



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 04:04 PM EDT

PDB ID : 8TX0
Title : IRAK4 in complex with compound
Authors : Metrick, C.M.; Chodaparambil, J.V.
Deposited on : 2023-08-21
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

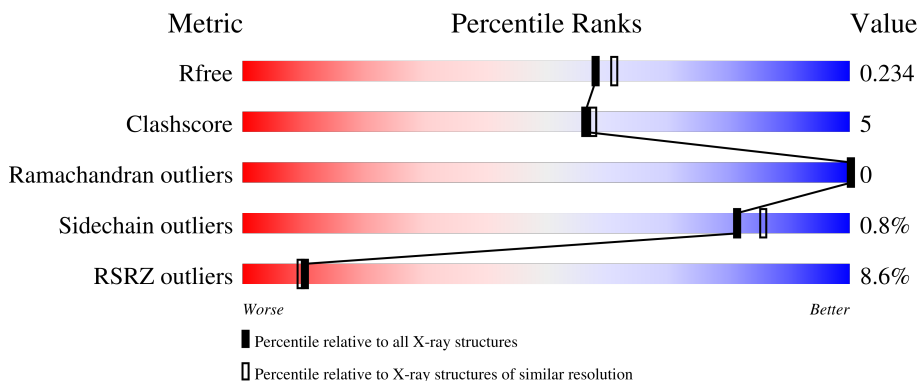
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	307	 9% 83% 10% 7%
1	B	307	 7% 83% 12% 5%

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
3	EDO	A	502	-	-	-	X

2 Entry composition [i](#)

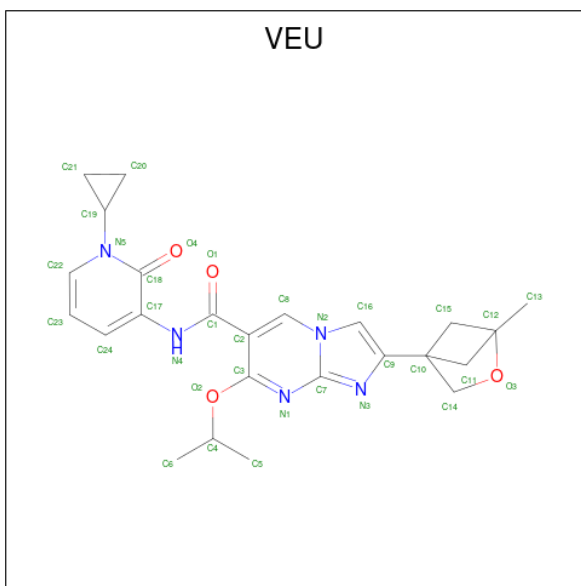
There are 5 unique types of molecules in this entry. The entry contains 4762 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	286	Total	C	N	O	P	S	0	0	0
			2206	1383	370	436	3	14			
1	B	292	Total	C	N	O	P	S	0	0	0
			2251	1412	377	444	3	15			

- Molecule 2 is {N}-(1-cyclopropyl-2-oxidanylidene-pyridin-3-yl)-2-(1-methyl-2-oxabicyclo [2.1.1]hexan-4-yl)-7-propan-2-yloxy-imidazo[1,2-a]pyrimidine-6-carboxamide (three-letter code: VEU) (formula: C₂₄H₂₇N₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			33	24	5	4		
2	B	1	Total	C	N	O	0	0
			33	24	5	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0

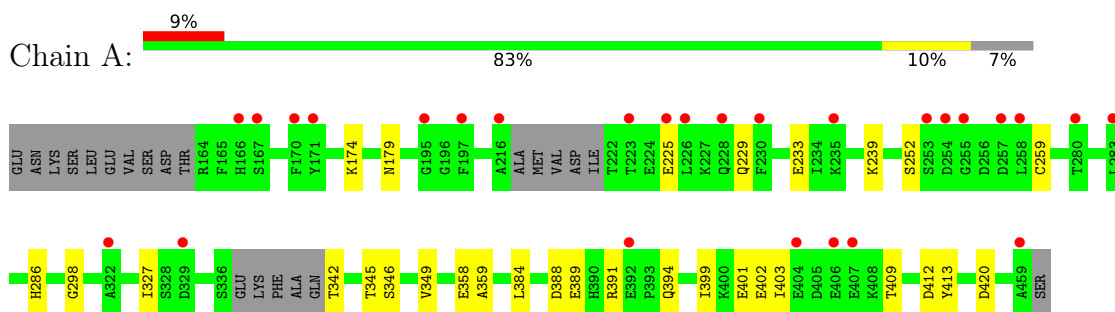
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	98	Total O 98 98	0	0
5	B	124	Total O 124 124	0	0

