



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:40 AM UTC

PDB ID : 7OIL / pdb_00007oil
Title : mPI3Kd in complex with compound 58
Authors : Petersen, J.
Deposited on : 2021-05-11
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

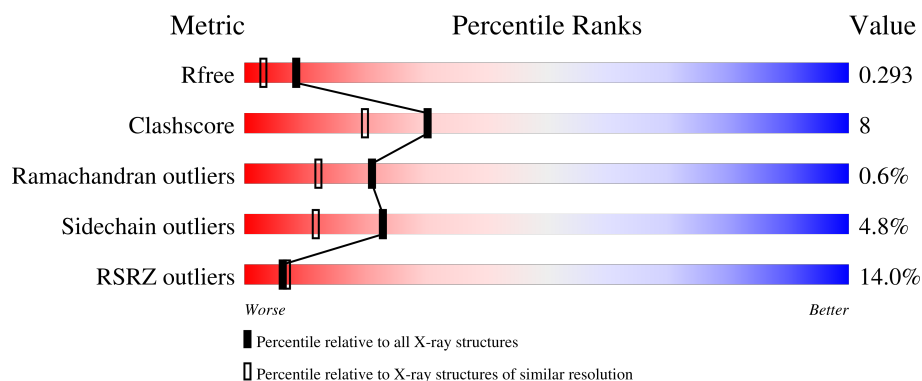
1 Overall quality at a glance

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	AAA	1084	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6958 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	827	Total	C	N	O	S	3	1	0
			6678	4281	1131	1211	55			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-39	MET	-	initiating methionine	UNP O35904
AAA	-38	SER	-	expression tag	UNP O35904
AAA	-37	TYR	-	expression tag	UNP O35904
AAA	-36	HIS	-	expression tag	UNP O35904
AAA	-35	ASN	-	expression tag	UNP O35904
AAA	-34	HIS	-	expression tag	UNP O35904
AAA	-33	ASN	-	expression tag	UNP O35904
AAA	-32	HIS	-	expression tag	UNP O35904
AAA	-31	ASN	-	expression tag	UNP O35904
AAA	-30	HIS	-	expression tag	UNP O35904
AAA	-29	ASN	-	expression tag	UNP O35904
AAA	-28	HIS	-	expression tag	UNP O35904
AAA	-27	ASN	-	expression tag	UNP O35904
AAA	-26	HIS	-	expression tag	UNP O35904
AAA	-25	ASN	-	expression tag	UNP O35904
AAA	-24	ASP	-	expression tag	UNP O35904
AAA	-23	TYR	-	expression tag	UNP O35904
AAA	-22	ASP	-	expression tag	UNP O35904
AAA	-21	ILE	-	expression tag	UNP O35904
AAA	-20	PRO	-	expression tag	UNP O35904
AAA	-19	THR	-	expression tag	UNP O35904
AAA	-18	THR	-	expression tag	UNP O35904
AAA	-17	GLU	-	expression tag	UNP O35904
AAA	-16	ASN	-	expression tag	UNP O35904
AAA	-15	LEU	-	expression tag	UNP O35904
AAA	-14	TYR	-	expression tag	UNP O35904

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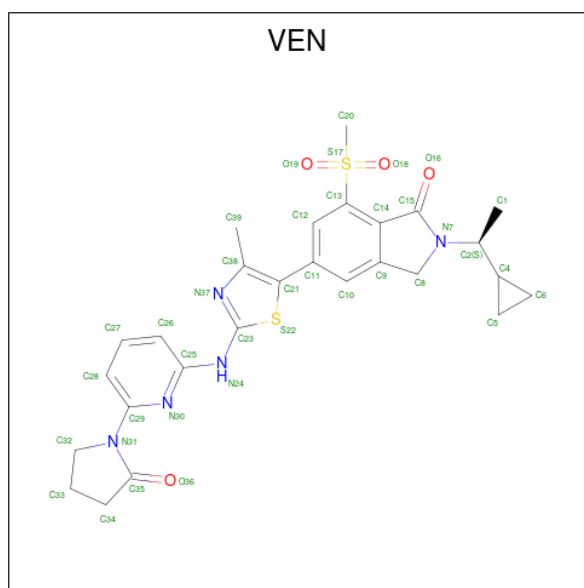
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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-13	PHE	-	expression tag	UNP O35904
AAA	-12	GLN	-	expression tag	UNP O35904
AAA	-11	GLY	-	expression tag	UNP O35904
AAA	-10	ALA	-	expression tag	UNP O35904
AAA	-9	MET	-	expression tag	UNP O35904
AAA	-8	ASP	-	expression tag	UNP O35904
AAA	-7	LEU	-	expression tag	UNP O35904
AAA	99	GLU	-	insertion	UNP O35904
AAA	100	ASN	-	insertion	UNP O35904
AAA	101	LEU	-	insertion	UNP O35904
AAA	102	TYR	-	insertion	UNP O35904
AAA	103	PHE	-	insertion	UNP O35904
AAA	104	GLN	-	insertion	UNP O35904
AAA	105	GLY	-	insertion	UNP O35904
AAA	510A	GLN	-	insertion	UNP O35904

