



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:04 PM UTC

PDB ID : 4BFV / pdb\_00004bfv  
Title : Crystal structure of Mycobacterium tuberculosis PanK in complex with a triazole inhibitory compound (1d) and phosphate  
Authors : Bjorkelid, C.; Bergfors, T.; Jones, T.A.  
Deposited on : 2013-03-22  
Resolution : 2.29 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

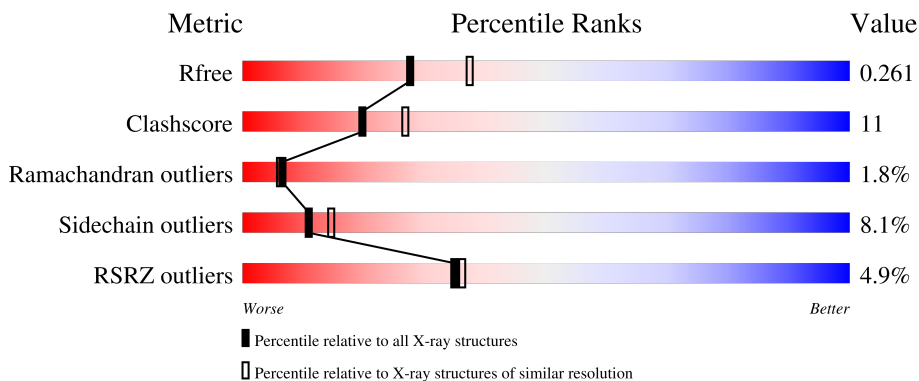
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

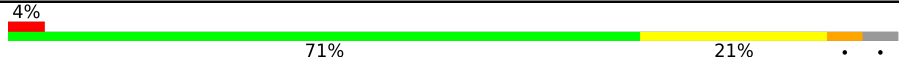
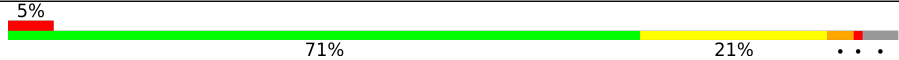
The reported resolution of this entry is 2.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	318	
1	B	318	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5229 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 PANTOTHENATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2471	1573	451	441	6	0	0	0
1	B	306	2471	1573	451	441	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

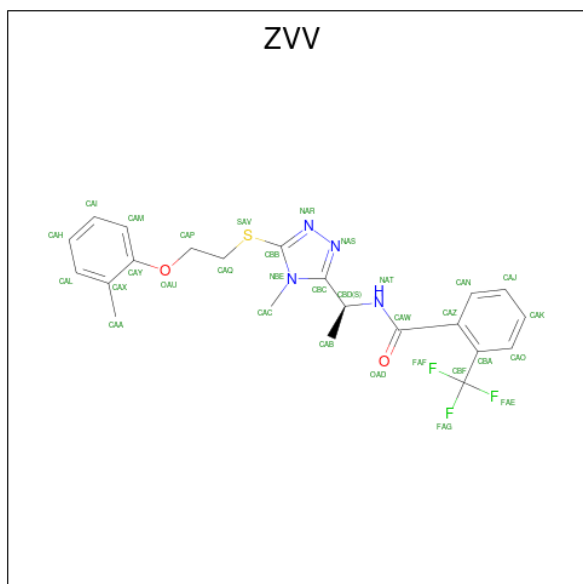
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P63810
A	-4	HIS	-	expression tag	UNP P63810
A	-3	HIS	-	expression tag	UNP P63810
A	-2	HIS	-	expression tag	UNP P63810
A	-1	HIS	-	expression tag	UNP P63810
A	0	HIS	-	expression tag	UNP P63810
B	-5	HIS	-	expression tag	UNP P63810
B	-4	HIS	-	expression tag	UNP P63810
B	-3	HIS	-	expression tag	UNP P63810
B	-2	HIS	-	expression tag	UNP P63810
B	-1	HIS	-	expression tag	UNP P63810
B	0	HIS	-	expression tag	UNP P63810

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is N-[1-(4-methyl-5-{[2-(2-methylphenoxy)ethyl]sulfanyl}-4H-1,2,4-triazol-3-yl)ethyl]-2-(trifluoromethyl)benzamide (CCD ID: ZVV) (formula: C<sub>22</sub>H<sub>23</sub>F<sub>3</sub>N<sub>4</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O S 32 22 3 4 2 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
3	B	1	32	22	3	4	2	1	0	0

