:LEU:CA	1:A:260:SER:C	2.89	0.42
1:B:419:ARG:NH2	3:B:620:HOH:O	2.49	0.42
1:A:172:PRO:HB2	1:A:175:GLN:HG3	2.02	0.41
1:A:345:VAL:HA	1:A:346:PRO:HD3	1.95	0.41
1:A:252:ARG:NH1	2:A:501:TYD:O2A	2.46	0.41
1:B:287:LEU:HD11	1:B:290:GLU:OE1	2.20	0.41
1:A:371:LEU:HD21	1:A:396:PHE:CZ	2.54	0.41
1:B:298:ASP:O	1:B:299:GLU:CB	2.68	0.41
1:A:212:TRP:CZ3	1:A:213:MET:HG3	2.55	0.41
1:A:179:PRO:O	1:A:180:LEU:C	2.59	0.41
1:A:195:PHE:CG	1:A:196:ASP:N	2.88	0.41
1:B:316:VAL:HG21	1:B:321:LEU:CD2	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLU:O	1:A:365:ALA:HB3	2.20	0.41
1:B:412:SER:O	1:B:413:PRO:C	2.58	0.41
1:B:4:LEU:HD23	1:B:127:VAL:CG2	2.50	0.41
1:A:298:ASP:O	1:A:299:GLU:HG3	2.20	0.41
1:A:322:LEU:HD11	1:A:328:ILE:CD1	2.50	0.41
1:B:141:ARG:CG	1:B:199:ILE:CD1	2.95	0.41
1:B:245:LYS:HG2	1:B:294:THR:HG22	2.02	0.41
1:B:128:VAL:HA	1:B:148:VAL:O	2.21	0.41
1:B:20:LEU:O	1:B:23:ALA:HB3	2.21	0.41
1:B:289:VAL:HG11	1:B:307:PRO:HG2	2.02	0.41
1:A:53:VAL:HG22	1:A:114:ASP:HB3	2.01	0.41
1:B:252:ARG:O	1:B:331:HIS:HB3	2.21	0.41
1:A:166:GLU:O	1:A:169:GLU:CB	2.70	0.40
1:B:253:GLY:H	1:B:254:LEU:CD2	2.22	0.40
1:B:55:ASP:OD2	1:B:110:ARG:HD3	2.20	0.40
1:A:223:SER:N	3:A:633:HOH:O	2.53	0.40
1:A:295:LEU:N	1:A:313:HIS:O	2.54	0.40
1:A:338:GLU:HA	1:A:341:THR:HB	2.02	0.40
1:A:119:ALA:HB1	1:A:143:LEU:CD1	2.51	0.40
1:B:12:SER:O	1:B:13:HIS:C	2.60	0.40
1:B:136:GLY:N	1:B:137:PRO:HD2	2.36	0.40
1:B:238:TRP:CH2	1:B:313:HIS:ND1	2.90	0.40
1:B:379:THR:HG22	1:B:382:ASP:CG	2.41	0.40
1:A:32:ARG:NH1	1:B:320:GLU:HG3	2.37	0.40
1:A:358:SER:O	1:A:362:GLU:N	2.50	0.40
1:B:364:LEU:HD13	1:B:369:ALA:HB3	2.04	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	365/455 (80%)	308 (84%)	42 (12%)	15 (4%)	3	18
1	B	367/455 (81%)	298 (81%)	56 (15%)	13 (4%)	3	21
All	All	732/910 (80%)	606 (83%)	98 (13%)	28 (4%)	3	19

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	SER
1	A	257	ARG
1	A	258	ARG
1	A	259	LEU
1	A	261	ARG
1	A	274	GLN
1	B	0	HIS
1	B	100	ALA
1	B	256	LYS
1	B	258	ARG
1	B	299	GLU
1	B	305	GLU
1	B	351	PRO
1	A	176	ARG
1	A	256	LYS
1	A	298	ASP
1	A	380	GLU
1	B	259	LEU
1	B	376	ALA
1	A	299	GLU
1	B	190	LYS
1	A	365	ALA
1	A	366	ASP
1	B	12	SER
1	B	298	ASP
1	A	173	PRO
1	A	217	VAL
1	B	304	GLY