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Na 1 1	0	0

- Molecule 3 is 2-[(1S)-1-cyclopropylethyl]-5-[4-methyl-2-[[6-(2-oxidanylidenepyrrolidin-1-yl)pyridin-2-yl]amino]-1,3-thiazol-5-yl]-7-methylsulfonyl-3H-isoindol-1-one (CCD ID: VEN) (formula: C₂₇H₂₉N₅O₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	S	0	0
			38	27	5	4	2		

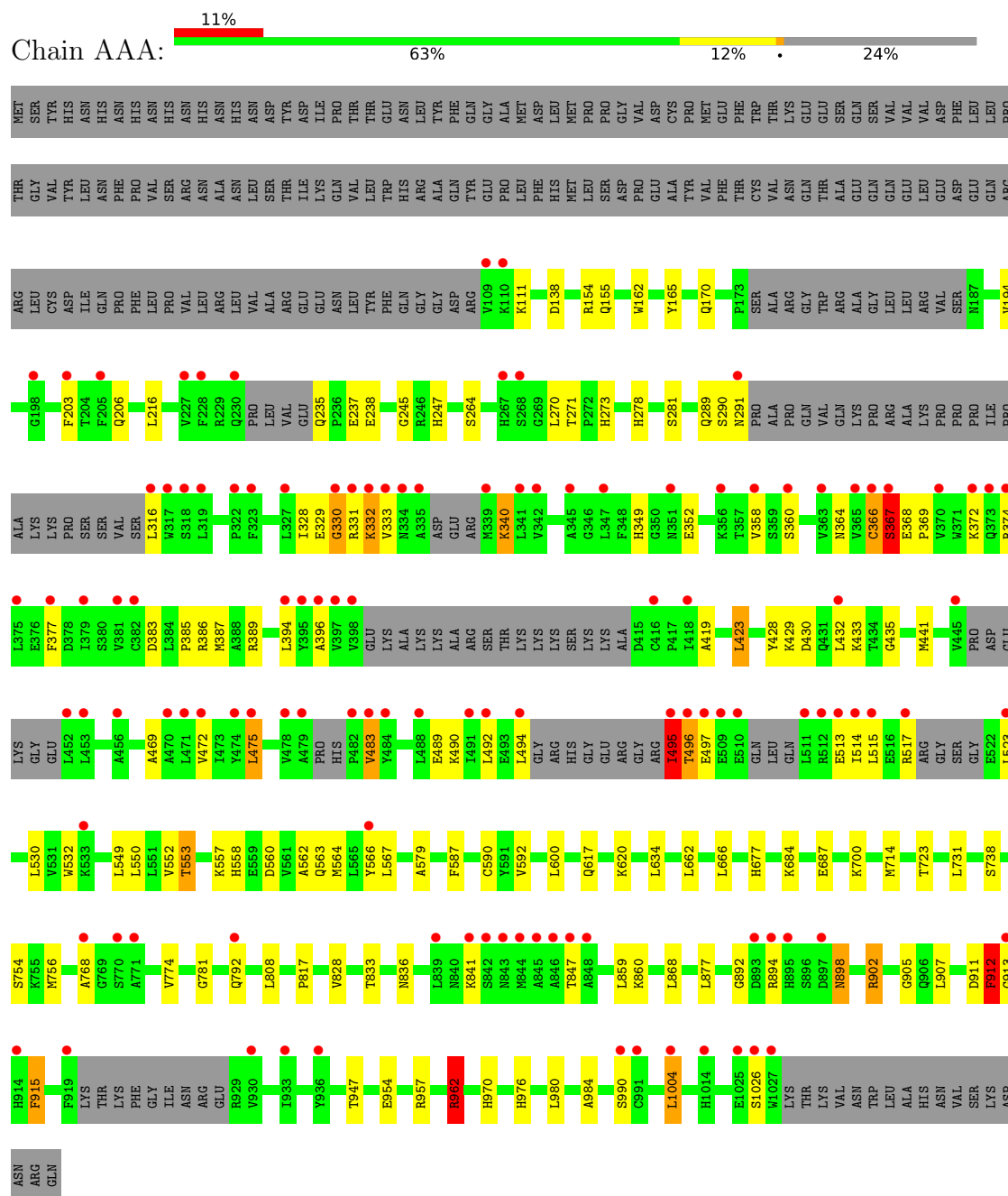
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	241	Total	O	0	0
			241	241		