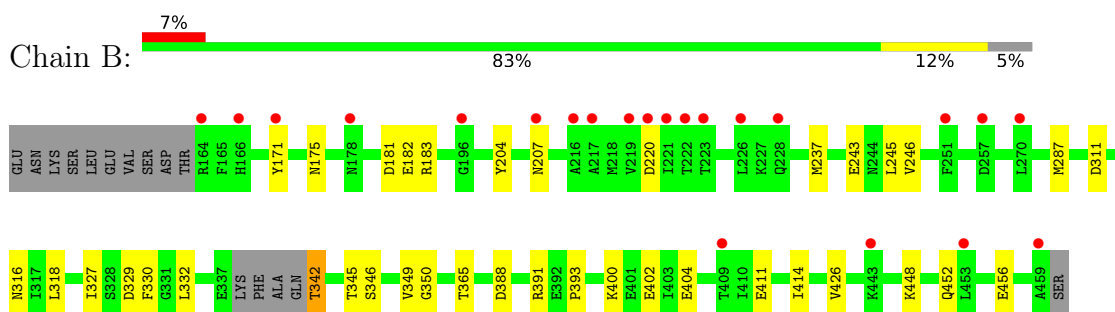
3 Residue-property plots [i](#)

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: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	89.51Å 118.91Å 139.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.66 – 2.00 46.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.66-2.00) 99.9 (46.66-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.238 0.203 , 0.234	Depositor DCC
R_{free} test set	2523 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtrriage
Anisotropy	0.240	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4762	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, NA, EDO, SEP, VEU

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	0.35	0/2209	0.56	0/2982
1	B	0.35	0/2256	0.57	0/3049
All	All	0.35	0/4465	0.56	0/6031

