



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 04:16 PM JST

PDB ID : 9XMJ / pdb\_00009xmj  
Title : A Potent and Selective ROR gamma Inhibitor for the Treatment of Autoimmune Diseases  
Authors : Nomura, A.; Akai, S.; Yamaguchi, K.; Adachi, T.  
Deposited on : 2025-11-10  
Resolution : 2.18 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.

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:

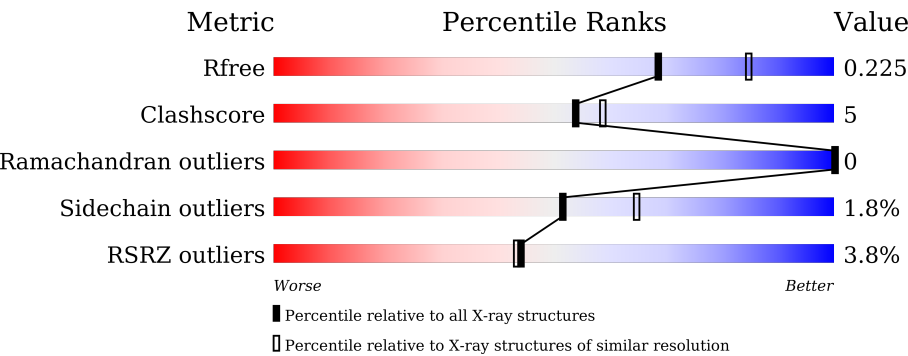
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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  $\geq 3$ , 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	258	<div><div>2%</div><div><div></div><div>78%</div><div>9%</div><div>•</div><div>12%</div></div></div>
1	C	258	<div><div>2%</div><div><div></div><div>75%</div><div>12%</div><div></div><div>12%</div></div></div>
1	E	258	<div><div>3%</div><div><div></div><div>79%</div><div>8%</div><div>•</div><div>12%</div></div></div>
1	G	258	<div><div>2%</div><div><div></div><div>76%</div><div>11%</div><div>•</div><div>12%</div></div></div>
2	B	22	<div><div>9%</div><div><div></div><div>59%</div><div>5%</div><div></div><div>36%</div></div></div>
2	D	22	<div><div>18%</div><div><div></div><div>50%</div><div>14%</div><div></div><div>36%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	22	<div><div><div></div><div></div><div></div></div><div>9%55%9%36%</div></div>
2	H	22	<div><div><div></div><div></div><div></div></div><div>9%41%23%36%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8058 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 Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1850	1173	333	330	14			
1	C	227	Total	C	N	O	S	0	0	0
			1850	1173	333	330	14			
1	E	227	Total	C	N	O	S	0	1	0
			1856	1176	334	331	15			
1	G	227	Total	C	N	O	S	0	0	0
			1850	1173	333	330	14			

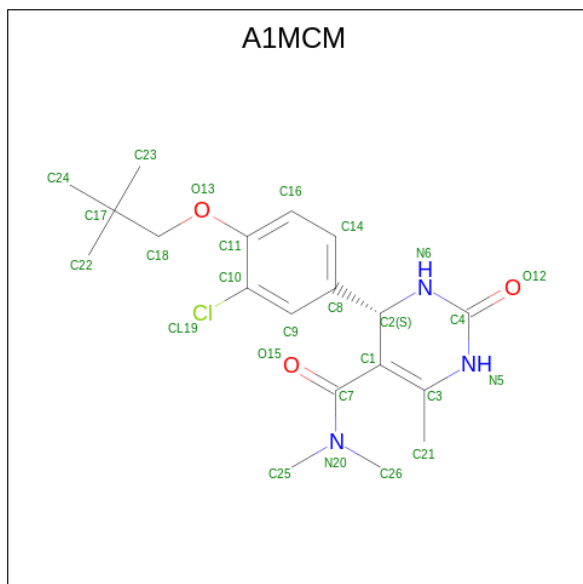
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	ALA	LYS	engineered mutation	UNP P51449
A	473	ALA	ARG	engineered mutation	UNP P51449
C	469	ALA	LYS	engineered mutation	UNP P51449
C	473	ALA	ARG	engineered mutation	UNP P51449
E	469	ALA	LYS	engineered mutation	UNP P51449
E	473	ALA	ARG	engineered mutation	UNP P51449
G	469	ALA	LYS	engineered mutation	UNP P51449
G	473	ALA	ARG	engineered mutation	UNP P51449

- Molecule 2 is a protein called Nuclear receptor corepressor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			106	67	19	18	2			
2	D	14	Total	C	N	O	S	0	0	0
			106	67	19	18	2			
2	F	14	Total	C	N	O	S	0	0	0
			106	67	19	18	2			
2	H	14	Total	C	N	O	S	0	0	0
			106	67	19	18	2			

- Molecule 3 is (4 {S})-4-[3-chloranyl-4-(2,2-dimethylpropoxy)phenyl]- {N}, {N},6-trimethyl-2-oxidanylidene-3,4-dihydro-1 {H}-pyrimidine-5-carboxamide (CCD ID: A1MCM) (formula: C<sub>19</sub>H<sub>26</sub>ClN<sub>3</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



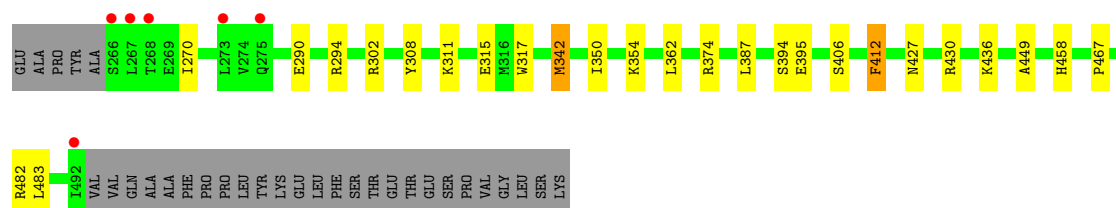
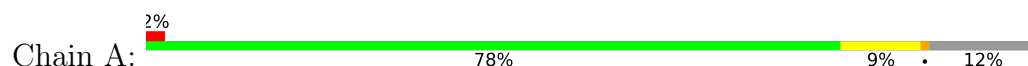
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	25	Total 25	O 25	0	0
4	H	1	Total 1	O 1	0	0

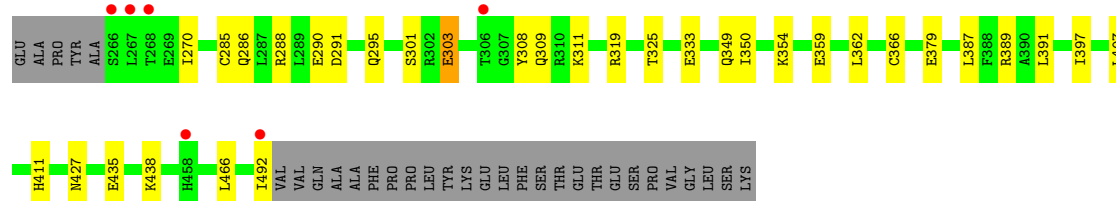
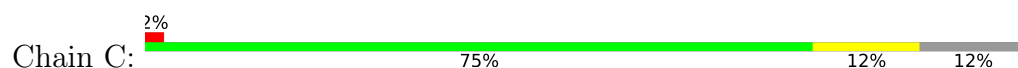
### 3 Residue-property plots [i](#)

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.

