Full wwPDB X-ray Structure Validation Report (i)

Jun 20, 2024 – 04:46 PM EDT

PDB ID	:	8TVM
Title	:	IRAK4 in complex with compound 24
Authors	:	Metrick, C.M.; Chodaparambil, J.V.
Deposited on	:	2023-08-18
Resolution	:	2.10 Å(reported)

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

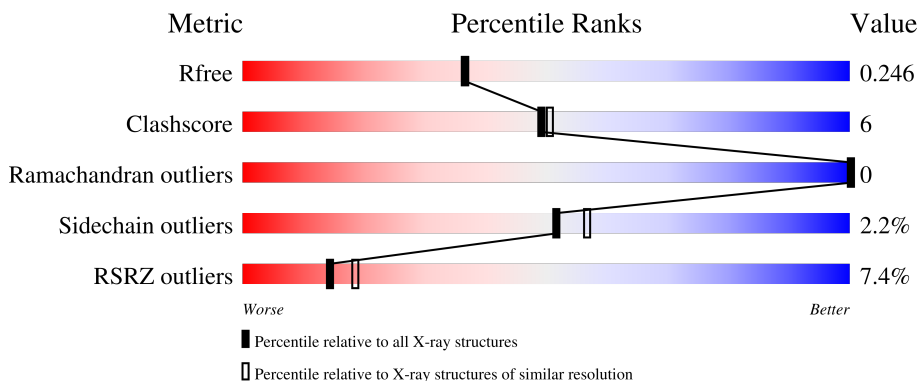|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.10 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		2.2%
RSRZ outliers		7.4%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	7% / 73% / 21% / 7%
1	B	307	6% / 80% / 14% / • 6%
1	C	307	6% / 79% / 12% / 8%
1	D	307	8% / 76% / 14% / 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9274 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
1	A	287	Total	C	N	O	P	S	0	1	0
			2261	1414	383	447	3	14			
1	B	289	Total	C	N	O	P	S	0	0	0
			2233	1397	377	442	3	14			
1	C	281	Total	C	N	O	P	S	0	3	0
			2215	1390	373	434	3	15			
1	D	277	Total	C	N	O	P	S	0	0	0
			2154	1353	362	422	3	14			

- Molecule 2 is N-{1-[(1R,2R)-2-fluorocyclopropyl]-2-oxo-1,2-dihydropyridin-3-yl}-2-[(1R,4r)-1-methyl-2-oxabicyclo[2.1.1]hexan-4-yl]-6-[(propan-2-yl)oxy]-2H-pyrazolo[3,4-b]pyridine-5-carboxamide (three-letter code: VDC) (formula: $C_{24}H_{26}FN_5O_4$) (labeled as "Ligand of Interest" by depositor).
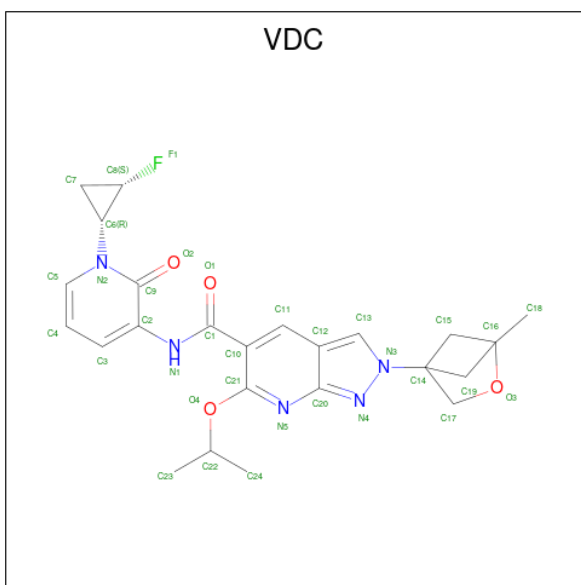
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			34	24	1	5	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			34	24	1	5	4		
2	C	1	Total	C	F	N	O	0	0
			34	24	1	5	4		
2	D	1	Total	C	F	N	O	0	0
			34	24	1	5	4		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	87	Total	O	0	0
			87	87		
3	C	58	Total	O	0	0
			58	58		
3	D	60	Total	O	0	0
			60	60		

3 Residue-property plots ⓘ

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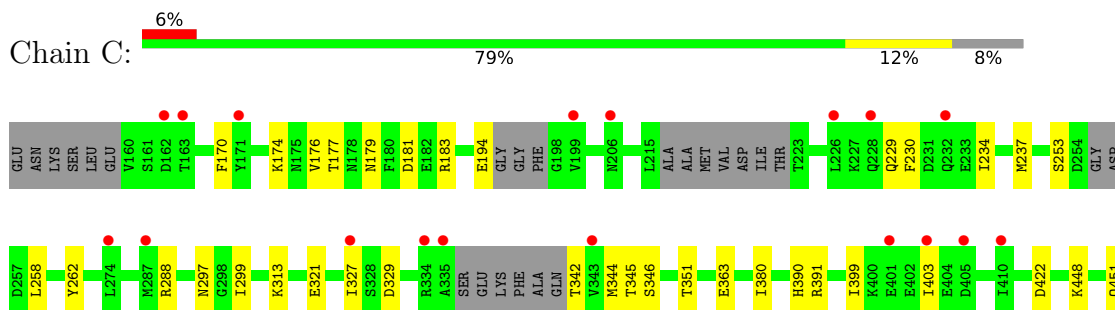
- Molecule 1: Interleukin-1 receptor-associated kinase 4
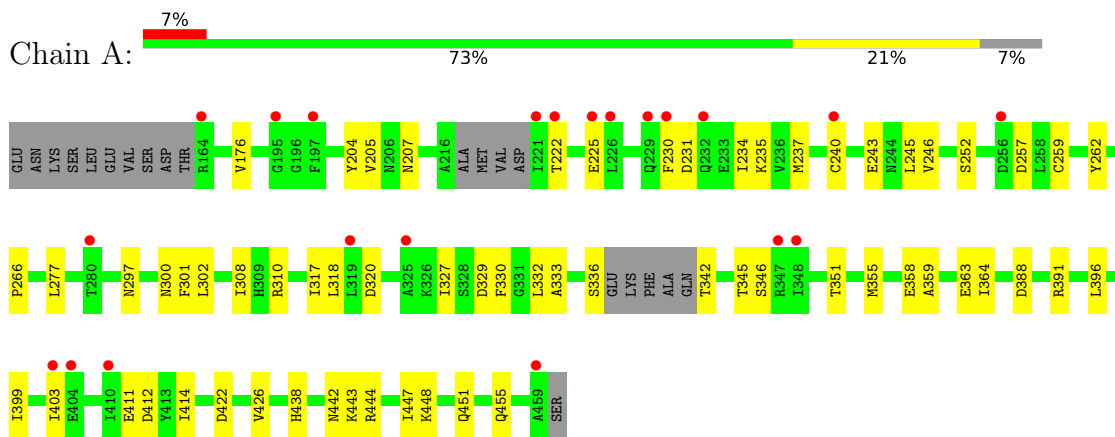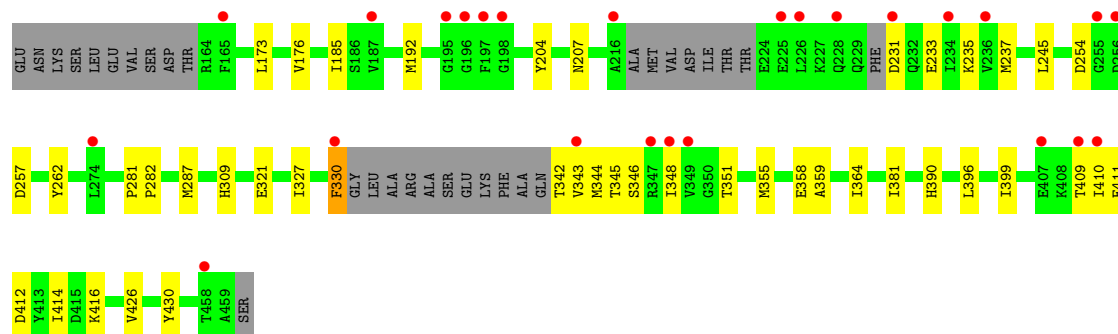