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2206	0	2133	17	0
1	B	2251	0	2178	26	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0
3	A	8	0	9	2	0
3	B	8	0	12	2	0
4	B	1	0	0	0	0
5	A	98	0	0	1	0
5	B	124	0	0	5	0
All	All	4762	0	4332	44	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 5.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:TPO:HG21	1:B:365:THR:HB	1.45	0.96
1:B:237:MET:HE3	5:B:645:HOH:O	1.74	0.88
1:B:245:LEU:HD22	1:B:330:PHE:CZ	2.32	0.64
1:A:389:GLU:HA	1:A:394:GLN:OE1	1.99	0.63
1:A:225:GLU:O	1:A:229:GLN:HG3	2.02	0.59
1:A:399:ILE:O	1:A:403:ILE:HG13	2.04	0.57
1:B:245:LEU:HD23	1:B:327:ILE:HB	1.86	0.57
1:B:350:GLY:HA2	3:B:503:EDO:H21	1.87	0.56
1:B:411:GLU:HA	1:B:414:ILE:HG13	1.88	0.55
1:B:245:LEU:HD22	1:B:330:PHE:HZ	1.70	0.54
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.89	0.53
1:B:316:ASN:OD1	1:B:329:ASP:OD2	2.28	0.52
1:A:286:HIS:ND1	1:A:420:ASP:OD2	2.41	0.52
1:A:349:VAL:H	3:A:503:EDO:H21	1.75	0.51
1:B:237:MET:CE	1:B:246:VAL:O	2.59	0.50
1:B:400:LYS:HE2	1:B:404:GLU:OE2	2.11	0.50
1:A:401:GLU:OE1	1:A:401:GLU:HA	2.12	0.49
1:B:287:MET:HG2	5:B:719:HOH:O	2.10	0.49
1:B:332:LEU:HD22	1:B:349:VAL:HG21	1.95	0.49
1:B:311:ASP:OD1	5:B:601:HOH:O	2.20	0.48
1:B:342:TPO:CG2	1:B:365:THR:HB	2.32	0.48
1:B:342:TPO:HG21	1:B:365:THR:CB	2.32	0.47
1:B:393:PRO:HG3	1:B:402:GLU:OE2	2.14	0.47
1:B:452:GLN:O	1:B:456:GLU:HG3	2.15	0.46
1:A:174:LYS:HG2	1:A:179:ASN:HA	1.96	0.46
1:A:388:ASP:HB3	1:A:391:ARG:HB3	1.98	0.46
1:A:402:GLU:OE1	1:A:413:TYR:OH	2.23	0.46
1:B:237:MET:HE3	1:B:246:VAL:O	2.16	0.46
1:A:349:VAL:H	3:A:503:EDO:C2	2.30	0.44
1:B:220:ASP:CB	5:B:712:HOH:O	2.64	0.44
1:B:204:TYR:CE2	1:B:207:ASN:HA	2.53	0.44
1:B:181:ASP:OD1	1:B:183:ARG:HD3	2.17	0.43
1:A:239:LYS:HA	1:A:239:LYS:HD3	1.82	0.43
1:B:414:ILE:CD1	1:B:426:VAL:HG11	2.48	0.43
3:B:502:EDO:O1	5:B:602:HOH:O	2.20	0.43
1:A:384:LEU:HB3	1:A:391:ARG:NH1	2.34	0.41
1:B:388:ASP:HB3	1:B:391:ARG:HB3	2.02	0.41
1:A:233:GLU:OE2	5:A:601:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:MET:HE1	1:B:246:VAL:O	2.21	0.41
1:A:358:GLU:HG2	1:A:359:ALA:N	2.36	0.40
1:A:409:THR:OG1	1:A:412:ASP:OD2	2.28	0.40
1:B:448:LYS:O	1:B:452:GLN:HG3	2.22	0.40
1:A:252:SER:HB3	1:A:259:CYS:HB2	2.02	0.40
1:A:298:GLY:HA3	1:A:327:ILE:HD12	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	278/307 (91%)	271 (98%)	7 (2%)	0	100	100
1	B	286/307 (93%)	279 (98%)	7 (2%)	0	100	100
All	All	564/614 (92%)	550 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	233/265 (88%)	233 (100%)	0	100	100
1	B	238/265 (90%)	234 (98%)	4 (2%)	60	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	471/530 (89%)	467 (99%)	4 (1%)	81	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	171	TYR
1	B	175	ASN
1	B	182	GLU
1	B	243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	438	HIS
1	A	455	GLN
1	B	241	GLN
1	B	452	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](#)

6 non-standard protein/DNA/RNA residues 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
1	TPO	A	342	1	8,10,11	1.60	1 (12%)	10,14,16	1.49	2 (20%)
1	TPO	B	345	1	8,10,11	1.58	1 (12%)	10,14,16	1.46	1 (10%)
1	SEP	A	346	1	8,9,10	1.62	1 (12%)	8,12,14	1.31	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	B	342	1	8,10,11	0.76	0	10,14,16	1.10	1 (10%)
1	TPO	A	345	1	8,10,11	0.76	0	10,14,16	0.98	1 (10%)
1	SEP	B	346	1	8,9,10	1.60	1 (12%)	8,12,14	0.85	0

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
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	B	345	1	-	2/9/11/13	-
1	SEP	A	346	1	-	4/5/8/10	-
1	TPO	B	342	1	-	5/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	SEP	P-O1P	3.53	1.61	1.50
1	B	346	SEP	P-O1P	3.50	1.61	1.50
1	A	342	TPO	P-O1P	3.32	1.61	1.50
1	B	345	TPO	P-O1P	3.21	1.60	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TPO	P-OG1-CB	-3.95	111.29	123.21
1	B	345	TPO	P-OG1-CB	-3.68	112.10	123.21
1	A	346	SEP	P-OG-CB	-2.48	111.47	118.30
1	B	342	TPO	O-C-CA	-2.43	118.40	124.78
1	A	345	TPO	O-C-CA	-2.31	118.71	124.78
1	A	342	TPO	O-C-CA	-2.03	119.46	124.78
1	A	346	SEP	OG-CB-CA	2.02	110.11	108.14