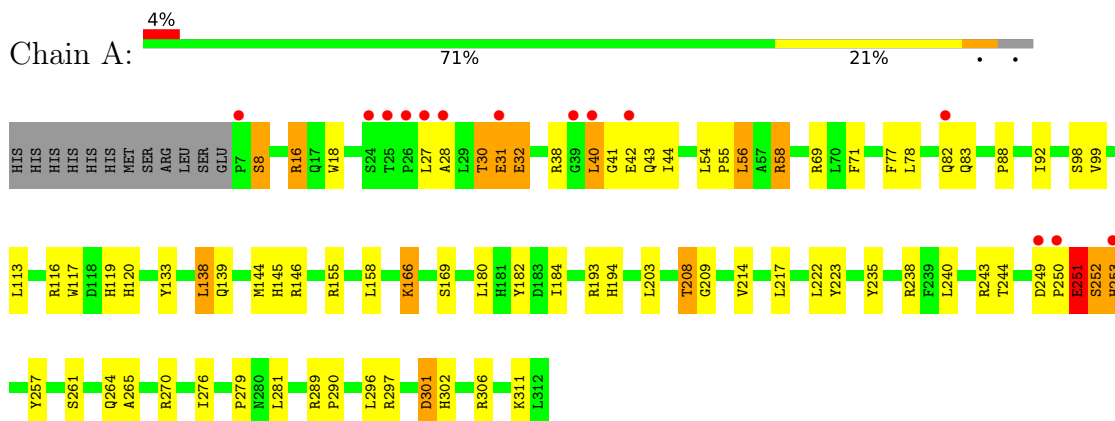
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	94	Total	O	0	0
			94	94		

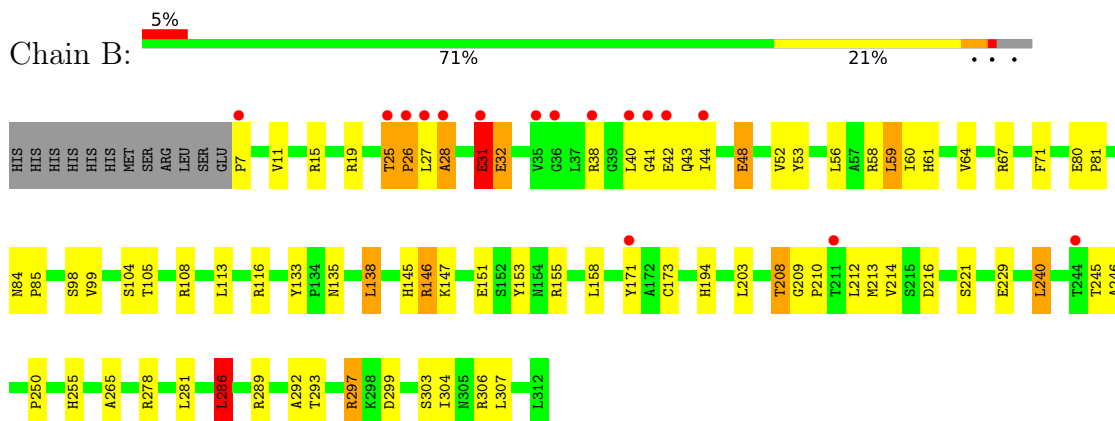
### 3 Residue-property plots [i](#)

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: PANTOTHENATE KINASE



- Molecule 1: PANTOTHENATE KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.33Å 151.77Å 63.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.29 39.51 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.51-2.29) 99.9 (39.51-2.29)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.03 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.203 , 0.262 0.203 , 0.261	Depositor DCC
$R_{free}$ test set	1946 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtrriage
Anisotropy	0.883	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7770e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PO4, ZVV

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	0.71	0/2531	0.97	3/3442 (0.1%)
1	B	0.69	0/2531	0.96	5/3442 (0.1%)
All	All	0.70	0/5062	0.97	8/6884 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	31	GLU	N-CA-C	7.26	126.27	110.80
1	B	31	GLU	CA-C-N	6.32	133.07	121.70
1	B	31	GLU	C-N-CA	6.32	133.07	121.70
1	A	31	GLU	CA-C-N	5.59	131.77	121.70
1	A	31	GLU	C-N-CA	5.59	131.77	121.70
1	B	53	TYR	N-CA-C	5.17	116.92	111.28
1	B	286	LEU	CA-C-N	-5.05	114.87	119.82
1	B	286	LEU	C-N-CA	-5.05	114.87	119.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	PRO	Peptide

## 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	2471	0	2473	61	0
1	B	2471	0	2473	63	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	32	0	23	1	0
3	B	32	0	23	0	0
4	A	119	0	0	9	0
4	B	94	0	0	8	0
All	All	5229	0	4992	115	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 11.

