



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:16 PM UTC

PDB ID : 8OG8 / pdb_00008og8
Title : Crystal structure of human DCAF1 WD40 repeats (Q1250L) in complex with compound 3
Authors : Schroeder, M.; Vulpetti, A.; Renatus, M.
Deposited on : 2023-03-19
Resolution : 2.11 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

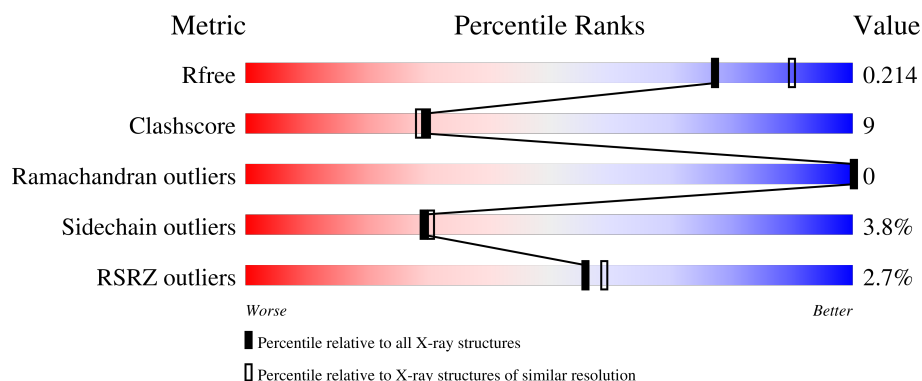
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

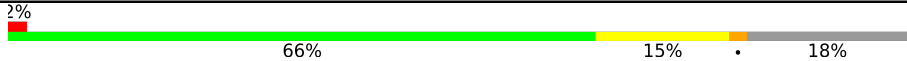
The reported resolution of this entry is 2.11 Å.

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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 $\leq 5\%$. 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	367	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5005 atoms, of which 2346 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.

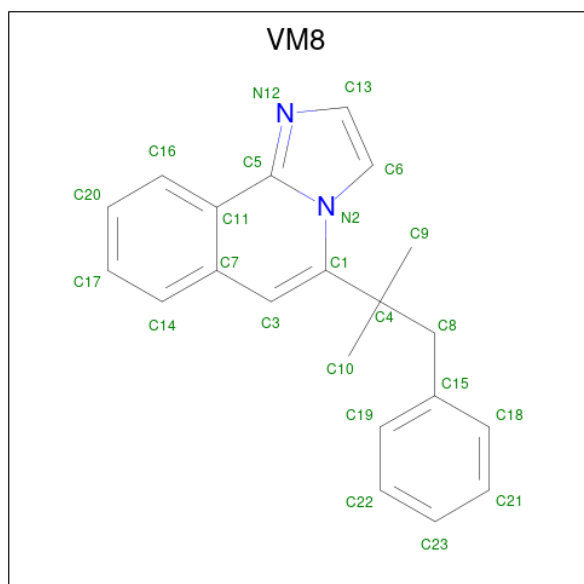
- Molecule 1 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	301	4746	1526	2337	409	456	18	86	3	0

There are 5 discrepancies between the modelled and reference sequences:

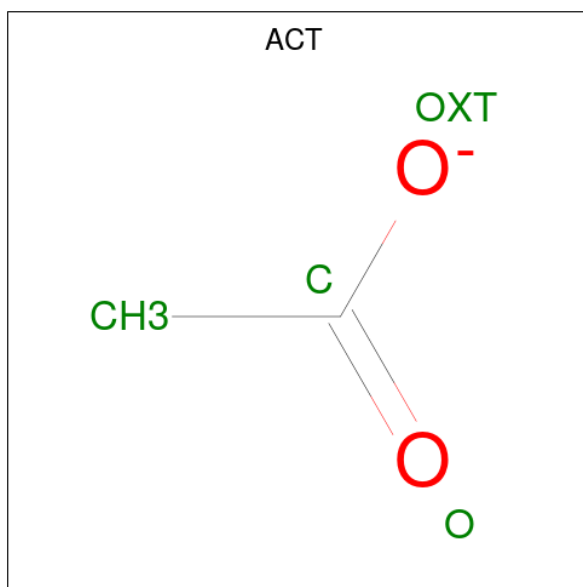
Chain	Residue	Modelled	Actual	Comment	Reference
A	1035	GLY	-	expression tag	UNP Q9Y4B6
A	1036	GLY	-	expression tag	UNP Q9Y4B6
A	1037	GLY	-	expression tag	UNP Q9Y4B6
A	1038	ARG	-	expression tag	UNP Q9Y4B6
A	1250	LEU	GLN	engineered mutation	UNP Q9Y4B6

- Molecule 2 is 5-(2-methyl-1-phenyl-propan-2-yl)imidazo[2,1-a]isoquinoline (CCD ID: VM8) (formula: C₂₁H₂₀N₂) (labeled as "Ligand of Interest" by depositor).