- Molecule 1: Interleukin-1 receptor-associated kinase 4
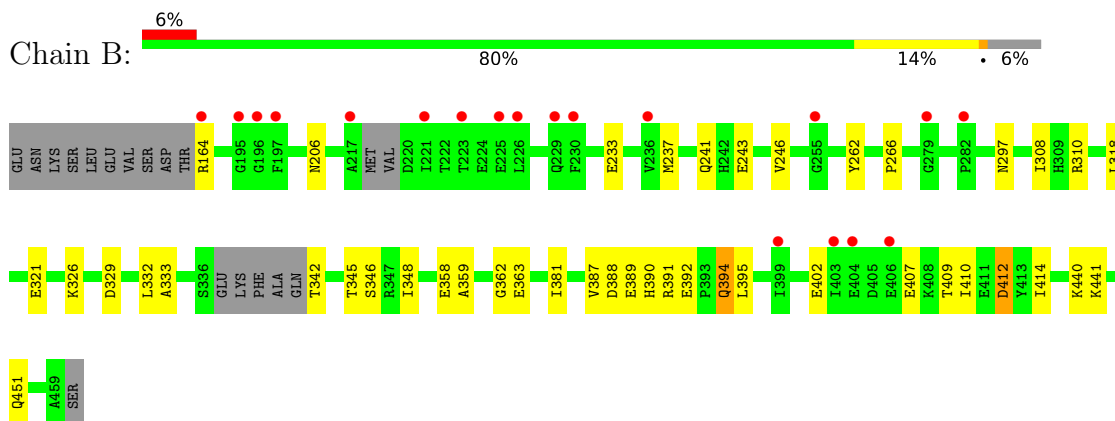
- Molecule 1: Interleukin-1 receptor-associated kinase 4

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

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.38Å 141.98Å 87.78Å 90.00° 126.37° 90.00°	Depositor
Resolution (Å)	48.52 – 2.10 48.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.52-2.10) 97.8 (48.52-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.221 , 0.246 0.220 , 0.246	Depositor DCC
R_{free} test set	3827 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9274	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SEP, VDC, TPO

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	0.30	0/2266	0.52	0/3054
1	B	0.27	0/2236	0.50	0/3018
1	C	0.28	0/2216	0.49	0/2987
1	D	0.30	0/2156	0.50	0/2906
All	All	0.29	0/8874	0.50	0/11965

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	2261	0	2200	36	0
1	B	2233	0	2157	26	0
1	C	2215	0	2148	19	0
1	D	2154	0	2095	28	0
2	A	34	0	0	0	0
2	B	34	0	0	0	0
2	C	34	0	0	0	0
2	D	34	0	0	0	0
3	A	70	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	87	0	0	3	0
3	C	58	0	0	3	0
3	D	60	0	0	1	0
All	All	9274	0	8600	103	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 6.