### 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	319/386 (83%)	276 (86%)	43 (14%)	4	17
1	B	316/386 (82%)	272 (86%)	44 (14%)	3	15
All	All	635/772 (82%)	548 (86%)	87 (14%)	3	16

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	44	THR
1	A	49	THR
1	A	53	VAL
1	A	57	LEU
1	A	104	LEU
1	A	109	ASP
1	A	110	ARG
1	A	132	MET
1	A	150	MET
1	A	157	SER
1	A	177	VAL
1	A	209	ILE
1	A	217	VAL
1	A	237	GLU
1	A	247	ARG
1	A	252	ARG
1	A	254	LEU
1	A	256	LYS
1	A	257	ARG
1	A	259	LEU
1	A	273	GLU
1	A	277	VAL
1	A	281	LEU
1	A	298	ASP
1	A	299	GLU
1	A	305	GLU
1	A	311	ARG
1	A	334	THR
1	A	335	THR
1	A	337	GLN
1	A	338	GLU
1	A	343	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	355	TRP
1	A	358	SER
1	A	363	LEU
1	A	371	LEU
1	A	381	ASP
1	A	382	ASP
1	A	389	ARG
1	A	395	SER
1	A	405	ARG
1	A	422	LYS
1	B	32	ARG
1	B	38	ASN
1	B	53	VAL
1	B	57	LEU
1	B	104	LEU
1	B	111	SER
1	B	112	LEU
1	B	141	ARG
1	B	150	MET
1	B	165	LEU
1	B	184	LEU
1	B	217	VAL
1	B	223	SER
1	B	235	LEU
1	B	239	LEU
1	B	245	LYS
1	B	247	ARG
1	B	254	LEU
1	B	257	ARG
1	B	258	ARG
1	B	279	ARG
1	B	280	LEU
1	B	282	ARG
1	B	287	LEU
1	B	288	ASP
1	B	291	VAL
1	B	294	THR
1	B	298	ASP
1	B	299	GLU
1	B	303	MET
1	B	306	LEU
1	B	311	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	314	GLU
1	B	316	VAL
1	B	333	SER
1	B	337	GLN
1	B	350	LEU
1	B	353	THR
1	B	359	ARG
1	B	364	LEU
1	B	377	THR
1	B	387	LEU
1	B	392	ASP
1	B	416	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	331	HIS
1	A	399	ASN
1	B	16	ASN
1	B	38	ASN
1	B	103	GLN
1	B	147	HIS
1	B	230	ASN
1	B	337	GLN
1	B	399	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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
2	TYD	A	501	-	23,26,26	2.35	4 (17%)	33,40,40	2.08	9 (27%)
2	TYD	B	501	-	23,26,26	2.65	3 (13%)	33,40,40	2.37	12 (36%)