All (115) 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:31:GLU:H	1:A:32:GLU:HB3	1.14	1.07
1:B:26:PRO:HB2	1:B:27:LEU:HA	1.06	1.05
1:A:209:GLY:O	1:B:208:THR:HG21	1.63	0.99
1:B:26:PRO:CB	1:B:27:LEU:HA	1.94	0.97
1:B:26:PRO:HB2	1:B:27:LEU:CA	1.92	0.96
1:A:261:SER:H	1:A:264:GLN:HE21	1.08	0.95
1:A:250:PRO:O	1:A:251:GLU:HB2	1.72	0.89
1:A:133:TYR:HB2	1:A:138:LEU:HD13	1.60	0.82
1:A:31:GLU:N	1:A:32:GLU:HB3	1.94	0.82
1:B:31:GLU:CB	1:B:32:GLU:HB2	2.10	0.82
1:A:261:SER:OG	1:A:264:GLN:HG3	1.81	0.80
1:B:31:GLU:HB2	1:B:32:GLU:HB2	1.64	0.79
1:A:182:TYR:HD2	1:A:253:HIS:HE1	1.30	0.79
1:B:133:TYR:HB2	1:B:138:LEU:HD13	1.67	0.76
1:B:286:LEU:HD11	1:B:289:ARG:HH21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:SER:H	1:A:264:GLN:NE2	1.85	0.72
1:A:182:TYR:CD2	1:A:253:HIS:HE1	2.08	0.71
1:B:15:ARG:HH22	1:B:48:GLU:HG2	1.56	0.71
1:B:27:LEU:HB2	1:B:116:ARG:HH12	1.57	0.69
1:A:41:GLY:HA2	1:A:44:ILE:HD12	1.75	0.68
1:A:31:GLU:H	1:A:32:GLU:CB	2.02	0.67
1:B:104:SER:HB3	4:B:2026:HOH:O	1.98	0.64
1:A:209:GLY:O	1:B:208:THR:CG2	2.44	0.64
1:A:261:SER:N	1:A:264:GLN:HE21	1.88	0.62
1:A:27:LEU:HD21	1:A:58:ARG:HD2	1.82	0.60
1:A:208:THR:HG21	1:B:209:GLY:O	2.03	0.59
4:A:2118:HOH:O	1:B:67:ARG:HD2	2.02	0.58
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.69	0.58
1:B:278:ARG:HD3	4:B:2086:HOH:O	2.04	0.56
1:A:92:ILE:HD12	1:A:166:LYS:HG2	1.87	0.56
1:A:301:ASP:O	1:A:302:HIS:HB2	2.04	0.56
1:B:158:LEU:HG	1:B:214:VAL:HG11	1.88	0.55
1:B:194:HIS:HE1	4:B:2022:HOH:O	1.90	0.54
1:A:240:LEU:HD22	1:A:265:ALA:HB3	1.89	0.54
1:A:113:LEU:O	1:A:116:ARG:HG2	2.08	0.53
1:A:194:HIS:HE1	4:A:2028:HOH:O	1.91	0.53
1:A:139:GLN:HG3	1:A:144:MET:HG2	1.90	0.53
1:A:249:ASP:O	1:A:252:SER:HB3	2.09	0.53
1:A:98:SER:HB2	1:A:281:LEU:HD13	1.90	0.52
1:A:208:THR:HG21	1:B:210:PRO:HA	1.91	0.52
1:B:52:VAL:HG11	1:B:304:ILE:HD13	1.92	0.52
1:A:223:TYR:CD1	1:A:289:ARG:HG3	2.44	0.52
1:B:99:VAL:HG23	1:B:203:LEU:HD21	1.92	0.52
1:B:146:ARG:HD3	1:B:151:GLU:OE2	2.09	0.52
1:A:117:TRP:HB2	1:A:120:HIS:CE1	2.45	0.51
1:B:135:ASN:OD1	1:B:147:LYS:NZ	2.44	0.51
1:B:27:LEU:O	1:B:28:ALA:O	2.29	0.50
1:A:240:LEU:HD22	1:A:265:ALA:CB	2.42	0.50
1:A:182:TYR:HD2	1:A:253:HIS:CE1	2.21	0.49
1:B:145:HIS:CE1	1:B:146:ARG:HG3	2.46	0.49
1:A:193:ARG:O	1:A:194:HIS:C	2.55	0.49
1:B:245:THR:OG1	1:B:246:ALA:N	2.46	0.49
4:A:2080:HOH:O	1:B:208:THR:HB	2.12	0.49
1:B:26:PRO:HD2	4:B:2009:HOH:O	2.13	0.49
1:B:145:HIS:CD2	4:B:2044:HOH:O	2.66	0.49
1:B:31:GLU:CA	1:B:32:GLU:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:CG2	1:B:203:LEU:HD21	2.43	0.48
1:B:286:LEU:CD1	1:B:289:ARG:HH21	2.21	0.48
1:A:78:LEU:HD21	1:B:59:LEU:HD11	1.96	0.48
1:B:145:HIS:HD2	4:B:2044:HOH:O	1.97	0.48
1:A:311:LYS:HD2	1:B:85:PRO:HG2	1.96	0.48