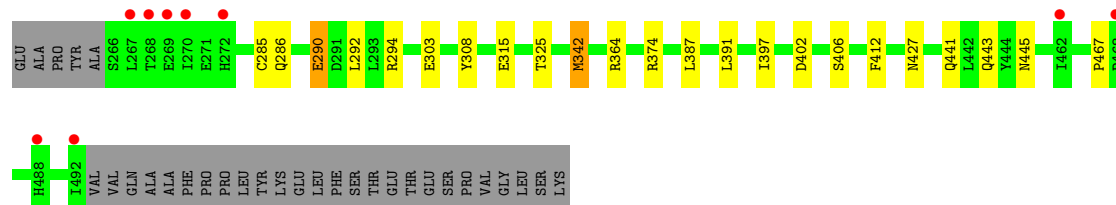
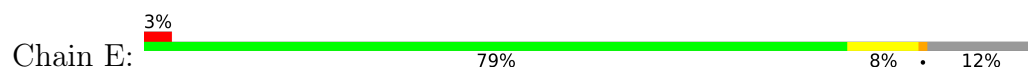
- Molecule 1: Nuclear receptor ROR-gamma



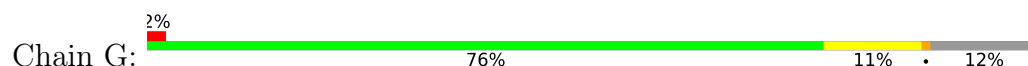
- Molecule 1: Nuclear receptor ROR-gamma

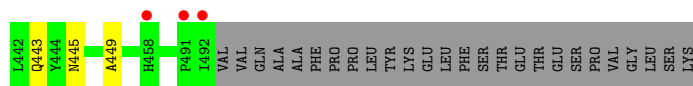


- Molecule 1: Nuclear receptor ROR-gamma

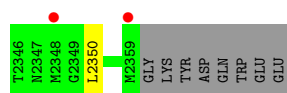


- Molecule 1: Nuclear receptor ROR-gamma

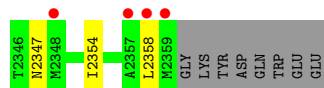




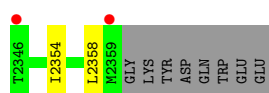
● Molecule 2: Nuclear receptor corepressor 2



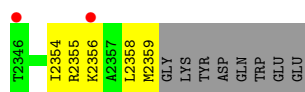
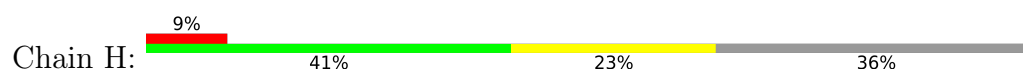
● Molecule 2: Nuclear receptor corepressor 2



● Molecule 2: Nuclear receptor corepressor 2



● Molecule 2: Nuclear receptor corepressor 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.26Å 72.16Å 98.36Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	49.18 – 2.18 49.18 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.18-2.18) 98.9 (49.18-2.18)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.179 , 0.218 0.188 , 0.225	Depositor DCC
$R_{free}$ test set	2903 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.14% 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: A1MCM

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	0.67	0/1888	1.12	2/2542 (0.1%)
1	C	0.66	0/1888	1.09	1/2542 (0.0%)
1	E	0.67	0/1894	1.13	2/2550 (0.1%)
1	G	0.66	0/1888	1.08	2/2542 (0.1%)
2	B	0.62	0/105	1.10	0/138
2	D	0.57	0/105	1.06	0/138
2	F	0.63	0/105	1.08	0/138
2	H	0.74	0/105	1.11	0/138
All	All	0.66	0/7978	1.11	7/10728 (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	E	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	PHE	CA-CB-CG	7.00	120.80	113.80
1	G	325	THR	CA-CB-OG1	-6.39	100.02	109.60
1	C	325	THR	CA-CB-OG1	-5.62	101.17	109.60
1	A	342	MET	CG-SD-CE	5.31	112.58	100.90
1	G	342	MET	CG-SD-CE	5.26	112.47	100.90
1	E	342	MET	CG-SD-CE	5.22	112.38	100.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	325	THR	CA-CB-OG1	-5.09	101.96	109.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	364	ARG	Sidechain
1	G	437	ARG	Sidechain

## 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	1850	0	1846	17	0
1	C	1850	0	1846	18	0
1	E	1856	0	1850	18	0
1	G	1850	0	1846	20	0
2	B	106	0	119	0	0
2	D	106	0	119	3	0
2	F	106	0	119	1	0
2	H	106	0	119	3	0
3	A	26	0	0	0	0
3	C	26	0	0	0	0
3	E	26	0	0	0	0
3	G	26	0	0	1	0
4	A	31	0	0	3	1
4	B	1	0	0	0	0
4	C	34	0	0	4	0
4	D	2	0	0	0	0
4	E	29	0	0	4	1
4	F	1	0	0	0	0
4	G	25	0	0	5	0
4	H	1	0	0	0	0
All	All	8058	0	7864	77	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 5.