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.01Å 64.75Å 116.38Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	31.13 – 1.95 31.13 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (31.13-1.95) 99.2 (31.13-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.239 , 0.289 0.244 , 0.293	Depositor DCC
R_{free} test set	3750 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6958	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: VEN, NA

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	AAA	1.12	4/6824 (0.1%)	1.47	11/9207 (0.1%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	330	GLY	N-CA	6.02	1.49	1.44
1	AAA	567	LEU	C-O	5.94	1.30	1.24
1	AAA	774	VAL	C-O	5.91	1.30	1.23
1	AAA	902	ARG	CD-NE	-5.13	1.39	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	912	PHE	CB-CA-C	7.50	125.36	110.42
1	AAA	723	THR	CA-CB-OG1	-6.82	99.37	109.60
1	AAA	915	PHE	CA-CB-CG	6.69	120.49	113.80
1	AAA	367	SER	CA-C-N	5.34	131.31	121.70
1	AAA	367	SER	C-N-CA	5.34	131.31	121.70
1	AAA	962	ARG	CG-CD-NE	5.32	123.71	112.00
1	AAA	264	SER	CA-C-N	5.13	127.16	120.28
1	AAA	264	SER	C-N-CA	5.13	127.16	120.28
1	AAA	495	ILE	CB-CA-C	-5.07	106.54	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	385	PRO	CA-C-N	5.04	127.28	120.38
1	AAA	385	PRO	C-N-CA	5.04	127.28	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	912	PHE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	6678	0	6656	111	1
2	AAA	1	0	0	0	0
3	AAA	38	0	0	1	0
4	AAA	241	0	0	15	0
All	All	6958	0	6656	112	1

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 8.