All (103) 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:411:GLU:HA	1:A:414:ILE:HD12	1.72	0.71
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.78	0.65
1:B:402:GLU:HG2	1:B:407:GLU:OE1	1.99	0.62
1:A:237:MET:HE3	1:A:262:TYR:HE2	1.62	0.62
1:B:326:LYS:NZ	3:B:602:HOH:O	2.20	0.60
1:A:231:ASP:HB3	1:A:235:LYS:HE2	1.83	0.60
1:C:297:ASN:OD1	1:C:451:GLN:NE2	2.28	0.60
1:B:233:GLU:OE1	1:B:262:TYR:OH	2.20	0.60
1:C:170:PHE:O	1:C:174:LYS:HG3	2.02	0.59
1:D:235:LYS:N	1:D:235:LYS:HD3	2.16	0.59
1:D:343:VAL:HG13	1:D:364:ILE:HB	1.84	0.59
1:D:309:HIS:CD2	1:D:330:PHE:HD1	2.20	0.59
1:B:381:ILE:HG21	1:B:410:ILE:HD11	1.85	0.59
1:D:414:ILE:HD11	1:D:426:VAL:HG11	1.85	0.58
1:B:389:GLU:O	1:B:394:GLN:NE2	2.37	0.58
1:A:243:GLU:HG3	1:C:321:GLU:O	2.04	0.58
1:D:233:GLU:OE1	1:D:262:TYR:OH	2.24	0.56
1:D:351:THR:O	1:D:355:MET:HG3	2.05	0.56
1:D:409:THR:HG23	1:D:411:GLU:H	1.71	0.55
1:B:310:ARG:HD3	1:B:332:LEU:O	2.06	0.55
1:A:297:ASN:ND2	1:A:451:GLN:HE21	2.05	0.55
1:D:245:LEU:HD22	1:D:330:PHE:CZ	2.42	0.55
1:A:245:LEU:HD22	1:A:330:PHE:HZ	1.72	0.55
1:C:313:LYS:NZ	3:C:601:HOH:O	2.39	0.55
1:B:390:HIS:O	1:C:391:ARG:HA	2.08	0.53
1:C:455:GLN:O	1:C:458:THR:OG1	2.23	0.53
1:A:451:GLN:O	1:A:455:GLN:HG2	2.08	0.53
1:C:176:VAL:HG23	1:C:177:THR:HG23	1.89	0.53
1:C:422:ASP:HB3	3:C:602:HOH:O	2.09	0.53
1:C:399:ILE:O	1:C:403:ILE:HG12	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ILE:HG12	1:A:426:VAL:HG11	1.89	0.52
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.11	0.51
1:B:391:ARG:HA	1:C:390:HIS:O	2.10	0.50
1:B:409:THR:HG23	1:B:412:ASP:H	1.78	0.49
1:A:277:LEU:HD13	1:D:416:LYS:HE3	1.95	0.49
1:B:409:THR:OG1	3:B:601:HOH:O	2.20	0.48
1:A:388:ASP:HB3	1:A:391:ARG:HB3	1.95	0.48
1:A:358:GLU:HG2	1:A:359:ALA:N	2.28	0.48
1:A:399:ILE:O	1:A:403:ILE:HG12	2.12	0.48
1:D:287:MET:HE1	3:D:659:HOH:O	2.12	0.48
1:D:409:THR:HG23	1:D:411:GLU:N	2.28	0.48
1:A:358:GLU:OE2	1:A:444:ARG:NH2	2.47	0.48
1:D:309:HIS:CD2	1:D:330:PHE:CD1	3.02	0.47
1:A:230:PHE:O	1:A:234:ILE:HG12	2.14	0.47
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.96	0.47
1:B:363:GLU:OE1	1:B:441:LYS:NZ	2.43	0.47
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.96	0.47
1:A:310:ARG:HD3	1:A:332:LEU:O	2.13	0.47
1:B:348:ILE:HG22	1:B:362:GLY:HA2	1.96	0.47
1:B:387:VAL:HG23	1:B:395:LEU:HD12	1.96	0.47
1:B:388:ASP:HB3	1:B:391:ARG:HB3	1.97	0.47
1:D:381:ILE:HG21	1:D:410:ILE:HD11	1.96	0.46
1:B:410:ILE:O	1:B:414:ILE:HG13	2.15	0.46
1:D:409:THR:HG22	1:D:412:ASP:OD2	2.16	0.46
1:D:358:GLU:HG2	1:D:359:ALA:N	2.31	0.45
1:A:308:ILE:O	1:A:333:ALA:HA	2.16	0.45
1:A:391:ARG:HA	1:D:390:HIS:O	2.17	0.45
1:A:302:LEU:HD11	1:A:330:PHE:HE2	1.82	0.45
1:A:266:PRO:HD2	1:A:320:ASP:HA	1.98	0.45
1:D:231:ASP:HB3	1:D:235:LYS:HE2	1.99	0.45
1:C:174:LYS:HE3	1:C:179:ASN:OD1	2.16	0.44
1:C:351:THR:OG1	3:C:601:HOH:O	2.21	0.44
1:A:438[A]:HIS:CD2	1:A:443:LYS:HB3	2.52	0.44
1:B:348:ILE:HD12	1:B:348:ILE:O	2.17	0.44
1:D:204:TYR:CE2	1:D:207:ASN:HA	2.52	0.44
1:D:348:ILE:HD12	1:D:348:ILE:H	1.81	0.44
1:C:253:SER:HA	1:C:258:LEU:HD23	2.00	0.44
1:B:206:ASN:OD1	3:B:603:HOH:O	2.21	0.43
1:B:440:LYS:HE2	1:B:440:LYS:H	1.83	0.43
1:A:240:CYS:HA	1:A:301:PHE:HE2	1.84	0.43
1:C:181:ASP:OD2	1:C:183:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.99	0.43
1:D:204:TYR:CZ	1:D:207:ASN:HA	2.54	0.43
1:D:396:LEU:O	1:D:399:ILE:HG12	2.18	0.43
1:C:299:ILE:HG13	1:C:327[B]:ILE:HD11	2.00	0.43
1:A:351:THR:O	1:A:355:MET:HG3	2.19	0.43
1:C:230:PHE:O	1:C:234:ILE:HG13	2.18	0.43
1:C:237:MET:CE	1:C:262:TYR:HE1	2.30	0.43
1:A:363:GLU:O	1:A:364:ILE:HD13	2.19	0.42
1:B:358:GLU:HG2	1:B:359:ALA:N	2.33	0.42
1:A:302:LEU:HD21	1:A:330:PHE:HE2	1.84	0.42
1:C:344:MET:HG2	1:C:363:GLU:HA	2.00	0.42
1:D:327:ILE:HG22	1:D:330:PHE:HE1	1.84	0.42
1:B:308:ILE:O	1:B:333:ALA:HA	2.19	0.42
1:D:185:ILE:CD1	1:D:192:MET:HG2	2.50	0.42
1:A:246:VAL:HG11	1:A:318:LEU:HD12	2.01	0.42
1:A:317:ILE:HG12	1:A:327:ILE:HD13	2.01	0.42
1:B:266:PRO:HG2	1:B:321:GLU:HG2	2.02	0.42
1:A:297:ASN:HD22	1:A:451:GLN:HE21	1.66	0.42
1:A:176:VAL:HG21	1:A:205:VAL:HG22	2.02	0.41
1:B:243:GLU:HG3	1:D:321:GLU:O	2.20	0.41
1:B:237:MET:HA	1:B:237:MET:HE2	2.02	0.41
1:A:235:LYS:N	1:A:235:LYS:HD3	2.35	0.41
1:B:297:ASN:ND2	1:B:451:GLN:HE21	2.19	0.41
1:D:173:LEU:HA	1:D:176:VAL:HG22	2.03	0.41
1:A:396:LEU:O	1:A:399:ILE:HG12	2.21	0.41
1:A:204:TYR:CZ	1:A:207:ASN:HA	2.56	0.41
1:B:409:THR:HG22	1:B:412:ASP:OD2	2.21	0.41
1:A:245:LEU:HD22	1:A:330:PHE:CZ	2.52	0.41
1:A:302:LEU:HD21	1:A:330:PHE:CE2	2.55	0.41
1:D:233:GLU:O	1:D:237:MET:HG2	2.20	0.41
1:D:281:PRO:HA	1:D:282:PRO:HD3	1.97	0.40
1:D:410:ILE:HD13	1:D:430:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/307 (91%)	276 (99%)	4 (1%)	0	100	100
1	B	281/307 (92%)	275 (98%)	6 (2%)	0	100	100
1	C	272/307 (89%)	262 (96%)	10 (4%)	0	100	100
1	D	267/307 (87%)	257 (96%)	10 (4%)	0	100	100
All	All	1100/1228 (90%)	1070 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/265 (92%)	236 (97%)	7 (3%)	42	46
1	B	235/265 (89%)	229 (97%)	6 (3%)	46	50
1	C	236/265 (89%)	232 (98%)	4 (2%)	60	67
1	D	229/265 (86%)	225 (98%)	4 (2%)	60	67
All	All	943/1060 (89%)	922 (98%)	21 (2%)	52	57

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ASP
1	A	329	ASP
1	A	336	SER
1	A	412	ASP
1	A	422	ASP
1	A	442	ASN
1	A	448	LYS
1	B	164	ARG

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Mol	Chain	Res	Type
1	B	241	GLN
1	B	329	ASP
1	B	392	GLU
1	B	394	GLN
1	B	412	ASP
1	C	194	GLU
1	C	229	GLN
1	C	329	ASP
1	C	448	LYS
1	D	254	ASP
1	D	257	ASP
1	D	330	PHE
1	D	344	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	297	ASN
1	A	305	ASN
1	B	297	ASN
1	B	394	GLN
1	B	455	GLN
1	C	241	GLN
1	D	241	GLN
1	D	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	SEP	B	346	1	8,9,10	1.57	1 (12%)	8,12,14	1.60	2 (25%)
1	TPO	C	345	1	8,10,11	1.21	0	10,14,16	1.79	1 (10%)
1	SEP	D	346	1	8,9,10	1.56	1 (12%)	8,12,14	1.32	2 (25%)
1	TPO	A	345	1	8,10,11	1.09	0	10,14,16	1.68	2 (20%)
1	SEP	C	346	1	8,9,10	1.55	1 (12%)	8,12,14	1.18	1 (12%)
1	TPO	C	342	1	8,10,11	1.20	0	10,14,16	1.29	1 (10%)
1	TPO	A	342	1	8,10,11	1.11	0	10,14,16	1.74	2 (20%)
1	TPO	D	345	1	8,10,11	1.11	0	10,14,16	1.72	2 (20%)
1	SEP	A	346	1	8,9,10	1.55	1 (12%)	8,12,14	1.48	2 (25%)
1	TPO	B	345	1	8,10,11	1.10	0	10,14,16	1.72	2 (20%)
1	TPO	D	342	1	8,10,11	1.16	0	10,14,16	1.42	1 (10%)
1	TPO	B	342	1	8,10,11	1.14	0	10,14,16	1.31	1 (10%)

