



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:24 pm BST

PDB ID : 2F98  
Title : Crystal structure of the polyketide cyclase AknH with bound substrate and product analogue: implications for catalytic mechanism and product stereoselectivity.  
Authors : Kallio, P.; Sultana, A.; Neimi, J.; Mantsala, P.; Schneider, G.  
Deposited on : 2005-12-05  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

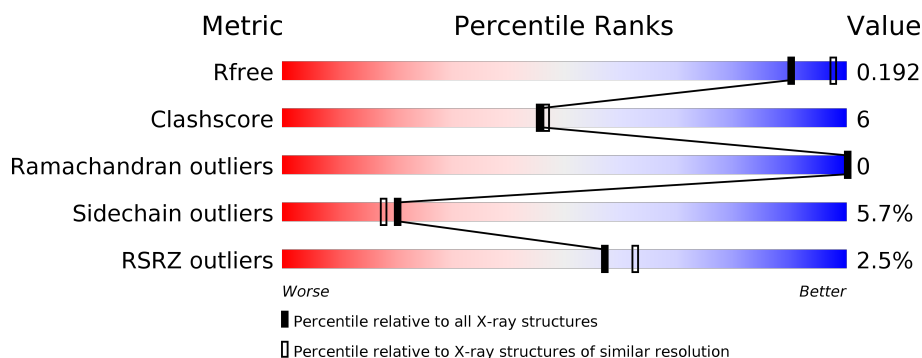
# 1 Overall quality at a glance

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	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	153	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 1%, yellow 15%, orange 8%, grey 76%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>75%</span> <span>15%</span> <span>• 8%</span> </div> </div>
1	B	153	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, green 1%, yellow 12%, orange 8%, grey 74%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>78%</span> <span>12%</span> <span>• 8%</span> </div> </div>
1	C	153	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 1%, yellow 16%, orange 7%, grey 73%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>76%</span> <span>16%</span> <span>• 7%</span> </div> </div>
1	D	153	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 1%, yellow 14%, orange 8%, grey 76%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>76%</span> <span>14%</span> <span>• 8%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5092 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 Aklanonic Acid methyl Ester Cyclase, AknH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	6	0
			1172	737	211	220	4			
1	B	141	Total	C	N	O	S	0	8	0
			1180	741	211	224	4			
1	C	143	Total	C	N	O	S	0	7	0
			1198	751	219	224	4			
1	D	140	Total	C	N	O	S	5	7	0
			1165	733	207	221	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	CLONING ARTIFACT	GB 7800671
A	-7	ALA	-	CLONING ARTIFACT	GB 7800671
A	-6	HIS	-	EXPRESSION TAG	GB 7800671
A	-5	HIS	-	EXPRESSION TAG	GB 7800671
A	-4	HIS	-	EXPRESSION TAG	GB 7800671
A	-3	HIS	-	EXPRESSION TAG	GB 7800671
A	-2	HIS	-	EXPRESSION TAG	GB 7800671
A	-1	HIS	-	EXPRESSION TAG	GB 7800671
A	0	HIS	-	EXPRESSION TAG	GB 7800671
A	1	ARG	-	CLONING ARTIFACT	GB 7800671
B	-8	MET	-	CLONING ARTIFACT	GB 7800671
B	-7	ALA	-	CLONING ARTIFACT	GB 7800671
B	-6	HIS	-	EXPRESSION TAG	GB 7800671
B	-5	HIS	-	EXPRESSION TAG	GB 7800671
B	-4	HIS	-	EXPRESSION TAG	GB 7800671
B	-3	HIS	-	EXPRESSION TAG	GB 7800671
B	-2	HIS	-	EXPRESSION TAG	GB 7800671
B	-1	HIS	-	EXPRESSION TAG	GB 7800671
B	0	HIS	-	EXPRESSION TAG	GB 7800671
B	1	ARG	-	CLONING ARTIFACT	GB 7800671
C	-8	MET	-	CLONING ARTIFACT	GB 7800671

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	CLONING ARTIFACT	GB 7800671
C	-6	HIS	-	EXPRESSION TAG	GB 7800671
C	-5	HIS	-	EXPRESSION TAG	GB 7800671
C	-4	HIS	-	EXPRESSION TAG	GB 7800671
C	-3	HIS	-	EXPRESSION TAG	GB 7800671
C	-2	HIS	-	EXPRESSION TAG	GB 7800671
C	-1	HIS	-	EXPRESSION TAG	GB 7800671
C	0	HIS	-	EXPRESSION TAG	GB 7800671
C	1	ARG	-	CLONING ARTIFACT	GB 7800671
D	-8	MET	-	CLONING ARTIFACT	GB 7800671
D	-7	ALA	-	CLONING ARTIFACT	GB 7800671
D	-6	HIS	-	EXPRESSION TAG	GB 7800671
D	-5	HIS	-	EXPRESSION TAG	GB 7800671
D	-4	HIS	-	EXPRESSION TAG	GB 7800671
D	-3	HIS	-	EXPRESSION TAG	GB 7800671
D	-2	HIS	-	EXPRESSION TAG	GB 7800671
D	-1	HIS	-	EXPRESSION TAG	GB 7800671
D	0	HIS	-	EXPRESSION TAG	GB 7800671
D	1	ARG	-	CLONING ARTIFACT	GB 7800671