All (112) 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:AAA:756:MET:HE2	1:AAA:781:GLY:HA3	1.29	1.11
1:AAA:549:LEU:HG	1:AAA:564:MET:HE1	1.51	0.92
1:AAA:700:LYS:HE2	1:AAA:756:MET:HE3	1.57	0.86
1:AAA:495:ILE:O	1:AAA:497:GLU:N	2.10	0.85
1:AAA:386:ARG:HG3	1:AAA:387:MET:HE2	1.61	0.82
1:AAA:235:GLN:N	4:AAA:1202:HOH:O	2.13	0.81
1:AAA:495:ILE:CG2	1:AAA:563:GLN:HA	2.12	0.79
1:AAA:495:ILE:HG12	1:AAA:562:ALA:C	2.08	0.78
1:AAA:495:ILE:HG23	1:AAA:563:GLN:HA	1.64	0.77
1:AAA:394:LEU:HD23	1:AAA:441:MET:HE1	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:367:SER:HB3	1:AAA:368:GLU:HB3	1.66	0.75
1:AAA:383:ASP:OD1	1:AAA:558:HIS:ND1	2.17	0.74
1:AAA:387:MET:HE3	1:AAA:590:CYS:HB3	1.69	0.73
1:AAA:549:LEU:CG	1:AAA:564:MET:HE1	2.19	0.73
1:AAA:271:THR:O	1:AAA:273:HIS:HD2	1.72	0.73
1:AAA:330:GLY:O	1:AAA:331:ARG:HG3	1.88	0.72
1:AAA:495:ILE:C	1:AAA:497:GLU:N	2.48	0.71
1:AAA:328:ILE:HB	1:AAA:472:VAL:HG23	1.73	0.70
1:AAA:817:PRO:HD2	4:AAA:1235:HOH:O	1.92	0.69
1:AAA:367:SER:HB2	1:AAA:368:GLU:C	2.19	0.68
1:AAA:495:ILE:O	1:AAA:496:THR:C	2.37	0.67
1:AAA:687:GLU:OE2	4:AAA:1201:HOH:O	2.12	0.66
1:AAA:332:LYS:HE3	1:AAA:333:VAL:N	2.10	0.66
1:AAA:387:MET:HE3	1:AAA:590:CYS:SG	2.35	0.66
1:AAA:432:LEU:HB3	1:AAA:483:VAL:HG23	1.78	0.66
1:AAA:394:LEU:CD2	1:AAA:441:MET:HE1	2.26	0.65
1:AAA:700:LYS:CE	1:AAA:756:MET:HE3	2.26	0.65
1:AAA:549:LEU:HG	1:AAA:564:MET:CE	2.25	0.64
3:AAA:1102:VEN:N30	3:AAA:1102:VEN:S22	2.70	0.64
1:AAA:367:SER:CB	1:AAA:368:GLU:C	2.72	0.63
1:AAA:435:GLY:O	1:AAA:475:LEU:N	2.25	0.62
1:AAA:495:ILE:CD1	1:AAA:562:ALA:O	2.48	0.61
1:AAA:387:MET:HE3	1:AAA:590:CYS:CB	2.30	0.61
1:AAA:833:THR:OG1	1:AAA:836:ASN:HB2	2.01	0.59
1:AAA:238:GLU:HG3	4:AAA:1386:HOH:O	2.02	0.59
1:AAA:358:VAL:HG22	1:AAA:377:PHE:CE1	2.36	0.59
1:AAA:495:ILE:HB	1:AAA:566:TYR:HB2	1.85	0.59
1:AAA:495:ILE:HD13	1:AAA:562:ALA:O	2.03	0.59
1:AAA:278:HIS:HE1	4:AAA:1386:HOH:O	1.85	0.58
1:AAA:892:GLY:O	1:AAA:894:ARG:NE	2.38	0.57
1:AAA:1004:LEU:HD11	4:AAA:1424:HOH:O	2.04	0.57
1:AAA:495:ILE:O	1:AAA:497:GLU:C	2.47	0.57
1:AAA:495:ILE:HG21	1:AAA:563:GLN:HA	1.86	0.57
1:AAA:419:ALA:HB3	1:AAA:441:MET:HE3	1.87	0.56
1:AAA:912:PHE:CB	1:AAA:913:GLY:HA3	2.36	0.55
1:AAA:954:GLU:OE1	1:AAA:957:ARG:NE	2.36	0.55
1:AAA:532:TRP:HZ3	1:AAA:564:MET:HE2	1.71	0.55
1:AAA:495:ILE:HD13	1:AAA:566:TYR:HB2	1.89	0.54
1:AAA:549:LEU:CD1	1:AAA:564:MET:HE1	2.38	0.53
1:AAA:495:ILE:HG12	1:AAA:562:ALA:O	2.06	0.53
1:AAA:330:GLY:C	1:AAA:331:ARG:HG3	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:245:GLY:HA3	1:AAA:768:ALA:HB2	1.90	0.52
1:AAA:662:LEU:O	1:AAA:666:LEU:HG	2.09	0.52
1:AAA:349:HIS:HE1	4:AAA:1265:HOH:O	1.92	0.52
1:AAA:331:ARG:O	1:AAA:469:ALA:HA	2.10	0.52
1:AAA:912:PHE:HB3	1:AAA:913:GLY:HA3	1.90	0.52