All (77) 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:G:443:GLN:NE2	4:G:701:HOH:O	2.12	0.77
1:A:458:HIS:CE1	4:A:724:HOH:O	2.42	0.73
1:C:359:GLU:OE1	4:C:701:HOH:O	2.12	0.68
1:C:349:GLN:OE1	2:D:2358:LEU:HD11	1.95	0.67
1:G:415:ASP:OD2	4:G:702:HOH:O	2.14	0.66
1:E:402:ASP:OD2	4:E:701:HOH:O	2.13	0.66
1:C:288:ARG:NH1	1:C:290:GLU:OE2	2.30	0.65
4:C:719:HOH:O	2:D:2347:ASN:HB2	1.97	0.64
1:A:311:LYS:HG2	1:A:315:GLU:OE2	2.00	0.60
1:E:374:ARG:HH11	1:E:374:ARG:HG3	1.66	0.60
1:C:333:GLU:OE1	4:C:702:HOH:O	2.17	0.60
1:C:319:ARG:NH1	1:C:379:GLU:OE1	2.35	0.59
1:E:315:GLU:OE1	4:E:702:HOH:O	2.16	0.59
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.67	0.59
1:G:311:LYS:NZ	1:G:315:GLU:OE1	2.35	0.58
1:G:286:GLN:OE1	4:G:703:HOH:O	2.17	0.57
1:C:366:CYS:SG	1:C:407:LEU:HB3	2.43	0.57
1:C:492:ILE:O	4:C:703:HOH:O	2.17	0.57
1:E:294:ARG:NH1	1:E:294:ARG:HG3	2.19	0.56
1:A:294:ARG:HG3	1:A:294:ARG:NH1	2.22	0.54
1:A:290:GLU:O	1:A:294:ARG:HG2	2.09	0.53
1:G:270:ILE:HG23	1:G:449:ALA:HA	1.93	0.51
1:C:435:GLU:OE1	1:C:438:LYS:HD2	2.10	0.51
1:E:443:GLN:NE2	4:E:704:HOH:O	2.42	0.51
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.75	0.51
1:C:411:HIS:O	1:E:294:ARG:CD	2.60	0.50
1:G:374:ARG:HG3	1:G:374:ARG:HH11	1.76	0.50
1:G:365:MET:HE2	3:G:601:A1MCM:C11	2.42	0.50
1:G:441:GLN:O	1:G:445:ASN:ND2	2.45	0.49
1:E:290:GLU:O	1:E:294:ARG:HG2	2.13	0.49
1:E:441:GLN:O	1:E:445:ASN:ND2	2.46	0.48
1:G:350:ILE:O	1:G:354:LYS:HB2	2.13	0.48
1:A:342:MET:HA	1:A:342:MET:HE2	1.95	0.47
1:G:302:ARG:HH11	1:G:302:ARG:HG3	1.79	0.47
1:E:294:ARG:HG3	1:E:294:ARG:HH11	1.79	0.47
1:G:391:LEU:HD12	1:G:397:ILE:HD11	1.97	0.47
1:A:350:ILE:O	1:A:354:LYS:HB2	2.14	0.46
2:F:2354:ILE:O	2:F:2358:LEU:HB2	2.16	0.46
1:E:342:MET:HA	1:E:342:MET:HE2	1.97	0.45
1:G:299:ILE:O	4:G:704:HOH:O	2.20	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HG23	1:A:449:ALA:HA	1.99	0.45
1:G:427:ASN:OD1	1:G:427:ASN:C	2.60	0.45
2:H:2354:ILE:O	2:H:2358:LEU:HB2	2.16	0.45
1:A:430:ARG:NE	4:A:705:HOH:O	2.36	0.45
1:C:350:ILE:O	1:C:354:LYS:HB2	2.17	0.45
1:A:374:ARG:HH11	1:A:374:ARG:CG	2.30	0.45
1:E:292:LEU:HB3	4:E:706:HOH:O	2.17	0.44
1:C:427:ASN:OD1	1:C:427:ASN:C	2.60	0.44
1:E:303:GLU:OE2	1:G:347:ASN:HB2	2.17	0.44
1:G:342:MET:HA	1:G:342:MET:HE2	1.98	0.44
1:C:391:LEU:HD12	1:C:397:ILE:HD11	2.00	0.44
1:A:302:ARG:HH11	1:A:302:ARG:HG3	1.82	0.44
1:A:427:ASN:C	1:A:427:ASN:OD1	2.61	0.44
1:A:406:SER:HB2	1:A:467:PRO:HG3	2.00	0.43
4:G:710:HOH:O	2:H:2356:LYS:HD2	2.19	0.43
1:E:391:LEU:HD12	1:E:397:ILE:HD11	2.01	0.42
1:E:308:TYR:CD2	1:E:387:LEU:HD11	2.55	0.42
1:G:327:ALA:O	1:G:331:VAL:HG23	2.18	0.42
1:E:374:ARG:HG3	1:E:374:ARG:NH1	2.34	0.42
1:G:308:TYR:CD2	1:G:387:LEU:HD11	2.55	0.42
1:G:395:GLU:HG2	1:G:396:LEU:N	2.35	0.41
1:C:285:CYS:O	1:C:286:GLN:HB3	2.20	0.41
1:E:285:CYS:O	1:E:286:GLN:HB3	2.19	0.41
1:G:374:ARG:HH11	1:G:374:ARG:CG	2.33	0.41
2:H:2355:ARG:O	2:H:2359:MET:HG2	2.20	0.41
1:C:291:ASP:O	1:C:295:GLN:HG2	2.20	0.41
1:A:308:TYR:CD2	1:A:387:LEU:HD11	2.56	0.41
1:C:308:TYR:HA	1:C:311:LYS:HD2	2.03	0.41
1:E:406:SER:HB2	1:E:467:PRO:HG3	2.02	0.41
1:C:301:SER:OG	1:C:303:GLU:HG2	2.20	0.41
1:C:309:GLN:HB3	1:C:389:ARG:NH2	2.36	0.41
1:C:308:TYR:CD2	1:C:387:LEU:HD11	2.55	0.41
1:E:427:ASN:OD1	1:E:427:ASN:C	2.63	0.41
1:G:302:ARG:HG3	1:G:302:ARG:NH1	2.36	0.41
1:A:317:TRP:HB3	1:A:483:LEU:HD21	2.02	0.40
1:A:482:ARG:NE	4:A:709:HOH:O	2.48	0.40
2:D:2354:ILE:O	2:D:2358:LEU:HB2	2.22	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)
4:A:709:HOH:O	4:E:708:HOH:O[2_454]	2.19	0.01

## 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	225/258 (87%)	222 (99%)	3 (1%)	0	100	100
1	C	225/258 (87%)	222 (99%)	3 (1%)	0	100	100
1	E	226/258 (88%)	223 (99%)	3 (1%)	0	100	100
1	G	225/258 (87%)	222 (99%)	3 (1%)	0	100	100
2	B	12/22 (54%)	12 (100%)	0	0	100	100
2	D	12/22 (54%)	12 (100%)	0	0	100	100
2	F	12/22 (54%)	12 (100%)	0	0	100	100
2	H	12/22 (54%)	12 (100%)	0	0	100	100
All	All	949/1120 (85%)	937 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	202/228 (89%)	197 (98%)	5 (2%)	42	53
1	C	202/228 (89%)	198 (98%)	4 (2%)	48	61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	203/228 (89%)	201 (99%)	2 (1%)	68	79
1	G	202/228 (89%)	199 (98%)	3 (2%)	57	70
2	B	11/18 (61%)	10 (91%)	1 (9%)	9	8
2	D	11/18 (61%)	11 (100%)	0	100	100
2	F	11/18 (61%)	11 (100%)	0	100	100
2	H	11/18 (61%)	11 (100%)	0	100	100
All	All	853/984 (87%)	838 (98%)	15 (2%)	51	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	LEU
1	A	394	SER
1	A	395	GLU
1	A	412	PHE
1	A	436	LYS
2	B	2350	LEU
1	C	270	ILE
1	C	303	GLU
1	C	362	LEU
1	C	466	LEU
1	E	290	GLU
1	E	412	PHE
1	G	354	LYS
1	G	362	LEU
1	G	366	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	298	ASN
1	A	445	ASN
1	A	478	GLN
1	A	487	GLN
1	C	286	GLN
1	C	484	GLN
1	C	490	HIS
1	E	298	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	443	GLN
1	E	445	ASN
1	G	434	GLN
1	G	445	ASN
1	G	453	HIS
1	G	478	GLN
1	G	487	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 ⓘ