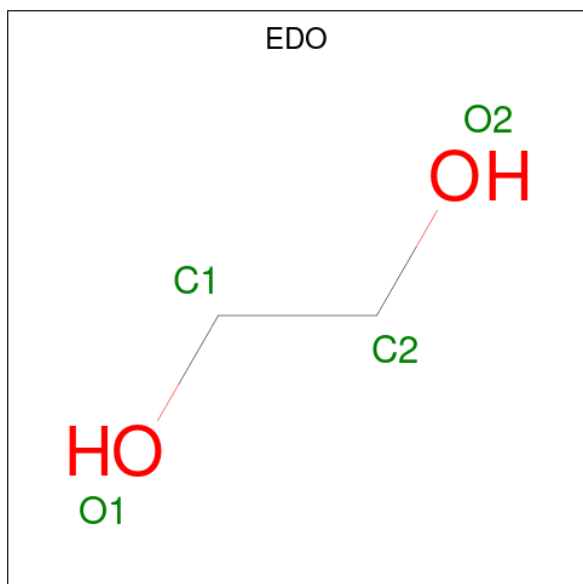
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			23	21	2		
2	A	1	Total	C	N	0	1
			46	42	4		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

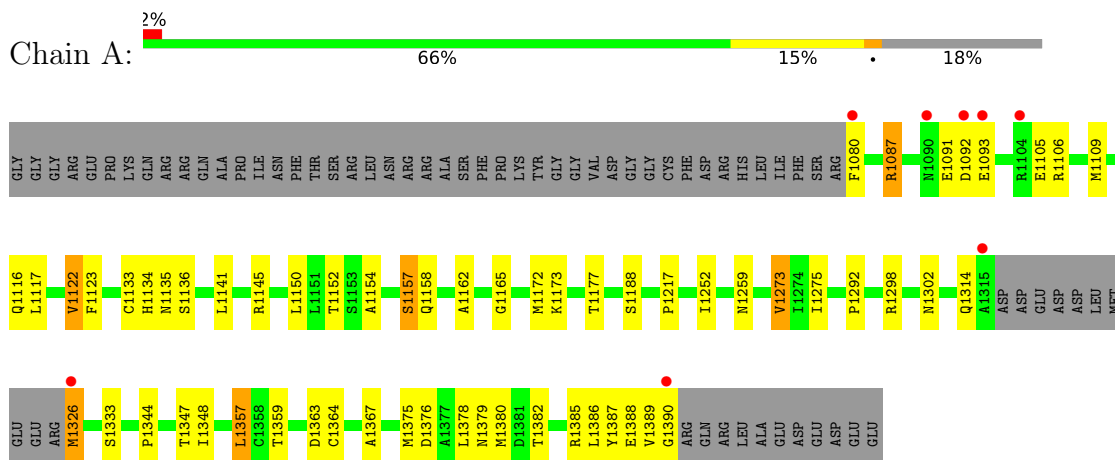


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		

- Molecule 1: DDB1- and CUL4-associated factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	81.81Å 81.81Å 232.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.03 – 2.11 45.03 – 2.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.03-2.11) 100.0 (45.03-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.174 , 0.212 0.174 , 0.214	Depositor DCC
R_{free} test set	1313 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5005	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VM8, ACT, EDO

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	1.30	8/2464 (0.3%)	1.41	12/3340 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1292	PRO	C-O	-6.61	1.15	1.24
1	A	1217	PRO	C-O	-6.49	1.16	1.24
1	A	1344	PRO	C-O	-6.48	1.16	1.23
1	A	1275	ILE	C-O	5.52	1.30	1.24
1	A	1188	SER	CA-CB	-5.48	1.45	1.53
1	A	1135	ASN	C-O	-5.21	1.17	1.24
1	A	1347	THR	C-O	-5.05	1.18	1.24
1	A	1376	ASP	C-O	-5.00	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1273	VAL	CB-CA-C	6.52	120.54	110.50
1	A	1092	ASP	CA-CB-CG	-6.49	106.11	112.60
1	A	1087	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	A	1145	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	A	1273	VAL	N-CA-CB	-6.23	101.23	111.44
1	A	1177	THR	CA-CB-OG1	-6.16	100.36	109.60
1	A	1252	ILE	N-CA-C	-5.96	106.69	111.81
1	A	1359	THR	CA-CB-OG1	-5.55	101.27	109.60
1	A	1388	GLU	CB-CA-C	5.25	118.42	109.80
1	A	1087	ARG	CB-CA-C	5.09	119.41	110.36
1	A	1379	ASN	CA-C-N	5.08	128.43	120.75
1	A	1379	ASN	C-N-CA	5.08	128.43	120.75

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	2409	2337	2319	39	0
2	A	69	0	0	2	0
3	A	4	3	3	0	0
4	A	4	6	6	0	0
5	A	173	0	0	4	1
All	All	2659	2346	2328	41	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 9.