1:AAA:617:GLN:NE2	1:AAA:984:ALA:HA	2.26	0.51
1:AAA:340:LYS:HG3	1:AAA:364:ASN:HA	1.92	0.51
1:AAA:194:VAL:HG21	1:AAA:216:LEU:HD21	1.92	0.51
1:AAA:492:LEU:HA	1:AAA:495:ILE:HD12	1.93	0.51
1:AAA:367:SER:HB3	1:AAA:368:GLU:CB	2.37	0.50
1:AAA:579:ALA:HB1	1:AAA:600:LEU:HG	1.93	0.50
1:AAA:289:GLN:HG2	1:AAA:677:HIS:CD2	2.46	0.50
1:AAA:329:GLU:HG2	1:AAA:472:VAL:CG2	2.42	0.50
1:AAA:329:GLU:O	1:AAA:472:VAL:HG22	2.11	0.50
1:AAA:792:GLN:HB3	4:AAA:1419:HOH:O	2.11	0.50
1:AAA:902:ARG:HD2	4:AAA:1305:HOH:O	2.10	0.49
1:AAA:162:TRP:NE1	4:AAA:1216:HOH:O	2.44	0.49
1:AAA:278:HIS:CE1	4:AAA:1386:HOH:O	2.63	0.49
1:AAA:550:LEU:O	1:AAA:553:THR:HG23	2.13	0.49
1:AAA:247:HIS:O	1:AAA:738:SER:HB2	2.12	0.48
1:AAA:962:ARG:HH11	1:AAA:962:ARG:HG2	1.79	0.48
1:AAA:170:GLN:HG3	4:AAA:1396:HOH:O	2.13	0.48
1:AAA:332:LYS:HE3	1:AAA:332:LYS:C	2.39	0.48
1:AAA:495:ILE:CG1	1:AAA:562:ALA:O	2.62	0.48
1:AAA:423:LEU:N	1:AAA:423:LEU:CD1	2.78	0.47
1:AAA:271:THR:O	1:AAA:273:HIS:CD2	2.60	0.47
1:AAA:495:ILE:CB	1:AAA:566:TYR:HB2	2.44	0.47
1:AAA:617:GLN:HE22	1:AAA:620:LYS:NZ	2.11	0.47
1:AAA:617:GLN:HE21	1:AAA:984:ALA:HA	1.80	0.47
1:AAA:970:HIS:HD2	4:AAA:1437:HOH:O	1.98	0.47
1:AAA:238:GLU:CG	4:AAA:1386:HOH:O	2.61	0.46
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CE2	2.51	0.46
1:AAA:329:GLU:HB2	1:AAA:369:PRO:O	2.15	0.46
1:AAA:549:LEU:O	1:AAA:552:VAL:HG22	2.16	0.46
1:AAA:828:VAL:CG1	1:AAA:902:ARG:HD3	2.46	0.46
1:AAA:138:ASP:OD2	1:AAA:428:TYR:OH	2.24	0.45
1:AAA:808:LEU:HA	1:AAA:877:LEU:HB3	1.98	0.45
1:AAA:235:GLN:HG3	1:AAA:237:GLU:OE1	2.17	0.45
1:AAA:859:LEU:HD21	1:AAA:905:GLY:HA2	1.98	0.45
1:AAA:489:GLU:HG3	1:AAA:490:LYS:N	2.32	0.44
1:AAA:907:LEU:C	1:AAA:907:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:976:HIS:O	1:AAA:980:LEU:HG	2.17	0.44
1:AAA:433:LYS:O	1:AAA:475:LEU:HD22	2.17	0.44
1:AAA:367:SER:HB3	1:AAA:368:GLU:C	2.42	0.44
1:AAA:860:LYS:HG2	1:AAA:868:LEU:HD22	2.00	0.44
1:AAA:700:LYS:HE3	1:AAA:756:MET:O	2.17	0.44
1:AAA:419:ALA:HB1	1:AAA:441:MET:HB3	1.99	0.43
1:AAA:495:ILE:CG1	1:AAA:562:ALA:HB1	2.48	0.43
1:AAA:494:LEU:O	1:AAA:494:LEU:HG	2.18	0.43
1:AAA:329:GLU:HG2	1:AAA:472:VAL:HG22	2.00	0.43
1:AAA:495:ILE:HG21	1:AAA:566:TYR:CB	2.49	0.43
1:AAA:366:CYS:O	1:AAA:367:SER:CB	2.66	0.42
1:AAA:553:THR:CG2	1:AAA:564:MET:HE3	2.49	0.42
1:AAA:684:LYS:CE	4:AAA:1257:HOH:O	2.68	0.42
1:AAA:367:SER:CB	1:AAA:368:GLU:CA	2.98	0.42
1:AAA:898:ASN:HB3	1:AAA:911:ASP:OD2	2.20	0.41
1:AAA:155:GLN:NE2	1:AAA:290:SER:HB3	2.36	0.41
1:AAA:429:LYS:O	1:AAA:430:ASP:HB2	2.21	0.41
1:AAA:340:LYS:O	1:AAA:396:ALA:HA	2.20	0.41
1:AAA:587:PHE:HB3	1:AAA:592:VAL:HG11	2.02	0.41
1:AAA:513:GLU:C	1:AAA:515:LEU:H	2.29	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:714:MET:SD	1:AAA:714:MET:SD[2_555]	1.78	0.42

