



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:37 am BST

PDB ID : 2Q59  
Title : Crystal Structure of PPARgamma LBD bound to full agonist MRL20  
Authors : Bruning, J.B.; Nettles, K.W.  
Deposited on : 2007-05-31  
Resolution : 2.20 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

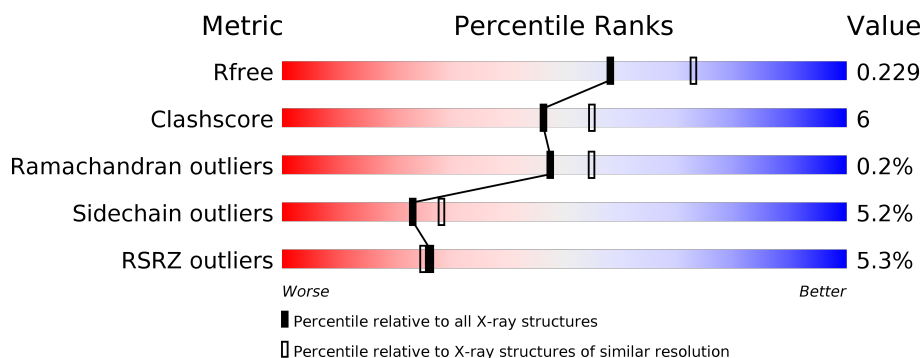
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	274	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div> </div>
2	B	274	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 8%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4396 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 Peroxisome Proliferator-Activated Receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	6	0
			2057	1328	332	384	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	SER	-	EXPRESSION TAG	UNP P37231
A	285	CME	CYS	MODIFIED RESIDUE	UNP P37231

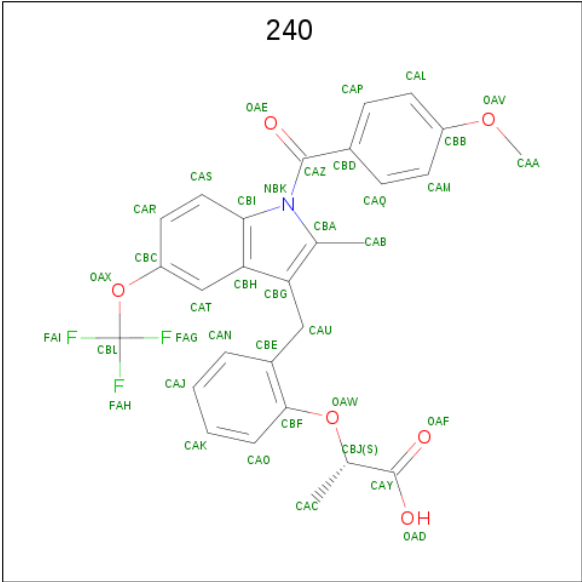
- Molecule 2 is a protein called Peroxisome Proliferator-Activated Receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	253	Total	C	N	O	S	0	4	0
			2019	1311	327	372	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	204	SER	-	EXPRESSION TAG	UNP P37231

- Molecule 3 is (2S)-2-(2-{[1-(4-METHOXYBENZOYL)-2-METHYL-5-(TRIFLUOROMETHOXY)-1H-INDOL-3-YL]METHYL}PHENOXY)PROPANOIC ACID (three-letter code: 240) (formula: C<sub>28</sub>H<sub>24</sub>F<sub>3</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	28	3	1	6		
3	B	1	Total	C	F	N	O	0	0
			38	28	3	1	6		

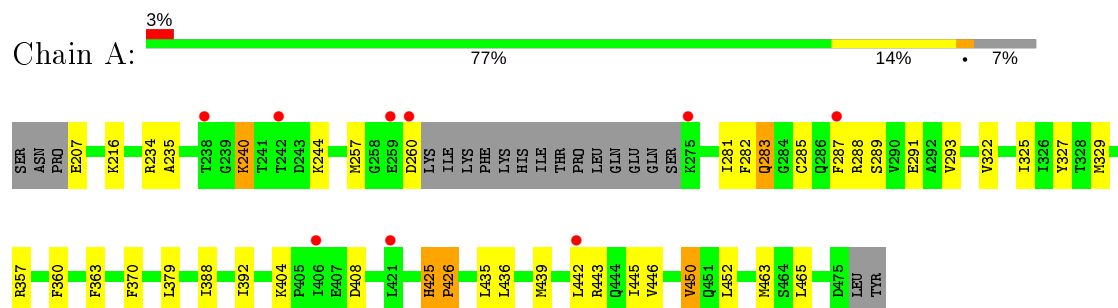
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	117	Total	O	0	0
			117	117		