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	346	SEP	CB-OG-P-O1P
1	A	346	SEP	CB-OG-P-O2P
1	A	346	SEP	CB-OG-P-O3P
1	B	342	TPO	N-CA-CB-CG2
1	B	342	TPO	N-CA-CB-OG1
1	B	342	TPO	C-CA-CB-CG2
1	B	342	TPO	CG2-CB-OG1-P
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	A	345	TPO	CB-OG1-P-O1P
1	A	346	SEP	N-CA-CB-OG
1	A	342	TPO	O-C-CA-CB
1	A	345	TPO	O-C-CA-CB
1	B	342	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	342	TPO	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	VEU	B	501	-	34,38,38	1.09	3 (8%)	34,60,60	1.72	7 (20%)
3	EDO	A	502	-	3,3,3	0.52	0	2,2,2	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	503	-	3,3,3	0.44	0	2,2,2	0.45	0
3	EDO	A	503	-	3,3,3	0.35	0	2,2,2	0.51	0
3	EDO	B	502	-	3,3,3	0.35	0	2,2,2	0.75	0
2	VEU	A	501	-	34,38,38	1.07	3 (8%)	34,60,60	1.58	6 (17%)

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	VEU	B	501	-	-	0/16/43/43	0/7/6/6
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
2	VEU	A	501	-	-	0/16/43/43	0/7/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	VEU	C17-C18	-3.55	1.39	1.47
2	B	501	VEU	C17-C18	-3.43	1.39	1.47
2	B	501	VEU	O3-C12	-3.17	1.41	1.45
2	A	501	VEU	O3-C12	-3.04	1.42	1.45
2	B	501	VEU	C10-C9	-2.25	1.48	1.53
2	A	501	VEU	C10-C9	-2.17	1.48	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	VEU	C18-C17-N4	5.15	117.01	112.30
2	A	501	VEU	C18-C17-N4	4.36	116.28	112.30
2	A	501	VEU	C14-O3-C12	-4.16	101.65	108.43
2	B	501	VEU	C14-O3-C12	-4.11	101.74	108.43
2	A	501	VEU	C13-C12-C11	3.03	123.83	115.57
2	B	501	VEU	C13-C12-C11	3.03	123.81	115.57
2	B	501	VEU	C11-C10-C15	-2.48	84.55	86.95
2	B	501	VEU	C24-C17-C18	-2.41	118.92	120.30
2	A	501	VEU	C24-C17-C18	-2.38	118.93	120.30
2	B	501	VEU	C24-C17-N4	-2.32	124.07	127.20
2	A	501	VEU	C3-N1-C7	2.22	118.50	116.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	VEU	C17-N4-C1	2.19	129.99	122.89
2	A	501	VEU	C11-C10-C15	-2.12	84.90	86.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

