



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:32 PM UTC

PDB ID : 2Q59 / pdb_00002q59
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

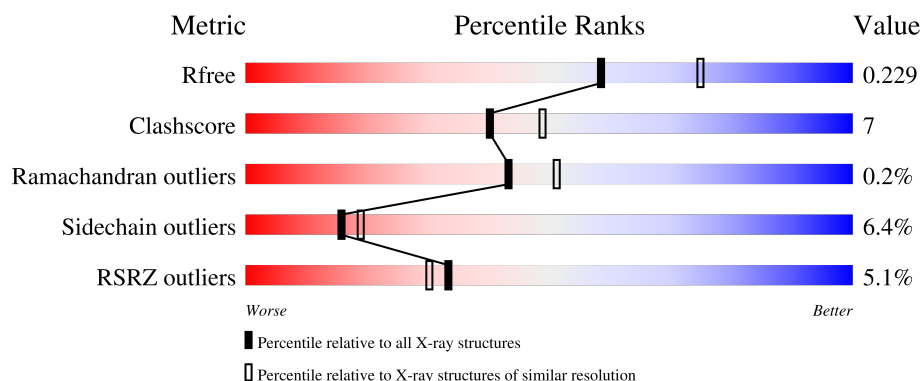
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	274	
2	B	274	

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

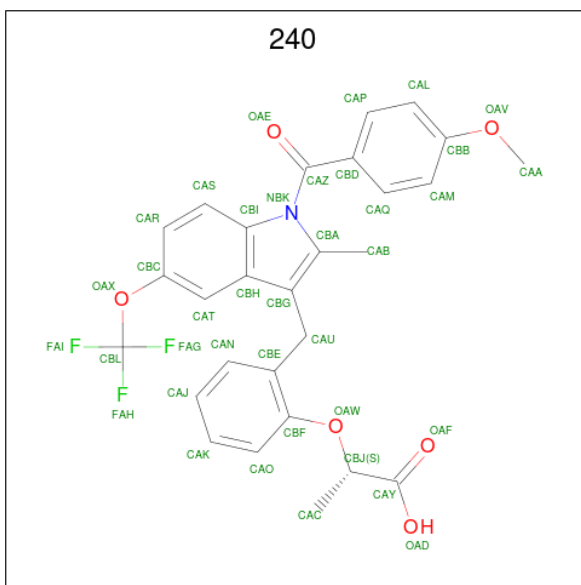
- Molecule 2 is a protein called Peroxisome Proliferator-Activated Receptor gamma.

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 (CCD ID: 240) (formula: C₂₈H₂₄F₃NO₆).



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

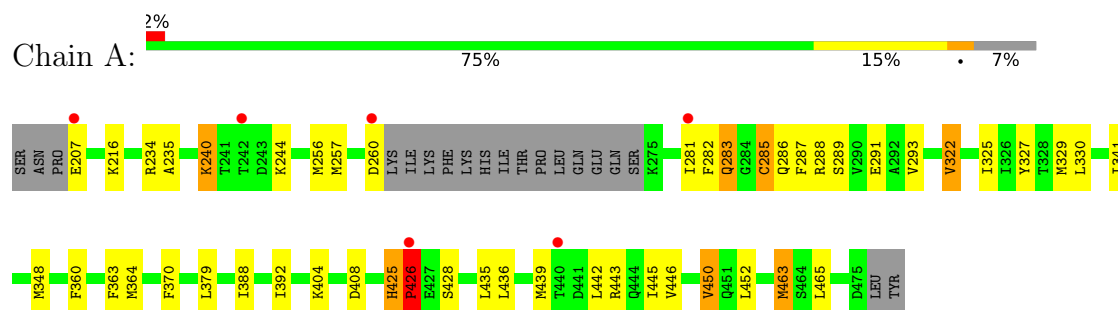
- Molecule 4 is water.