All (41) 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:1117[A]:LEU:CD2	1:A:1150:LEU:HD21	1.92	0.98
1:A:1117[A]:LEU:HD23	1:A:1150:LEU:HD21	1.55	0.88
1:A:1117[A]:LEU:HD21	1:A:1150:LEU:HD21	1.63	0.80
1:A:1093:GLU:HB3	1:A:1380:MET:O	1.82	0.80
2:A:1502[B]:VM8:C6	2:A:1502[B]:VM8:C9	2.61	0.79
1:A:1117[A]:LEU:CD2	1:A:1150:LEU:CD2	2.64	0.76
1:A:1117[A]:LEU:HD23	1:A:1150:LEU:CD2	2.15	0.75
1:A:1116:GLN:NE2	5:A:1602:HOH:O	2.22	0.73
1:A:1109:MET:HE2	1:A:1117[B]:LEU:HD21	1.75	0.67
1:A:1091:GLU:HB3	1:A:1093:GLU:O	1.96	0.65
1:A:1141:LEU:C	1:A:1141:LEU:HD12	2.22	0.65
1:A:1165:GLY:HA3	1:A:1173:LYS:HE2	1.85	0.58
1:A:1326:MET:O	1:A:1326:MET:HG3	2.05	0.56
1:A:1123:PHE:O	5:A:1601:HOH:O	2.18	0.56
1:A:1117[A]:LEU:HD22	1:A:1133:CYS:SG	2.49	0.52
1:A:1109:MET:CE	1:A:1117[B]:LEU:HD21	2.40	0.52
1:A:1380:MET:HE2	1:A:1382:THR:HG23	1.93	0.51
1:A:1162:ALA:CB	1:A:1172:MET:HE2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117[A]:LEU:HD13	1:A:1133:CYS:SG	2.51	0.50
1:A:1389:VAL:HG23	1:A:1390:GLY:HA2	1.94	0.49
1:A:1158:GLN:HG2	5:A:1718:HOH:O	2.12	0.48
1:A:1385:ARG:HD3	1:A:1387:TYR:OH	2.13	0.48
1:A:1162:ALA:HB2	1:A:1172:MET:HE2	1.95	0.48
1:A:1357:LEU:HA	1:A:1367:ALA:O	2.14	0.47
1:A:1117[B]:LEU:HD13	1:A:1150:LEU:HD21	1.96	0.47
1:A:1117[A]:LEU:HD21	1:A:1152:THR:CG2	2.45	0.47
1:A:1326:MET:HG2	1:A:1380:MET:SD	2.54	0.46
1:A:1389:VAL:CG2	1:A:1390:GLY:HA2	2.46	0.46
1:A:1389:VAL:N	1:A:1390:GLY:HA3	2.29	0.46
1:A:1389:VAL:H	1:A:1390:GLY:HA3	1.80	0.46
1:A:1134:HIS:CG	1:A:1154:ALA:HB2	2.51	0.45
1:A:1136:SER:HG	1:A:1157[A]:SER:HB2	1.81	0.45
2:A:1502[A]:VM8:C10	2:A:1502[A]:VM8:C19	2.97	0.43
1:A:1105:GLU:O	1:A:1106:ARG:HB2	2.19	0.43
1:A:1333:SER:HA	1:A:1348:ILE:O	2.19	0.43
1:A:1385:ARG:NH1	5:A:1615:HOH:O	2.54	0.41
1:A:1087:ARG:HH11	1:A:1087:ARG:HD2	1.45	0.41
1:A:1364:CYS:O	1:A:1390:GLY:HA3	2.21	0.40
1:A:1080:PHE:CE2	1:A:1389:VAL:HG12	2.57	0.40
1:A:1122:VAL:HG13	1:A:1386:LEU:HD22	2.03	0.40
1:A:1302:ASN:HB2	1:A:1363:ASP:CG	2.46	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)
5:A:1601:HOH:O	5:A:1688:HOH:O[8_445]	2.17	0.03

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	300/367 (82%)	291 (97%)	9 (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	267/321 (83%)	256 (96%)	11 (4%)	27	27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1122	VAL
1	A	1157[A]	SER
1	A	1157[B]	SER
1	A	1259	ASN
1	A	1273	VAL
1	A	1298	ARG
1	A	1314	GLN
1	A	1326	MET
1	A	1357	LEU
1	A	1375	MET
1	A	1378	LEU

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

Mol	Chain	Res	Type
1	A	1090	ASN
1	A	1126	GLN
1	A	1132	ASN
1	A	1303	HIS
1	A	1314	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	VM8	A	1502[A]	-	25,26,26	2.92	9 (36%)	28,38,38	2.09	8 (28%)
4	EDO	A	1504	-	3,3,3	0.14	0	2,2,2	0.65	0
2	VM8	A	1501	-	25,26,26	3.42	15 (60%)	28,38,38	2.18	8 (28%)
3	ACT	A	1503	-	3,3,3	1.14	0	3,3,3	0.86	0
2	VM8	A	1502[B]	-	25,26,26	2.97	9 (36%)	28,38,38	2.59	8 (28%)