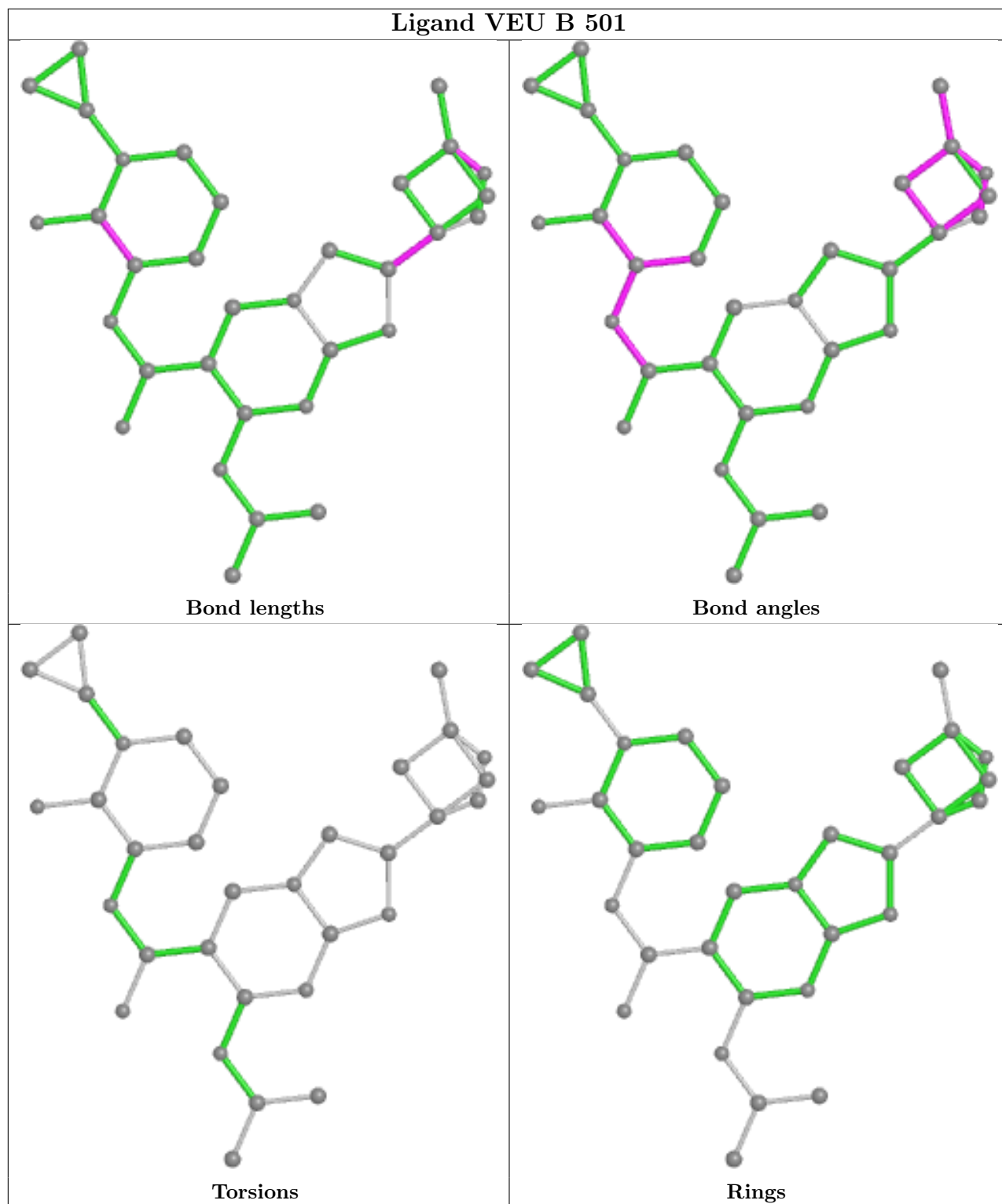
Mol	Chain	Res	Type	Atoms
3	A	502	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2