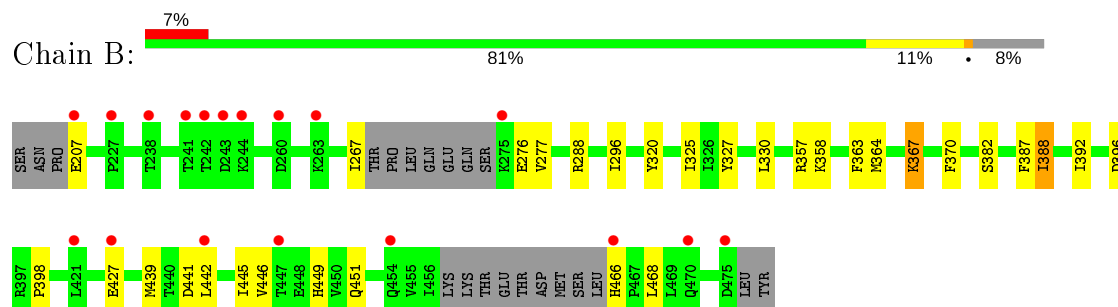
### 3 Residue-property plots [i](#)

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: Peroxisome Proliferator-Activated Receptor gamma



- Molecule 2: Peroxisome Proliferator-Activated Receptor gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.16 Å   63.94 Å   119.19 Å 90.00°   103.43°   90.00°	Depositor
Resolution (Å)	15.00 – 2.20 14.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.20) 99.2 (14.94-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.183   ,   0.230 0.181   ,   0.229	Depositor DCC
$R_{free}$ test set	1667 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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: CME, 240