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



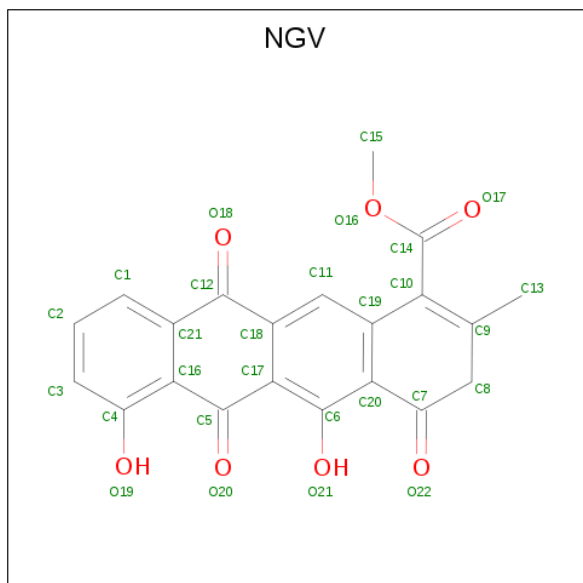
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is METHYL 5,7-DIHYDROXY-2-METHYL-4,6,11-TRIOXO-3,4,6,11-TETRAHYDROTETRACENE-1-CARBOXYLATE (three-letter code: NGV) (formula: C<sub>21</sub>H<sub>14</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	21	7		
3	B	1	Total	C	O	0	0
			28	21	7		
3	C	1	Total	C	O	0	0
			28	21	7		
3	D	1	Total	C	O	0	0
			28	21	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	48	Total	O	0	0
			48	48		
4	C	71	Total	O	0	0
			71	71		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	50	Total	O	0	0
			50	50		

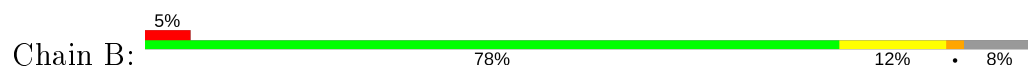
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Aklanonic Acid methyl Ester Cyclase, AknH



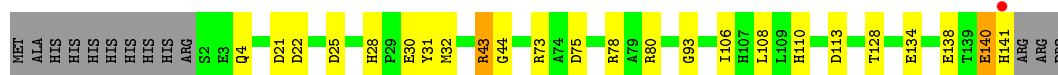
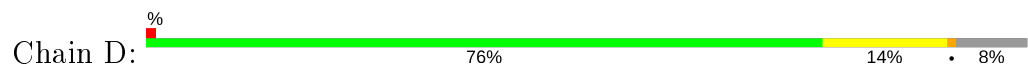
- Molecule 1: Aklanonic Acid methyl Ester Cyclase, AknH



- Molecule 1: Aklanonic Acid methyl Ester Cyclase, AknH



- Molecule 1: Aklanonic Acid methyl Ester Cyclase, AknH



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.27Å 152.27Å 109.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.48 – 2.10 56.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.48-2.10) 100.0 (56.48-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.193 , 0.218 0.199 , 0.192	Depositor DCC
$R_{free}$ test set	2758 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NGV, SO4

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	0.49	0/1237	0.74	4/1676 (0.2%)
1	B	0.51	0/1255	0.73	5/1700 (0.3%)
1	C	0.51	0/1268	0.74	5/1716 (0.3%)
1	D	0.49	0/1235	0.73	3/1674 (0.2%)
All	All	0.50	0/4995	0.74	17/6766 (0.3%)

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	D	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	113	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	113	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	25	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	113	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	25	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	21[A]	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	21[B]	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	21[A]	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	21[B]	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	78	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	121	ASP	CB-CG-OD2	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	21[A]	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	21[B]	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	78	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	22	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	140	GLU	Peptide