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
4	EDO	A	1504	-	-	0/1/1/1	-
2	VM8	A	1502[A]	-	-	4/9/11/11	0/4/4/4
2	VM8	A	1502[B]	-	-	6/9/11/11	0/4/4/4
2	VM8	A	1501	-	-	1/9/11/11	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1502[A]	VM8	C6-C13	9.66	1.57	1.35
2	A	1502[B]	VM8	C6-C13	9.41	1.56	1.35
2	A	1501	VM8	C6-C13	9.31	1.56	1.35
2	A	1501	VM8	C6-N2	7.14	1.51	1.39
2	A	1501	VM8	C5-N2	-5.41	1.30	1.38
2	A	1501	VM8	C13-N12	5.00	1.47	1.38
2	A	1502[B]	VM8	C5-N2	-4.94	1.31	1.38
2	A	1502[A]	VM8	C5-N2	-4.61	1.31	1.38
2	A	1502[B]	VM8	C7-C3	4.42	1.52	1.43
2	A	1502[A]	VM8	C6-N2	4.36	1.46	1.39
2	A	1502[B]	VM8	C6-N2	4.16	1.46	1.39
2	A	1502[A]	VM8	C7-C3	3.80	1.51	1.43
2	A	1502[B]	VM8	C5-N12	-3.70	1.27	1.33
2	A	1502[B]	VM8	C13-N12	3.57	1.44	1.38
2	A	1502[B]	VM8	C11-C5	3.55	1.52	1.45
2	A	1501	VM8	C7-C3	3.54	1.50	1.43
2	A	1502[A]	VM8	C13-N12	3.50	1.44	1.38
2	A	1502[A]	VM8	C11-C5	3.45	1.52	1.45
2	A	1502[A]	VM8	C5-N12	-3.12	1.28	1.33
2	A	1501	VM8	C17-C14	2.97	1.44	1.38
2	A	1501	VM8	C11-C5	2.83	1.51	1.45
2	A	1501	VM8	C8-C4	2.78	1.59	1.56
2	A	1502[A]	VM8	C8-C15	2.67	1.55	1.51
2	A	1501	VM8	C11-C7	2.62	1.45	1.41
2	A	1501	VM8	C9-C4	2.57	1.58	1.53
2	A	1501	VM8	C20-C16	2.56	1.43	1.38
2	A	1501	VM8	C20-C17	2.55	1.43	1.38
2	A	1501	VM8	C8-C15	2.49	1.55	1.51
2	A	1502[B]	VM8	C8-C15	2.38	1.55	1.51
2	A	1501	VM8	C5-N12	-2.29	1.29	1.33
2	A	1501	VM8	C21-C18	2.28	1.42	1.38
2	A	1502[B]	VM8	C8-C4	2.27	1.58	1.56
2	A	1502[A]	VM8	C8-C4	2.19	1.58	1.56

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1502[B]	VM8	C4-C8-C15	8.97	122.05	114.94
2	A	1501	VM8	C6-C13-N12	-6.43	102.32	110.74
2	A	1502[A]	VM8	C6-C13-N12	-5.74	103.22	110.74
2	A	1502[B]	VM8	C6-C13-N12	-4.90	104.33	110.74
2	A	1502[B]	VM8	C11-C5-N12	-4.83	120.05	128.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1502[A]	VM8	C11-C5-N12	-4.66	120.36	128.44
2	A	1502[B]	VM8	C13-C6-N2	-4.43	100.24	105.02
2	A	1502[A]	VM8	C4-C1-N2	4.34	128.67	120.41
2	A	1502[A]	VM8	C13-C6-N2	-4.09	100.60	105.02
2	A	1501	VM8	C13-N12-C5	4.09	110.56	105.08
2	A	1501	VM8	C14-C7-C11	3.57	122.62	118.82
2	A	1501	VM8	C11-C5-N12	-3.56	122.27	128.44
2	A	1501	VM8	C17-C14-C7	-3.18	116.14	120.95
2	A	1502[B]	VM8	C11-C7-C3	-3.14	115.38	119.06
2	A	1501	VM8	C11-C7-C3	-3.04	115.49	119.06
2	A	1502[A]	VM8	C11-C7-C3	-2.49	116.14	119.06
2	A	1502[B]	VM8	C9-C4-C8	-2.41	106.28	109.75
2	A	1502[B]	VM8	C4-C1-N2	2.39	124.95	120.41
2	A	1501	VM8	C13-C6-N2	-2.37	102.46	105.02
2	A	1502[A]	VM8	C10-C4-C8	-2.32	106.41	109.75
2	A	1502[A]	VM8	C14-C7-C11	2.31	121.28	118.82
2	A	1501	VM8	C4-C8-C15	-2.22	113.19	114.94
2	A	1502[A]	VM8	C4-C8-C15	2.09	116.60	114.94
2	A	1502[B]	VM8	C13-N12-C5	2.01	107.78	105.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1502[A]	VM8	N2-C1-C4-C9
2	A	1502[A]	VM8	N2-C1-C4-C10
2	A	1502[B]	VM8	N2-C1-C4-C9
2	A	1502[B]	VM8	C1-C4-C8-C15
2	A	1502[B]	VM8	C9-C4-C8-C15
2	A	1502[B]	VM8	C10-C4-C8-C15
2	A	1502[A]	VM8	C19-C15-C8-C4
2	A	1502[A]	VM8	C18-C15-C8-C4
2	A	1502[B]	VM8	N2-C1-C4-C10
2	A	1502[B]	VM8	C3-C1-C4-C9
2	A	1501	VM8	C1-C4-C8-C15

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1502[A]	VM8	1	0

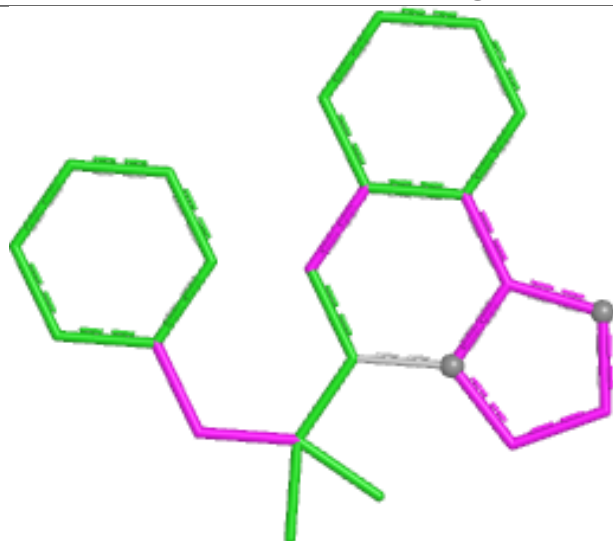
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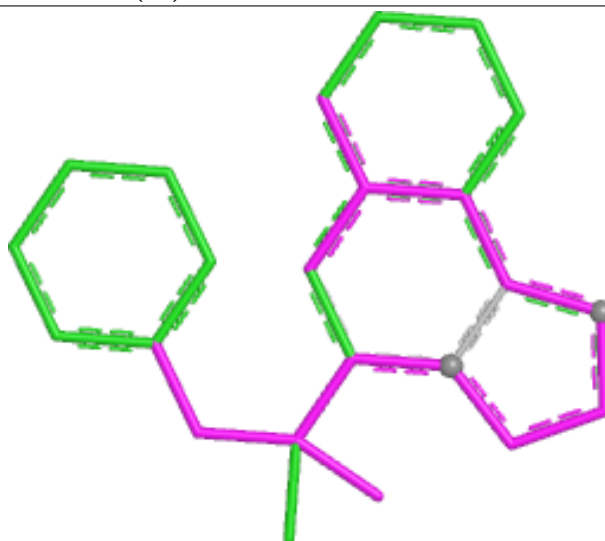
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1502[B]	VM8	1	0