1:B:212:LEU:HD12	1:B:216:ASP:OD2	2.14	0.48
1:B:60:ILE:O	1:B:64:VAL:HG23	2.14	0.48
4:A:2078:HOH:O	1:B:208:THR:HG22	2.13	0.47
1:A:243:ARG:HG2	1:A:257:TYR:O	2.15	0.47
1:A:139:GLN:HG3	1:A:144:MET:CG	2.44	0.47
1:B:58:ARG:O	1:B:61:HIS:HB3	2.15	0.47
1:B:240:LEU:HD22	1:B:265:ALA:HB3	1.96	0.46
1:A:311:LYS:HD2	1:B:85:PRO:CG	2.45	0.46
1:A:180:LEU:HD12	1:A:252:SER:HB2	1.97	0.46
1:A:289:ARG:N	1:A:290:PRO:HD2	2.30	0.46
1:B:44:ILE:HD11	1:B:105:THR:HG23	1.97	0.46
1:B:19:ARG:HD3	4:B:2006:HOH:O	2.15	0.46
1:A:145:HIS:HE1	4:A:2055:HOH:O	1.99	0.46
1:B:240:LEU:HD22	1:B:265:ALA:CB	2.46	0.46
1:B:27:LEU:HB2	1:B:116:ARG:NH1	2.29	0.45
1:B:221:SER:OG	1:B:292:ALA:HA	2.16	0.45
1:A:145:HIS:CE1	4:A:2055:HOH:O	2.70	0.45
1:A:302:HIS:HE1	4:A:2032:HOH:O	2.00	0.45
1:B:145:HIS:CD2	1:B:145:HIS:H	2.34	0.45
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.54	0.44
1:A:56:LEU:HD21	1:A:296:LEU:HD21	1.98	0.44
1:A:270:ARG:HD3	4:A:2101:HOH:O	2.16	0.44
1:A:77:PHE:CE1	1:B:58:ARG:HD3	2.52	0.44
1:A:8:SER:O	1:A:311:LYS:HE2	2.17	0.44
1:A:69:ARG:HB3	4:A:2018:HOH:O	2.17	0.44
1:B:15:ARG:NH1	1:B:48:GLU:OE2	2.50	0.44
1:B:31:GLU:CA	1:B:32:GLU:CB	2.96	0.43
1:B:98:SER:HB2	1:B:281:LEU:HD13	1.99	0.43
1:B:41:GLY:O	1:B:43:GLN:N	2.51	0.43
1:A:30:THR:OG1	1:A:32:GLU:HB3	2.18	0.43
1:A:158:LEU:HG	1:A:214:VAL:HG11	1.99	0.43
1:B:108:ARG:HH11	1:B:108:ARG:HG3	1.84	0.43
1:A:27:LEU:HB3	1:A:54:LEU:HD21	2.00	0.42
1:B:81:PRO:HG2	1:B:84:ASN:HB2	2.00	0.42
1:B:113:LEU:O	1:B:116:ARG:HD2	2.20	0.42
1:B:229:GLU:H	1:B:229:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:HIS:H	1:A:119:HIS:CD2	2.36	0.42
1:A:18:TRP:HZ2	1:A:55:PRO:HB2	1.85	0.42
1:B:250:PRO:HA	1:B:255:HIS:CD2	2.55	0.42
1:A:40:LEU:H	1:A:40:LEU:HG	1.57	0.42
1:A:71:PHE:CD2	1:A:88:PRO:HD3	2.55	0.41
1:A:208:THR:OG1	1:B:213:MET:HE1	2.19	0.41
1:A:99:VAL:HG23	1:A:203:LEU:HD21	2.02	0.41
1:B:307:LEU:HD12	1:B:307:LEU:N	2.35	0.41
1:B:153:TYR:OH	1:B:203:LEU:HD12	2.20	0.41
1:A:235:TYR:OH	3:A:501:ZVV:NAR	2.46	0.41
1:B:297:ARG:HD3	4:B:2092:HOH:O	2.20	0.41
1:B:299:ASP:HB2	1:B:303:SER:O	2.21	0.41
1:A:16:ARG:HH11	1:A:16:ARG:CG	2.32	0.41
1:B:171:TYR:CE1	1:B:173:CYS:SG	3.13	0.41
1:A:276:ILE:C	1:A:279:PRO:HD2	2.46	0.41
1:B:71:PHE:CD2	1:B:71:PHE:C	2.98	0.40
1:A:145:HIS:H	1:A:145:HIS:CD2	2.40	0.40
1:A:166:LYS:HG3	1:A:217:LEU:HB3	2.02	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	304/318 (96%)	289 (95%)	10 (3%)	5 (2%)	7	7
1	B	304/318 (96%)	288 (95%)	10 (3%)	6 (2%)	6	5
All	All	608/636 (96%)	577 (95%)	20 (3%)	11 (2%)	6	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ALA
1	A	30	THR
1	B	25	THR
1	B	28	ALA
1	B	32	GLU
1	B	42	GLU
1	A	251	GLU
1	B	26	PRO
1	B	31	GLU
1	A	32	GLU
1	A	42	GLU