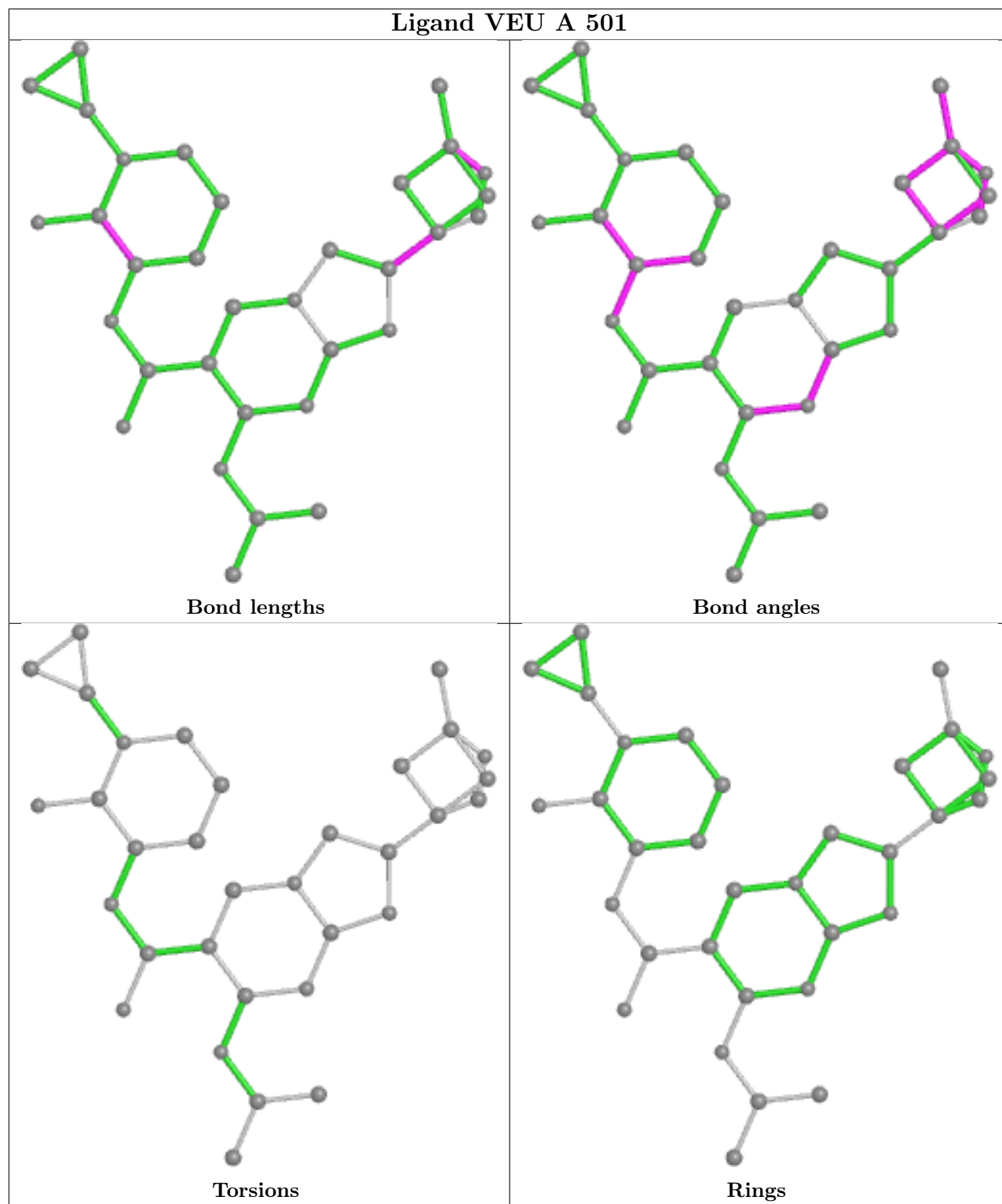
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	EDO	1	0
3	A	503	EDO	2	0
3	B	502	EDO	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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/307 (92%)	0.58	27 (9%) 8 7	28, 46, 83, 107	0
1	B	289/307 (94%)	0.61	22 (7%) 13 13	29, 48, 83, 111	0
All	All	572/614 (93%)	0.59	49 (8%) 10 9	28, 47, 83, 111	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	THR	5.4
1	A	223	THR	4.4
1	A	255	GLY	4.4
1	B	226	LEU	4.4
1	A	216	ALA	4.2
1	A	226	LEU	4.1
1	B	220	ASP	4.1
1	A	195	GLY	4.1
1	B	228	GLN	3.9
1	B	171	TYR	3.9
1	B	164	ARG	3.9
1	B	459	ALA	3.9
1	A	170	PHE	3.9
1	A	459	ALA	3.7
1	A	254	ASP	3.7
1	B	217	ALA	3.7
1	A	230	PHE	3.5
1	A	167	SER	3.3
1	A	253	SER	3.3
1	B	196	GLY	3.2
1	A	225	GLU	3.0
1	B	223	THR	3.0
1	A	197	PHE	2.9
1	A	406	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	453	LEU	2.9
1	B	219	VAL	2.7
1	B	409	THR	2.7
1	B	443	LYS	2.7
1	A	258	LEU	2.7
1	B	251	PHE	2.7
1	A	235	LYS	2.5
1	A	280	THR	2.5
1	B	257	ASP	2.4
1	A	404	GLU	2.4
1	B	178	ASN	2.3
1	A	283	LEU	2.3
1	B	270	LEU	2.2
1	B	221	ILE	2.2
1	A	257	ASP	2.2
1	B	216	ALA	2.2
1	A	329	ASP	2.2
1	A	392	GLU	2.1
1	A	407	GLU	2.1
1	A	166	HIS	2.1
1	A	171	TYR	2.1
1	A	228	GLN	2.1
1	A	322	ALA	2.1
1	B	166	HIS	2.1
1	B	207	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	B	342	11/12	0.74	0.24	69,85,100,107	0
1	SEP	B	346	10/11	0.82	0.19	60,72,104,118	0
1	TPO	A	342	11/12	0.89	0.20	59,84,96,97	0
1	TPO	B	345	11/12	0.91	0.11	54,61,69,72	0
1	SEP	A	346	10/11	0.91	0.19	62,77,114,122	0
1	TPO	A	345	11/12	0.93	0.13	54,65,82,86	0