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
3	A1MCM	E	601	-	27,27,27	1.83	10 (37%)	40,40,40	1.99	11 (27%)
3	A1MCM	G	601	-	27,27,27	1.16	3 (11%)	40,40,40	3.06	9 (22%)
3	A1MCM	A	601	-	27,27,27	1.66	4 (14%)	40,40,40	2.83	13 (32%)
3	A1MCM	C	601	-	27,27,27	1.71	7 (25%)	40,40,40	2.55	15 (37%)

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	A1MCM	E	601	-	-	1/18/34/34	0/2/2/2
3	A1MCM	G	601	-	-	2/18/34/34	0/2/2/2
3	A1MCM	A	601	-	-	0/18/34/34	0/2/2/2
3	A1MCM	C	601	-	-	2/18/34/34	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	A1MCM	C2-C1	-5.44	1.47	1.51
3	C	601	A1MCM	C2-N6	4.31	1.51	1.47
3	E	601	A1MCM	C16-C14	4.00	1.46	1.38
3	A	601	A1MCM	C7-C1	3.95	1.54	1.49
3	E	601	A1MCM	C9-C8	3.53	1.44	1.39
3	E	601	A1MCM	C4-N5	-3.36	1.31	1.37
3	C	601	A1MCM	C7-N20	3.19	1.38	1.34
3	C	601	A1MCM	C4-N6	3.10	1.41	1.34
3	C	601	A1MCM	C9-C8	3.10	1.43	1.39
3	E	601	A1MCM	C16-C11	2.72	1.45	1.39
3	E	601	A1MCM	C2-C1	-2.42	1.49	1.51
3	C	601	A1MCM	C9-C10	2.40	1.42	1.38
3	E	601	A1MCM	C9-C10	2.38	1.42	1.38
3	E	601	A1MCM	O15-C7	2.28	1.27	1.23
3	G	601	A1MCM	C2-C1	-2.19	1.49	1.51
3	A	601	A1MCM	C9-C8	2.15	1.42	1.39
3	G	601	A1MCM	C16-C14	2.11	1.42	1.38
3	E	601	A1MCM	O12-C4	-2.10	1.19	1.23
3	E	601	A1MCM	C8-C2	2.07	1.56	1.52
3	G	601	A1MCM	C7-N20	2.06	1.36	1.34
3	A	601	A1MCM	C7-N20	2.05	1.36	1.34
3	E	601	A1MCM	C7-N20	2.05	1.36	1.34
3	C	601	A1MCM	C2-C1	-2.04	1.50	1.51
3	C	601	A1MCM	C11-C10	-2.03	1.36	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	601	A1MCM	C1-C7-N20	15.23	128.97	119.92
3	A	601	A1MCM	C1-C7-N20	10.51	126.16	119.92
3	C	601	A1MCM	C1-C7-N20	8.07	124.71	119.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	A1MCM	C8-C2-N6	-7.35	102.55	110.87
3	G	601	A1MCM	C8-C2-N6	-7.19	102.73	110.87
3	C	601	A1MCM	C8-C2-C1	-6.44	104.06	112.84
3	A	601	A1MCM	C1-C2-N6	6.10	113.96	109.09
3	C	601	A1MCM	C8-C2-N6	-5.86	104.24	110.87
3	A	601	A1MCM	C8-C2-C1	-5.43	105.43	112.84
3	C	601	A1MCM	C1-C2-N6	4.88	112.98	109.09
3	A	601	A1MCM	C8-C2-N6	-4.78	105.45	110.87
3	A	601	A1MCM	O15-C7-N20	-4.43	114.81	122.64
3	A	601	A1MCM	C21-C3-N5	-3.97	108.74	113.45
3	E	601	A1MCM	C21-C3-C1	3.87	131.49	127.62
3	C	601	A1MCM	C3-N5-C4	3.57	126.49	123.71
3	A	601	A1MCM	C21-C3-C1	3.55	131.17	127.62
3	E	601	A1MCM	C9-C10-CL19	3.46	124.08	118.49
3	A	601	A1MCM	C9-C10-CL19	3.30	123.81	118.49
3	E	601	A1MCM	C21-C3-N5	-3.26	109.58	113.45
3	G	601	A1MCM	C9-C10-CL19	3.13	123.54	118.49
3	A	601	A1MCM	O13-C18-C17	-2.94	99.75	109.58
3	E	601	A1MCM	C10-C9-C8	2.87	124.46	120.29
3	C	601	A1MCM	C26-N20-C7	-2.87	113.03	121.75
3	G	601	A1MCM	O15-C7-N20	-2.79	117.70	122.64
3	C	601	A1MCM	C9-C10-CL19	2.78	122.97	118.49
3	A	601	A1MCM	C9-C10-C11	-2.76	117.33	121.02
3	G	601	A1MCM	C10-C9-C8	2.74	124.27	120.29
3	E	601	A1MCM	C18-O13-C11	-2.72	111.03	117.67
3	G	601	A1MCM	O15-C7-C1	-2.70	113.12	119.94
3	A	601	A1MCM	C9-C8-C2	2.59	124.32	119.78
3	G	601	A1MCM	C7-C1-C3	-2.57	117.81	123.02
3	E	601	A1MCM	O12-C4-N5	-2.56	116.98	121.82
3	C	601	A1MCM	C9-C8-C2	2.55	124.26	119.78
3	A	601	A1MCM	C14-C8-C9	-2.49	115.90	118.76
3	C	601	A1MCM	C14-C8-C9	-2.45	115.94	118.76
3	E	601	A1MCM	C9-C10-C11	-2.39	117.82	121.02
3	G	601	A1MCM	C14-C8-C9	-2.33	116.08	118.76
3	C	601	A1MCM	O12-C4-N5	-2.28	117.51	121.82
3	E	601	A1MCM	O13-C18-C17	-2.24	102.07	109.58
3	C	601	A1MCM	O12-C4-N6	2.23	127.38	122.92
3	C	601	A1MCM	C2-C1-C3	2.21	122.28	119.95
3	E	601	A1MCM	C2-C1-C3	2.18	122.25	119.95
3	C	601	A1MCM	C11-C10-CL19	-2.15	116.91	119.43
3	E	601	A1MCM	C14-C8-C9	-2.12	116.32	118.76
3	A	601	A1MCM	C16-C11-C10	2.12	122.18	118.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	A1MCM	O15-C7-C1	-2.09	114.66	119.94
3	G	601	A1MCM	C11-C10-CL19	-2.06	117.01	119.43
3	C	601	A1MCM	C14-C16-C11	2.04	123.95	120.06