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.

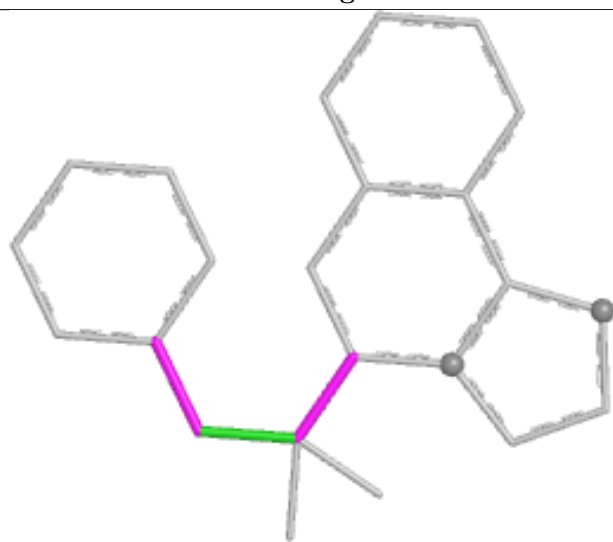
Ligand VM8 A 1502 (A)



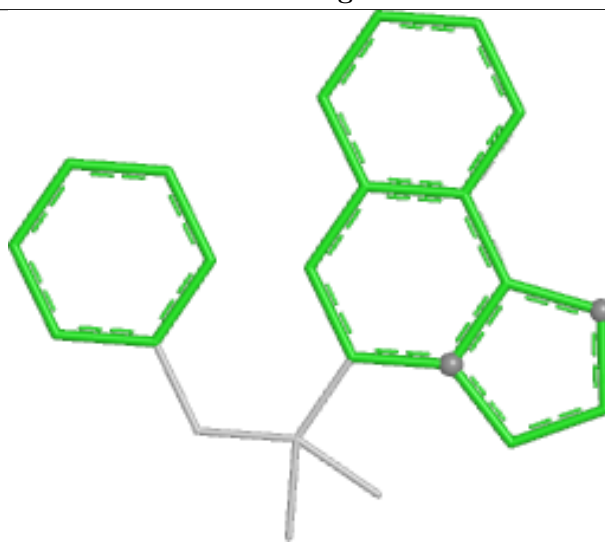
Bond lengths



Bond angles

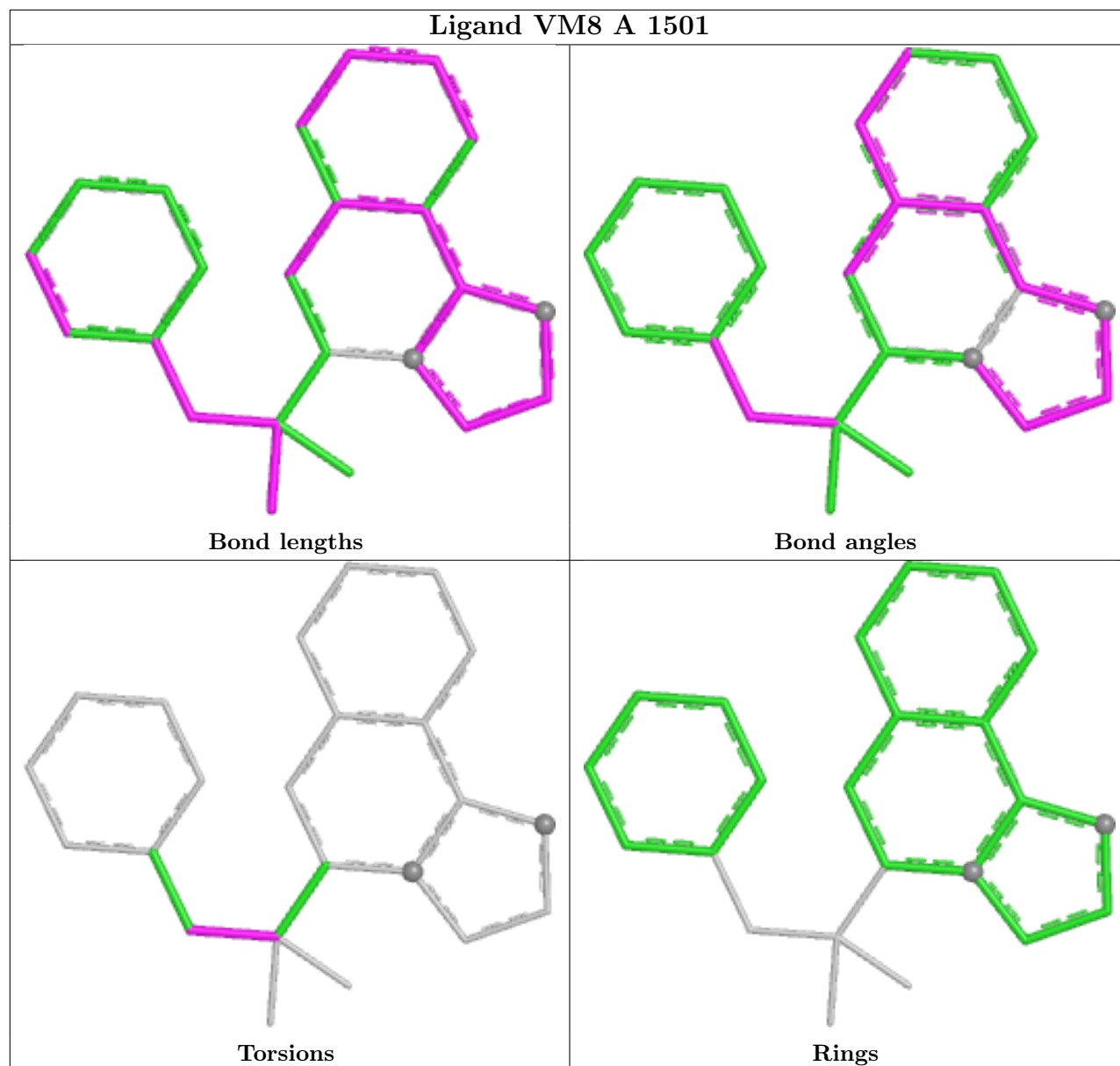


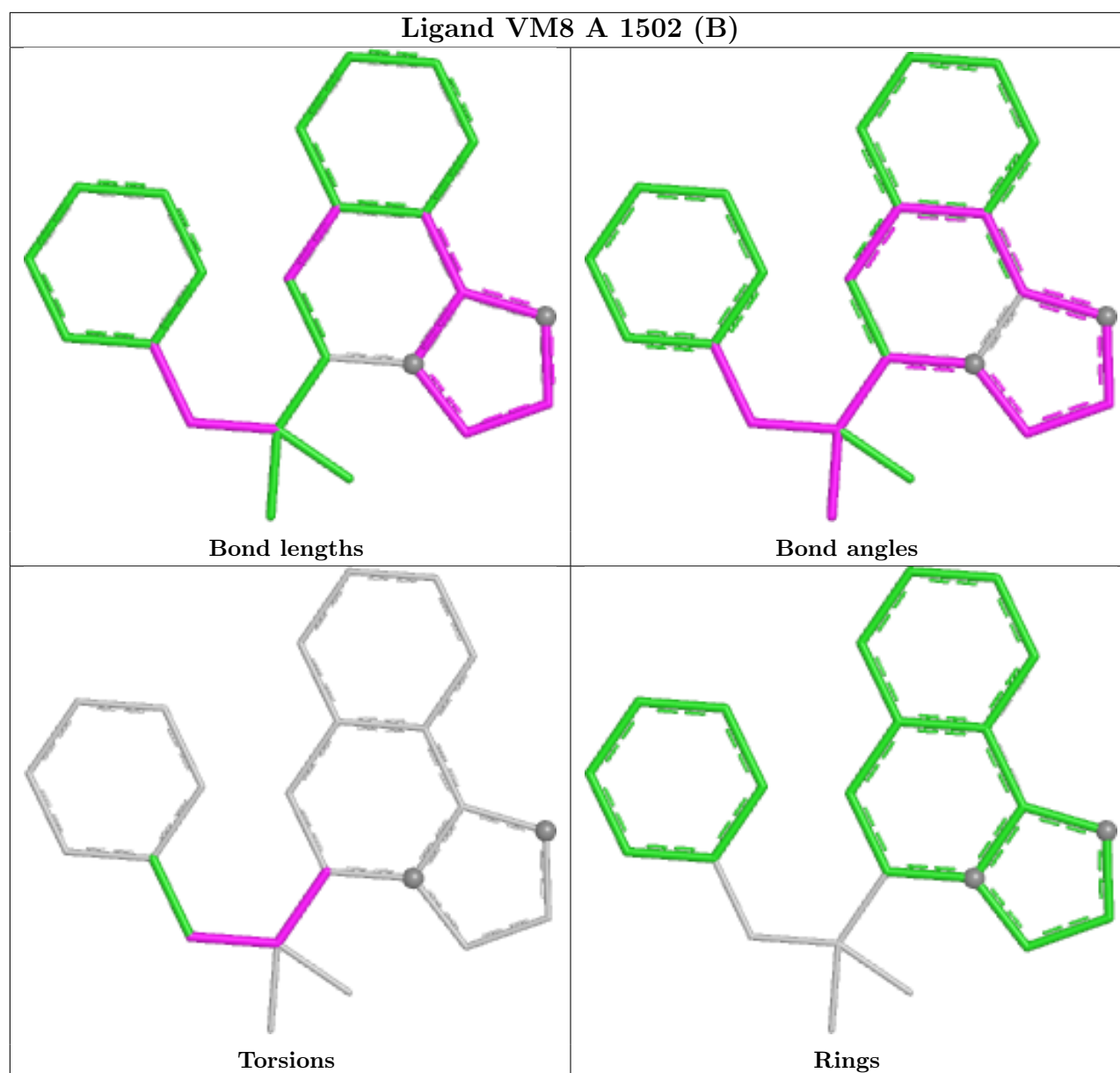
Torsions



Rings

Ligand VM8 A 1501