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	AAA	806/1084 (74%)	766 (95%)	35 (4%)	5 (1%)	21 12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	367	SER
1	AAA	496	THR
1	AAA	1026	SER
1	AAA	372	LYS
1	AAA	514	ILE

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	AAA	734/962 (76%)	699 (95%)	35 (5%)	23	12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	111	LYS
1	AAA	203	PHE
1	AAA	206	GLN
1	AAA	270	LEU
1	AAA	281	SER
1	AAA	291	ASN
1	AAA	316	LEU
1	AAA	332	LYS
1	AAA	340	LYS
1	AAA	352	GLU
1	AAA	360	SER
1	AAA	366	CYS
1	AAA	374	ARG
1	AAA	389	ARG
1	AAA	423	LEU
1	AAA	475	LEU
1	AAA	483	VAL
1	AAA	495	ILE
1	AAA	517	ARG
1	AAA	523	LEU

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Mol	Chain	Res	Type
1	AAA	530	LEU
1	AAA	553	THR
1	AAA	557	LYS
1	AAA	560	ASP
1	AAA	634	LEU
1	AAA	731	LEU
1	AAA	754	SER
1	AAA	841	LYS
1	AAA	847	THR
1	AAA	898	ASN
1	AAA	915	PHE
1	AAA	947	THR
1	AAA	962	ARG
1	AAA	990	SER
1	AAA	1004	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
3	VEN	AAA	1102	-	41,43,43	1.34	8 (19%)	57,66,66	3.61	22 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VEN	AAA	1102	-	-	1/26/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	1102	VEN	C10-C9	-3.14	1.34	1.39
3	AAA	1102	VEN	C20-S17	2.61	1.84	1.75
3	AAA	1102	VEN	C23-N24	2.46	1.40	1.36
3	AAA	1102	VEN	C38-N37	-2.36	1.33	1.38
3	AAA	1102	VEN	C28-C29	2.29	1.44	1.39
3	AAA	1102	VEN	C32-N31	2.06	1.50	1.47
3	AAA	1102	VEN	C8-N7	2.05	1.49	1.47
3	AAA	1102	VEN	C8-C9	-2.02	1.47	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	1102	VEN	C8-N7-C15	-14.76	106.93	113.15
3	AAA	1102	VEN	C23-N37-C38	9.03	115.89	110.38
3	AAA	1102	VEN	C9-C8-N7	8.94	107.06	102.31
3	AAA	1102	VEN	S22-C23-N37	-6.42	110.04	115.78
3	AAA	1102	VEN	C34-C35-N31	5.97	112.21	108.17
3	AAA	1102	VEN	C32-N31-C29	5.96	126.52	120.61
3	AAA	1102	VEN	C25-N30-C29	5.25	123.01	117.62
3	AAA	1102	VEN	C33-C32-N31	4.93	108.80	103.32
3	AAA	1102	VEN	C8-N7-C2	4.43	128.28	124.24
3	AAA	1102	VEN	C23-S22-C21	4.25	91.00	88.35
3	AAA	1102	VEN	O19-S17-O18	4.21	125.13	117.99
3	AAA	1102	VEN	O16-C15-N7	-3.77	122.34	125.34
3	AAA	1102	VEN	O19-S17-C13	-3.62	104.04	108.24
3	AAA	1102	VEN	C25-N24-C23	-3.47	122.35	126.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	1102	VEN	C38-C21-S22	-3.45	107.81	109.91
3	AAA	1102	VEN	O19-S17-C20	-3.23	103.72	108.47
3	AAA	1102	VEN	C12-C13-C14	-3.18	117.29	120.69
3	AAA	1102	VEN	C8-C9-C14	-3.15	107.67	109.96
3	AAA	1102	VEN	C32-N31-C35	-3.13	109.88	112.85
3	AAA	1102	VEN	C1-C2-C4	-2.56	108.21	113.47
3	AAA	1102	VEN	C28-C29-N30	-2.11	120.17	123.62
3	AAA	1102	VEN	O16-C15-C14	-2.05	126.04	129.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