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	A1MCM	C1-C7-N20-C26
3	G	601	A1MCM	C1-C7-N20-C26
3	E	601	A1MCM	O15-C7-N20-C26
3	G	601	A1MCM	O15-C7-N20-C26
3	C	601	A1MCM	C3-C1-C7-N20

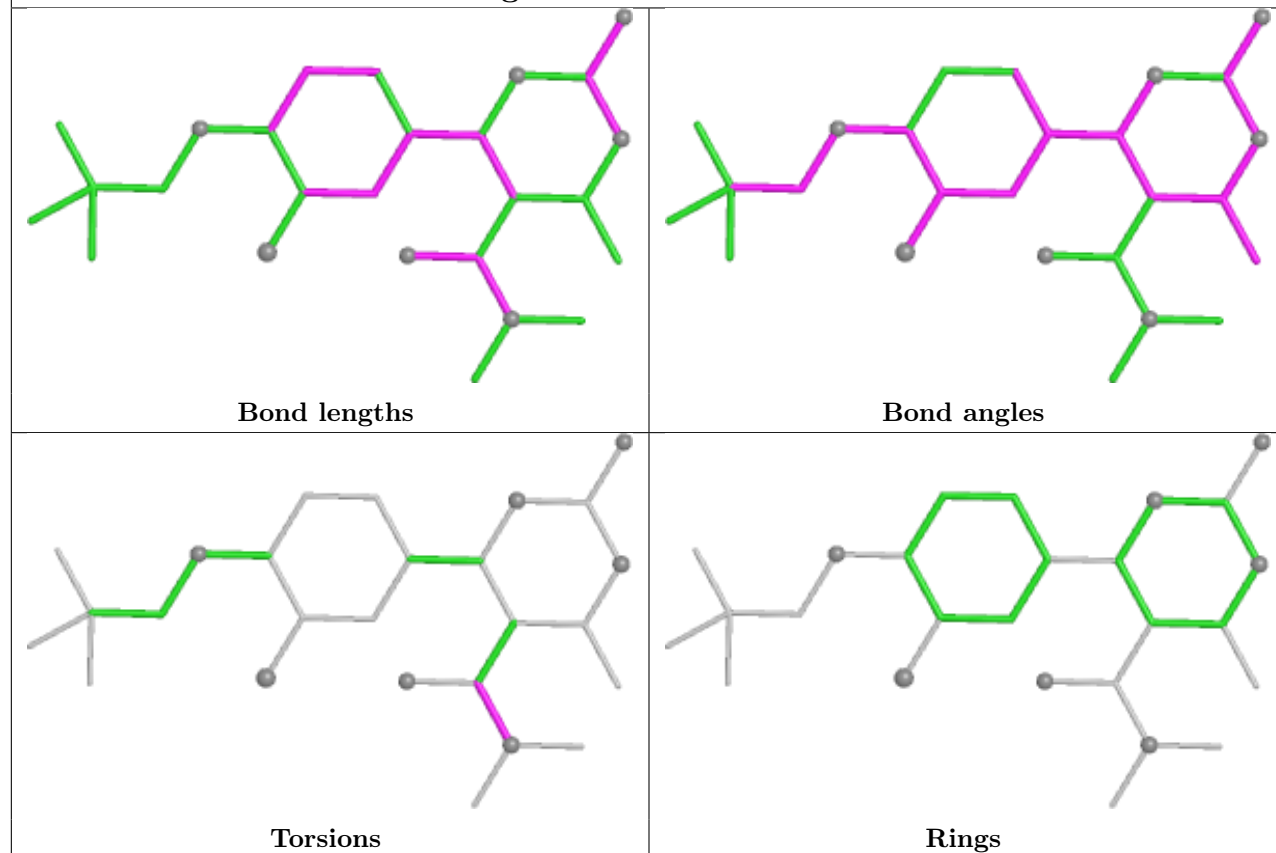
There are no ring outliers.

1 monomer is involved in 1 short contact:

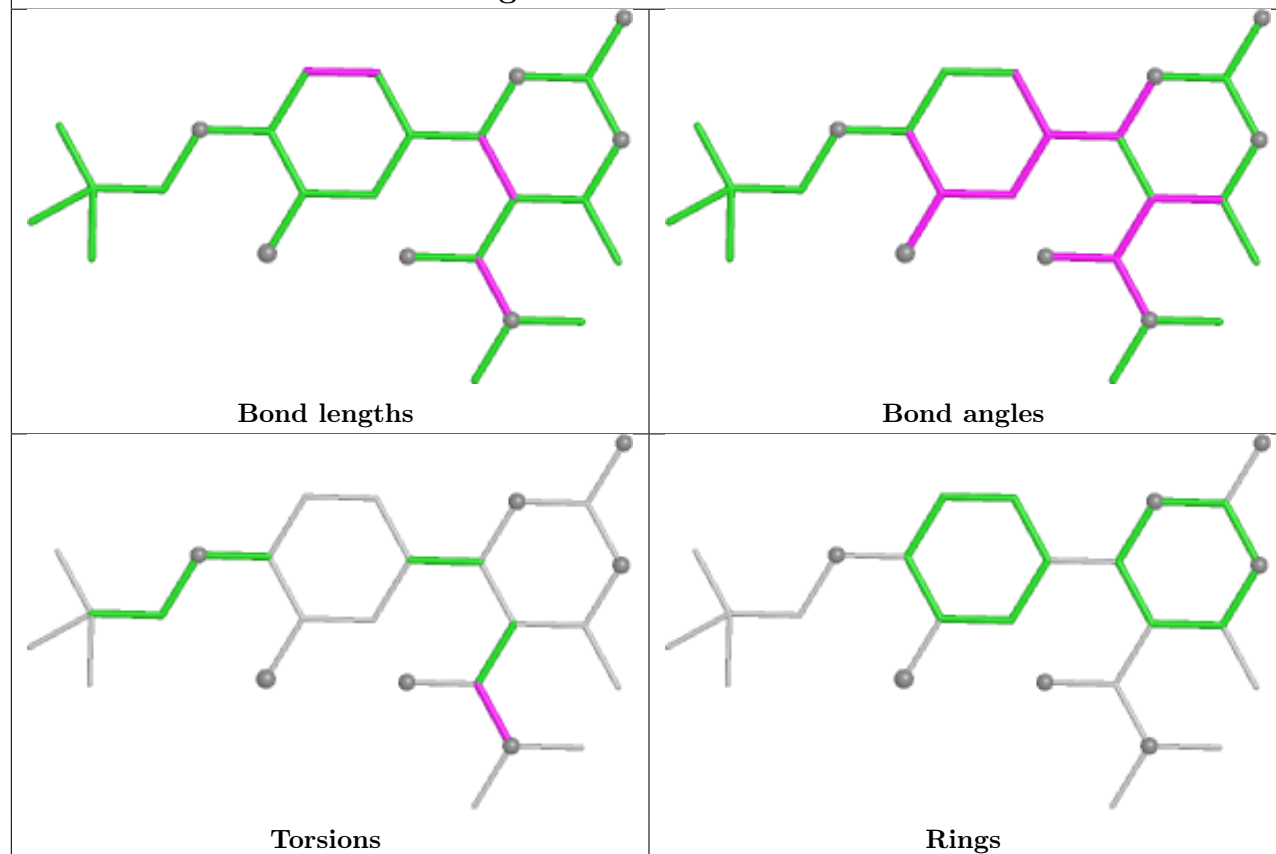
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	601	A1MCM	1	0