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	301/367 (82%)	-0.39	8 (2%) 56 59	10, 29, 56, 83	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1315	ALA	4.1
1	A	1080	PHE	3.8
1	A	1093	GLU	3.4
1	A	1090	ASN	3.2
1	A	1092	ASP	3.1
1	A	1104	ARG	2.9
1	A	1390	GLY	2.9
1	A	1326	MET	2.2

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](#)

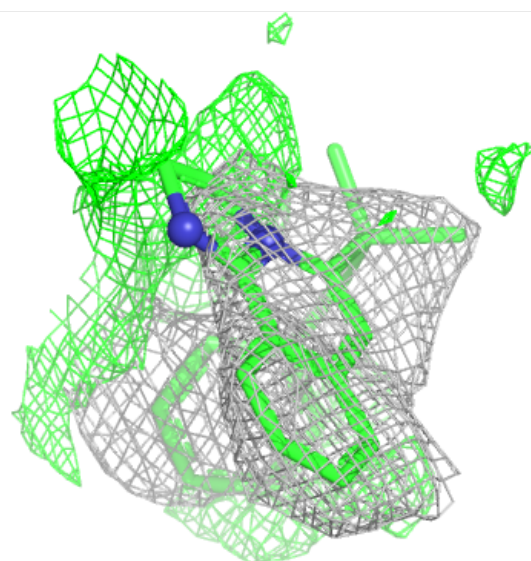
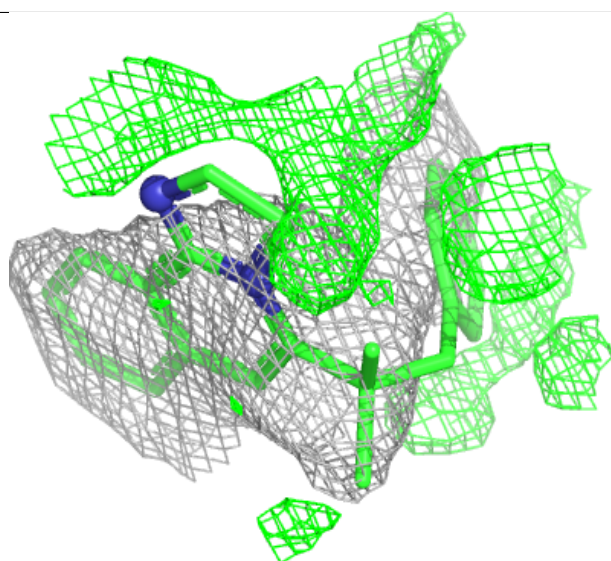