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	SEP	B	346	1	-	4/5/8/10	-
1	TPO	C	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-
1	SEP	C	346	1	-	3/5/8/10	-
1	TPO	C	342	1	-	5/9/11/13	-
1	TPO	A	342	1	-	4/9/11/13	-
1	TPO	D	345	1	-	2/9/11/13	-
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	B	345	1	-	2/9/11/13	-
1	TPO	D	342	1	-	7/9/11/13	-
1	TPO	B	342	1	-	2/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	346	SEP	P-O1P	3.41	1.61	1.50
1	D	346	SEP	P-O1P	3.39	1.61	1.50
1	A	346	SEP	P-O1P	3.37	1.61	1.50
1	C	346	SEP	P-O1P	3.35	1.61	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	345	TPO	P-OG1-CB	-4.99	108.12	123.21
1	B	345	TPO	P-OG1-CB	-4.62	109.25	123.21
1	A	345	TPO	P-OG1-CB	-4.47	109.72	123.21
1	D	345	TPO	P-OG1-CB	-4.44	109.80	123.21
1	A	342	TPO	P-OG1-CB	-4.34	110.10	123.21
1	D	342	TPO	P-OG1-CB	-3.87	111.52	123.21
1	B	342	TPO	P-OG1-CB	-3.62	112.29	123.21
1	C	342	TPO	P-OG1-CB	-3.36	113.07	123.21
1	B	346	SEP	P-OG-CB	-2.88	110.37	118.30
1	A	346	SEP	P-OG-CB	-2.81	110.56	118.30
1	B	346	SEP	OG-CB-CA	2.80	110.87	108.14
1	D	345	TPO	CG2-CB-CA	-2.43	108.37	113.16
1	A	342	TPO	CG2-CB-CA	-2.42	108.39	113.16
1	A	346	SEP	OG-CB-CA	2.30	110.39	108.14
1	D	346	SEP	P-OG-CB	-2.25	112.10	118.30
1	C	346	SEP	P-OG-CB	-2.19	112.27	118.30
1	D	346	SEP	OG-CB-CA	2.15	110.24	108.14
1	B	345	TPO	CG2-CB-CA	-2.15	108.93	113.16
1	A	345	TPO	CG2-CB-CA	-2.13	108.96	113.16

There are no chirality outliers.

All (34) torsion outliers are listed below:

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

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
2	VDC	B	501	-	35,39,39	0.99	2 (5%)	33,62,62	2.11	10 (30%)
2	VDC	C	501	-	35,39,39	0.98	2 (5%)	33,62,62	2.48	11 (33%)
2	VDC	A	501	-	35,39,39	0.98	2 (5%)	33,62,62	2.11	10 (30%)
2	VDC	D	501	-	35,39,39	0.98	2 (5%)	33,62,62	2.44	13 (39%)

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	VDC	B	501	-	-	2/14/46/46	0/7/6/6
2	VDC	C	501	-	-	2/14/46/46	0/7/6/6
2	VDC	A	501	-	-	2/14/46/46	0/7/6/6
2	VDC	D	501	-	-	2/14/46/46	0/7/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	VDC	C2-C9	-3.42	1.39	1.47
2	C	501	VDC	C2-C9	-3.42	1.39	1.47
2	D	501	VDC	C2-C9	-3.42	1.39	1.47
2	A	501	VDC	C2-C9	-3.40	1.39	1.47
2	C	501	VDC	F1-C8	-2.15	1.35	1.40
2	D	501	VDC	F1-C8	-2.15	1.35	1.40
2	B	501	VDC	F1-C8	-2.14	1.35	1.40
2	A	501	VDC	F1-C8	-2.12	1.35	1.40

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	VDC	C9-C2-N1	7.03	118.72	112.30
2	C	501	VDC	C9-C2-N1	6.96	118.65	112.30
2	D	501	VDC	C13-N3-C14	6.84	129.38	124.18
2	C	501	VDC	C13-N3-C14	6.80	129.35	124.18
2	B	501	VDC	C9-C2-N1	6.23	117.99	112.30
2	A	501	VDC	C9-C2-N1	6.19	117.95	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	VDC	C17-O3-C16	-4.29	101.44	108.43
2	A	501	VDC	C17-O3-C16	-4.28	101.45	108.43
2	C	501	VDC	C17-O3-C16	-4.23	101.54	108.43
2	D	501	VDC	C17-O3-C16	-4.22	101.55	108.43
2	C	501	VDC	C19-C14-N3	-3.77	116.92	126.42
2	C	501	VDC	C3-C2-N1	-3.70	122.21	127.20
2	D	501	VDC	C3-C2-N1	-3.70	122.21	127.20
2	B	501	VDC	C19-C14-N3	-3.57	117.44	126.42
2	A	501	VDC	C19-C14-N3	-3.56	117.45	126.42
2	B	501	VDC	C3-C2-N1	-3.33	122.71	127.20
2	A	501	VDC	C3-C2-N1	-3.30	122.75	127.20
2	D	501	VDC	C19-C14-N3	-3.10	118.63	126.42
2	C	501	VDC	C13-N3-N4	3.07	113.54	111.69
2	A	501	VDC	C18-C16-C15	3.03	123.83	115.57
2	B	501	VDC	C18-C16-C15	3.02	123.79	115.57
2	B	501	VDC	C13-N3-C14	2.99	126.45	124.18
2	A	501	VDC	C13-N3-C14	2.96	126.43	124.18
2	A	501	VDC	C13-N3-N4	2.95	113.47	111.69
2	B	501	VDC	C13-N3-N4	2.92	113.45	111.69
2	C	501	VDC	C18-C16-C15	2.75	123.04	115.57
2	D	501	VDC	C13-N3-N4	2.73	113.34	111.69
2	C	501	VDC	C5-N2-C9	-2.68	120.25	122.24
2	C	501	VDC	O3-C17-C14	-2.61	99.51	106.52
2	D	501	VDC	O3-C17-C14	-2.58	99.59	106.52
2	D	501	VDC	C18-C16-C15	2.56	122.55	115.57
2	D	501	VDC	C21-N5-C20	2.53	118.77	116.61
2	A	501	VDC	O3-C17-C14	-2.50	99.81	106.52
2	B	501	VDC	O3-C17-C14	-2.50	99.81	106.52
2	A	501	VDC	C21-N5-C20	2.41	118.66	116.61
2	B	501	VDC	C21-N5-C20	2.40	118.66	116.61
2	C	501	VDC	C21-N5-C20	2.38	118.64	116.61
2	B	501	VDC	C5-N2-C9	-2.33	120.51	122.24
2	A	501	VDC	C5-N2-C9	-2.32	120.52	122.24
2	D	501	VDC	C5-N2-C9	-2.25	120.57	122.24
2	D	501	VDC	C3-C2-C9	-2.18	119.05	120.30
2	D	501	VDC	C18-C16-C19	2.06	121.18	115.57
2	C	501	VDC	C3-C2-C9	-2.05	119.12	120.30
2	D	501	VDC	C10-C21-N5	-2.05	122.51	124.45