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	0.43	1/2087 (0.0%)	0.56	1/2812 (0.0%)
2	B	0.39	0/2065	0.50	0/2787
All	All	0.41	1/4152 (0.0%)	0.53	1/5599 (0.0%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	ASP	C-O	6.00	1.34	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	HIS	C-N-CD	-5.38	108.76	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	425	HIS	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	2057	0	2114	24	0
2	B	2019	0	2052	23	0
3	A	38	0	23	9	0
3	B	38	0	23	7	0
4	A	127	0	0	0	0
4	B	117	0	0	0	0
All	All	4396	0	4212	53	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 (53) 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:327:TYR:HE1	3:A:5001:240:HAK	1.33	0.93
1:A:327:TYR:CE1	3:A:5001:240:HAK	2.20	0.74
1:A:235:ALA:HA	1:A:240:LYS:HG3	1.76	0.68
2:B:325[A]:ILE:HD11	2:B:392:ILE:CG1	2.26	0.66
2:B:357:ARG:HG2	2:B:358:LYS:H	1.60	0.64
2:B:363:PHE:HE1	2:B:449:HIS:HE1	1.45	0.64
2:B:288:ARG:CZ	3:B:7001:240:HAQ	2.31	0.59
2:B:325[B]:ILE:HD12	2:B:388[B]:ILE:HB	1.84	0.59
2:B:327:TYR:CE2	2:B:367:LYS:HG3	2.37	0.59
2:B:325[A]:ILE:HD11	2:B:392:ILE:HG13	1.85	0.59
3:B:7001:240:HAS	3:B:7001:240:OAE	2.04	0.58
2:B:441:ASP:O	2:B:445:ILE:HG13	2.04	0.57
1:A:329:MET:HB2	3:A:5001:240:HAA3	1.87	0.56
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.88	0.55
3:A:5001:240:HAS	3:A:5001:240:OAE	2.06	0.55
1:A:327:TYR:HE1	3:A:5001:240:CAK	2.14	0.54
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.89	0.53
1:A:404:LYS:HE2	1:A:408:ASP:OD1	2.10	0.52
1:A:288:ARG:CZ	3:A:5001:240:HAQ	2.41	0.51
2:B:296:ILE:HD11	3:B:7001:240:HAA2	1.92	0.51
2:B:296:ILE:HD11	3:B:7001:240:CAA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:5001:240:CBD	3:A:5001:240:HAB1	2.40	0.51
1:A:282:PHE:HA	1:A:285[A]:CME:SD	2.51	0.50
1:A:216:LYS:HE2	1:A:216:LYS:HA	1.92	0.50
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.41	0.50
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.94	0.50
2:B:276:GLU:OE1	2:B:357:ARG:HD3	2.12	0.49
3:A:5001:240:CAP	3:A:5001:240:HAB1	2.44	0.48
2:B:396:ASP:O	2:B:396:ASP:CG	2.52	0.48
1:A:287:PHE:CE2	1:A:291:GLU:OE1	2.67	0.47
2:B:325[A]:ILE:HD11	2:B:392:ILE:HG12	1.97	0.46
1:A:283:GLN:HE21	1:A:283:GLN:HA	1.80	0.46
3:A:5001:240:CAS	3:A:5001:240:OAE	2.62	0.46
1:A:281:ILE:HG22	1:A:285[B]:CME:HE2	1.97	0.46
3:B:7001:240:CBD	3:B:7001:240:HAB1	2.45	0.46
2:B:327:TYR:OH	2:B:367:LYS:HE2	2.16	0.46
1:A:325:ILE:HD13	1:A:388[A]:ILE:HG23	1.99	0.45
2:B:442:LEU:HA	2:B:445:ILE:HD12	1.99	0.44
1:A:360:PHE:HA	1:A:363:PHE:HD2	1.82	0.44
1:A:327:TYR:HE2	1:A:446:VAL:HG22	1.83	0.44
2:B:370:PHE:CD1	2:B:445:ILE:HD11	2.53	0.43
1:A:234[A]:ARG:HD3	1:A:234[A]:ARG:HA	1.86	0.43
2:B:320:TYR:CZ	2:B:398:PRO:HG2	2.54	0.43
2:B:327:TYR:CE2	2:B:445:ILE:CG2	3.02	0.43
2:B:327:TYR:CE2	2:B:445:ILE:HG21	2.54	0.43
1:A:289:SER:O	1:A:293:VAL:HG23	2.20	0.42
2:B:330:LEU:HD22	3:B:7001:240:HAJ	2.02	0.42
2:B:387:PHE:CE1	2:B:439:MET:HG2	2.54	0.42
1:A:436:LEU:O	1:A:439:MET:HG2	2.21	0.41
1:A:446:VAL:O	1:A:450:VAL:HG13	2.20	0.41
2:B:442:LEU:O	2:B:446:VAL:HG23	2.21	0.41
2:B:364:MET:HE1	3:B:7001:240:HAT	2.01	0.41
1:A:325:ILE:HD11	1:A:392:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/274 (93%)	253 (99%)	1 (0%)	1 (0%)	34	37
2	B	251/274 (92%)	243 (97%)	8 (3%)	0	100	100
All	All	506/548 (92%)	496 (98%)	9 (2%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	PRO

### 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	227/246 (92%)	214 (94%)	13 (6%)	20	24
2	B	221/247 (90%)	210 (95%)	11 (5%)	24	30
All	All	448/493 (91%)	424 (95%)	24 (5%)	23	26

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	240	LYS
1	A	244	LYS
1	A	257	MET
1	A	283	GLN
1	A	357	ARG
1	A	426	PRO
1	A	442	LEU
1	A	443	ARG
1	A	450	VAL
1	A	452	LEU