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	TYD	A	501	-	-	3/16/28/28	0/2/2/2
2	TYD	B	501	-	-	7/16/28/28	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	TYD	C6-N1	-9.93	1.34	1.46
2	A	501	TYD	C6-N1	-8.85	1.35	1.46
2	B	501	TYD	C2-N1	5.86	1.44	1.35
2	A	501	TYD	C6-C5	-4.27	1.38	1.51
2	A	501	TYD	C2-N1	3.62	1.40	1.35
2	B	501	TYD	C6-C5	-3.61	1.40	1.51
2	A	501	TYD	C2-N3	-2.25	1.33	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	TYD	N3-C2-N1	6.35	123.37	116.65
2	A	501	TYD	C2'-C1'-N1	-5.68	108.66	115.61
2	B	501	TYD	C4-N3-C2	-5.25	120.44	126.86
2	B	501	TYD	O4'-C1'-N1	4.97	114.75	108.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TYD	O4'-C1'-N1	4.58	114.25	108.41
2	A	501	TYD	C5-C6-N1	4.55	120.06	111.11
2	B	501	TYD	C5-C6-N1	4.32	119.61	111.11
2	A	501	TYD	C4-N3-C2	-3.48	122.61	126.86
2	B	501	TYD	C5M-C5-C6	3.47	119.75	112.34
2	B	501	TYD	C6-C5-C4	3.11	120.45	111.53
2	A	501	TYD	C5M-C5-C6	3.10	118.96	112.34
2	B	501	TYD	O2-C2-N3	-2.91	116.07	121.50
2	A	501	TYD	N3-C2-N1	2.67	119.48	116.65
2	B	501	TYD	C1'-N1-C2	2.54	121.87	118.50
2	B	501	TYD	C3'-C2'-C1'	2.26	108.21	102.54
2	B	501	TYD	C2'-C1'-N1	-2.22	112.89	115.61
2	B	501	TYD	PA-O3A-PB	-2.21	125.25	132.83
2	A	501	TYD	C6-C5-C4	2.12	117.63	111.53
2	A	501	TYD	O2-C2-N1	-2.07	120.51	123.11
2	A	501	TYD	O2B-PB-O1B	2.05	118.71	110.68
2	B	501	TYD	O2-C2-N1	-2.03	120.55	123.11

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	TYD	C5'-O5'-PA-O1A
2	B	501	TYD	C5'-O5'-PA-O2A
2	B	501	TYD	C3'-C4'-C5'-O5'
2	B	501	TYD	O4'-C4'-C5'-O5'
2	B	501	TYD	C2'-C1'-N1-C2
2	B	501	TYD	C2'-C1'-N1-C6
2	A	501	TYD	C5'-O5'-PA-O3A
2	B	501	TYD	C5'-O5'-PA-O3A
2	A	501	TYD	PA-O3A-PB-O3B
2	A	501	TYD	O4'-C4'-C5'-O5'

There are no ring outliers.

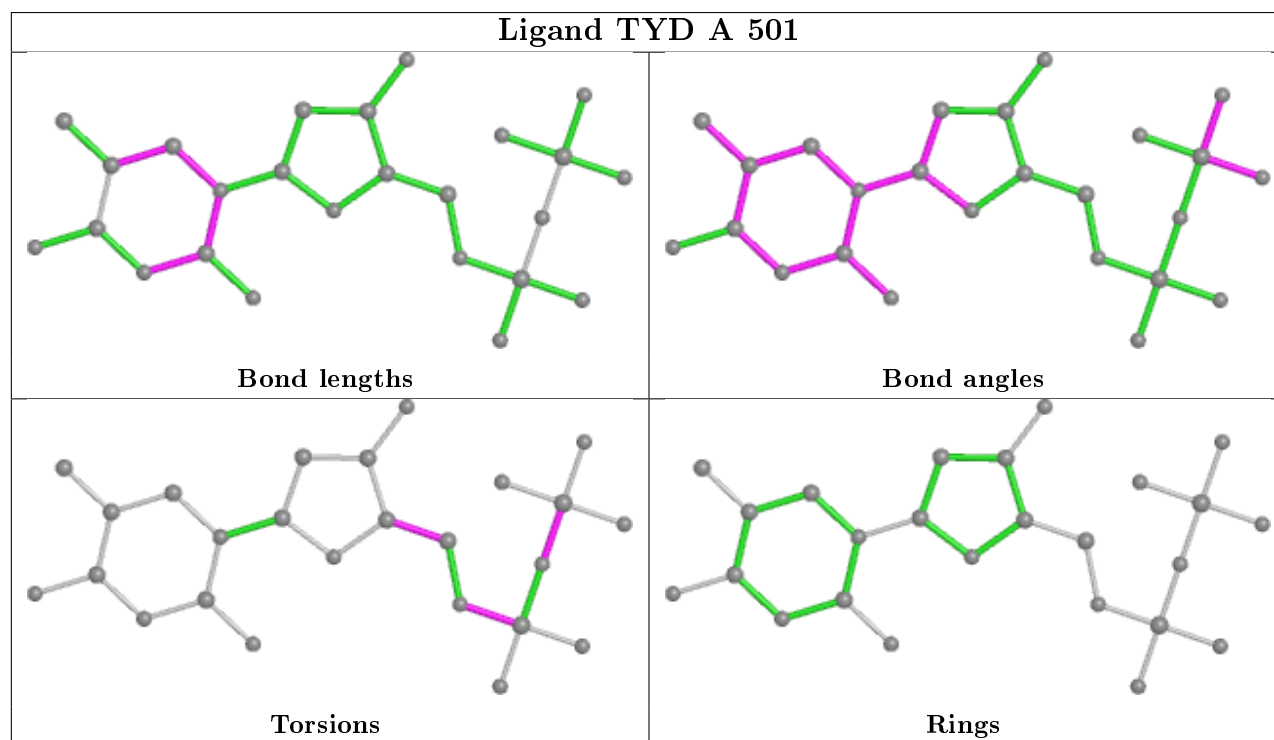
2 monomers are involved in 15 short contacts:

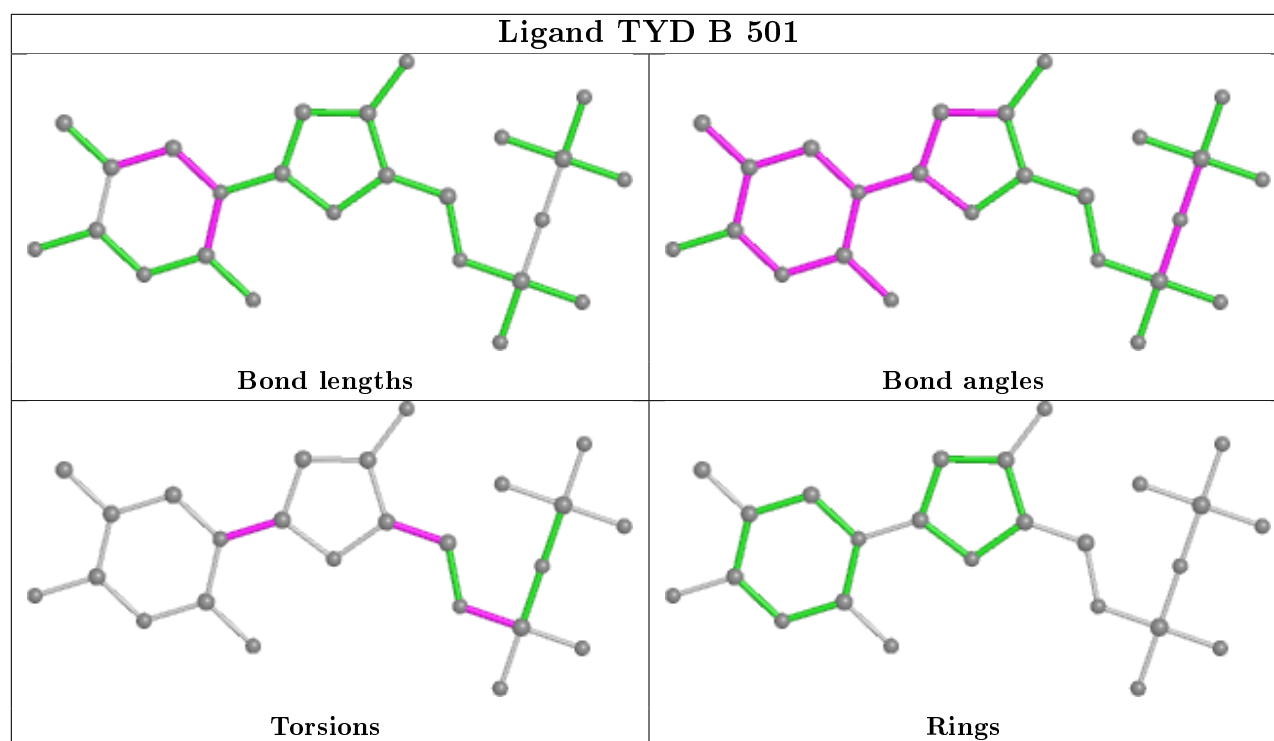
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TYD	5	0
2	B	501	TYD	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	375/455 (82%)	-0.10	8 (2%) 63 49	32, 59, 91, 119	0
1	B	373/455 (81%)	-0.27	2 (0%) 91 86	29, 53, 95, 116	0
All	All	748/910 (82%)	-0.18	10 (1%) 77 66	29, 56, 94, 119	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	PHE	3.4
1	A	60	ILE	3.0
1	A	255	THR	2.9
1	A	373	LEU	2.8
1	A	170	SER	2.6
1	A	262	VAL	2.5
1	B	303	MET	2.2
1	A	274	GLN	2.1
1	B	287	LEU	2.1
1	A	281	LEU	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](#)