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.

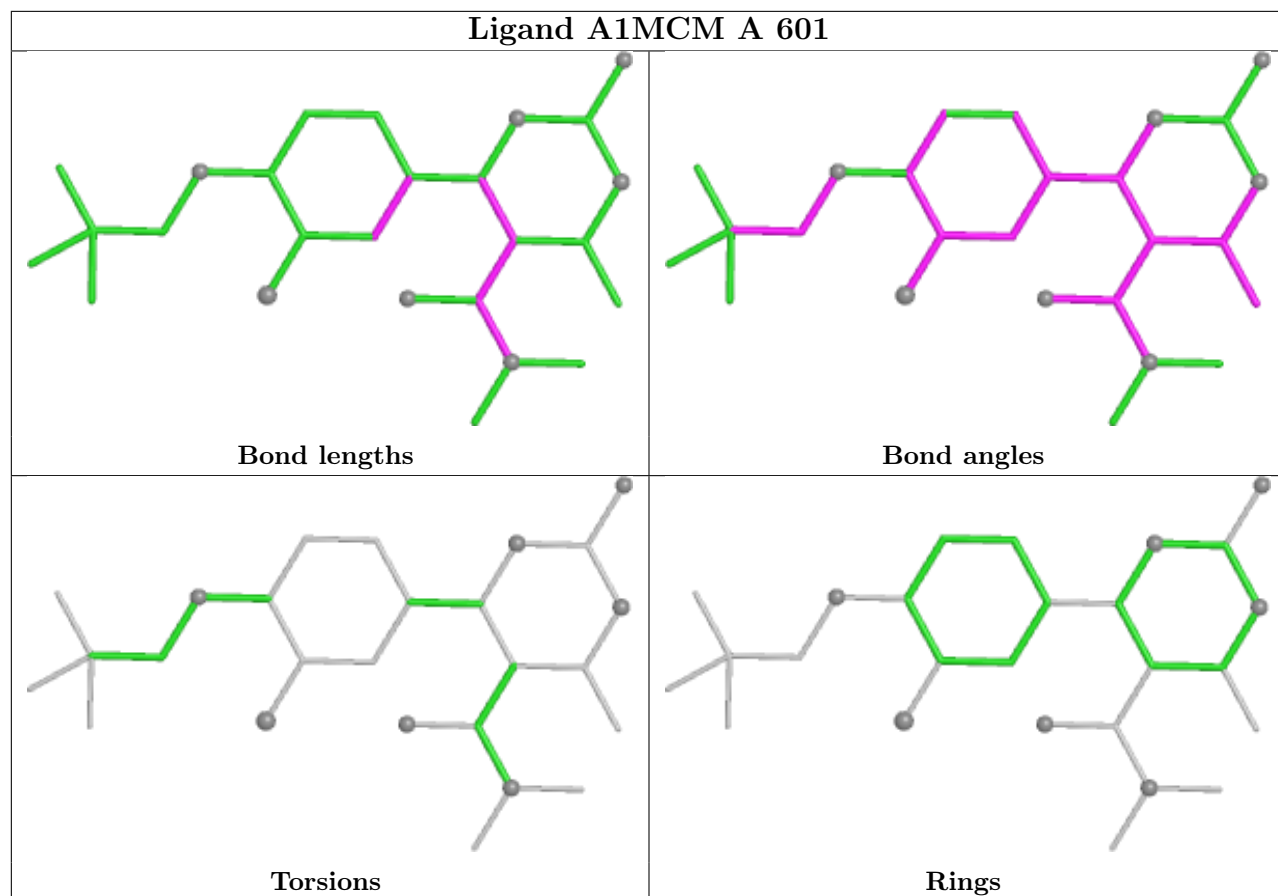
## Ligand A1MCM E 601



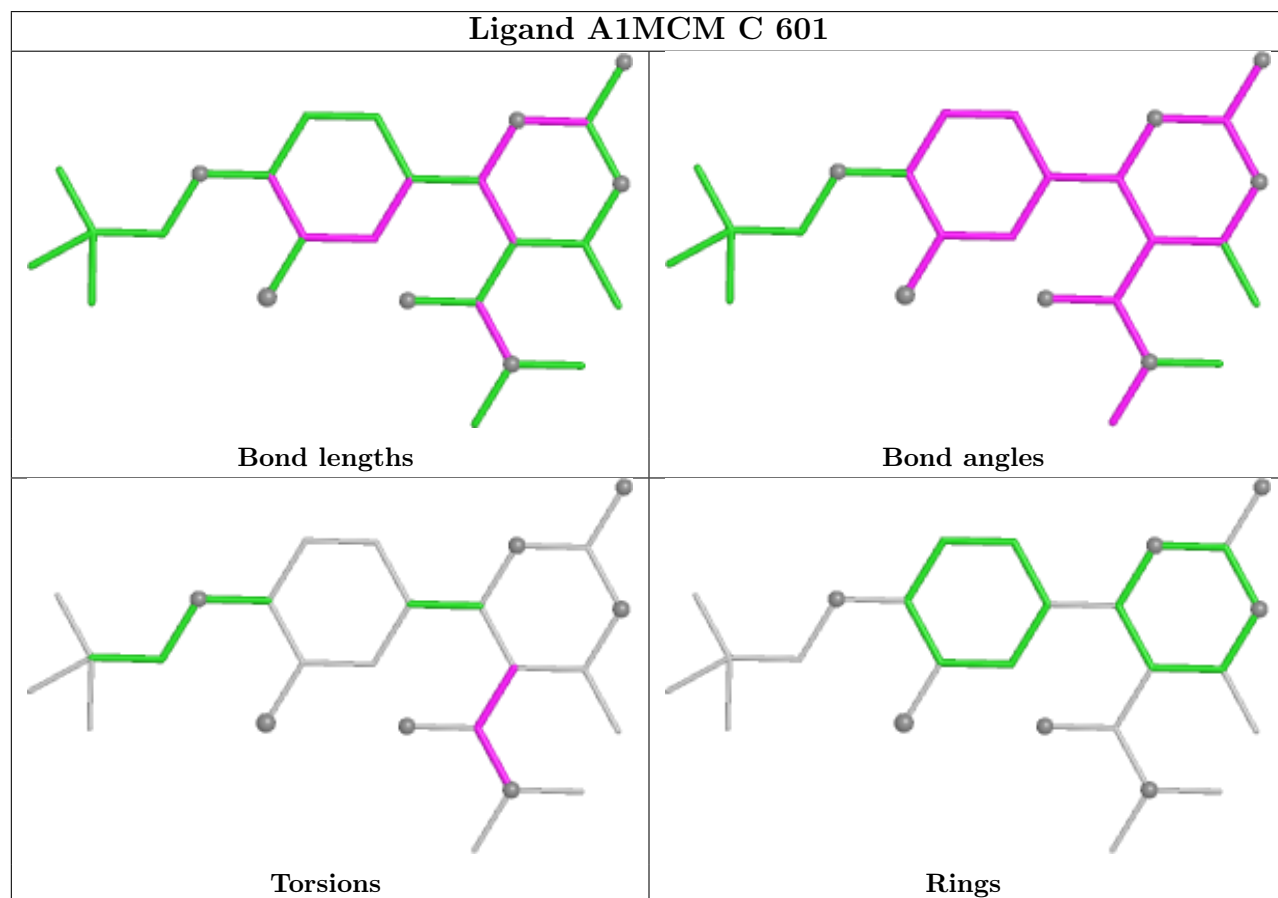
## Ligand A1MCM G 601



## Ligand A1MCM A 601



## Ligand A1MCM C 601



## 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	227/258 (87%)	0.44	6 (2%) 57 56	23, 42, 65, 89	0
1	C	227/258 (87%)	0.53	6 (2%) 57 56	28, 46, 70, 108	0
1	E	227/258 (87%)	0.39	9 (3%) 42 41	21, 41, 65, 105	1 (0%)
1	G	227/258 (87%)	0.44	6 (2%) 57 56	24, 44, 66, 84	0
2	B	14/22 (63%)	1.24	2 (14%) 6 5	39, 55, 78, 91	0
2	D	14/22 (63%)	1.49	4 (28%) 1 1	49, 64, 82, 94	0
2	F	14/22 (63%)	0.73	2 (14%) 6 5	33, 46, 55, 82	0
2	H	14/22 (63%)	0.87	2 (14%) 6 5	38, 42, 51, 60	0
All	All	964/1120 (86%)	0.48	37 (3%) 44 43	21, 44, 69, 108	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	492	ILE	5.8
1	A	492	ILE	5.8
1	C	492	ILE	4.9
1	E	268	THR	4.8
1	E	492	ILE	4.7
1	C	267	LEU	3.9
1	C	268	THR	3.9
1	A	267	LEU	3.8
2	B	2359	MET	3.2
1	G	267	LEU	3.1
1	A	266	SER	3.0
2	D	2348	MET	3.0