There are no chirality outliers.
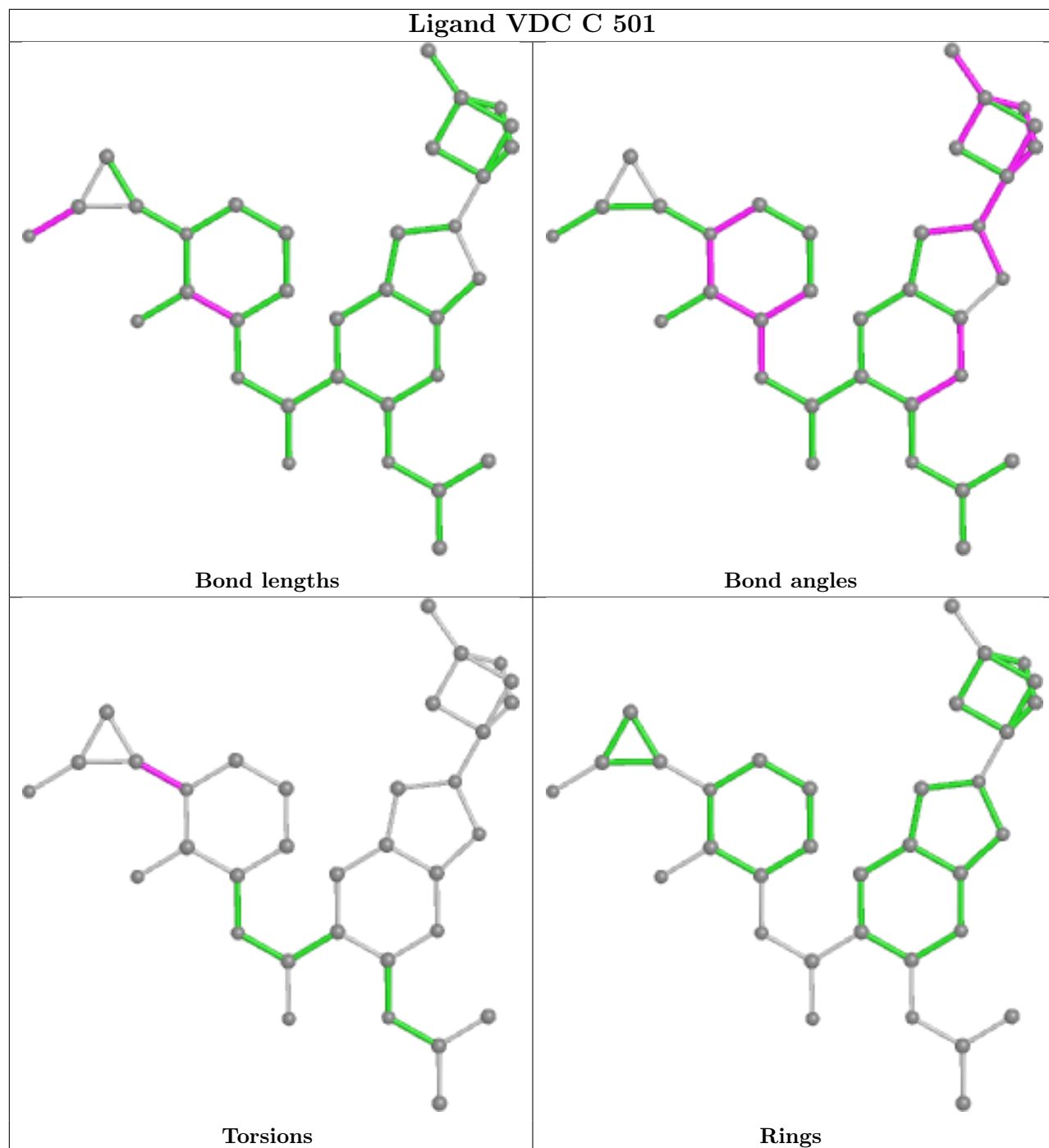
All (8) torsion outliers are listed below:

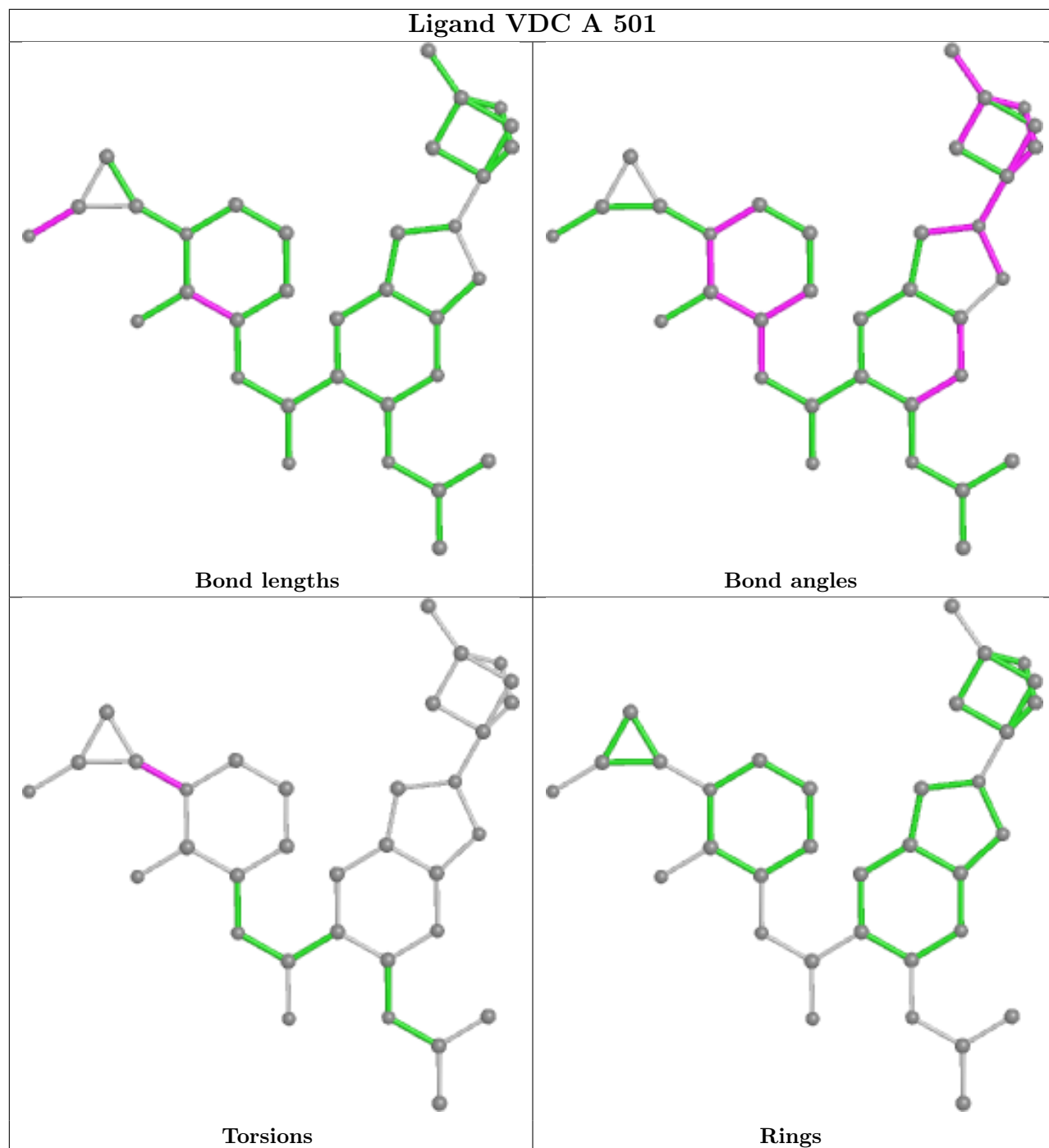| Mol	Chain	Res	Type	Atoms
2	A	501	VDC	C7-C6-N2-C5
2	B	501	VDC	C7-C6-N2-C5
2	C	501	VDC	C7-C6-N2-C5
2	A	501	VDC	C7-C6-N2-C9
2	B	501	VDC	C7-C6-N2-C9
2	C	501	VDC	C7-C6-N2-C9
2	D	501	VDC	C7-C6-N2-C5
2	D	501	VDC	C7-C6-N2-C9