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

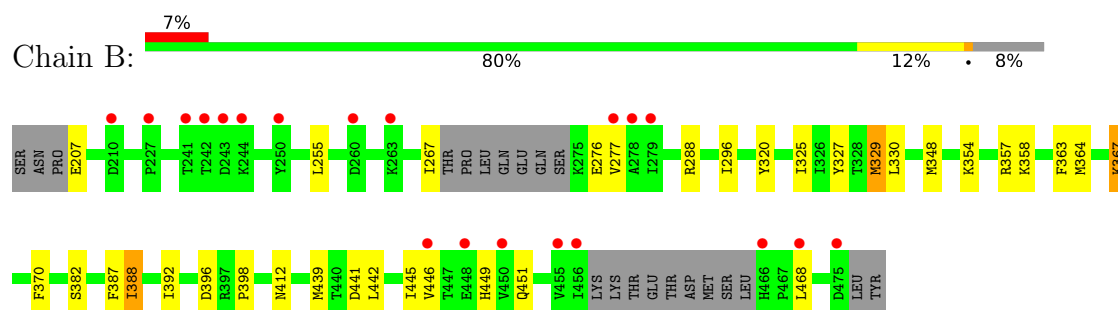
3 Residue-property plots [i](#)

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: 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, α , β , γ	89.16Å 63.94Å 119.19Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.20) 98.8 (15.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.20Å)	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4396	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.55	1/2087 (0.0%)	0.98	4/2812 (0.1%)
2	B	0.50	0/2065	0.85	0/2787
All	All	0.52	1/4152 (0.0%)	0.92	4/5599 (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	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	5.60	1.34	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	HIS	CA-C-N	17.84	142.13	119.84
1	A	425	HIS	C-N-CA	17.84	142.13	119.84
1	A	428	SER	N-CA-C	5.68	117.47	111.28
1	A	426	PRO	CA-CB-CG	-5.11	94.80	104.50

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	27	0
2	B	2019	0	2052	24	0
3	A	38	0	23	7	0
3	B	38	0	23	6	0
4	A	127	0	0	0	0
4	B	117	0	0	0	0
All	All	4396	0	4212	55	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 7.

All (55) 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:OAE	3:B:7001:240:HAS	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:OAE	3:A:5001:240:HAS	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:7001:240:CAP	3:B:7001:240:HAB1	2.39	0.52
2:B:396:ASP:CG	2:B:396:ASP:O	2.52	0.52
1:A:404:LYS:HE2	1:A:408:ASP:OD1	2.10	0.52
2:B:363:PHE:CE2	2:B:364:MET:HE2	2.45	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
1:A:282:PHE:HA	1:A:285[A]:CME:SD	2.51	0.50
1:A:216:LYS:HA	1:A:216:LYS:HE2	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
1:A:463:MET:HB3	1:A:463:MET:HE2	1.80	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:OAE	3:A:5001:240:CAS	2.62	0.46
1:A:281:ILE:HG22	1:A:285[B]:CME:HE2	1.97	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
2:B:329:MET:HE2	2:B:329:MET:HA	1.99	0.44
1:A:327:TYR:HE2	1:A:446:VAL:HG22	1.83	0.44
1:A:360:PHE:HA	1:A:363:PHE:HD2	1.82	0.44
1:A:341:ILE:HD13	1:A:348:MET:HE3	2.00	0.43
2:B:370:PHE:CD1	2:B:445:ILE:HD11	2.53	0.43
1:A:234[A]:ARG:HA	1:A:234[A]:ARG:HD3	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
1:A:330:LEU:HD21	1:A:364:MET:HE1	2.03	0.40
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%)	30	34
2	B	251/274 (92%)	243 (97%)	8 (3%)	0	100	100
All	All	506/548 (92%)	496 (98%)	9 (2%)	1 (0%)	43	51

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%)	212 (93%)	15 (7%)	15	18
2	B	221/247 (90%)	207 (94%)	14 (6%)	16	19
All	All	448/493 (91%)	419 (94%)	29 (6%)	16	18

All (29) 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	256	MET
1	A	257	MET