## 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	1172	0	1108	15	0
1	B	1180	0	1112	13	0
1	C	1198	0	1136	15	0
1	D	1165	0	1094	25	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	28	0	12	1	0
3	B	28	0	12	1	0
3	C	28	0	12	1	0
3	D	28	0	12	1	0
4	A	76	0	0	1	0
4	B	48	0	0	1	0
4	C	71	0	0	1	0
4	D	50	0	0	2	0
All	All	5092	0	4498	60	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 (60) 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:D:43:ARG:HG2	1:D:43:ARG:HH11	1.07	1.10
1:D:141:HIS:O	4:D:380:HOH:O	1.85	0.93
1:D:43:ARG:CG	1:D:43:ARG:HH11	1.80	0.92
1:D:43:ARG:HG2	1:D:43:ARG:NH1	1.69	0.88
1:D:32:MET:HE3	1:D:43:ARG:NH1	1.89	0.88
1:D:32:MET:CE	1:D:43:ARG:NH1	2.40	0.84
1:D:32:MET:CE	1:D:43:ARG:HH11	1.95	0.79
1:C:139:THR:HG21	1:C:143:ARG:HA	1.68	0.76
1:D:32:MET:HB2	1:D:43:ARG:HH12	1.51	0.76
1:D:32:MET:HE2	1:D:43:ARG:HH11	1.53	0.71
1:C:110:HIS:HD2	1:D:140:GLU:OE1	1.79	0.65
1:C:50:ILE:HB	4:C:365:HOH:O	1.96	0.64
1:B:140:GLU:O	1:B:141:HIS:HB2	1.97	0.64
1:C:47:LEU:O	1:C:50:ILE:HG22	1.98	0.63
1:B:32:MET:CE	1:B:43:ARG:HG2	2.30	0.61
1:D:32:MET:HE2	1:D:43:ARG:NH1	2.12	0.61
1:B:75:ASP:OD2	1:B:110:HIS:HE1	1.84	0.59
1:D:4:GLN:HE22	1:D:75:ASP:HA	1.69	0.58
1:C:140:GLU:OE1	1:D:110:HIS:HD2	1.87	0.57
1:C:75:ASP:OD2	1:C:110:HIS:HE1	1.88	0.57
1:B:4:GLN:HE22	1:B:75:ASP:HA	1.69	0.56
1:C:78:ARG:NH2	1:D:134:GLU:O	2.40	0.54
1:B:32:MET:HE1	1:B:43:ARG:HG2	1.89	0.54
1:A:32:MET:CE	1:A:43:ARG:HG2	2.40	0.52
1:D:80[B]:ARG:HG2	1:D:106:ILE:HD13	1.90	0.52
1:A:11:MET:HG3	1:A:48:PHE:CE1	2.45	0.51
1:B:56:LYS:HG3	1:B:61:GLU:HA	1.92	0.51
1:C:40:THR:OG1	1:C:42:LEU:HG	2.11	0.50
1:C:47:LEU:O	1:C:50:ILE:CG2	2.61	0.49
1:D:75:ASP:OD2	1:D:110:HIS:HE1	1.95	0.49
1:A:140:GLU:OE1	1:B:110:HIS:HD2	1.96	0.48
1:B:128:THR:HG21	3:B:336:NGV:H82	1.96	0.47
1:C:134:GLU:O	1:D:78:ARG:NH2	2.48	0.47
1:A:76:TRP:CZ3	1:A:110:HIS:HB2	2.49	0.47
1:A:80[B]:ARG:HD2	4:A:345:HOH:O	2.14	0.47
1:A:134:GLU:O	1:B:78:ARG:NH2	2.48	0.47
1:C:4:GLN:HE22	1:C:75:ASP:HA	1.80	0.47
1:D:140:GLU:O	1:D:141:HIS:HB2	2.14	0.47
1:A:80[B]:ARG:HG2	1:A:106:ILE:CD1	2.46	0.46
1:B:32:MET:HE2	1:B:43:ARG:HG2	1.97	0.46
1:A:80[B]:ARG:HD3	4:B:363:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:THR:HG21	3:C:335:NGV:H82	1.98	0.46
1:D:128:THR:HG21	3:D:334:NGV:H82	1.98	0.46
1:A:140:GLU:O	1:A:141:HIS:HB2	2.15	0.46
1:C:32:MET:CE	1:C:43:ARG:HG2	2.46	0.45
1:D:28:HIS:CE1	1:D:30[B]:GLU:HG3	2.52	0.44
1:D:32:MET:HE2	1:D:43:ARG:HG2	1.99	0.44
1:C:42:LEU:HD12	1:C:50:ILE:HG21	2.00	0.43
1:B:76:TRP:CZ3	1:B:110:HIS:HB2	2.53	0.43
1:A:54:TRP:CH2	1:A:58:THR:HG21	2.53	0.43
1:A:4:GLN:HE22	1:A:75:ASP:HA	1.84	0.42
1:A:78:ARG:NH2	1:B:134:GLU:O	2.52	0.42
1:C:126:GLN:HG2	1:D:106:ILE:HG13	2.01	0.42
1:A:128:THR:HG21	3:A:333:NGV:H82	2.01	0.42
1:A:8:VAL:HG21	1:A:77:VAL:HG11	2.01	0.41
1:D:80[B]:ARG:HD2	4:D:369:HOH:O	2.21	0.41
1:A:32:MET:HE2	1:A:43:ARG:HG2	2.01	0.41
1:B:11:MET:HG3	1:B:48:PHE:CZ	2.56	0.41
1:D:93:GLY:O	1:D:138:GLU:HG2	2.20	0.41
1:D:31:TYR:HB3	1:D:44:GLY:HA2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	145/153 (95%)	142 (98%)	3 (2%)	0	100	100
1	B	147/153 (96%)	144 (98%)	3 (2%)	0	100	100
1	C	148/153 (97%)	145 (98%)	3 (2%)	0	100	100
1	D	145/153 (95%)	142 (98%)	3 (2%)	0	100	100
All	All	585/612 (96%)	573 (98%)	12 (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	125/130 (96%)	117 (94%)	8 (6%)	17	14
1	B	127/130 (98%)	119 (94%)	8 (6%)	18	15
1	C	128/130 (98%)	116 (91%)	12 (9%)	8	5
1	D	125/130 (96%)	120 (96%)	5 (4%)	31	32
All	All	505/520 (97%)	472 (94%)	33 (6%)	20	14