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Mol	Chain	Res	Type
1	A	463	MET
1	A	465	LEU
2	B	207	GLU
2	B	267	ILE
2	B	277	VAL
2	B	367	LYS
2	B	382	SER
2	B	388[A]	ILE
2	B	388[B]	ILE
2	B	427	GLU
2	B	451	GLN
2	B	466	HIS
2	B	468	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CME	A	285[B]	-	8,9,10	0.93	0	5,9,11	1.67	1 (20%)
1	CME	A	285[A]	-	8,9,10	0.78	0	5,9,11	1.67	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	285[B]	-	-	2/5/8/10	-
1	CME	A	285[A]	-	-	3/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	285[B]	CME	CE-SD-SG	3.30	118.66	103.45
1	A	285[A]	CME	CE-SD-SG	3.26	118.45	103.45

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	285[B]	CME	SD-CE-CZ-OH
1	A	285[A]	CME	SD-CE-CZ-OH
1	A	285[B]	CME	CE-SD-SG-CB
1	A	285[A]	CME	CZ-CE-SD-SG
1	A	285[A]	CME	CA-CB-SG-SD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285[B]	CME	1	0
1	A	285[A]	CME	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	240	A	5001	-	35,41,41	1.04	2 (5%)	46,60,60	2.72	13 (28%)
3	240	B	7001	-	35,41,41	0.99	1 (2%)	46,60,60	2.52	11 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	240	A	5001	-	-	7/19/27/27	0/4/4/4
3	240	B	7001	-	-	7/19/27/27	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5001	240	CBI-NBK	-3.83	1.34	1.39
3	B	7001	240	CBI-NBK	-3.63	1.34	1.39
3	A	5001	240	CAT-CBC	2.10	1.40	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	7001	240	CBD-CAZ-NBK	9.81	129.41	117.95
3	A	5001	240	CBD-CAZ-NBK	9.19	128.69	117.95
3	A	5001	240	CAP-CBD-CAZ	-7.09	104.97	120.26
3	A	5001	240	CAQ-CBD-CAZ	6.87	135.08	120.26
3	B	7001	240	CAP-CBD-CAZ	-5.89	107.55	120.26
3	B	7001	240	CAB-CBA-NBK	5.58	129.41	122.37
3	B	7001	240	CAQ-CBD-CAZ	5.47	132.06	120.26
3	A	5001	240	CAB-CBA-NBK	5.42	129.19	122.37
3	A	5001	240	OAE-CAZ-CBD	-5.17	110.16	120.23
3	B	7001	240	OAE-CAZ-CBD	-4.69	111.08	120.23
3	A	5001	240	CBL-OAX-CBC	3.84	130.69	118.01
3	B	7001	240	CAC-CBJ-CAY	-3.44	108.90	113.35
3	B	7001	240	CBF-OAW-CBJ	3.40	124.16	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5001	240	CAL-CAP-CBD	3.08	124.36	120.78
3	A	5001	240	CAM-CAQ-CBD	-2.97	117.32	120.78
3	B	7001	240	CBL-OAX-CBC	2.96	127.78	118.01
3	A	5001	240	CAQ-CAM-CBB	2.94	123.33	119.73
3	A	5001	240	CBF-OAW-CBJ	2.92	123.31	118.17
3	A	5001	240	CAC-CBJ-CAY	-2.85	109.67	113.35
3	A	5001	240	CAP-CAL-CBB	-2.78	116.33	119.73
3	B	7001	240	CAM-CAQ-CBD	-2.45	117.93	120.78
3	A	5001	240	OAW-CBF-CBE	2.35	120.17	116.04
3	B	7001	240	OAW-CBF-CBE	2.16	119.85	116.04
3	B	7001	240	CAT-CBH-CBG	-2.04	130.65	134.17

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	7001	240	FAG-CBL-OAX-CBC
3	B	7001	240	FAH-CBL-OAX-CBC
3	B	7001	240	CAM-CBB-OAV-CAA
3	B	7001	240	CAL-CBB-OAV-CAA
3	B	7001	240	FAI-CBL-OAX-CBC
3	A	5001	240	FAH-CBL-OAX-CBC
3	A	5001	240	CBG-CAU-CBE-CBF
3	B	7001	240	CBG-CAU-CBE-CBF
3	A	5001	240	CBG-CAU-CBE-CAN
3	B	7001	240	CBG-CAU-CBE-CAN
3	A	5001	240	FAG-CBL-OAX-CBC
3	A	5001	240	FAI-CBL-OAX-CBC
3	A	5001	240	CAR-CBC-OAX-CBL
3	A	5001	240	CAT-CBC-OAX-CBL

There are no ring outliers.