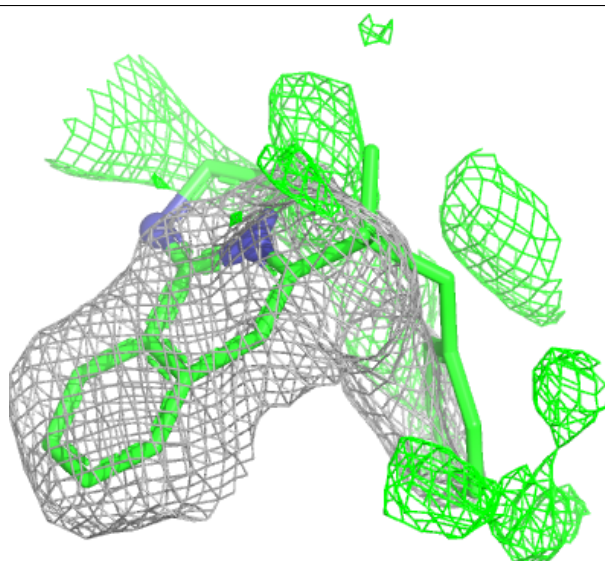
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	EDO	A	1504	4/4	0.81	0.16	41,44,47,48	1
2	VM8	A	1502[B]	23/23	0.87	0.27	48,58,73,75	23
2	VM8	A	1502[A]	23/23	0.87	0.27	53,58,63,64	23
2	VM8	A	1501	23/23	0.94	0.09	23,26,32,34	0
3	ACT	A	1503	4/4	0.97	0.06	22,23,23,24	7

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.

