



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:03 AM UTC

PDB ID : 8TVN / pdb_00008tvn
Title : IRAK4 in complex with compound 23
Authors : Metrick, C.M.; Chodaparambil, J.V.
Deposited on : 2023-08-18
Resolution : 1.95 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

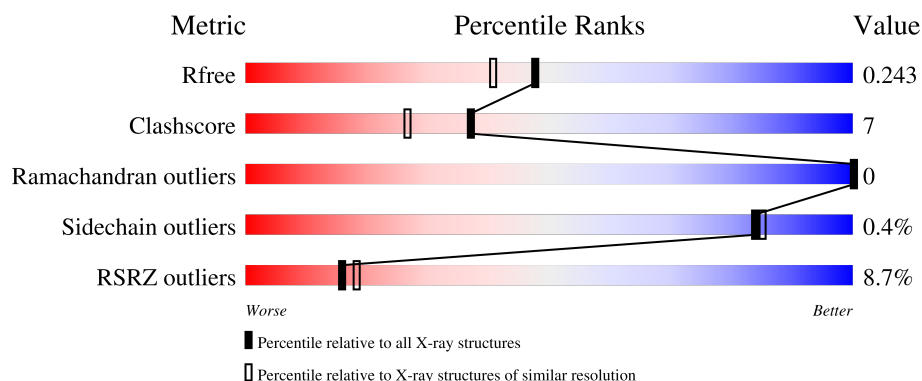
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	7% 78% 14% 8%
1	B	307	9% 82% 10% 7%
1	C	307	7% 80% 12% 7%
1	D	307	9% 76% 17% 7%

2 Entry composition [i](#)

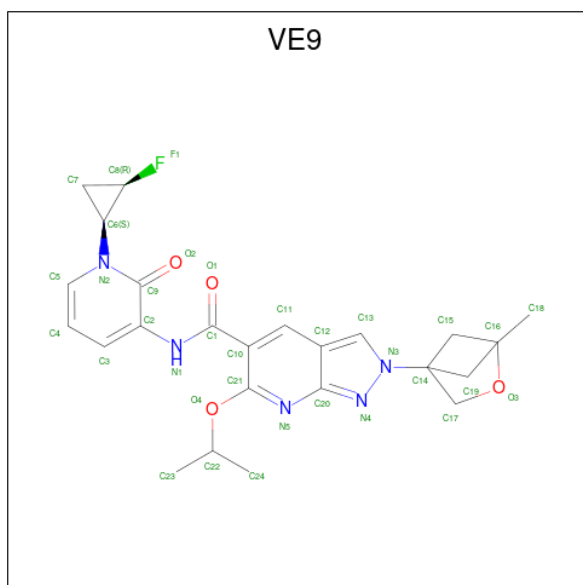
There are 3 unique types of molecules in this entry. The entry contains 9437 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	282	Total	C	N	O	P	S	0	0	0
			2184	1367	364	436	3	14			
1	B	286	Total	C	N	O	P	S	0	1	0
			2208	1382	370	439	3	14			
1	C	286	Total	C	N	O	P	S	0	0	0
			2236	1403	377	439	3	14			
1	D	286	Total	C	N	O	P	S	0	1	0
			2228	1392	376	443	3	14			

- Molecule 2 is N-{1-[(1R,2S)-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 (CCD ID: VE9) (formula: C₂₄H₂₆FN₅O₄) (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		

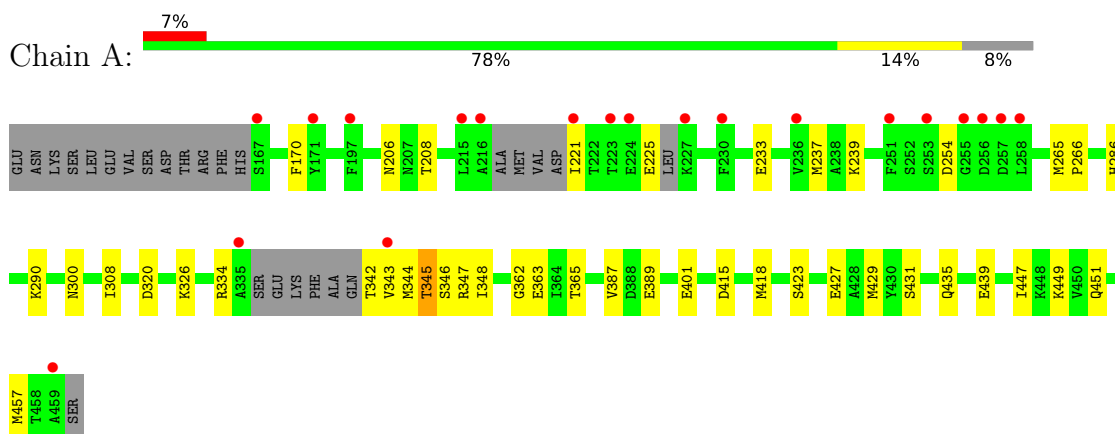
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		
3	B	143	Total	O	0	0
			143	143		
3	C	111	Total	O	0	0
			111	111		
3	D	65	Total	O	0	0
			65	65		

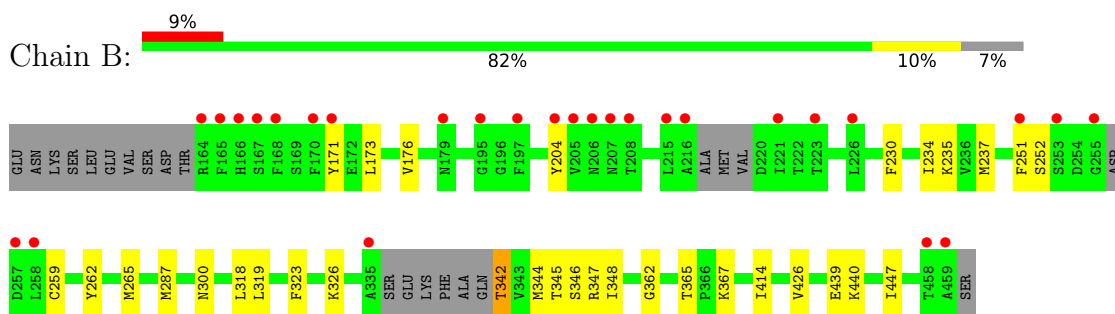
3 Residue-property plots [i](#)

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.