### 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	264/276 (96%)	239 (90%)	25 (10%)	<b>8</b> <b>10</b>
1	B	264/276 (96%)	246 (93%)	18 (7%)	<b>14</b> <b>20</b>
All	All	528/552 (96%)	485 (92%)	43 (8%)	<b>11</b> <b>14</b>

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	16	ARG
1	A	38	ARG
1	A	40	LEU
1	A	43	GLN
1	A	56	LEU
1	A	58	ARG
1	A	82	GLN
1	A	83	GLN
1	A	138	LEU
1	A	146	ARG
1	A	155	ARG
1	A	166	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	169	SER
1	A	184	ILE
1	A	208	THR
1	A	222	LEU
1	A	238	ARG
1	A	244	THR
1	A	251	GLU
1	A	252	SER
1	A	253	HIS
1	A	297	ARG
1	A	301	ASP
1	A	306	ARG
1	B	11	VAL
1	B	25	THR
1	B	31	GLU
1	B	38	ARG
1	B	40	LEU
1	B	48	GLU
1	B	56	LEU
1	B	59	LEU
1	B	80	GLU
1	B	138	LEU
1	B	146	ARG
1	B	155	ARG
1	B	208	THR
1	B	240	LEU
1	B	286	LEU
1	B	293	THR
1	B	297	ARG
1	B	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	82	GLN
1	A	119	HIS
1	A	145	HIS
1	A	194	HIS
1	A	233	GLN
1	A	253	HIS
1	A	264	GLN
1	A	302	HIS

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Mol	Chain	Res	Type
1	B	119	HIS
1	B	145	HIS
1	B	179	HIS
1	B	233	GLN
1	B	253	HIS
1	B	255	HIS
1	B	264	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](#)

4 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	ZVV	A	501	-	34,34,34	0.99	2 (5%)	44,48,48	1.58	5 (11%)
2	PO4	B	401	-	4,4,4	1.33	0	6,6,6	1.17	1 (16%)
2	PO4	A	401	-	4,4,4	1.21	0	6,6,6	1.01	0
3	ZVV	B	501	-	34,34,34	0.95	2 (5%)	44,48,48	1.91	8 (18%)

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	ZVV	A	501	-	-	5/25/25/25	0/3/3/3
3	ZVV	B	501	-	-	6/25/25/25	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ZVV	CBC-NAS	3.50	1.35	1.32
3	B	501	ZVV	CBC-NAS	3.10	1.35	1.32
3	B	501	ZVV	CBB-NBE	-2.35	1.32	1.37
3	A	501	ZVV	CBB-NBE	-2.12	1.32	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	ZVV	NBE-CBB-NAR	9.03	114.90	111.03
3	A	501	ZVV	NBE-CBB-NAR	6.60	113.86	111.03
3	A	501	ZVV	CAQ-SAV-CBB	4.45	107.62	100.57
3	B	501	ZVV	SAV-CBB-NAR	-3.50	122.73	127.78
3	B	501	ZVV	CAP-OAU-CAY	3.01	124.94	117.69
3	A	501	ZVV	SAV-CBB-NAR	-2.66	123.95	127.78
3	B	501	ZVV	CBB-NAR-NAS	-2.44	102.27	107.08
2	B	401	PO4	O3-P-O2	2.39	115.35	107.91
3	B	501	ZVV	OAU-CAY-CAX	2.28	119.85	114.94
3	B	501	ZVV	CAQ-SAV-CBB	2.26	104.16	100.57
3	A	501	ZVV	CBB-NAR-NAS	-2.26	102.62	107.08
3	B	501	ZVV	FAF-CBF-CBA	-2.25	108.65	112.65
3	B	501	ZVV	FAE-CBF-CBA	-2.08	108.96	112.65
3	A	501	ZVV	CAB-CBD-CBC	2.00	114.24	111.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ZVV	CAP-CAQ-SAV-CBB
3	B	501	ZVV	CAP-CAQ-SAV-CBB
3	B	501	ZVV	NAR-CBB-SAV-CAQ
3	A	501	ZVV	NAR-CBB-SAV-CAQ
3	A	501	ZVV	NAS-CBC-CBD-NAT