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand VDC B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand VDC C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand VDC A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand VDC D 501

Bond lengths

Bond angles

Torsions

Rings
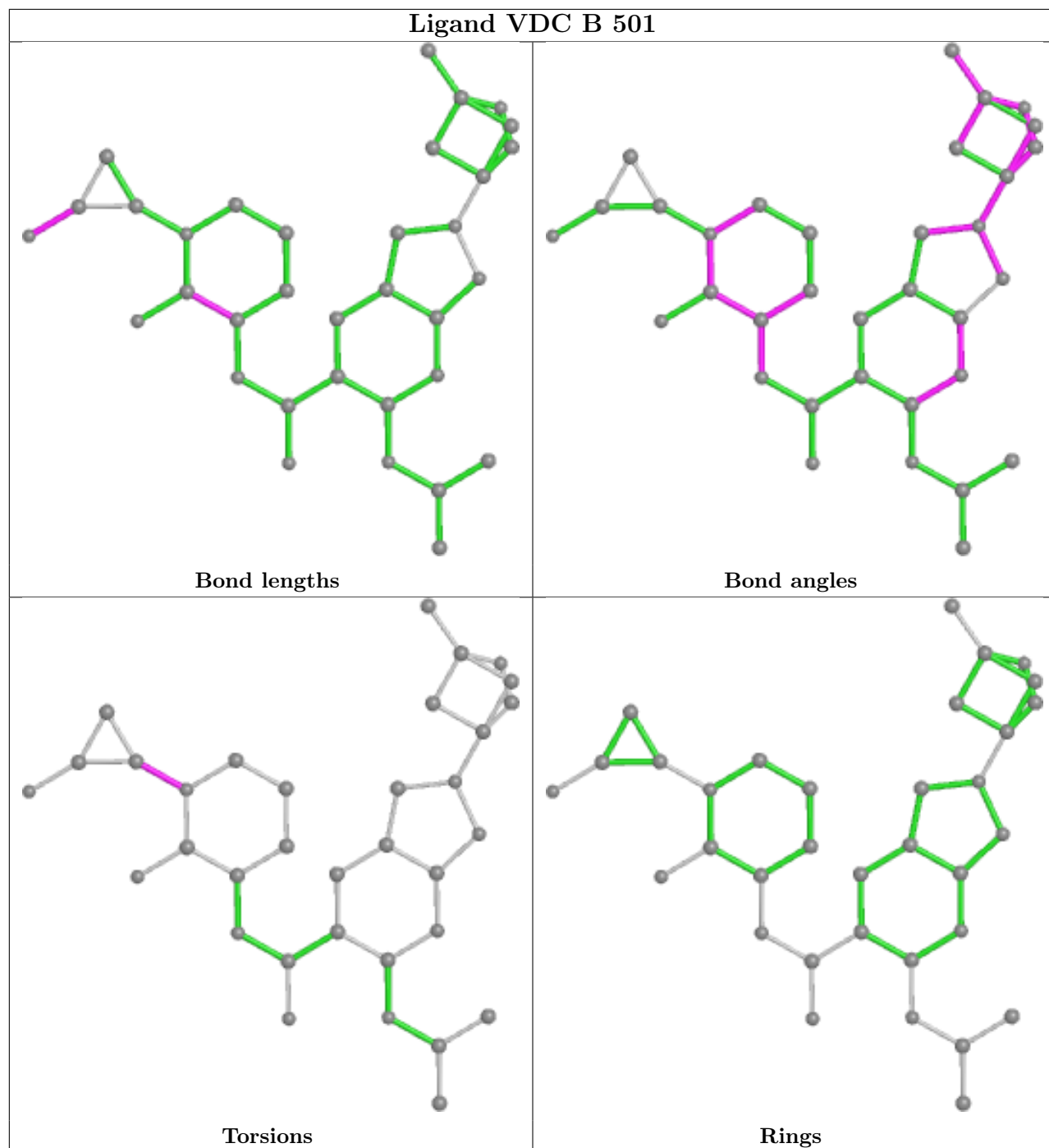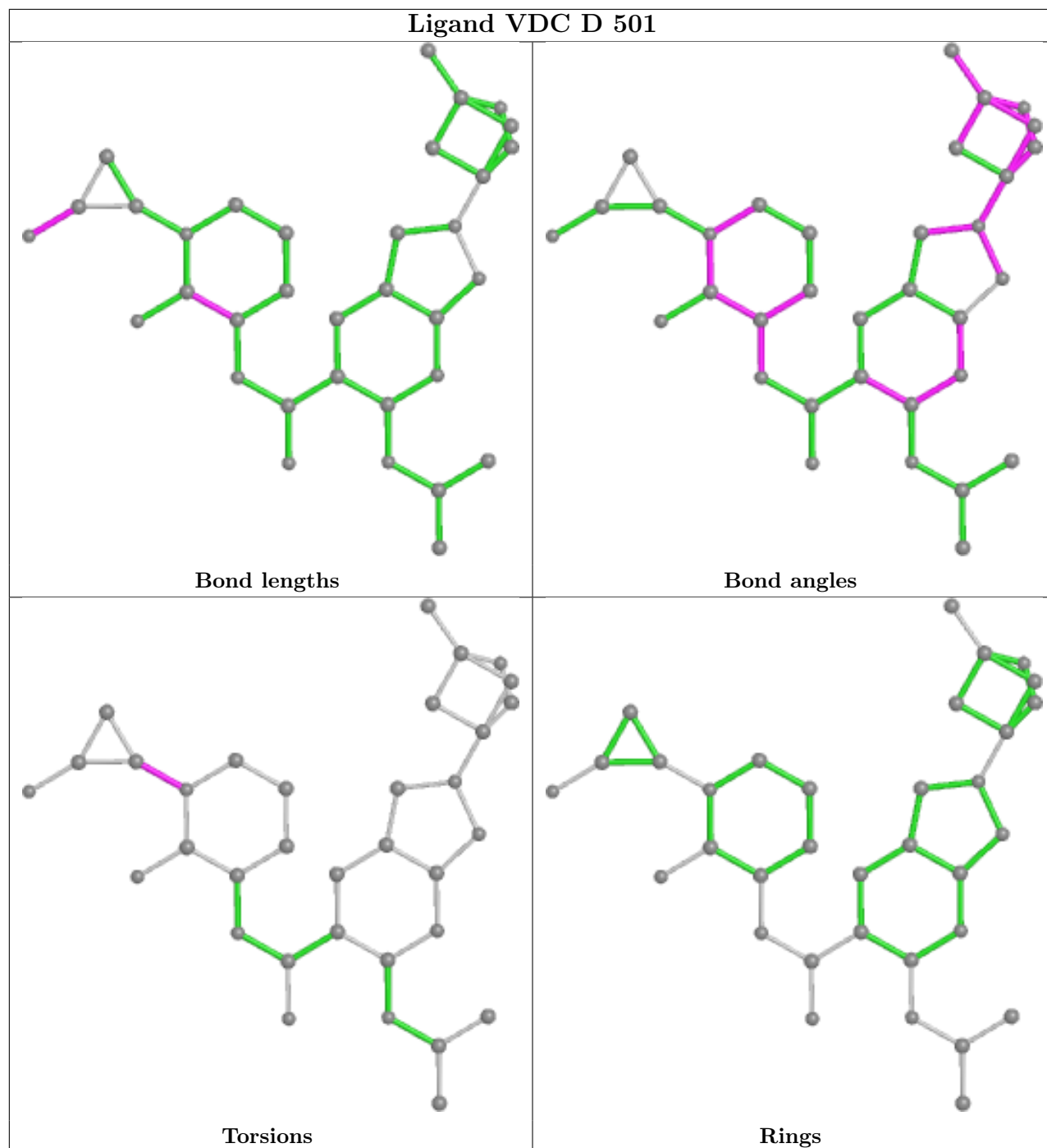
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	284/307 (92%)	0.51	21 (7%)	14	18	35, 58, 104, 137	0
1	B	286/307 (93%)	0.48	19 (6%)	18	23	35, 55, 99, 137	0
1	C	278/307 (90%)	0.50	18 (6%)	18	23	36, 60, 101, 120	0
1	D	274/307 (89%)	0.42	25 (9%)	9	12	37, 59, 109, 173	0
All	All	1122/1228 (91%)	0.48	83 (7%)	14	18	35, 58, 102, 173	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	GLN	4.9
1	A	459	ALA	4.8
1	C	343	VAL	4.7
1	D	216	ALA	4.5
1	A	226	LEU	4.3
1	C	162	ASP	4.1
1	B	230	PHE	4.0
1	D	330	PHE	3.9
1	A	230	PHE	3.9
1	D	197	PHE	3.7
1	B	195	GLY	3.7
1	B	226	LEU	3.6
1	B	403	ILE	3.6
1	D	236	VAL	3.6
1	D	226	LEU	3.5
1	B	399	ILE	3.4
1	A	229	GLN	3.4
1	A	221	ILE	3.4
1	C	226	LEU	3.4
1	C	163	THR	3.3
1	A	197	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	236	VAL	3.2
1	D	343	VAL	3.2
1	A	164	ARG	3.2
1	A	348	ILE	3.1
1	B	196	GLY	3.0
1	D	256	ASP	3.0
1	B	223	THR	3.0
1	B	197	PHE	3.0
1	A	256	ASP	3.0
1	D	195	GLY	2.9
1	D	349	VAL	2.9
1	B	164	ARG	2.8
1	B	221	ILE	2.8
1	A	232	GLN	2.8
1	A	222	THR	2.8
1	D	409	THR	2.8
1	D	196	GLY	2.8
1	C	410	ILE	2.8
1	D	255	GLY	2.8
1	A	195	GLY	2.7
1	B	255	GLY	2.7
1	B	406	GLU	2.6
1	D	348	ILE	2.6
1	D	187	VAL	2.6
1	D	165	PHE	2.6
1	C	334	ARG	2.6
1	A	404	GLU	2.6
1	B	404	GLU	2.6
1	B	279	GLY	2.6
1	A	403	ILE	2.6
1	D	458	THR	2.5
1	D	274	LEU	2.5
1	C	171	TYR	2.5
1	A	347	ARG	2.5
1	A	325	ALA	2.5
1	D	347	ARG	2.5
1	B	217	ALA	2.4
1	C	228	GLN	2.4
1	D	231	ASP	2.4
1	C	335	ALA	2.4
1	C	287[A]	MET	2.4
1	C	403	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	206	ASN	2.3
1	C	232	GLN	2.3
1	C	327[A]	ILE	2.3
1	D	198	GLY	2.3
1	D	228	GLN	2.3
1	A	410	ILE	2.3
1	B	225	GLU	2.2
1	C	401	GLU	2.2
1	B	282	PRO	2.2
1	A	225	GLU	2.1
1	D	234	ILE	2.1
1	C	199	VAL	2.1
1	C	405	ASP	2.1
1	A	240	CYS	2.1
1	C	274	LEU	2.0
1	D	225	GLU	2.0
1	A	319	LEU	2.0
1	A	280	THR	2.0
1	D	407	GLU	2.0
1	D	410	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