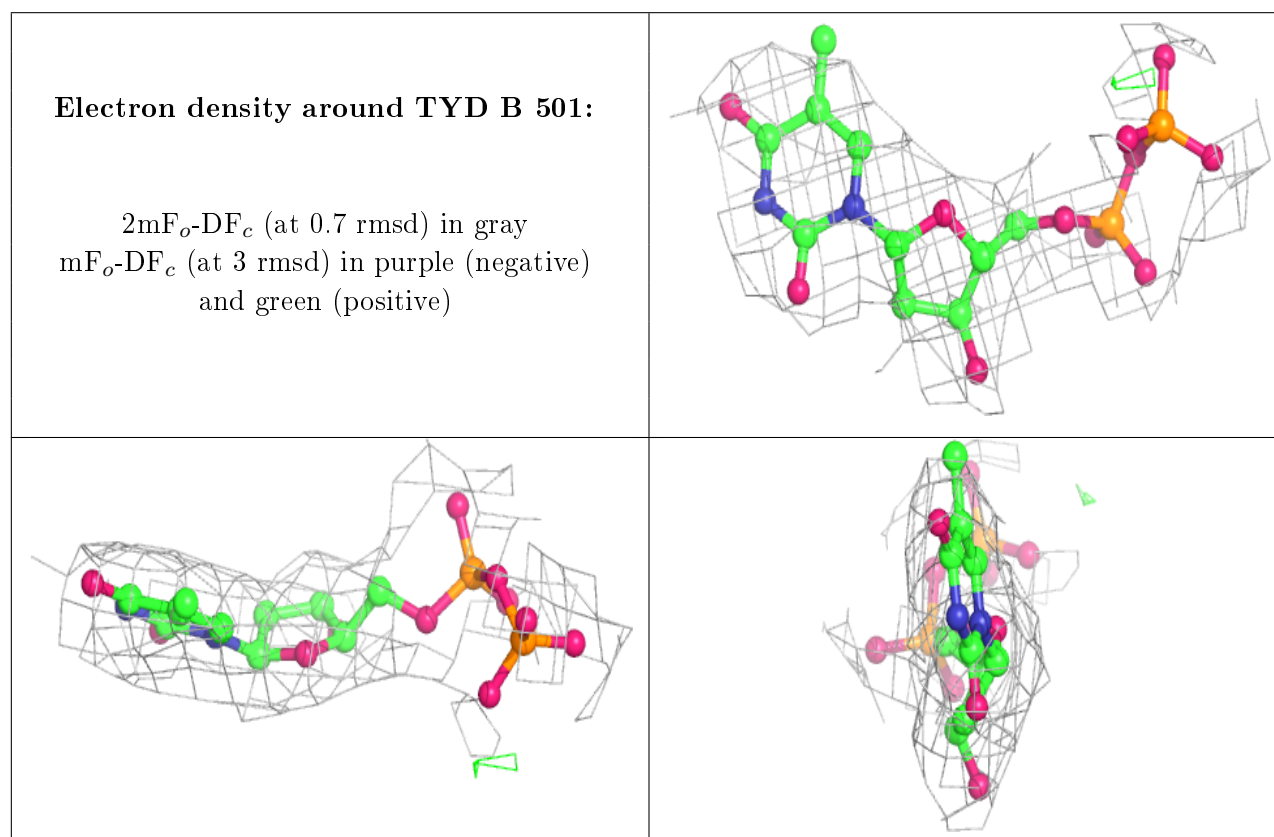
There are no carbohydrates in this entry.