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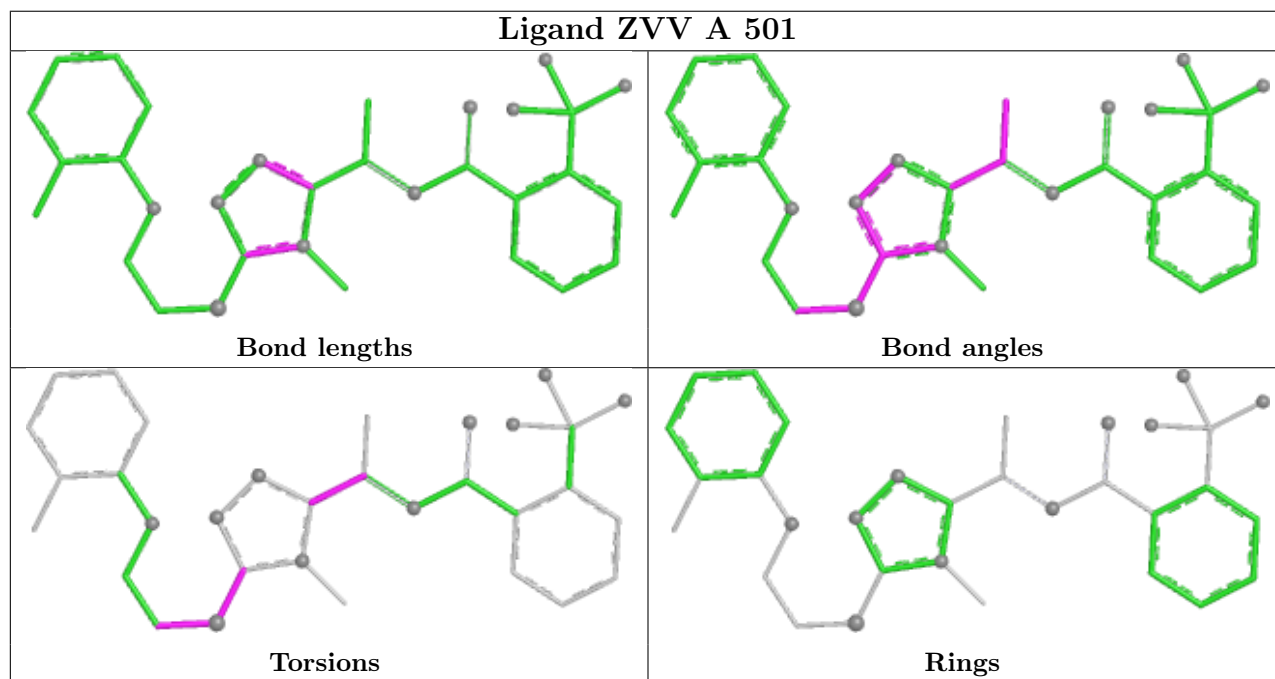
Mol	Chain	Res	Type	Atoms
3	A	501	ZVV	NAS-CBC-CBD-CAB
3	B	501	ZVV	NBE-CBB-SAV-CAQ
3	B	501	ZVV	NAS-CBC-CBD-NAT
3	B	501	ZVV	NAS-CBC-CBD-CAB
3	B	501	ZVV	NBE-CBC-CBD-CAB
3	A	501	ZVV	NBE-CBB-SAV-CAQ

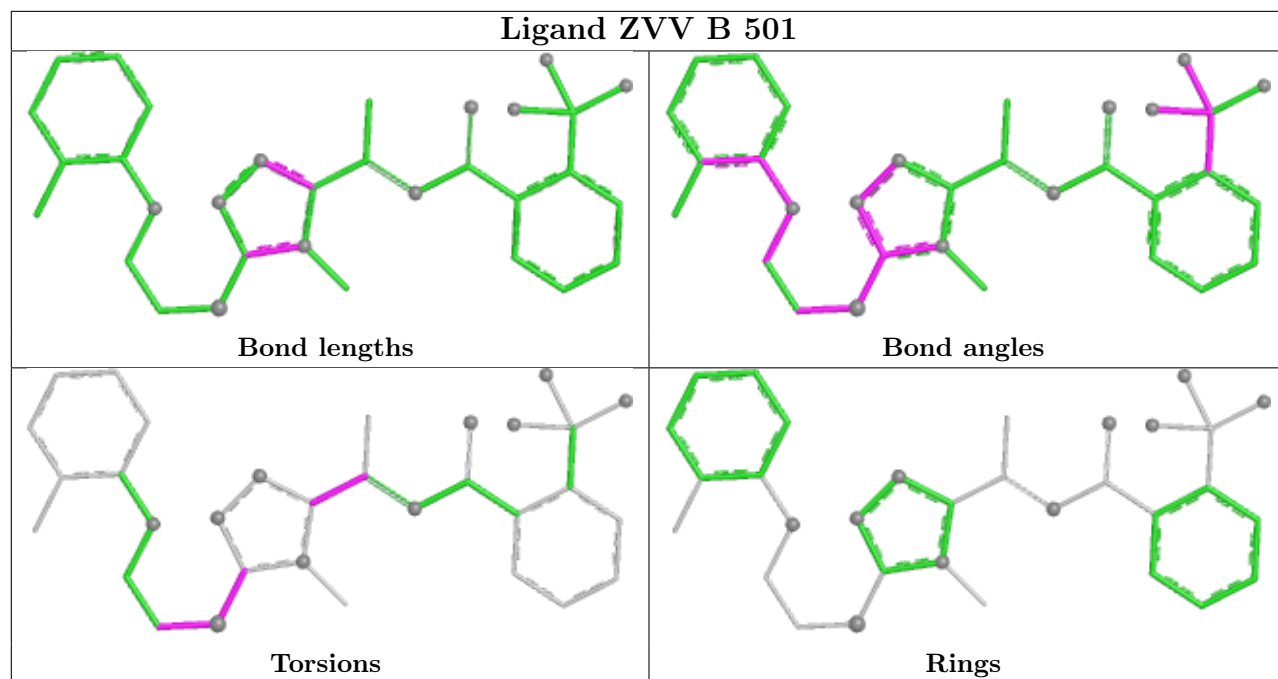
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ZVV	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	306/318 (96%)	0.02	14 (4%) 37 39	13, 27, 62, 99	0
1	B	306/318 (96%)	0.03	16 (5%) 33 34	14, 27, 64, 99	0
All	All	612/636 (96%)	0.02	30 (4%) 35 36	13, 27, 64, 99	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	LEU	6.9
1	A	26	PRO	6.0
1	A	25	THR	5.7
1	B	26	PRO	5.4
1	A	27	LEU	4.7
1	B	7	PRO	4.6
1	A	7	PRO	4.2
1	B	41	GLY	4.1
1	B	25	THR	3.9
1	B	42	GLU	3.4
1	B	211	THR	3.2
1	A	28	ALA	3.2
1	B	28	ALA	3.2
1	B	35	VAL	3.2
1	A	253	HIS	3.2
1	A	24	SER	3.1
1	A	42	GLU	2.7
1	A	40	LEU	2.6
1	B	171	TYR	2.6
1	B	31	GLU	2.5
1	A	39	GLY	2.5
1	B	44	ILE	2.4
1	A	250	PRO	2.4
1	B	40	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	31	GLU	2.3
1	A	82	GLN	2.2
1	B	36	GLY	2.1
1	B	38	ARG	2.1
1	B	244	THR	2.1
1	A	249	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