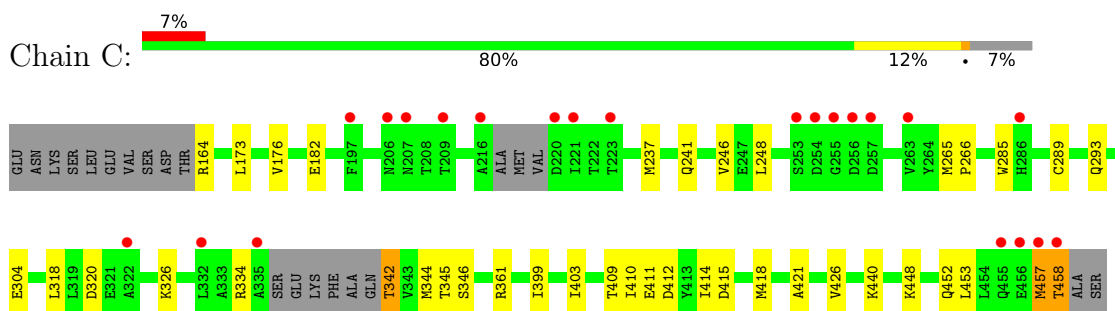
- Molecule 1: Interleukin-1 receptor-associated kinase 4



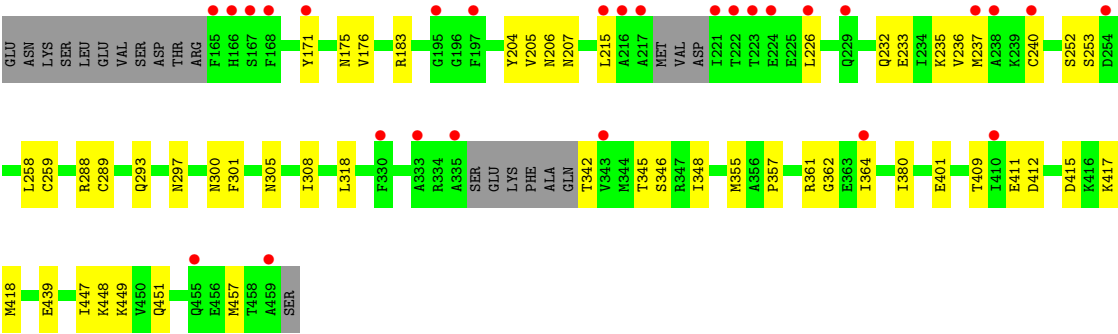
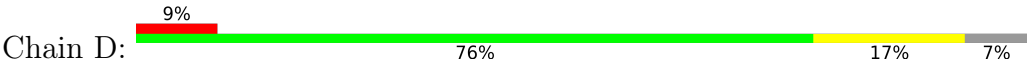
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.92Å 94.18Å 98.92Å 90.00° 108.47° 90.00°	Depositor
Resolution (Å)	47.09 – 1.95 47.09 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.09-1.95) 99.7 (47.09-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.242 0.206 , 0.243	Depositor DCC
R_{free} test set	4733 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9437	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, VE9, 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	0.69	0/2185	0.79	0/2949
1	B	0.69	0/2210	0.78	0/2982
1	C	0.58	0/2240	0.76	0/3020
1	D	0.52	0/2229	0.71	0/3006
All	All	0.63	0/8864	0.76	0/11957

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 [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	2184	0	2111	30	0
1	B	2208	0	2117	38	0
1	C	2236	0	2183	28	0
1	D	2228	0	2177	35	0
2	A	34	0	0	1	0
2	B	34	0	0	0	0
2	C	34	0	0	1	0
2	D	34	0	0	2	0
3	A	126	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	143	0	0	2	0
3	C	111	0	0	2	0
3	D	65	0	0	1	0
All	All	9437	0	8588	124	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 7.