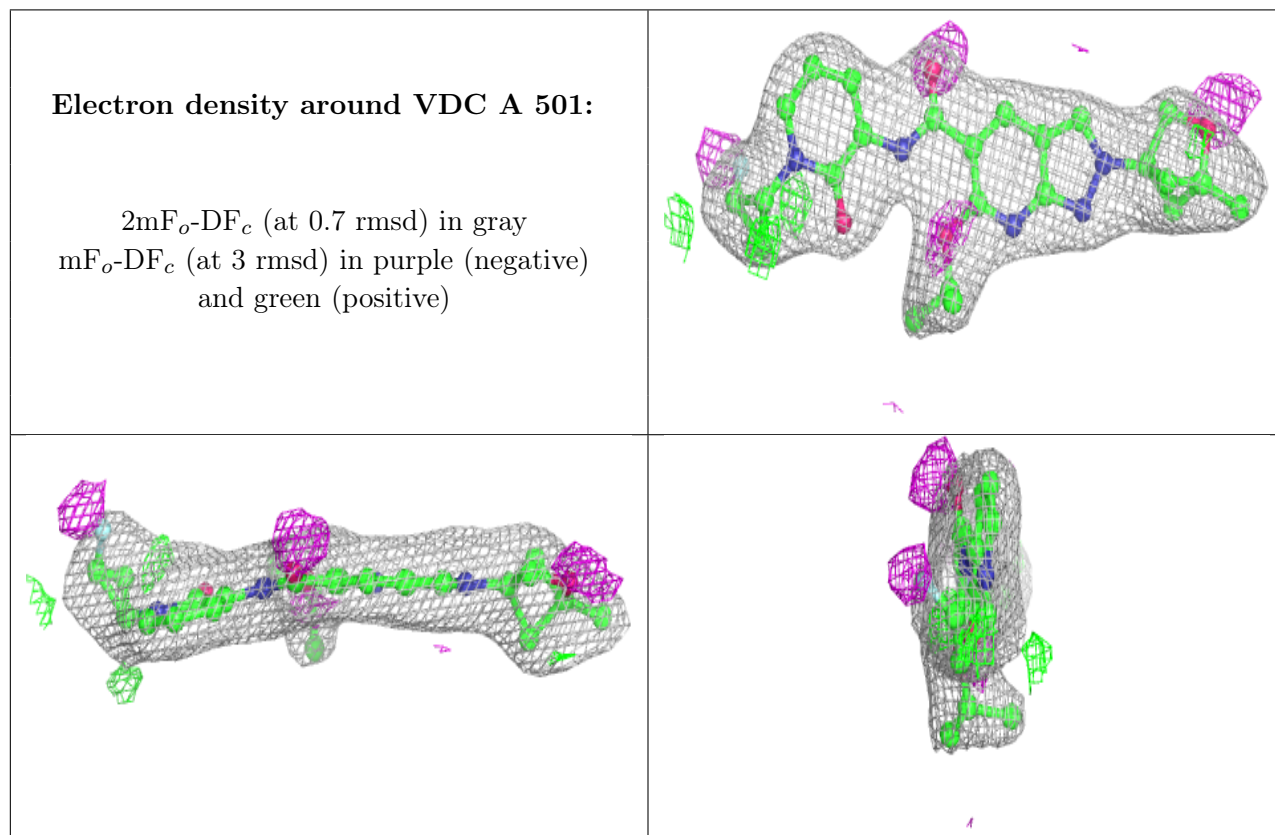| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	A	342	11/12	0.27	0.39	116,123,148,154	0
1	TPO	C	342	11/12	0.63	0.21	96,105,126,137	0
1	SEP	C	346	10/11	0.70	0.36	112,118,129,133	0
1	TPO	D	342	11/12	0.74	0.20	97,108,122,132	0
1	TPO	B	342	11/12	0.75	0.21	100,109,117,134	0
1	TPO	D	345	11/12	0.78	0.23	96,104,115,119	0
1	SEP	B	346	10/11	0.80	0.18	103,112,138,167	0
1	SEP	D	346	10/11	0.80	0.32	105,114,129,141	0
1	SEP	A	346	10/11	0.82	0.23	116,122,126,136	0
1	TPO	A	345	11/12	0.82	0.21	101,111,118,124	0
1	TPO	C	345	11/12	0.83	0.25	100,108,121,122	0
1	TPO	B	345	11/12	0.90	0.17	91,98,114,117	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VDC	A	501	34/34	0.94	0.16	35,41,54,59	0
2	VDC	B	501	34/34	0.95	0.14	35,41,54,59	0
2	VDC	C	501	34/34	0.95	0.12	45,50,58,65	0
2	VDC	D	501	34/34	0.96	0.11	39,47,55,67	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.
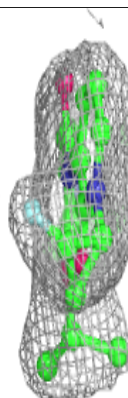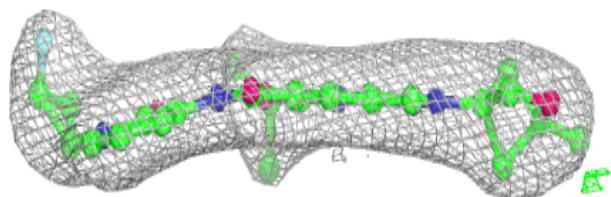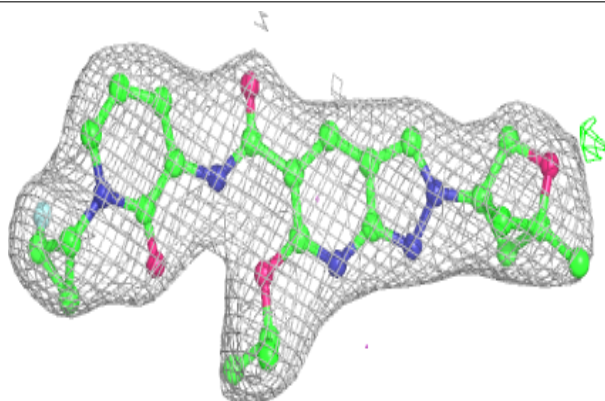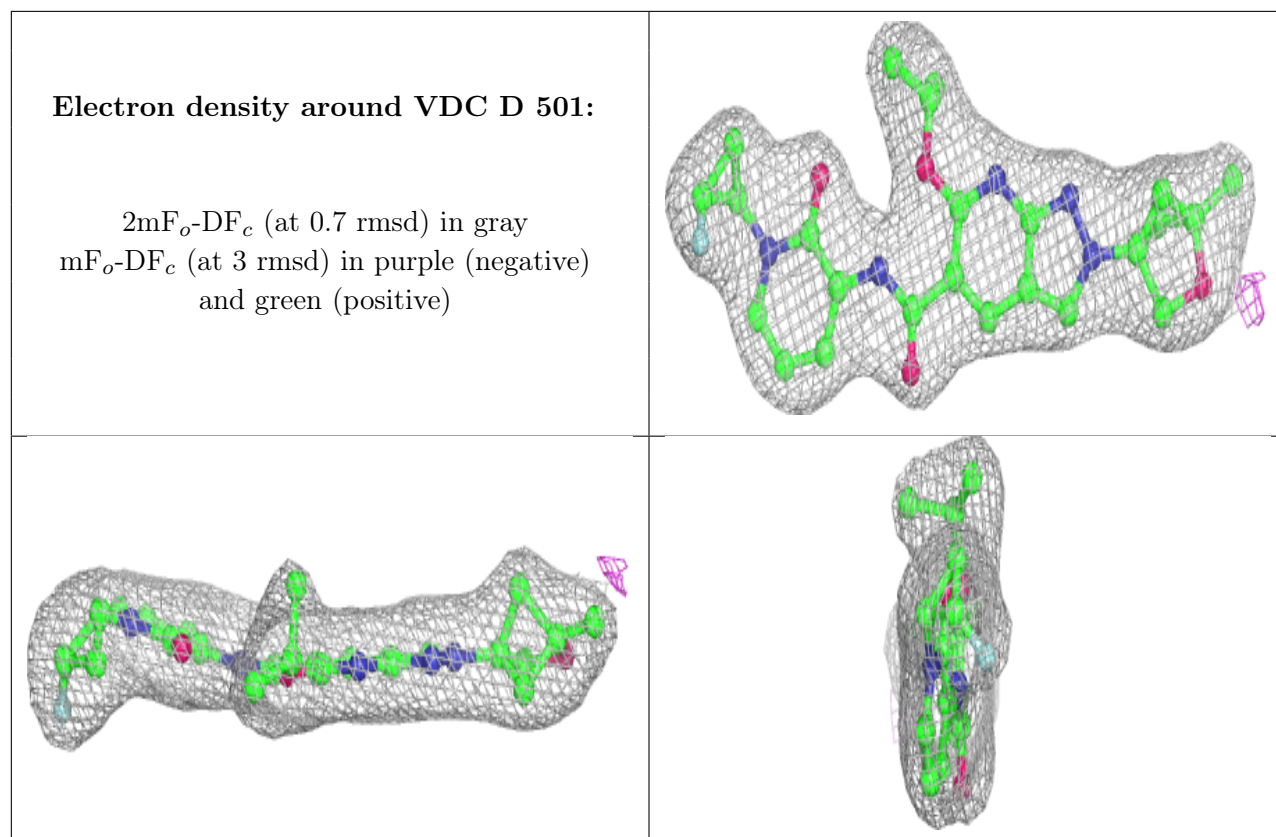