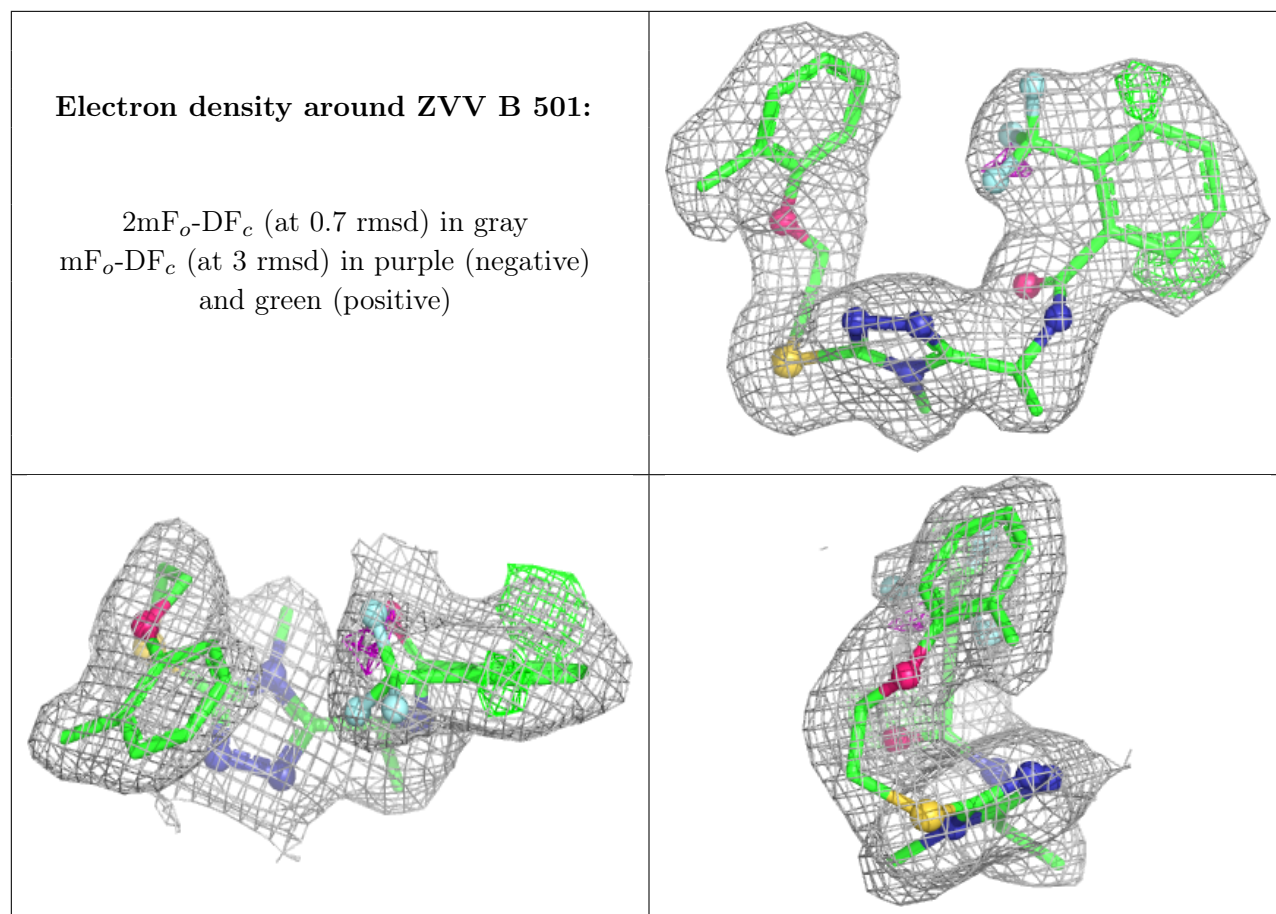
There are no oligosaccharides in this entry.