1	G	491	PRO	3.0
1	E	270	ILE	2.9
1	A	273	LEU	2.8
1	A	268	THR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	2359	MET	2.7
1	E	267	LEU	2.7
1	E	468	PRO	2.7
2	H	2356	LYS	2.6
1	C	266	SER	2.5
2	F	2359	MET	2.5
2	F	2346	THR	2.4
2	B	2348	MET	2.4
2	D	2358	LEU	2.4
1	E	488	HIS	2.4
1	A	275	GLN	2.4
1	E	272	HIS	2.4
1	G	273	LEU	2.3
1	C	458	HIS	2.2
1	C	306	THR	2.2
1	E	462	ILE	2.1
1	G	458	HIS	2.1
2	H	2346	THR	2.1
1	G	270	ILE	2.1
1	E	269	GLU	2.0
2	D	2357	ALA	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, 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( $\text{\AA}^2$ )	Q<0.9
3	A1MCM	C	601	26/26	0.93	0.09	27,35,42,45	0
3	A1MCM	A	601	26/26	0.96	0.07	24,28,37,39	0

*Continued on next page...*



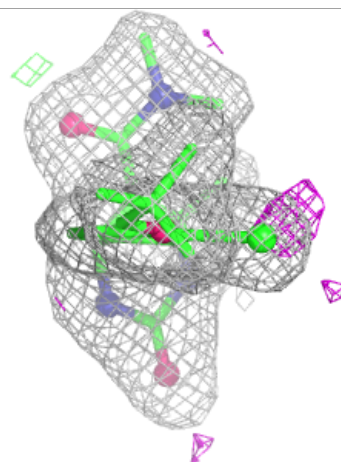
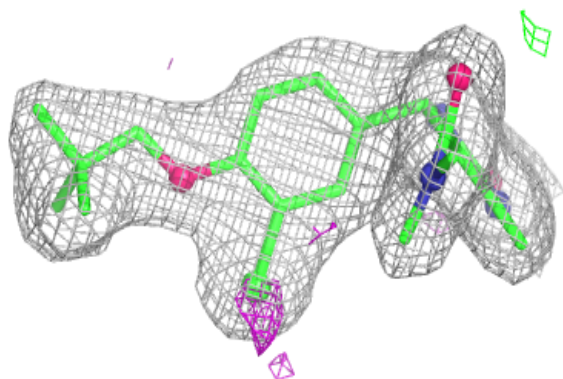
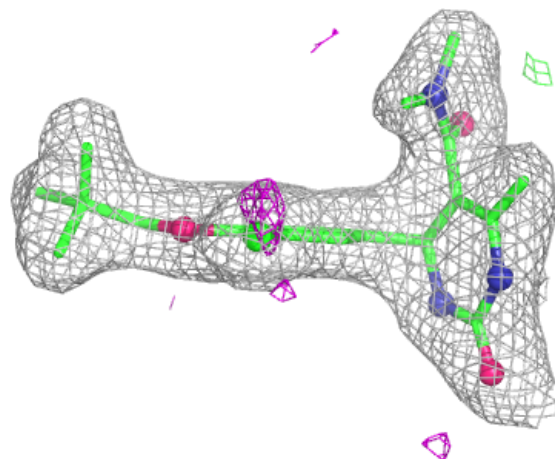
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1MCM	E	601	26/26	0.96	0.07	26,33,37,40	0
3	A1MCM	G	601	26/26	0.96	0.07	21,28,42,46	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.