All (124) 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:287:MET:CE	1:B:323:PHE:HB2	1.88	1.03
1:C:237:MET:HE3	1:C:248:LEU:HB2	1.51	0.91
1:C:409:THR:HG23	1:C:412:ASP:H	1.54	0.72
1:B:287:MET:CE	1:B:323:PHE:CB	2.67	0.71
1:B:287:MET:HE1	1:B:323:PHE:HB2	1.72	0.70
1:A:439:GLU:HG3	1:B:439:GLU:HG3	1.75	0.69
1:D:233:GLU:O	1:D:237:MET:HG3	1.92	0.69
1:A:423:SER:O	1:A:427:GLU:HG3	1.91	0.69
1:D:289:CYS:O	1:D:293:GLN:HG3	1.94	0.68
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.75	0.68
1:C:411:GLU:HA	1:C:414:ILE:HG13	1.77	0.66
1:C:265:MET:HE1	1:C:326:LYS:HG3	1.79	0.64
1:C:457:MET:O	1:C:458:THR:C	2.41	0.64
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.80	0.64
1:C:164:ARG:HH12	1:C:241:GLN:HE22	1.46	0.63
1:C:289:CYS:O	1:C:293:GLN:HG3	1.99	0.63
1:B:176:VAL:HG12	1:B:204:TYR:O	1.99	0.62
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.80	0.62
1:B:342:TPO:HG22	1:B:365:THR:HB	1.81	0.61
1:D:301:PHE:O	1:D:305:ASN:ND2	2.32	0.61
1:A:344:MET:HE1	1:A:363:GLU:HG3	1.82	0.61
1:A:347:ARG:HB3	1:A:347:ARG:NH1	2.16	0.61
1:A:206:ASN:O	1:A:208:THR:HG23	2.00	0.60
1:B:234:ILE:HD13	1:B:251:PHE:CD2	2.37	0.59
1:B:235:LYS:NZ	3:B:606:HOH:O	2.37	0.58
1:A:265:MET:HE1	1:A:326:LYS:HG3	1.86	0.57
1:A:389:GLU:HG2	1:B:344:MET:HG3	1.86	0.57
1:B:265:MET:CE	1:B:326:LYS:HG3	2.35	0.56
1:A:334:ARG:HH22	1:A:345:TPO:P	2.28	0.56
1:B:287:MET:HE3	1:B:323:PHE:HB2	1.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:NZ	3:A:602:HOH:O	2.21	0.55
1:A:334:ARG:NH2	1:A:345:TPO:O3P	2.39	0.55
1:A:431:SER:O	1:A:435:GLN:HG3	2.07	0.55
1:B:237:MET:HE1	1:B:262:TYR:HE2	1.71	0.55
1:D:176:VAL:HG21	1:D:205:VAL:HG12	1.87	0.55
1:D:409:THR:HG23	1:D:411:GLU:N	2.23	0.54
1:D:240:CYS:HB3	1:D:301:PHE:HE1	1.72	0.54
1:D:409:THR:HG22	1:D:412:ASP:CG	2.33	0.53
1:A:347:ARG:HB3	1:A:347:ARG:HH11	1.73	0.53
1:C:403:ILE:HD13	1:C:410:ILE:HG13	1.91	0.53
1:D:357:PRO:HG2	1:D:439:GLU:HG3	1.91	0.53
1:B:287:MET:HE2	1:B:323:PHE:HB2	1.86	0.52
1:D:253:SER:HA	1:D:258:LEU:HD23	1.92	0.52
1:D:171:TYR:O	1:D:175:ASN:ND2	2.35	0.52
1:D:409:THR:HG23	1:D:412:ASP:H	1.75	0.51
1:D:204:TYR:CZ	1:D:207:ASN:HA	2.46	0.51
1:B:287:MET:HE3	1:B:323:PHE:CB	2.40	0.51
1:D:232:GLN:O	1:D:236:VAL:HG23	2.10	0.51
1:D:409:THR:CG2	1:D:412:ASP:H	2.24	0.50
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.94	0.50
1:C:440:LYS:HD2	1:D:401:GLU:CD	2.37	0.49
1:C:342:TPO:O3P	3:C:601:HOH:O	2.20	0.49
1:B:265:MET:HE3	1:B:319:LEU:C	2.38	0.49
1:D:206:ASN:O	1:D:206:ASN:ND2	2.42	0.49
1:B:230:PHE:O	1:B:234:ILE:HG13	2.13	0.48
1:A:401:GLU:HG3	1:B:440:LYS:HE2	1.94	0.48
1:A:300:ASN:HD22	1:A:451:GLN:HE22	1.61	0.48
1:D:297:ASN:OD1	1:D:451:GLN:NE2	2.41	0.48
1:A:401:GLU:HG3	1:B:440:LYS:CE	2.44	0.48
1:D:318:LEU:HD11	2:D:501:VE9:C9	2.43	0.48
1:C:448:LYS:O	1:C:452:GLN:HG2	2.14	0.48
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.95	0.48
1:C:246:VAL:HG11	1:C:318:LEU:HD12	1.96	0.48
1:D:448:LYS:HA	1:D:448:LYS:HD2	1.69	0.47
1:A:308:ILE:HD13	1:A:365:THR:C	2.39	0.47
1:D:409:THR:HG23	1:D:411:GLU:H	1.79	0.47
1:D:308:ILE:HD12	1:D:364:ILE:HG22	1.96	0.47
1:C:266:PRO:HD2	1:C:320:ASP:HA	1.97	0.47
1:B:173:LEU:HA	1:B:176:VAL:HG22	1.97	0.47
1:D:215:LEU:O	1:D:226:LEU:HD21	2.15	0.47
1:A:233:GLU:O	1:A:237:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.98	0.46
1:A:449:LYS:HD3	1:A:449:LYS:HA	1.64	0.46
1:A:401:GLU:CG	1:B:440:LYS:HE2	2.46	0.46
1:A:286:HIS:O	1:A:290:LYS:HG2	2.15	0.45
1:D:348:ILE:HG12	1:D:362:GLY:HA2	1.98	0.45
1:C:164:ARG:HH12	1:C:241:GLN:NE2	2.13	0.45
1:A:266:PRO:HD2	1:A:320:ASP:HA	1.97	0.45
1:A:170:PHE:HB2	1:A:254:ASP:O	2.16	0.45
1:C:182:GLU:O	1:C:182:GLU:HG3	2.17	0.45
1:D:417[A]:LYS:HE3	3:D:625:HOH:O	2.17	0.45
1:C:265:MET:CE	1:C:326:LYS:HG3	2.46	0.45
1:D:457:MET:HE2	1:D:457:MET:HB3	1.87	0.45
1:C:457:MET:HE3	1:C:457:MET:HB3	1.60	0.44
1:B:348:ILE:HG12	1:B:362:GLY:HA2	2.00	0.44
1:B:342:TPO:CG2	1:B:365:THR:HB	2.47	0.44
1:B:347:ARG:HG3	1:B:347:ARG:HH11	1.83	0.44
1:B:287:MET:HE2	1:B:323:PHE:CD1	2.52	0.44
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.00	0.44
1:D:449:LYS:HD3	1:D:449:LYS:HA	1.84	0.44
1:D:288:ARG:HB3	1:D:380:ILE:CG2	2.48	0.44
1:A:237:MET:HA	1:A:237:MET:HE3	2.00	0.44
1:B:171:TYR:HB3	1:D:183:ARG:HG2	1.99	0.44
1:B:265:MET:HB2	1:B:318:LEU:HD12	2.00	0.44
1:B:347:ARG:HG3	1:B:347:ARG:NH1	2.31	0.44
1:B:237:MET:CE	1:B:262:TYR:HE2	2.31	0.44
1:A:429:MET:HB2	1:A:457:MET:SD	2.58	0.43
1:A:221:ILE:HG13	1:A:225:GLU:HB3	1.99	0.43
1:B:342:TPO:HG22	1:B:342:TPO:O1P	2.19	0.43
1:C:173:LEU:HA	1:C:176:VAL:HG22	2.01	0.43
1:C:334:ARG:HD3	1:C:334:ARG:HA	1.91	0.43
1:D:252:SER:HB3	1:D:259:CYS:HB2	2.01	0.43
1:A:348:ILE:HG12	1:A:362:GLY:HA2	2.00	0.43
1:C:414:ILE:CD1	1:C:426:VAL:HG11	2.49	0.42
1:B:367:LYS:NZ	3:B:603:HOH:O	2.48	0.42
1:C:164:ARG:NH1	1:C:241:GLN:HE22	2.15	0.42
1:C:293:GLN:NE2	1:C:458:THR:OG1	2.45	0.42
1:C:440:LYS:HD2	1:D:401:GLU:HG3	2.01	0.42
1:B:287:MET:HE2	1:B:323:PHE:CG	2.54	0.42
1:D:415:ASP:HB3	1:D:418:MET:HE2	2.01	0.42
1:A:387:VAL:HG21	1:B:344:MET:HE2	2.01	0.42
1:D:357:PRO:O	1:D:361:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:TRP:HB2	1:C:421:ALA:HB2	2.02	0.42
1:A:343:VAL:C	1:A:344:MET:HE2	2.44	0.42
1:B:342:TPO:P	1:B:367:LYS:NZ	2.93	0.42
1:B:173:LEU:HA	1:B:176:VAL:CG2	2.49	0.42
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.02	0.41
2:A:501:VE9:N1	2:A:501:VE9:O4	2.54	0.41
1:C:304:GLU:OE1	3:C:602:HOH:O	2.22	0.41
1:C:399:ILE:O	1:C:403:ILE:HG13	2.21	0.41
1:D:232:GLN:HA	1:D:235:LYS:HG2	2.03	0.41
2:D:501:VE9:O4	2:D:501:VE9:N1	2.54	0.41
2:C:501:VE9:O4	2:C:501:VE9:N1	2.54	0.41
1:C:361:ARG:NH2	1:D:355:MET:O	2.47	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	272/307 (89%)	267 (98%)	5 (2%)	0	100	100
1	B	277/307 (90%)	272 (98%)	5 (2%)	0	100	100
1	C	278/307 (91%)	272 (98%)	6 (2%)	0	100	100
1	D	279/307 (91%)	271 (97%)	8 (3%)	0	100	100
All	All	1106/1228 (90%)	1082 (98%)	24 (2%)	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	232/265 (88%)	232 (100%)	0	100	100
1	B	231/265 (87%)	231 (100%)	0	100	100
1	C	239/265 (90%)	235 (98%)	4 (2%)	53	49
1	D	238/265 (90%)	238 (100%)	0	100	100
All	All	940/1060 (89%)	936 (100%)	4 (0%)	84	85