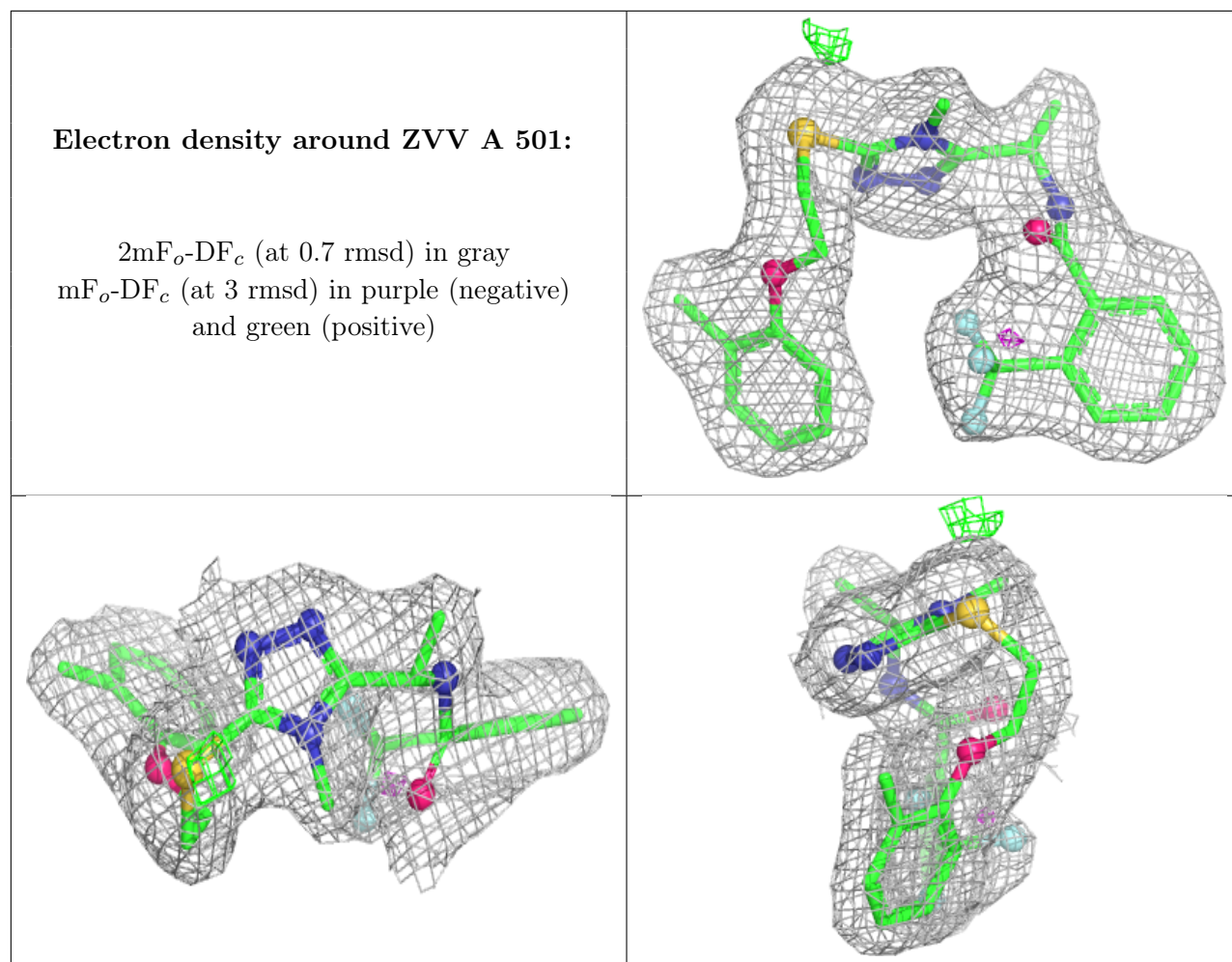
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	ZVV	B	501	32/32	0.92	0.10	26,32,50,55	0
3	ZVV	A	501	32/32	0.96	0.08	27,31,51,57	0
2	PO4	B	401	5/5	0.98	0.06	25,25,27,28	0
2	PO4	A	401	5/5	0.99	0.05	21,21,22,24	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.