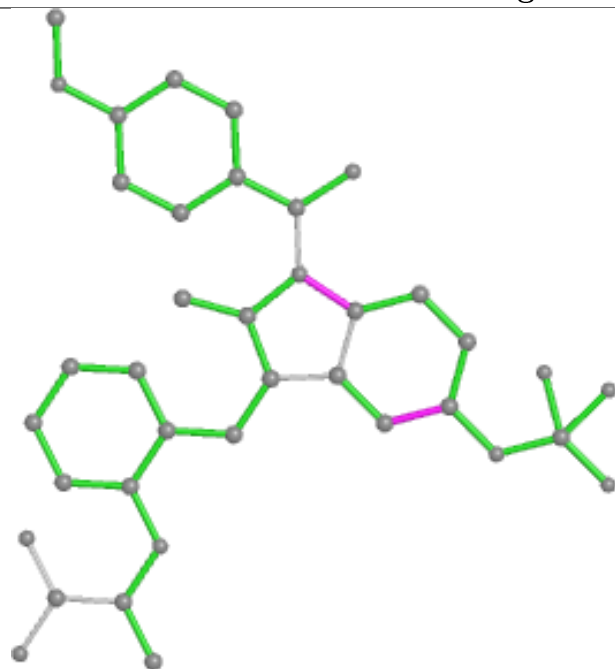
2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5001	240	9	0
3	B	7001	240	7	0

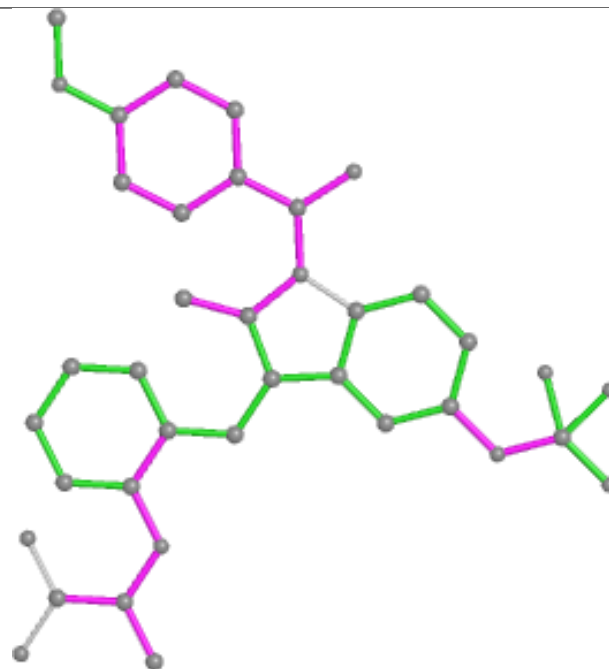
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