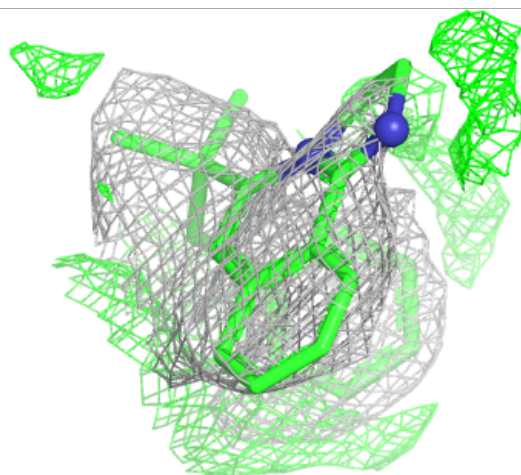
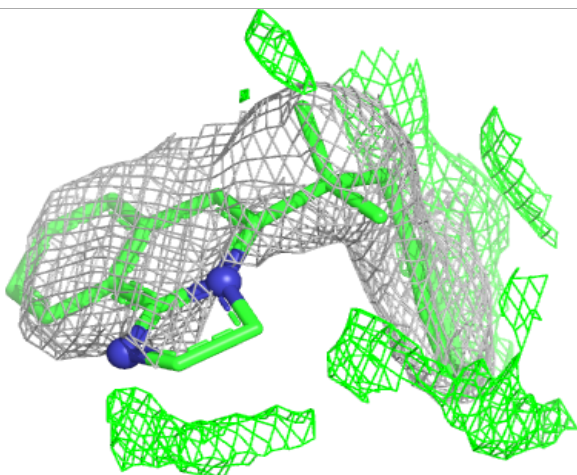
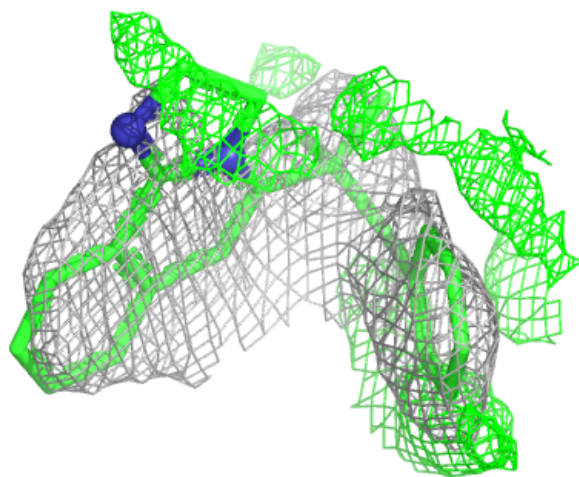
Electron density around VM8 A 1502 (B):

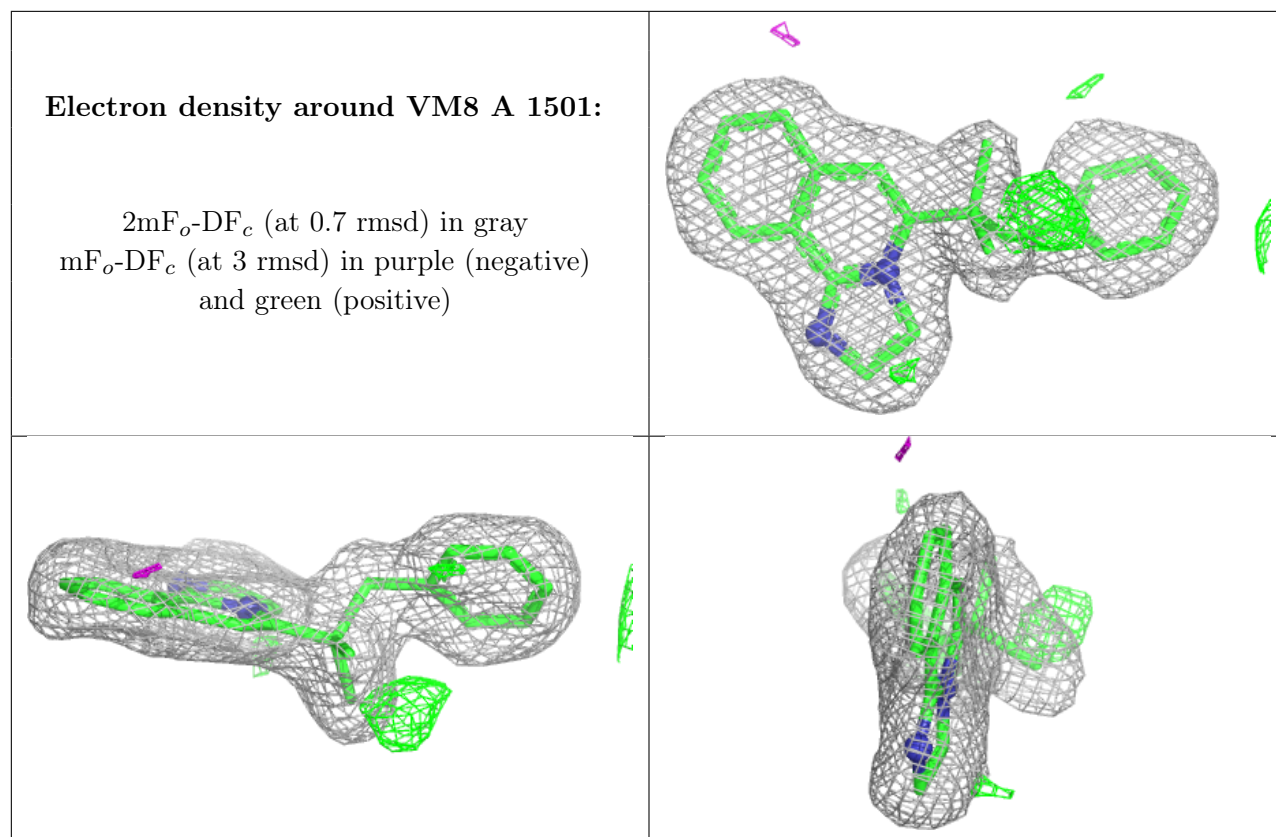
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VM8 A 1502 (A):

$2mF_o-DF_c$ (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.