6.3 Carbohydrates [i](#)

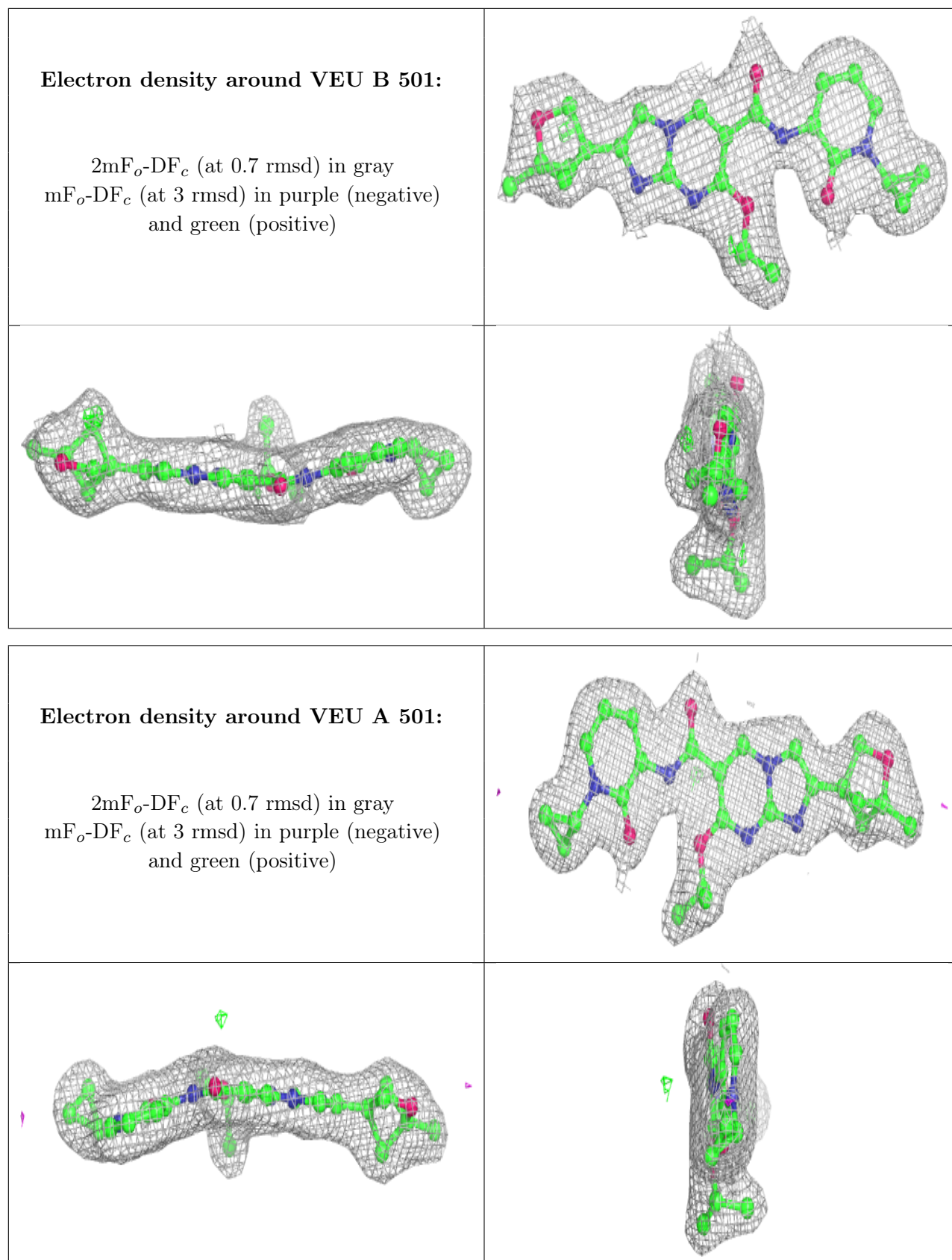
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	502	4/4	0.24	0.44	64,66,67,70	0
3	EDO	B	502	4/4	0.74	0.34	57,63,64,64	0
3	EDO	A	503	4/4	0.84	0.30	54,55,59,61	0
3	EDO	B	503	4/4	0.84	0.18	53,60,62,64	0
4	NA	B	504	1/1	0.87	0.30	60,60,60,60	0
2	VEU	B	501	33/33	0.94	0.14	32,37,43,48	0
2	VEU	A	501	33/33	0.96	0.13	31,36,40,42	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.