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

Mol	Chain	Res	Type
1	C	344	MET
1	C	453	LEU
1	C	457	MET
1	C	458	THR

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

Mol	Chain	Res	Type
1	A	286	HIS
1	A	300	ASN
1	A	442	ASN
1	B	435	GLN
1	C	241	GLN
1	C	267	ASN
1	C	442	ASN
1	D	232	GLN
1	D	241	GLN
1	D	394	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	TPO	C	345	1	8,10,11	1.58	2 (25%)	10,14,16	1.45	1 (10%)
1	TPO	D	345	1	8,10,11	1.35	1 (12%)	10,14,16	1.61	2 (20%)
1	TPO	C	342	1	8,10,11	1.26	0	10,14,16	2.05	3 (30%)
1	SEP	C	346	1	8,9,10	1.64	1 (12%)	7,12,14	1.12	1 (14%)
1	SEP	D	346	1	8,9,10	1.67	1 (12%)	7,12,14	0.99	0
1	TPO	D	342	1	8,10,11	1.62	2 (25%)	10,14,16	1.76	4 (40%)
1	SEP	A	346	1	8,9,10	1.57	1 (12%)	7,12,14	0.51	0
1	TPO	A	345	1	8,10,11	1.39	1 (12%)	10,14,16	1.50	2 (20%)
1	TPO	B	345	1	8,10,11	1.26	1 (12%)	10,14,16	1.90	2 (20%)
1	SEP	B	346	1	8,9,10	1.60	1 (12%)	7,12,14	0.98	0
1	TPO	A	342	1	8,10,11	1.62	2 (25%)	10,14,16	1.55	2 (20%)
1	TPO	B	342	1	8,10,11	0.68	0	10,14,16	1.02	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	TPO	C	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	C	342	1	-	4/9/11/13	-
1	SEP	C	346	1	-	2/6/8/10	-
1	SEP	D	346	1	-	2/6/8/10	-
1	TPO	D	342	1	-	2/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	A	345	1	-	4/9/11/13	-
1	TPO	B	345	1	-	2/9/11/13	-
1	SEP	B	346	1	-	3/6/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	342	1	-	4/9/11/13	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	346	SEP	P-O1P	3.60	1.61	1.50
1	C	346	SEP	P-O1P	3.54	1.61	1.50
1	B	346	SEP	P-O1P	3.48	1.61	1.50
1	A	346	SEP	P-O1P	3.47	1.61	1.50
1	C	345	TPO	CB-CA	3.06	1.60	1.53
1	A	342	TPO	P-OG1	3.00	1.64	1.59
1	D	342	TPO	P-OG1	2.67	1.64	1.59
1	B	345	TPO	P-OG1	2.25	1.63	1.59
1	D	345	TPO	P-O2P	2.15	1.62	1.54
1	A	345	TPO	P-OG1	2.10	1.63	1.59
1	A	342	TPO	P-O3P	2.04	1.62	1.54
1	D	342	TPO	P-O3P	2.03	1.62	1.54
1	C	345	TPO	P-O2P	2.03	1.62	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	TPO	P-OG1-CB	-4.53	111.02	123.33
1	C	342	TPO	CG2-CB-CA	-4.01	105.45	113.26
1	D	345	TPO	P-OG1-CB	-3.85	112.86	123.33
1	C	342	TPO	P-OG1-CB	-3.71	113.25	123.33
1	C	345	TPO	P-OG1-CB	-3.62	113.50	123.33
1	D	342	TPO	P-OG1-CB	-2.90	115.45	123.33
1	D	342	TPO	CG2-CB-CA	-2.78	107.85	113.26
1	A	345	TPO	P-OG1-CB	-2.65	116.13	123.33
1	A	342	TPO	CG2-CB-CA	-2.65	108.11	113.26
1	D	342	TPO	O3P-P-OG1	2.64	116.13	105.85
1	B	342	TPO	O-C-CA	-2.48	118.40	124.77
1	A	342	TPO	P-OG1-CB	-2.37	116.88	123.33
1	A	345	TPO	CG2-CB-CA	-2.35	108.67	113.26
1	D	345	TPO	CG2-CB-CA	-2.30	108.79	113.26
1	B	345	TPO	CG2-CB-CA	-2.28	108.82	113.26
1	C	342	TPO	O-C-CA	-2.16	119.20	124.77
1	C	346	SEP	OG-P-O1P	2.12	112.16	106.44
1	D	342	TPO	O-C-CA	-2.05	119.49	124.77

There are no chirality outliers.

All (31) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	342	TPO	1	0
1	A	345	TPO	2	0
1	B	342	TPO	4	0

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	$\# Z > 2$
2	VE9	D	501	-	35,39,39	1.22	3 (8%)	34,62,62	2.03	8 (23%)
2	VE9	A	501	-	35,39,39	1.21	3 (8%)	34,62,62	2.03	8 (23%)
2	VE9	B	501	-	35,39,39	1.02	3 (8%)	34,62,62	2.17	9 (26%)
2	VE9	C	501	-	35,39,39	1.22	3 (8%)	34,62,62	2.02	8 (23%)

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	VE9	D	501	-	-	2/20/46/46	0/7/6/6
2	VE9	A	501	-	-	2/20/46/46	0/7/6/6
2	VE9	B	501	-	-	2/20/46/46	0/7/6/6
2	VE9	C	501	-	-	2/20/46/46	0/7/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	VE9	C2-C9	-3.75	1.39	1.48
2	D	501	VE9	C2-C9	-3.64	1.39	1.48
2	C	501	VE9	C2-C9	-3.62	1.39	1.48
2	A	501	VE9	C2-C9	-3.61	1.39	1.48
2	A	501	VE9	O3-C16	-3.15	1.41	1.45
2	C	501	VE9	O3-C16	-3.14	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	VE9	O3-C16	-3.12	1.41	1.45
2	C	501	VE9	C3-C2	2.47	1.42	1.37
2	D	501	VE9	C3-C2	2.47	1.41	1.37
2	A	501	VE9	C3-C2	2.44	1.41	1.37
2	B	501	VE9	F1-C8	-2.08	1.36	1.40
2	B	501	VE9	C3-C2	2.06	1.41	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	VE9	C19-C14-C15	-6.37	84.48	88.59
2	B	501	VE9	C9-C2-N1	6.33	117.88	112.00
2	A	501	VE9	C12-C20-N5	-5.47	121.91	126.31
2	C	501	VE9	C12-C20-N5	-5.47	121.91	126.31
2	D	501	VE9	C12-C20-N5	-5.47	121.92	126.31
2	C	501	VE9	C19-C14-C15	-5.33	85.15	88.59
2	A	501	VE9	C19-C14-C15	-5.30	85.17	88.59
2	D	501	VE9	C19-C14-C15	-5.29	85.17	88.59
2	B	501	VE9	C12-C20-N5	-4.79	122.47	126.31
2	D	501	VE9	C9-C2-N1	3.41	115.17	112.00
2	A	501	VE9	C9-C2-N1	3.39	115.15	112.00
2	C	501	VE9	C9-C2-N1	3.36	115.12	112.00
2	A	501	VE9	O3-C17-C14	-3.09	98.20	106.40
2	D	501	VE9	O3-C17-C14	-3.08	98.21	106.40
2	C	501	VE9	O3-C17-C14	-3.06	98.27	106.40
2	B	501	VE9	C3-C2-N1	-2.99	123.34	127.12
2	B	501	VE9	C19-C14-N3	-2.93	119.49	126.04
2	C	501	VE9	C19-C14-N3	-2.87	119.63	126.04
2	D	501	VE9	C18-C16-C15	2.85	126.15	116.07
2	D	501	VE9	C19-C14-N3	-2.85	119.67	126.04
2	C	501	VE9	C18-C16-C15	2.85	126.14	116.07
2	A	501	VE9	C18-C16-C15	2.85	126.14	116.07
2	A	501	VE9	C19-C14-N3	-2.84	119.69	126.04
2	B	501	VE9	O3-C17-C14	-2.77	99.03	106.40
2	D	501	VE9	C10-C21-N5	-2.71	121.85	124.40
2	A	501	VE9	C10-C21-N5	-2.70	121.86	124.40
2	C	501	VE9	C10-C21-N5	-2.67	121.89	124.40
2	B	501	VE9	C18-C16-C15	2.51	124.93	116.07
2	B	501	VE9	C3-C2-C9	-2.33	118.76	120.46
2	A	501	VE9	C14-N3-N4	-2.20	116.77	119.65
2	B	501	VE9	O2-C9-N2	-2.17	118.12	122.45
2	D	501	VE9	C14-N3-N4	-2.16	116.82	119.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	VE9	C14-N3-N4	-2.15	116.84	119.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	VE9	C17-C14-N3-C13
2	A	501	VE9	C17-C14-N3-N4
2	B	501	VE9	C17-C14-N3-C13
2	B	501	VE9	C17-C14-N3-N4
2	C	501	VE9	C17-C14-N3-C13
2	C	501	VE9	C17-C14-N3-N4
2	D	501	VE9	C17-C14-N3-C13
2	D	501	VE9	C17-C14-N3-N4