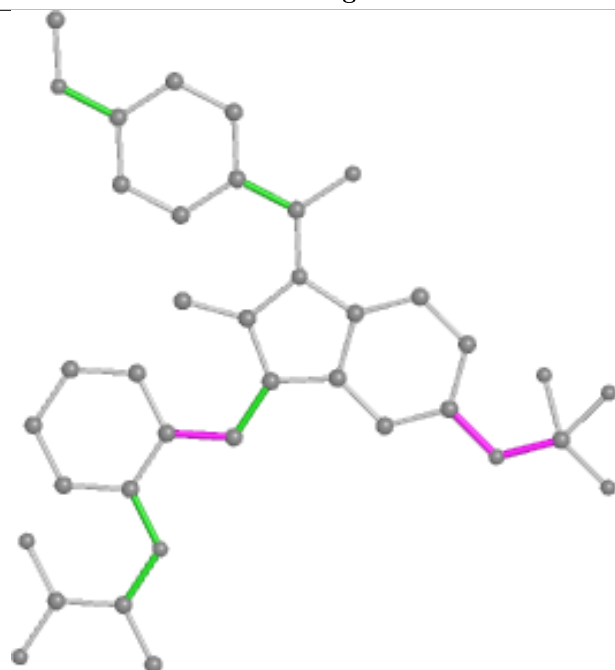
## Ligand 240 A 5001



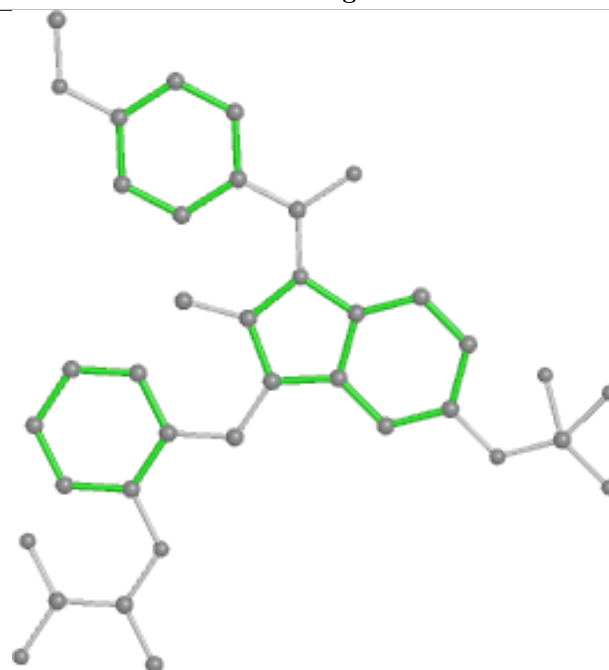
Bond lengths



Bond angles

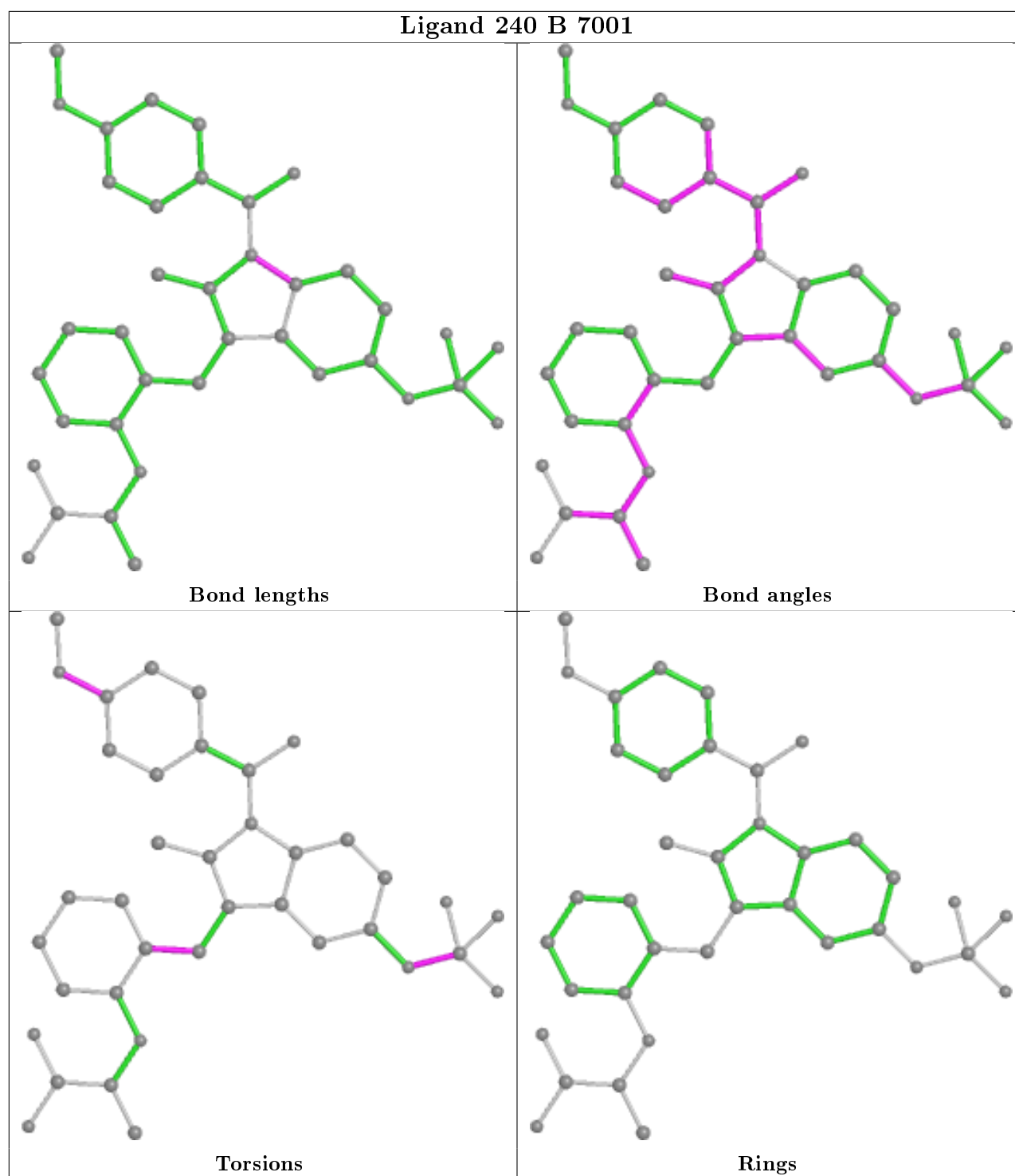


Torsions



Rings





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	254/274 (92%)	0.18	9 (3%) 44 42	7, 17, 27, 35	6 (2%)
2	B	253/274 (92%)	0.33	18 (7%) 16 14	11, 22, 38, 40	0
All	All	507/548 (92%)	0.25	27 (5%) 26 25	7, 19, 37, 40	6 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	242	THR	6.0
2	B	243	ASP	5.5
2	B	475	ASP	4.8
1	A	260	ASP	4.4
1	A	275	LYS	3.8
2	B	263	LYS	3.5
2	B	244	LYS	3.4
2	B	241	THR	3.2
2	B	275	LYS	2.9
2	B	454	GLN	2.9
1	A	242	THR	2.9
2	B	207	GLU	2.8
1	A	287	PHE	2.7
2	B	466	HIS	2.6
1	A	238	THR	2.5
1	A	442	LEU	2.5
2	B	470	GLN	2.4
2	B	260	ASP	2.3
2	B	447	THR	2.3
1	A	406	ILE	2.2
2	B	427	GLU	2.2
1	A	259	GLU	2.2
2	B	238	THR	2.1
2	B	227	PRO	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	421	LEU	2.1
1	A	421	LEU	2.1
2	B	442	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	A	285[B]	10/11	0.73	0.32	22,23,26,27	7
1	CME	A	285[A]	10/11	0.73	0.32	21,23,23,23	7