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	21[A]	ASP
1	A	21[B]	ASP
1	A	56	LYS
1	A	73	ARG
1	A	108	LEU
1	A	121	ASP
1	A	141	HIS
1	B	1	ARG
1	B	21[A]	ASP
1	B	21[B]	ASP
1	B	56	LYS
1	B	73	ARG
1	B	80[A]	ARG
1	B	80[B]	ARG
1	B	108	LEU
1	C	1	ARG
1	C	21[A]	ASP
1	C	21[B]	ASP
1	C	50	ILE
1	C	57	LYS
1	C	73	ARG

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Mol	Chain	Res	Type
1	C	80[A]	ARG
1	C	80[B]	ARG
1	C	91	MET
1	C	108	LEU
1	C	142	ARG
1	C	143	ARG
1	D	21[A]	ASP
1	D	21[B]	ASP
1	D	43	ARG
1	D	73	ARG
1	D	108	LEU

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

Mol	Chain	Res	Type
1	A	51	ASN
1	B	4	GLN
1	B	51	ASN
1	B	110	HIS
1	C	4	GLN
1	C	51	ASN
1	C	110	HIS
1	D	4	GLN
1	D	51	ASN
1	D	110	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

8 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
3	NGV	C	335	-	30,31,31	2.69	11 (36%)	44,48,48	1.12	3 (6%)
2	SO4	B	279	-	4,4,4	0.15	0	6,6,6	0.10	0
3	NGV	D	334	-	30,31,31	2.64	12 (40%)	44,48,48	1.24	6 (13%)
3	NGV	A	333	-	30,31,31	2.68	10 (33%)	44,48,48	1.24	4 (9%)
3	NGV	B	336	-	30,31,31	2.65	11 (36%)	44,48,48	1.16	2 (4%)
2	SO4	D	277	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	C	278	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	A	276	-	4,4,4	0.14	0	6,6,6	0.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NGV	C	335	-	-	0/6/38/38	0/4/4/4
3	NGV	D	334	-	-	0/6/38/38	0/4/4/4
3	NGV	A	333	-	-	2/6/38/38	0/4/4/4
3	NGV	B	336	-	-	0/6/38/38	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	335	NGV	O18-C12	6.69	1.35	1.22
3	B	336	NGV	C8-C9	-6.55	1.38	1.50
3	A	333	NGV	O18-C12	6.31	1.34	1.22
3	A	333	NGV	C8-C9	-6.28	1.39	1.50
3	C	335	NGV	C8-C9	-6.27	1.39	1.50
3	D	334	NGV	C8-C9	-6.11	1.39	1.50
3	B	336	NGV	O18-C12	6.04	1.33	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	334	NGV	O18-C12	6.02	1.33	1.22
3	A	333	NGV	O16-C14	5.93	1.46	1.33
3	C	335	NGV	O16-C14	5.70	1.46	1.33
3	B	336	NGV	O16-C14	5.55	1.45	1.33
3	D	334	NGV	O16-C14	5.54	1.45	1.33
3	D	334	NGV	C21-C12	-4.27	1.39	1.48
3	B	336	NGV	C20-C6	4.19	1.49	1.41
3	C	335	NGV	C20-C6	4.10	1.49	1.41
3	A	333	NGV	C20-C6	4.04	1.49	1.41
3	B	336	NGV	C21-C12	-4.02	1.40	1.48
3	A	333	NGV	C21-C12	-3.83	1.40	1.48
3	B	336	NGV	C18-C12	-3.75	1.40	1.48
3	D	334	NGV	C20-C6	3.71	1.48	1.41
3	A	333	NGV	C18-C12	-3.65	1.40	1.48
3	C	335	NGV	C18-C12	-3.63	1.40	1.48
3	C	335	NGV	C21-C12	-3.59	1.40	1.48
3	D	334	NGV	C18-C12	-3.47	1.41	1.48
3	C	335	NGV	C20-C7	-3.28	1.39	1.46
3	B	336	NGV	C20-C7	-3.22	1.39	1.46
3	C	335	NGV	C17-C5	-3.20	1.40	1.47
3	A	333	NGV	C16-C5	-3.15	1.40	1.47
3	C	335	NGV	C19-C10	-3.11	1.40	1.46
3	D	334	NGV	C19-C10	-3.11	1.40	1.46
3	D	334	NGV	C20-C7	-3.07	1.39	1.46
3	A	333	NGV	C20-C7	-3.06	1.39	1.46
3	B	336	NGV	C16-C5	-3.02	1.40	1.47
3	D	334	NGV	C16-C5	-2.98	1.40	1.47
3	A	333	NGV	C17-C5	-2.97	1.40	1.47
3	C	335	NGV	C16-C5	-2.88	1.40	1.47
3	B	336	NGV	C17-C5	-2.87	1.40	1.47
3	D	334	NGV	C17-C5	-2.86	1.40	1.47
3	A	333	NGV	C19-C10	-2.83	1.40	1.46
3	B	336	NGV	C19-C10	-2.82	1.40	1.46
3	D	334	NGV	O22-C7	2.43	1.26	1.22
3	B	336	NGV	O20-C5	2.28	1.27	1.22
3	C	335	NGV	O22-C7	2.10	1.25	1.22
3	D	334	NGV	O20-C5	2.10	1.26	1.22