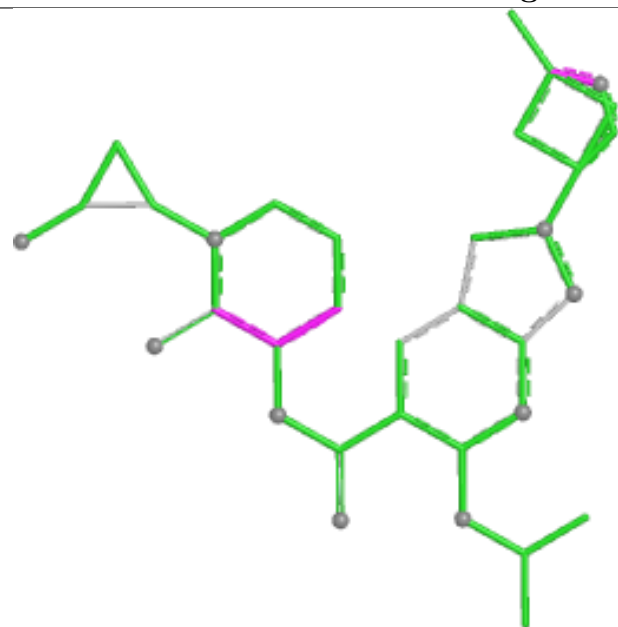
There are no ring outliers.

3 monomers are involved in 4 short contacts:

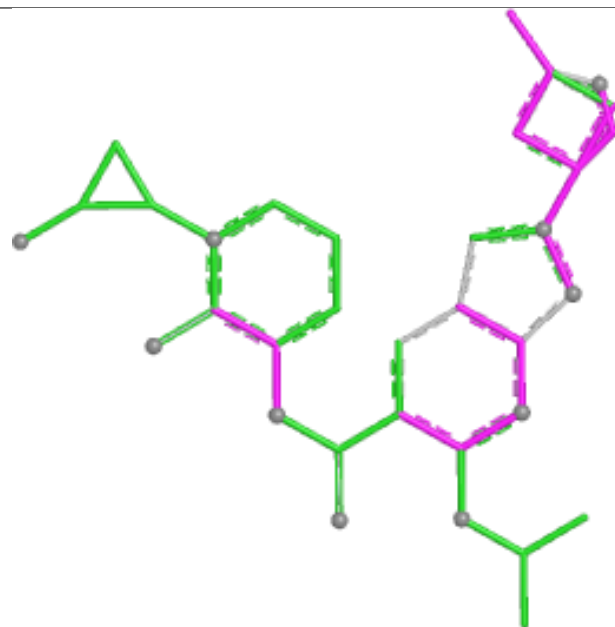
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	VE9	2	0
2	A	501	VE9	1	0
2	C	501	VE9	1	0

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.