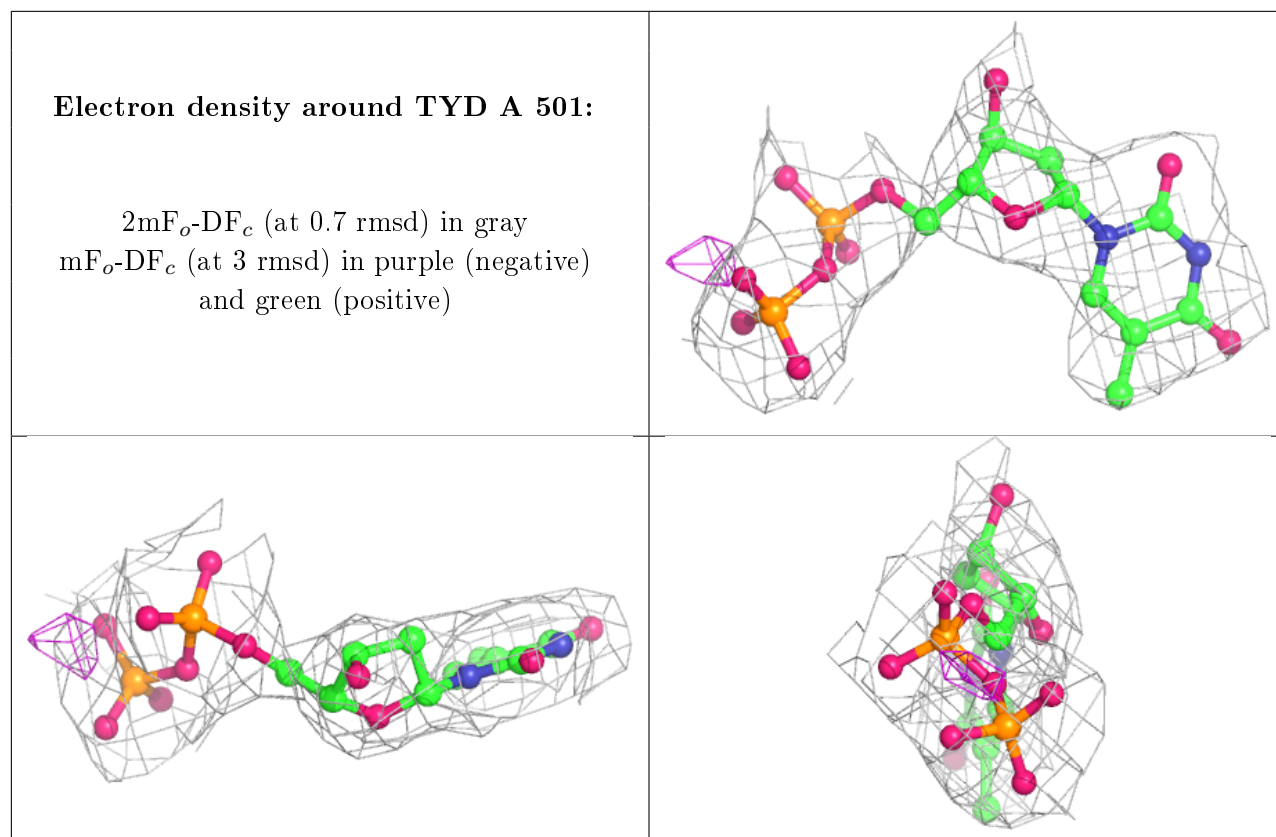
## 6.4 Ligands ⓘ

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
2	TYD	B	501	25/25	0.95	0.14	59,72,78,80	0
2	TYD	A	501	25/25	0.96	0.15	50,65,71,77	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.