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	336	NGV	C15-O16-C14	4.60	124.56	115.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	333	NGV	C15-O16-C14	4.49	124.35	115.86
3	D	334	NGV	O16-C14-C10	3.62	117.09	112.09
3	C	335	NGV	C15-O16-C14	3.57	122.62	115.86
3	D	334	NGV	C15-O16-C14	3.29	122.08	115.86
3	A	333	NGV	O16-C14-C10	2.60	115.69	112.09
3	C	335	NGV	C13-C9-C8	2.57	118.09	113.69
3	A	333	NGV	C13-C9-C8	2.45	117.89	113.69
3	D	334	NGV	O18-C12-C21	-2.30	117.54	120.91
3	D	334	NGV	C13-C9-C8	2.26	117.56	113.69
3	B	336	NGV	C8-C7-C20	2.19	120.68	116.74
3	D	334	NGV	O16-C14-O17	-2.15	119.40	123.53
3	D	334	NGV	C21-C12-C18	2.02	120.99	117.60
3	A	333	NGV	C8-C7-C20	2.01	120.36	116.74
3	C	335	NGV	C8-C7-C20	2.00	120.35	116.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	333	NGV	C10-C14-O16-C15
3	A	333	NGV	O17-C14-O16-C15

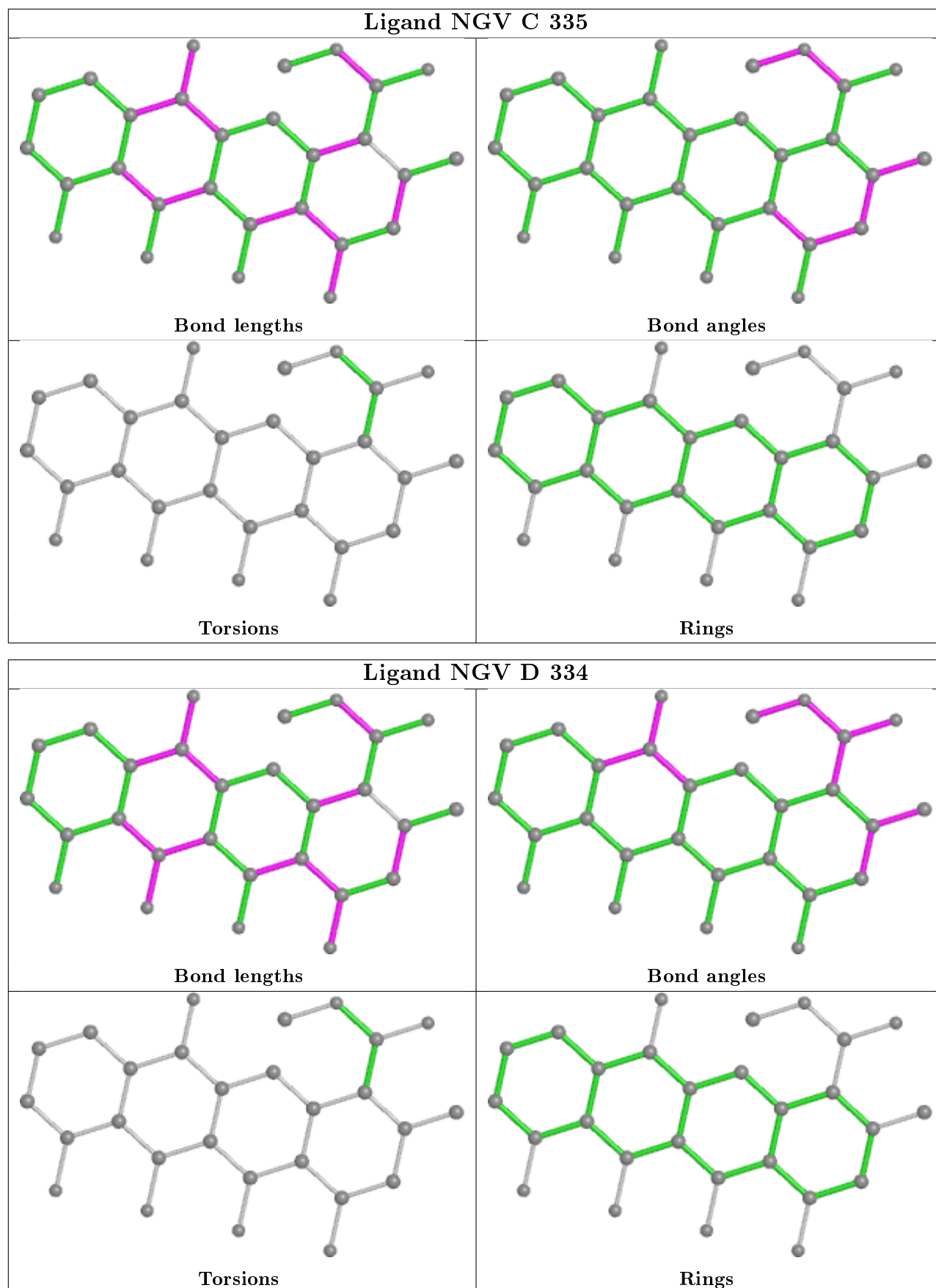
There are no ring outliers.