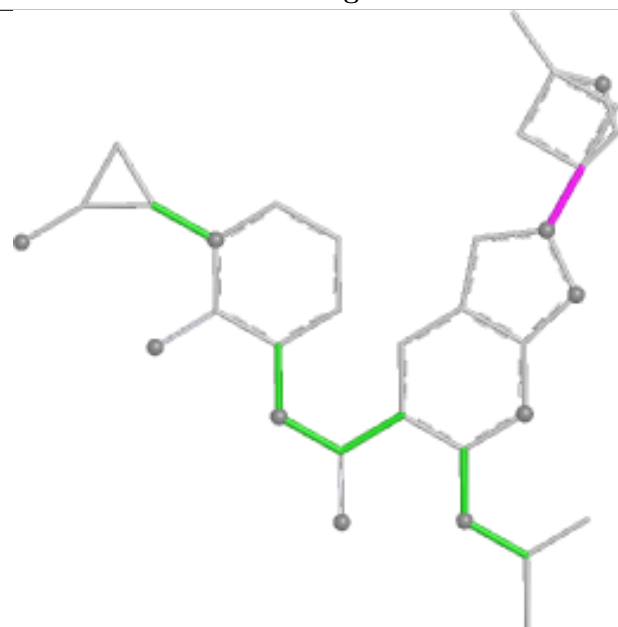
Ligand VE9 D 501



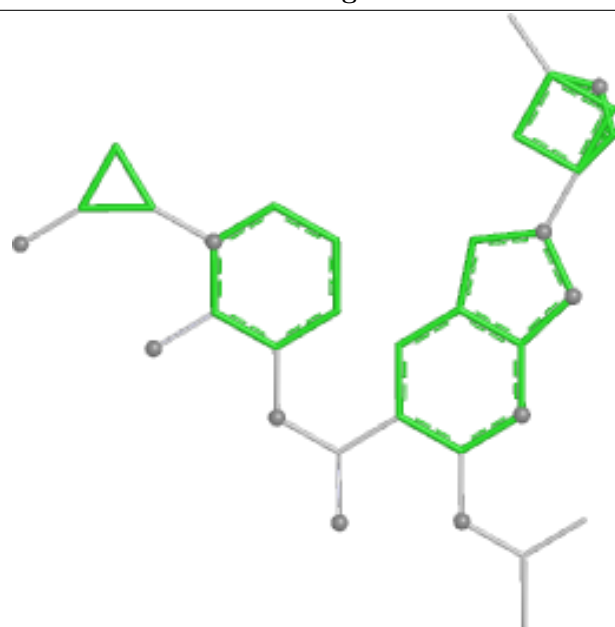
Bond lengths



Bond angles

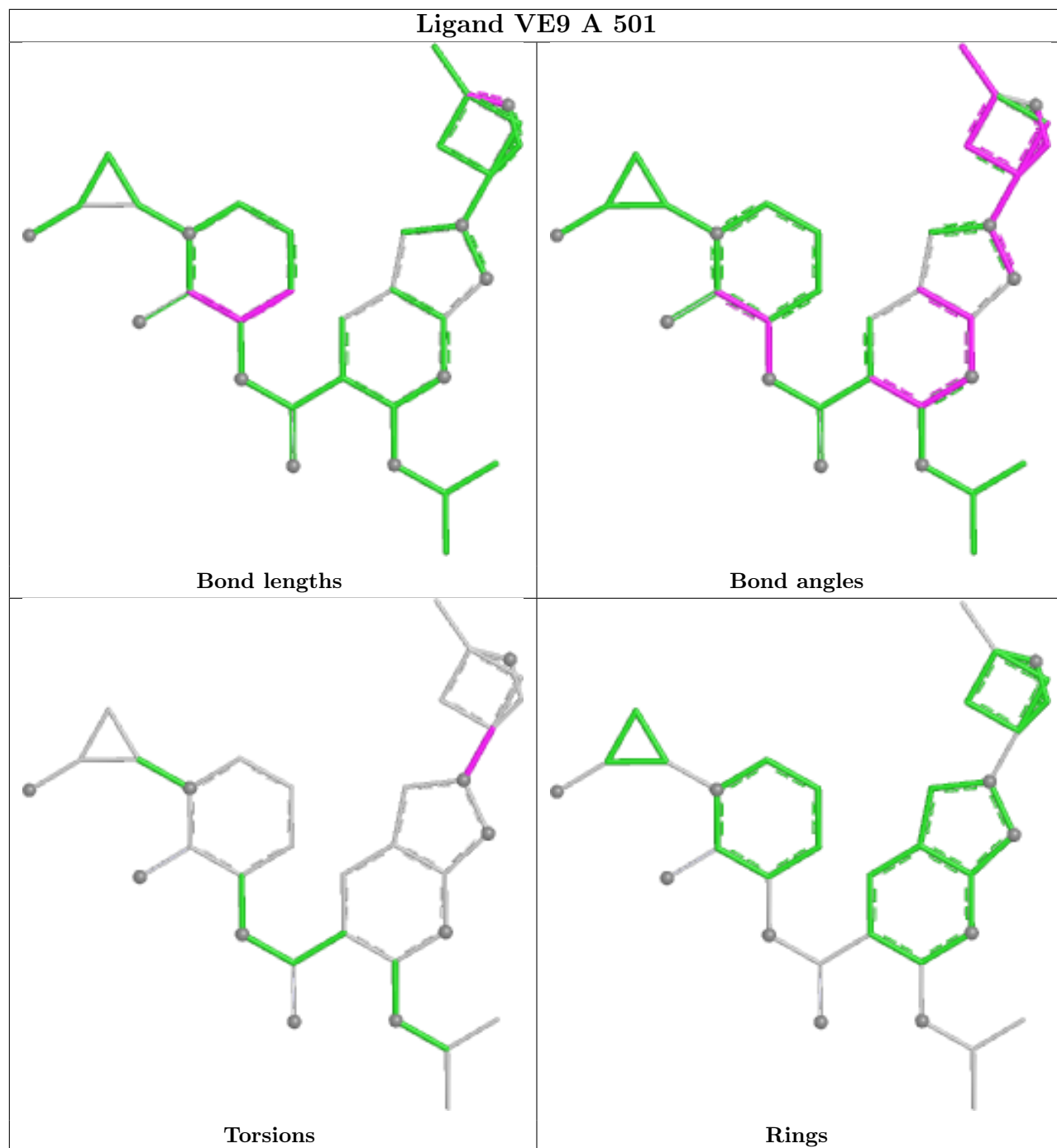


Torsions

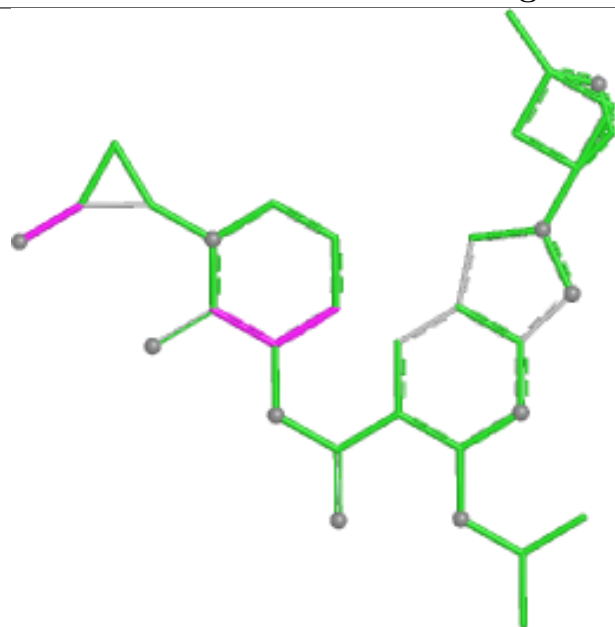


Rings

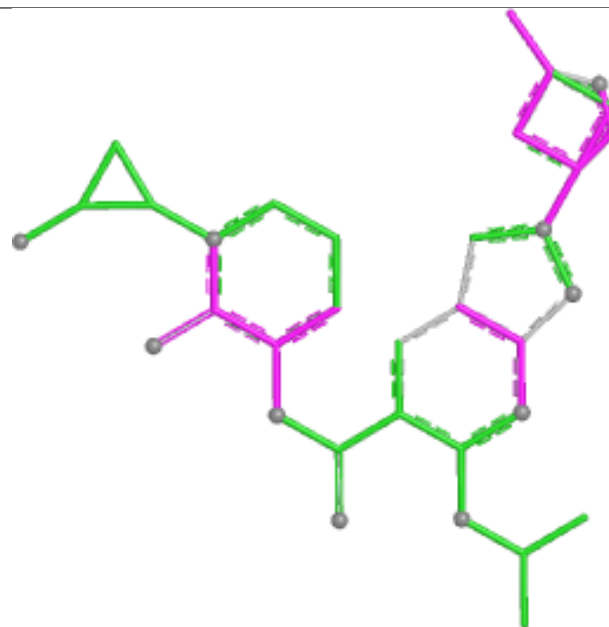
Ligand VE9 A 501



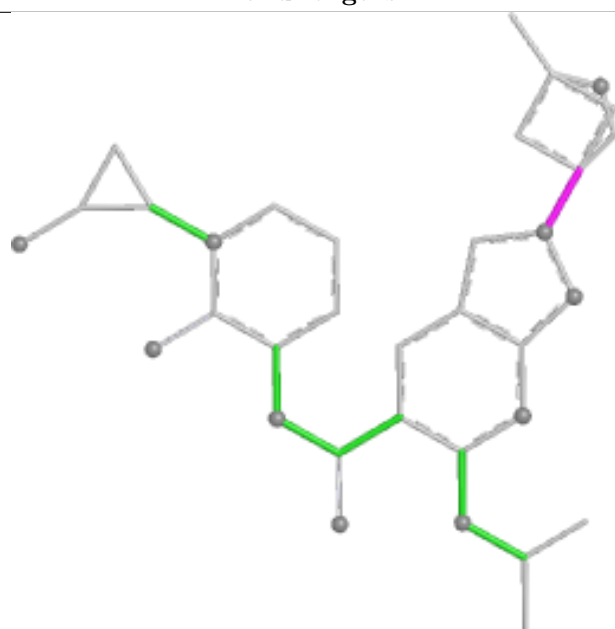
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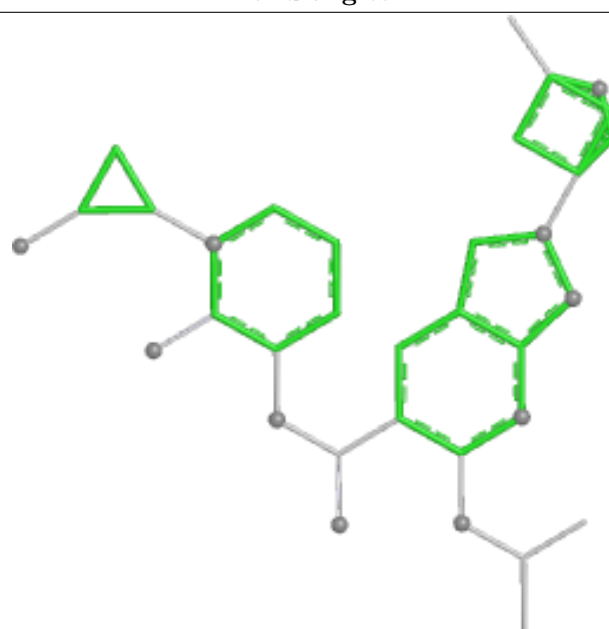
Bond lengths