Electron density around VDC A 501:

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

Electron density around VDC B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
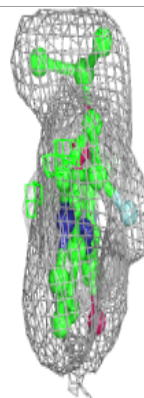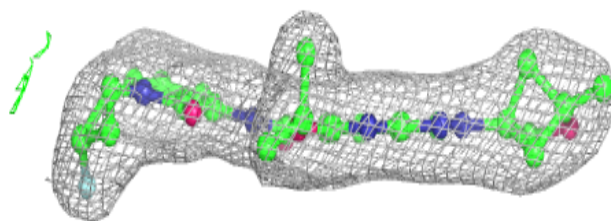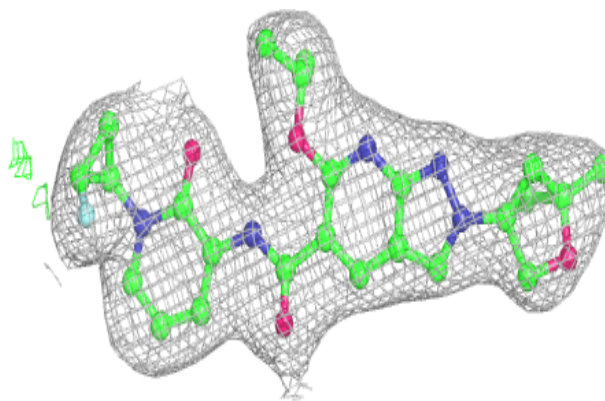
Electron density around VDC C 501:

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

Electron density around VDC D 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.