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

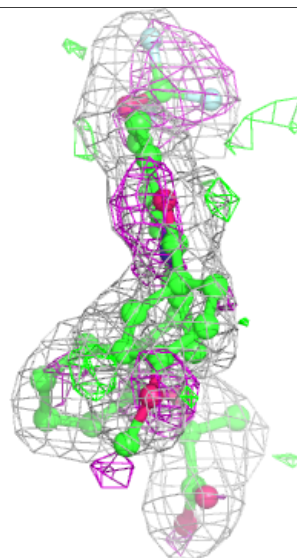
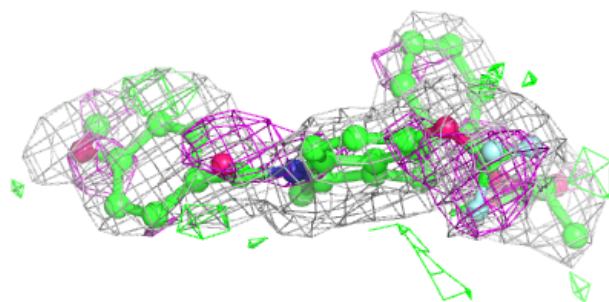
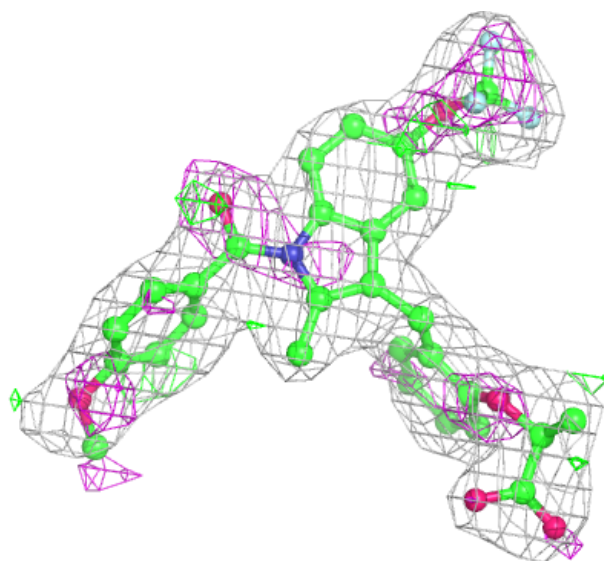
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	240	B	7001	38/38	0.85	0.24	38,41,46,47	0
3	240	A	5001	38/38	0.93	0.20	24,25,29,31	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.

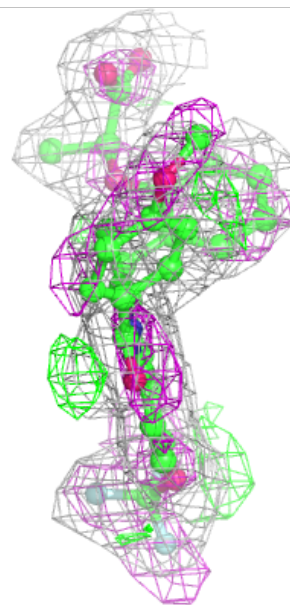
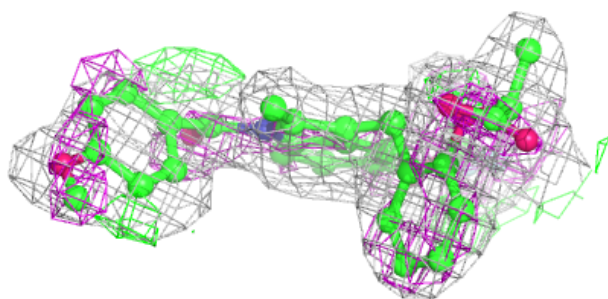
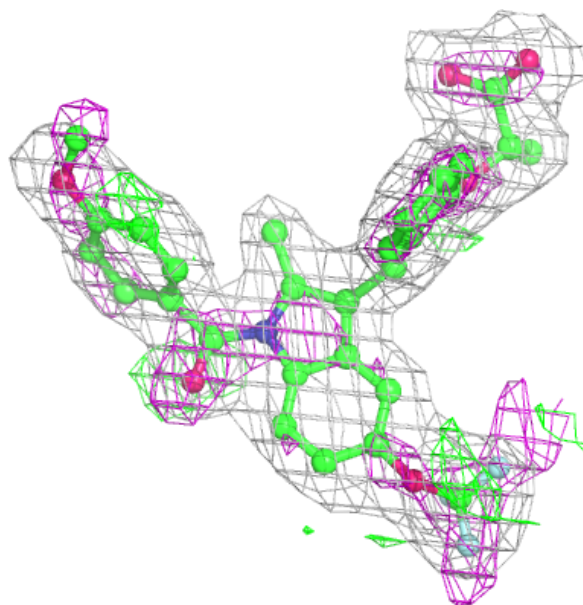
**Electron density around 240 B 7001:**

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



**Electron density around 240 A 5001:**

$2mF_o-DF_c$  (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.