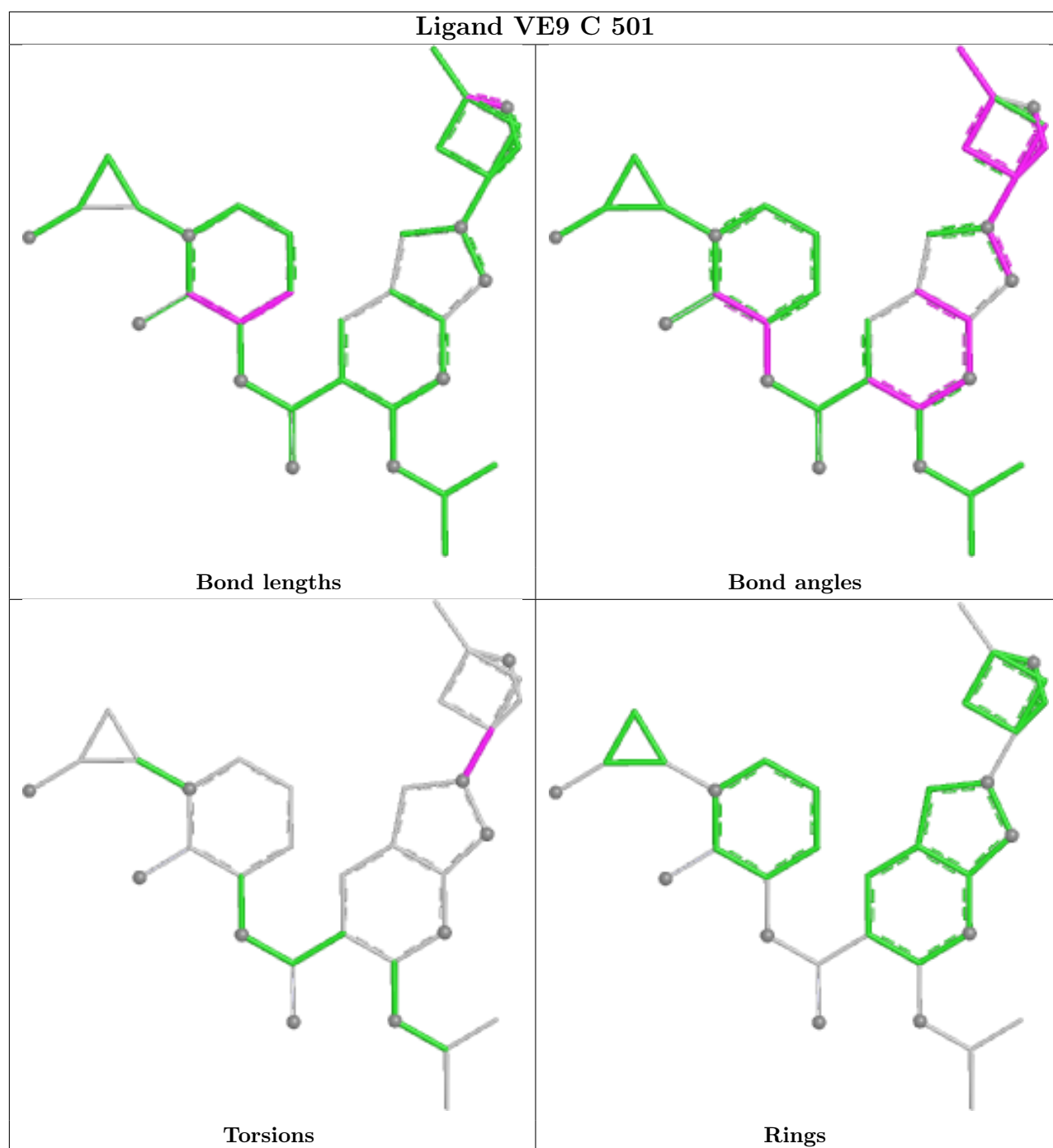
Bond angles



Torsions



Rings



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, 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	279/307 (90%)	0.52	20 (7%) 21 25	32, 54, 95, 124	0
1	B	283/307 (92%)	0.41	28 (9%) 13 14	28, 46, 94, 116	1 (0%)
1	C	283/307 (92%)	0.53	22 (7%) 19 22	35, 54, 86, 107	0
1	D	283/307 (92%)	0.75	28 (9%) 13 14	22, 63, 93, 119	1 (0%)
All	All	1128/1228 (91%)	0.55	98 (8%) 16 18	22, 55, 93, 124	2 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	PHE	5.0
1	B	458	THR	4.6
1	D	222	THR	4.5
1	D	165	PHE	4.5
1	C	335	ALA	4.5
1	C	458	THR	4.2
1	C	221	ILE	4.2
1	A	258	LEU	4.1
1	D	238	ALA	4.0
1	B	335	ALA	3.9
1	D	217	ALA	3.8
1	B	216	ALA	3.7
1	D	459	ALA	3.7
1	B	257	ASP	3.6
1	A	171	TYR	3.6
1	B	206	ASN	3.5
1	A	459	ALA	3.5
1	C	216	ALA	3.5
1	A	197	PHE	3.5
1	C	197	PHE	3.4
1	A	167	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	227	LYS	3.4
1	B	221	ILE	3.2
1	D	221	ILE	3.2
1	C	254	ASP	3.1
1	D	335	ALA	3.1
1	B	255	GLY	3.1
1	C	207	ASN	3.1
1	A	335	ALA	3.1
1	B	226	LEU	3.0
1	B	179	ASN	3.0
1	B	171	TYR	3.0
1	D	197	PHE	3.0
1	C	456	GLU	3.0
1	D	330	PHE	2.9
1	B	164	ARG	2.9
1	C	220	ASP	2.9
1	C	322	ALA	2.9
1	C	457	MET	2.9
1	C	209	THR	2.8
1	C	257	ASP	2.8
1	B	459	ALA	2.7
1	D	224	GLU	2.7
1	C	255	GLY	2.7
1	A	216	ALA	2.6
1	A	251	PHE	2.6
1	B	207	ASN	2.6
1	D	167	SER	2.6
1	A	221	ILE	2.6
1	D	254	ASP	2.6
1	B	197	PHE	2.5
1	A	343	VAL	2.5
1	D	343	VAL	2.5
1	B	208	THR	2.5
1	A	215	LEU	2.5
1	A	253	SER	2.5
1	C	253	SER	2.5
1	D	168	PHE	2.4
1	D	410	ILE	2.4
1	A	257	ASP	2.4
1	B	258	LEU	2.4
1	A	236	VAL	2.4
1	D	455	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	167	SER	2.4
1	C	206	ASN	2.3
1	D	240	CYS	2.3
1	C	263	VAL	2.3
1	D	166	HIS	2.3
1	B	165	PHE	2.3
1	D	364	ILE	2.3
1	A	256	ASP	2.3
1	D	229	GLN	2.3
1	B	205	VAL	2.3
1	B	166	HIS	2.3
1	C	332	LEU	2.3
1	B	253	SER	2.2
1	D	333	ALA	2.2
1	B	168	PHE	2.2
1	B	170	PHE	2.2
1	D	171	TYR	2.2
1	D	237	MET	2.2
1	C	455	GLN	2.2
1	C	256	ASP	2.2
1	B	215	LEU	2.2