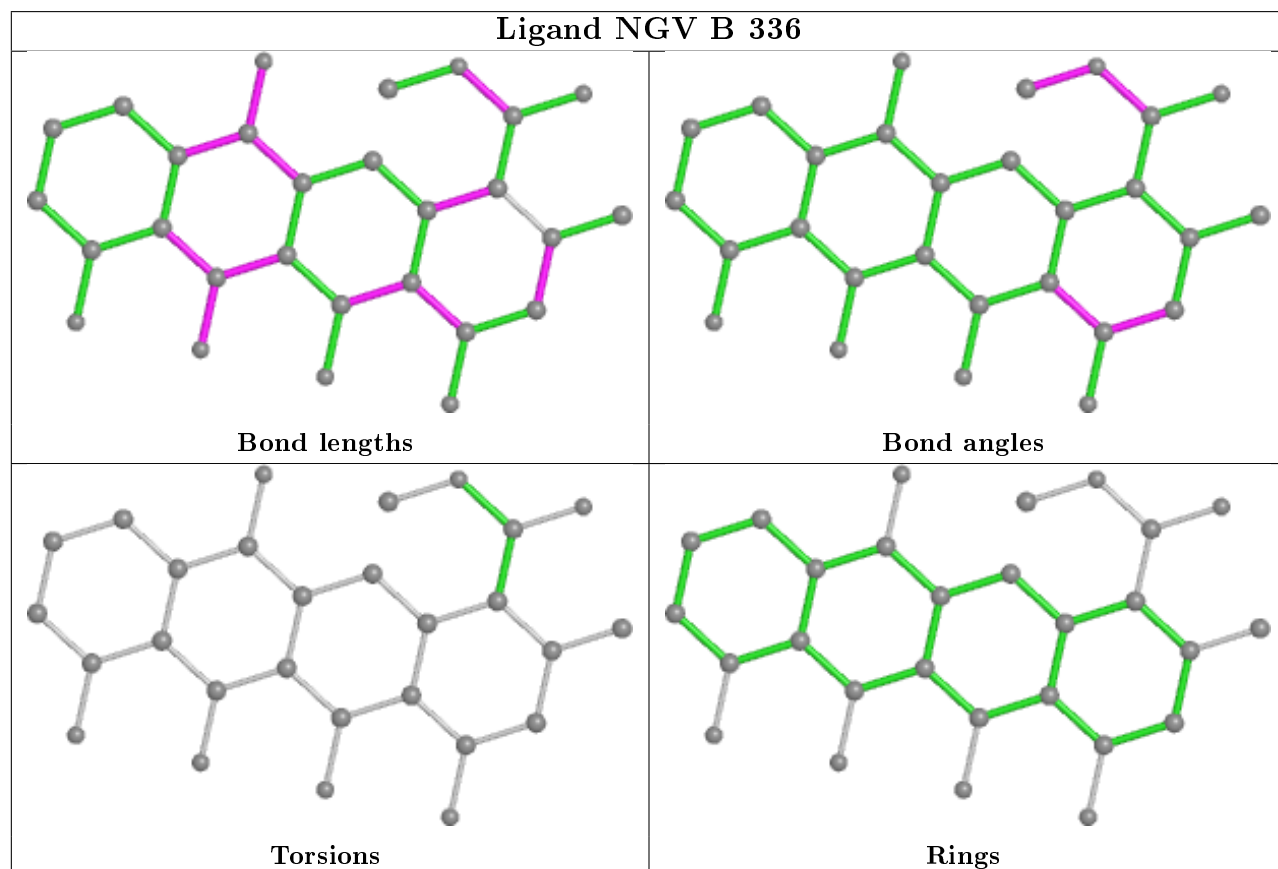
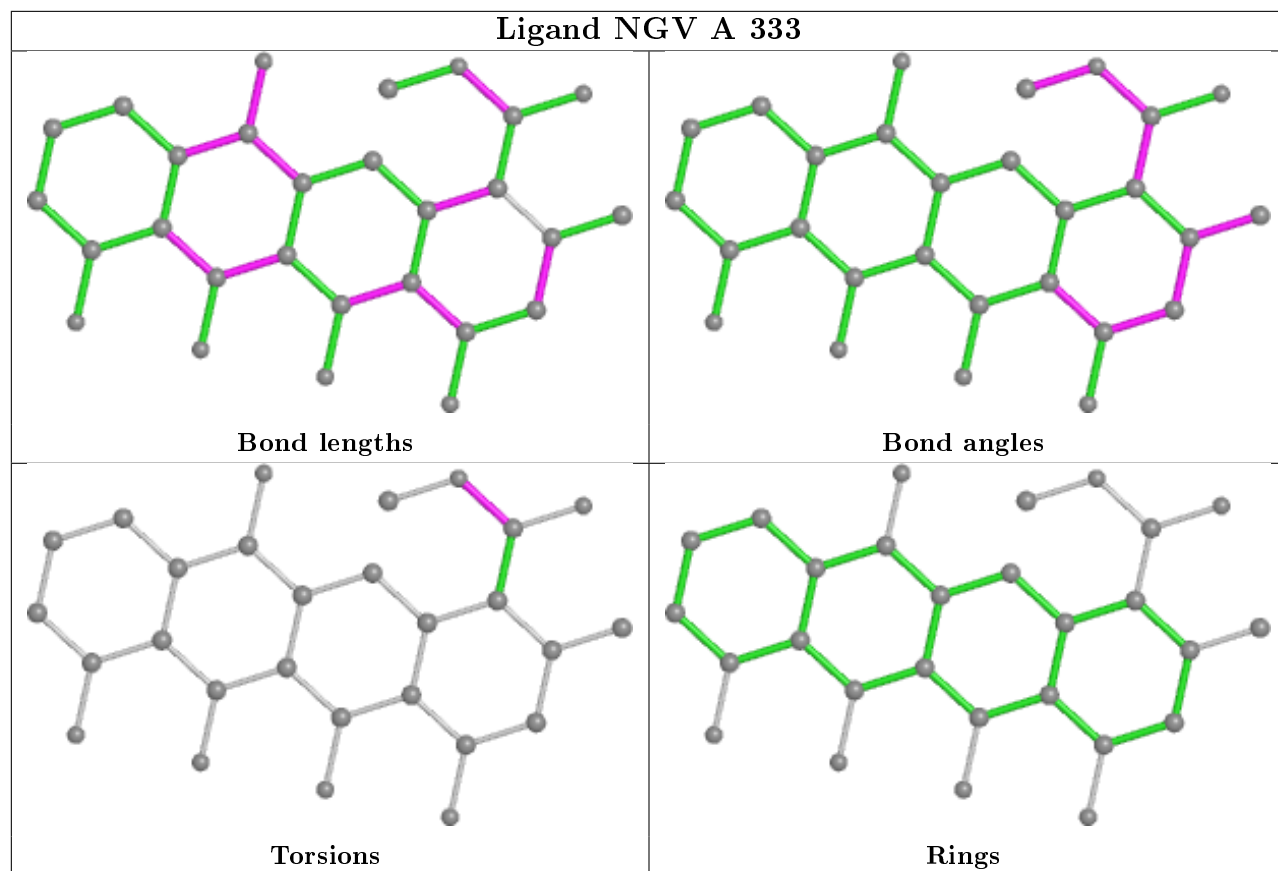
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	335	NGV	1	0
3	D	334	NGV	1	0
3	A	333	NGV	1	0
3	B	336	NGV	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	141/153 (92%)	-0.28	1 (0%) 87 89	20, 28, 38, 51	1 (0%)
1	B	141/153 (92%)	0.14	8 (5%) 23 29	20, 29, 38, 56	1 (0%)
1	C	143/153 (93%)	-0.18	4 (2%) 53 59	18, 27, 39, 62	3 (2%)
1	D	140/153 (91%)	-0.35	1 (0%) 87 89	21, 29, 38, 50	5 (3%)
All	All	565/612 (92%)	-0.17	14 (2%) 57 62	18, 28, 39, 62	10 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ARG	5.4
1	A	141	HIS	3.0
1	B	112	VAL	3.0
1	B	141	HIS	3.0
1	B	7	ALA	2.7
1	D	141	HIS	2.6
1	B	5	ILE	2.6
1	C	1	ARG	2.5
1	B	113	ASP	2.4
1	B	3	GLU	2.4
1	C	142	ARG	2.3
1	C	143	ARG	2.2
1	C	50	ILE	2.1
1	B	2	SER	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