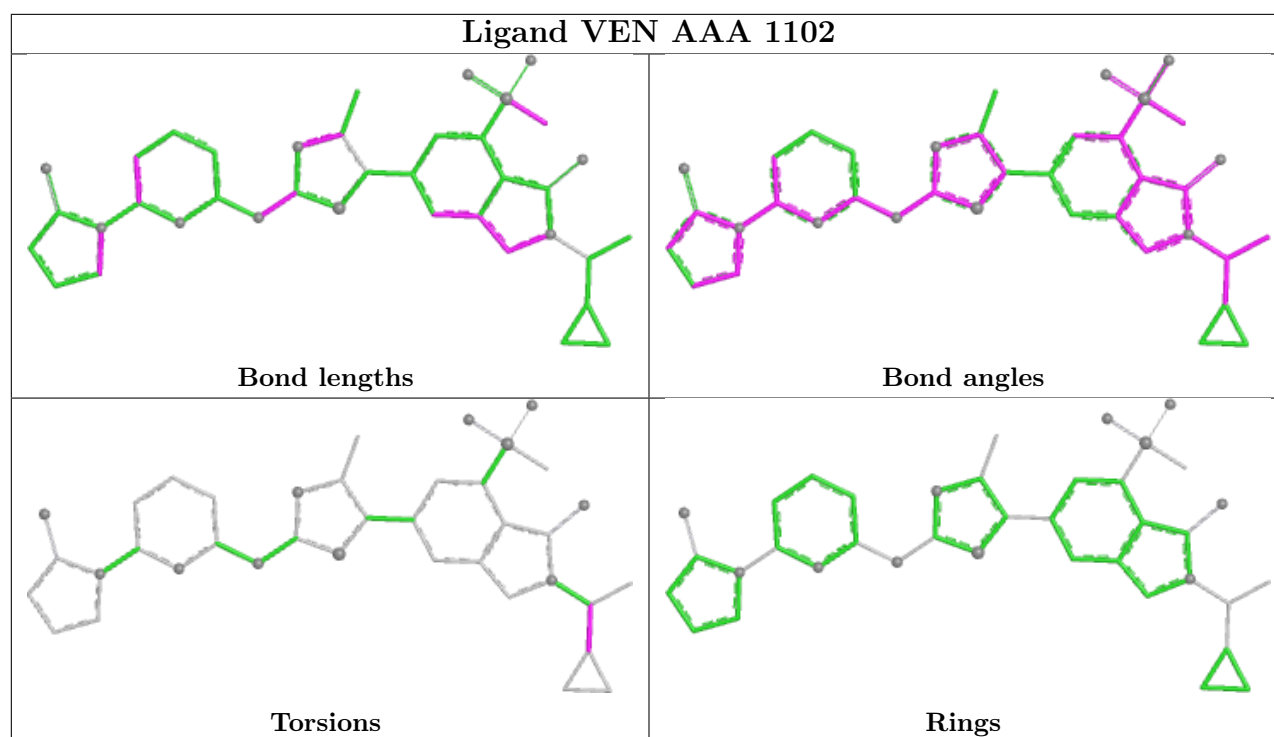
Mol	Chain	Res	Type	Atoms
3	AAA	1102	VEN	C1-C2-C4-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	1102	VEN	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AAA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AAA	497:GLU	C	509:GLU	N	21.72