1	D	195	GLY	2.2
1	A	224	GLU	2.1
1	D	226	LEU	2.1
1	B	251	PHE	2.1
1	B	223	THR	2.1
1	D	223	THR	2.1
1	A	255	GLY	2.1
1	B	195	GLY	2.1
1	D	216	ALA	2.1
1	C	286	HIS	2.1
1	B	204	TYR	2.0
1	A	223	THR	2.0
1	C	223	THR	2.0
1	D	215	LEU	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($\text{\AA}^2$)	Q<0.9
1	TPO	D	342	11/12	0.56	0.15	85,103,129,132	0
1	SEP	D	346	10/11	0.63	0.12	96,101,120,131	0
1	TPO	A	342	11/12	0.67	0.18	78,86,103,114	0
1	TPO	C	342	11/12	0.74	0.14	76,85,99,102	0
1	SEP	A	346	10/11	0.76	0.12	76,82,114,126	0
1	SEP	C	346	10/11	0.77	0.10	74,88,96,117	0
1	TPO	B	342	11/12	0.78	0.15	58,73,79,82	0
1	SEP	B	346	10/11	0.81	0.11	66,78,108,124	0
1	TPO	D	345	11/12	0.91	0.09	85,92,101,101	0
1	TPO	A	345	11/12	0.92	0.09	64,70,79,87	0
1	TPO	C	345	11/12	0.93	0.09	62,69,76,79	0
1	TPO	B	345	11/12	0.94	0.07	55,63,70,72	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

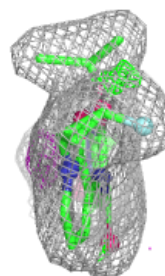
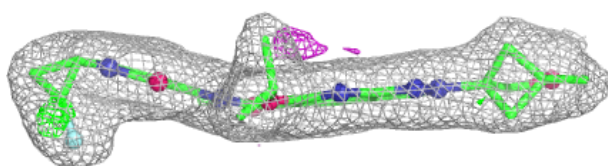
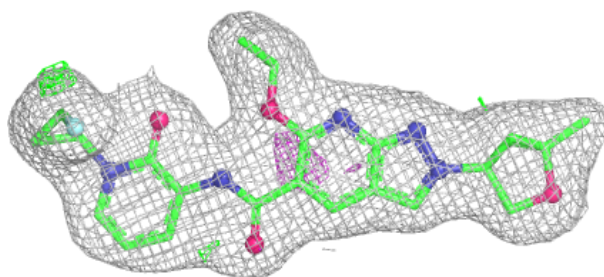
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	VE9	B	501	34/34	0.94	0.09	35,41,50,56	0
2	VE9	C	501	34/34	0.94	0.09	32,41,49,51	0
2	VE9	D	501	34/34	0.94	0.08	32,41,49,51	0
2	VE9	A	501	34/34	0.96	0.07	32,41,49,51	0

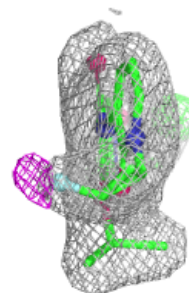
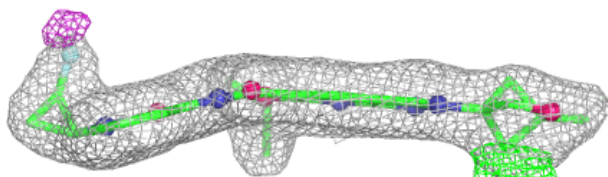
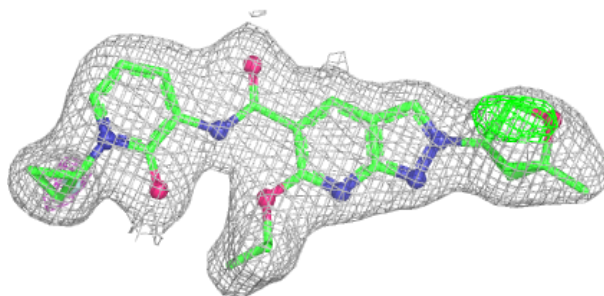
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VE9 B 501:

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

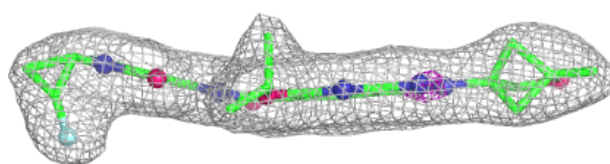
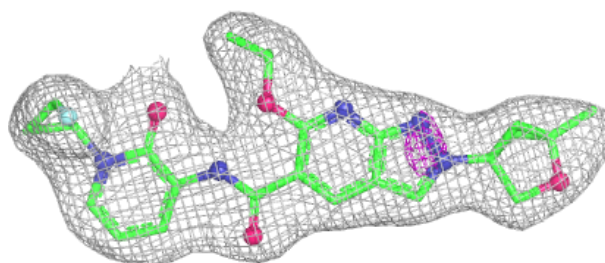
**Electron density around VE9 C 501:**

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

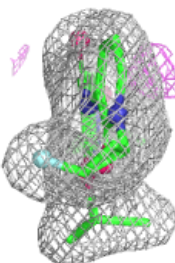
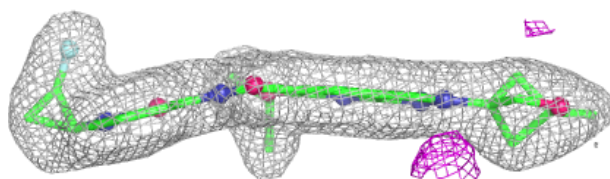
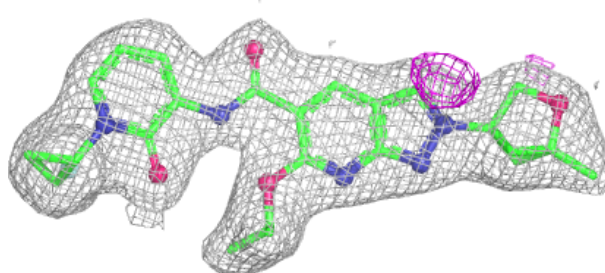


Electron density around VE9 D 501:

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

**Electron density around VE9 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.