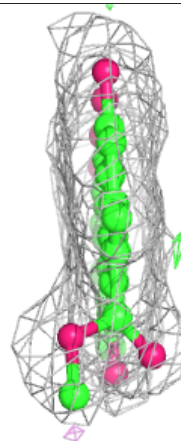
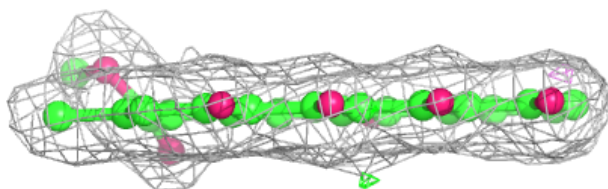
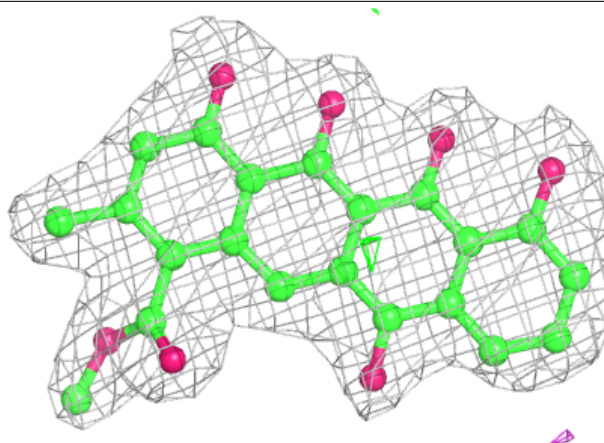
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NGV	D	334	28/28	0.91	0.12	27,33,35,37	0
3	NGV	B	336	28/28	0.92	0.11	26,31,35,36	0
3	NGV	A	333	28/28	0.93	0.10	32,36,39,40	0
3	NGV	C	335	28/28	0.93	0.10	25,29,32,33	0
2	SO4	A	276	5/5	0.95	0.22	53,53,54,54	5
2	SO4	D	277	5/5	0.98	0.09	40,41,41,41	5
2	SO4	C	278	5/5	0.98	0.12	46,48,48,49	5
2	SO4	B	279	5/5	0.98	0.07	48,48,48,48	5