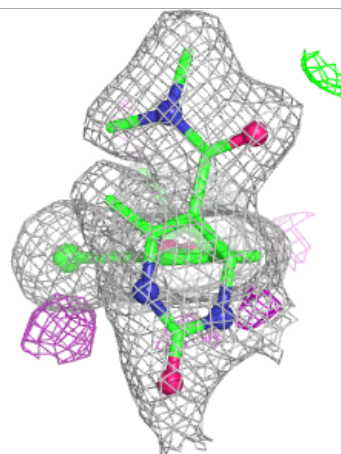
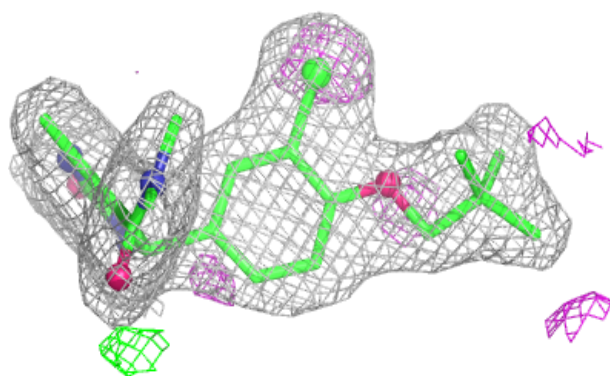
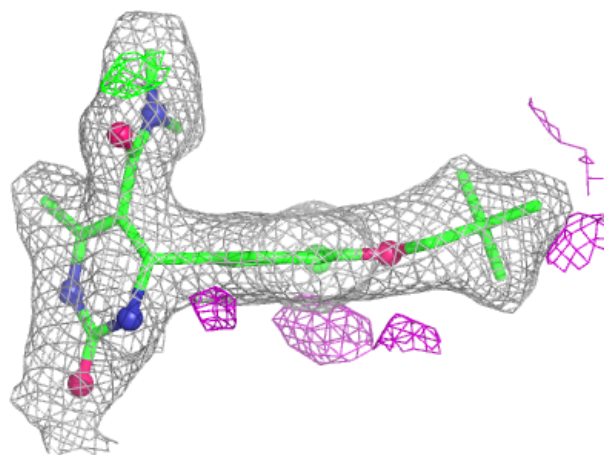
**Electron density around A1MCM C 601:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



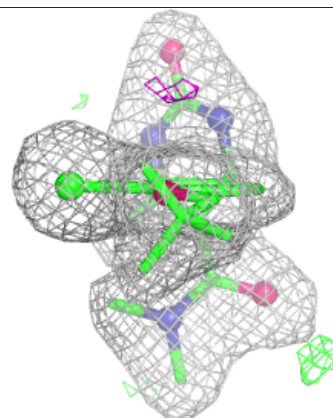
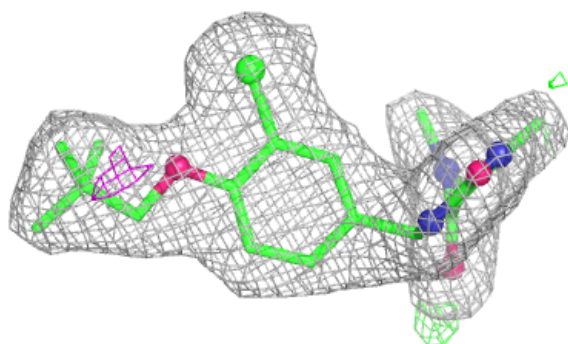
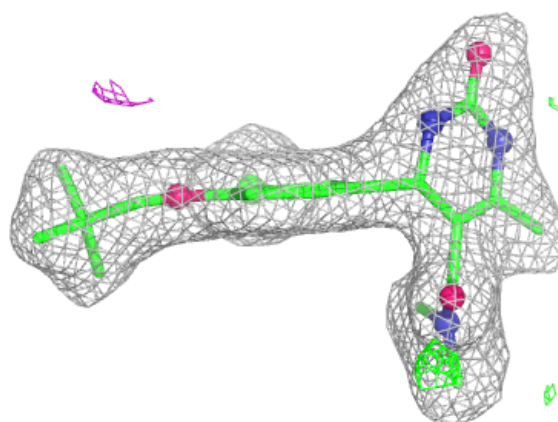
**Electron density around A1MCM A 601:**

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

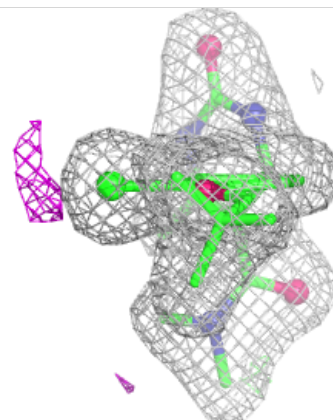
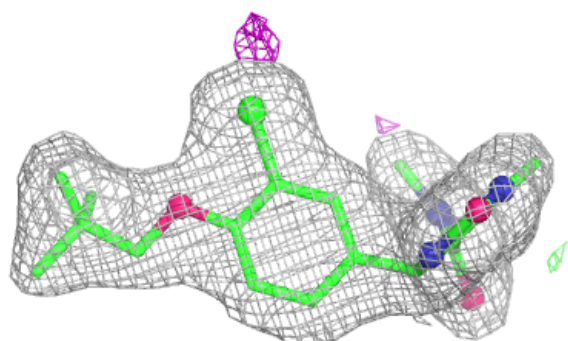
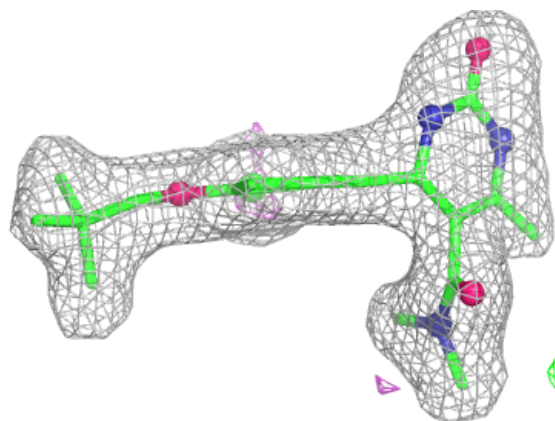


**Electron density around A1MCM E 601:**

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

**Electron density around A1MCM G 601:**

$2mF_o-DF_c$  (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.