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	AAA	827/1084 (76%)	0.77	116 (14%) 6 7	11, 39, 74, 115	2 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	495	ILE	7.0
1	AAA	1027	TRP	6.8
1	AAA	317	TRP	6.7
1	AAA	445	VAL	6.6
1	AAA	333	VAL	6.4
1	AAA	335	ALA	6.1
1	AAA	847	THR	5.8
1	AAA	846	ALA	5.7
1	AAA	366	CYS	5.6
1	AAA	919	PHE	5.2
1	AAA	316	LEU	5.1
1	AAA	523	LEU	4.9
1	AAA	478	VAL	4.7
1	AAA	514	ILE	4.7
1	AAA	367	SER	4.7
1	AAA	397	VAL	4.7
1	AAA	515	LEU	4.5
1	AAA	511	LEU	4.4
1	AAA	377	PHE	4.3
1	AAA	845	ALA	4.2
1	AAA	512	ARG	4.2
1	AAA	479	ALA	4.0
1	AAA	228	PHE	4.0
1	AAA	894	ARG	4.0
1	AAA	332	LYS	3.9
1	AAA	496	THR	3.9
1	AAA	375	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	334	ASN	3.7
1	AAA	453	LEU	3.7
1	AAA	913	GLY	3.5
1	AAA	365	VAL	3.4
1	AAA	452	LEU	3.4
1	AAA	203	PHE	3.4
1	AAA	517	ARG	3.4
1	AAA	488	LEU	3.3
1	AAA	330	GLY	3.3
1	AAA	109	VAL	3.2
1	AAA	227	VAL	3.1
1	AAA	475	LEU	3.1
1	AAA	513	GLU	3.0
1	AAA	374	ARG	3.0
1	AAA	319	LEU	3.0
1	AAA	370	VAL	3.0
1	AAA	474	TYR	3.0
1	AAA	398	VAL	2.9
1	AAA	930	VAL	2.9
1	AAA	363	VAL	2.8
1	AAA	1004	LEU	2.8
1	AAA	483	VAL	2.8
1	AAA	842	SER	2.8
1	AAA	848	ALA	2.8
1	AAA	841	LYS	2.7
1	AAA	510	GLU	2.7
1	AAA	990	SER	2.7
1	AAA	1026	SER	2.7
1	AAA	395	TYR	2.7
1	AAA	323	PHE	2.7
1	AAA	416	CYS	2.7
1	AAA	379	ILE	2.7
1	AAA	472	VAL	2.7
1	AAA	267	HIS	2.6
1	AAA	322	PRO	2.6
1	AAA	291	ASN	2.6
1	AAA	492	LEU	2.6
1	AAA	482	PRO	2.5
1	AAA	372	LYS	2.5
1	AAA	768	ALA	2.5
1	AAA	770	SER	2.5
1	AAA	566	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	471	LEU	2.5
1	AAA	356	LYS	2.5
1	AAA	936	TYR	2.5
1	AAA	347	LEU	2.5
1	AAA	331	ARG	2.5
1	AAA	341	LEU	2.4
1	AAA	230	GLN	2.4
1	AAA	382	CYS	2.4
1	AAA	914	HIS	2.4
1	AAA	484	TYR	2.4
1	AAA	205	PHE	2.4
1	AAA	418	ILE	2.4
1	AAA	339	MET	2.4
1	AAA	933	ILE	2.4
1	AAA	198	GLY	2.4
1	AAA	991	CYS	2.4
1	AAA	897	ASP	2.3
1	AAA	456	ALA	2.3
1	AAA	771	ALA	2.3
1	AAA	1025	GLU	2.3
1	AAA	533	LYS	2.3
1	AAA	396	ALA	2.3
1	AAA	470	ALA	2.3
1	AAA	360	SER	2.2
1	AAA	358	VAL	2.2
1	AAA	895	HIS	2.2
1	AAA	844	MET	2.2
1	AAA	839	LEU	2.2
1	AAA	345	ALA	2.2
1	AAA	1014	HIS	2.2
1	AAA	394	LEU	2.2
1	AAA	110	LYS	2.2
1	AAA	327	LEU	2.2
1	AAA	351	ASN	2.1
1	AAA	381	VAL	2.1
1	AAA	373	GLN	2.1
1	AAA	893	ASP	2.1
1	AAA	843	ASN	2.1
1	AAA	792	GLN	2.1
1	AAA	432	LEU	2.1
1	AAA	268	SER	2.0
1	AAA	491	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	AAA	342	VAL	2.0
1	AAA	494	LEU	2.0
1	AAA	497	GLU	2.0
1	AAA	509	GLU	2.0
1	AAA	318	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

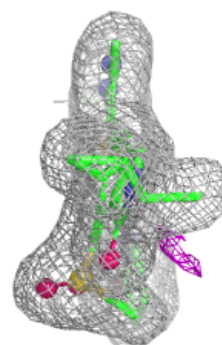
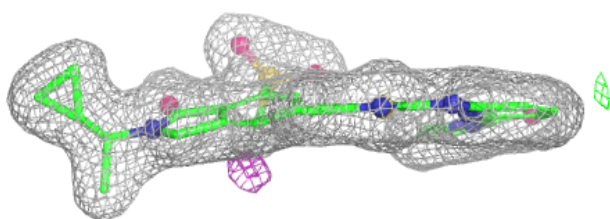
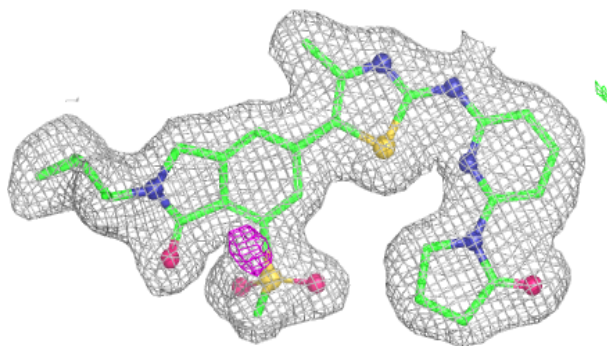
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NA	AAA	1101	1/1	0.94	0.28	45,45,45,45	0
3	VEN	AAA	1102	38/38	0.98	0.05	19,21,27,30	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 VEN AAA 1102:

$2mF_o-DF_c$ (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.