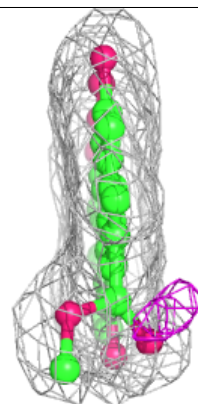
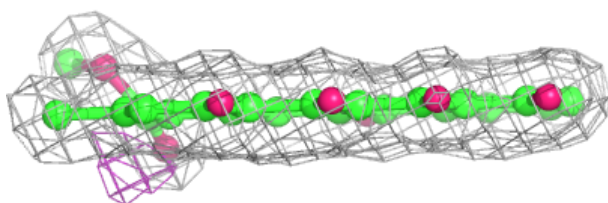
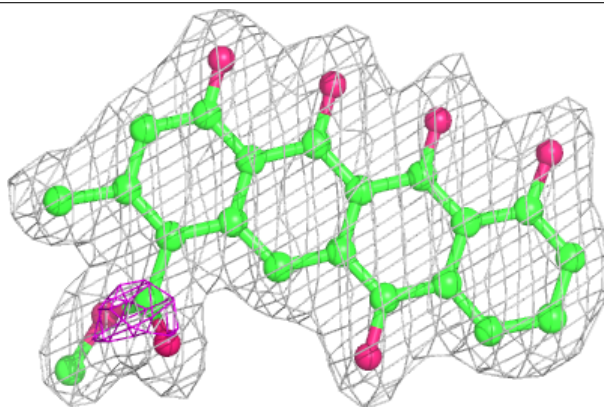
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NGV D 334:**

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

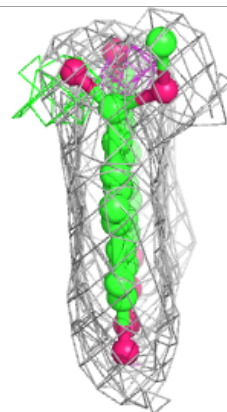
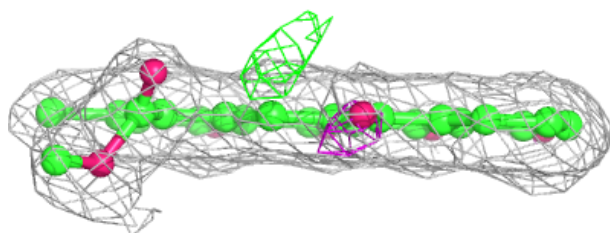
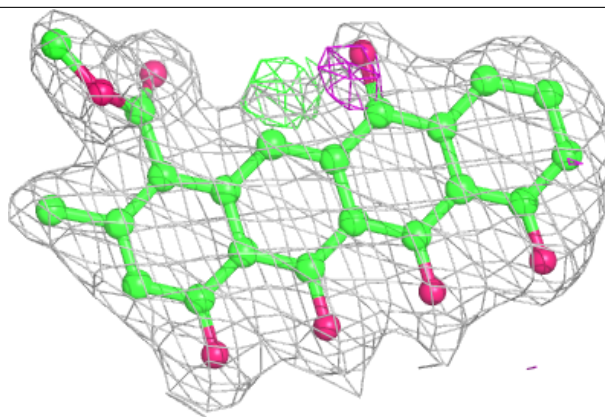
**Electron density around NGV B 336:**

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

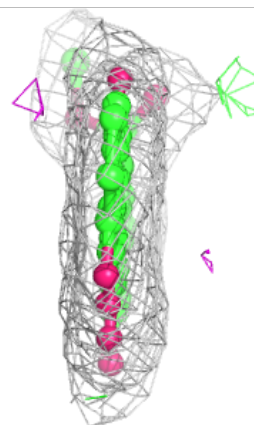
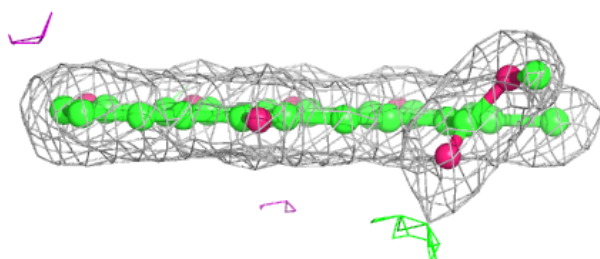
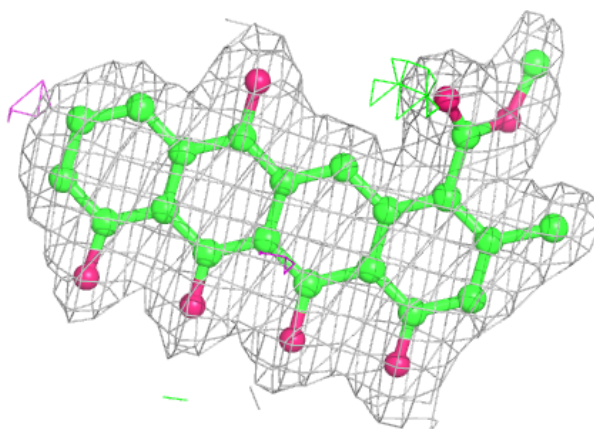


**Electron density around NGV A 333:**

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

**Electron density around NGV C 335:**

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





## 6.5 Other polymers

There are no such residues in this entry.