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Mol	Chain	Res	Type
1	A	283	GLN
1	A	286	GLN
1	A	322	VAL
1	A	426	PRO
1	A	442	LEU
1	A	443	ARG
1	A	450	VAL
1	A	452	LEU
1	A	463	MET
1	A	465	LEU
2	B	207	GLU
2	B	255	LEU
2	B	267	ILE
2	B	277	VAL
2	B	329	MET
2	B	348	MET
2	B	354	LYS
2	B	367	LYS
2	B	382	SER
2	B	388[A]	ILE
2	B	388[B]	ILE
2	B	412	ASN
2	B	451	GLN
2	B	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
2	B	266	HIS
2	B	286	GLN
2	B	345	GLN
2	B	449	HIS
2	B	451	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	0.94	0	6,9,11	1.60	1 (16%)
1	CME	A	285[A]	-	8,9,10	0.79	0	6,9,11	1.63	1 (16%)

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]	-	-	3/5/8/10	-
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(°)	Ideal(°)
1	A	285[B]	CME	CE-SD-SG	3.46	118.66	103.46
1	A	285[A]	CME	CE-SD-SG	3.42	118.45	103.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	285[A]	CME	SD-CE-CZ-OH
1	A	285[B]	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
1	A	285[B]	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 oligosaccharides 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	-	41,41,41	1.21	3 (7%)	60,60,60	2.39	15 (25%)
3	240	B	7001	-	41,41,41	1.19	4 (9%)	60,60,60	2.20	14 (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	-	-	8/27/27/27	0/4/4/4
3	240	B	7001	-	-	7/27/27/27	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5001	240	CBI-NBK	-4.42	1.34	1.41
3	B	7001	240	CBI-NBK	-4.27	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5001	240	CBA-NBK	-2.51	1.35	1.40
3	B	7001	240	CBA-NBK	-2.46	1.35	1.40
3	B	7001	240	CBA-CBG	2.34	1.40	1.36
3	A	5001	240	CBA-CBG	2.27	1.40	1.36
3	B	7001	240	CBH-CBG	-2.19	1.40	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5001	240	CBI-NBK-CBA	7.70	114.08	107.80
3	B	7001	240	CBI-NBK-CBA	7.48	113.90	107.80
3	B	7001	240	CBD-CAZ-NBK	5.98	129.41	117.92
3	A	5001	240	CAP-CBD-CAZ	-5.97	104.97	120.28
3	A	5001	240	CAQ-CBD-CAZ	5.77	135.08	120.28
3	A	5001	240	CBD-CAZ-NBK	5.61	128.69	117.92
3	A	5001	240	OAE-CAZ-CBD	-5.11	110.16	120.29
3	B	7001	240	CAP-CBD-CAZ	-4.96	107.55	120.28
3	B	7001	240	CAB-CBA-NBK	4.90	129.41	122.07
3	A	5001	240	CAB-CBA-NBK	4.75	129.19	122.07
3	B	7001	240	OAE-CAZ-CBD	-4.64	111.08	120.29
3	B	7001	240	CAQ-CBD-CAZ	4.59	132.06	120.28
3	B	7001	240	CBG-CBA-NBK	-4.06	104.99	108.85
3	A	5001	240	CBL-OAX-CBC	4.02	130.69	118.14
3	A	5001	240	CBG-CBA-NBK	-3.94	105.11	108.85
3	A	5001	240	CAL-CAP-CBD	3.33	124.36	120.80
3	A	5001	240	CAM-CAQ-CBD	-3.26	117.32	120.80
3	B	7001	240	CBI-NBK-CAZ	-3.22	117.34	125.02
3	A	5001	240	CAQ-CAM-CBB	3.15	123.33	119.73
3	B	7001	240	CBL-OAX-CBC	3.09	127.78	118.14
3	A	5001	240	CAP-CAL-CBB	-2.97	116.33	119.73
3	A	5001	240	CBI-NBK-CAZ	-2.89	118.12	125.02
3	B	7001	240	CBF-OAW-CBJ	2.80	124.16	118.01
3	B	7001	240	CAM-CAQ-CBD	-2.69	117.93	120.80
3	A	5001	240	CBF-OAW-CBJ	2.41	123.31	118.01
3	A	5001	240	OAW-CBF-CBE	2.41	120.17	115.99
3	B	7001	240	OAW-CBF-CBE	2.22	119.85	115.99
3	B	7001	240	CBH-CBI-NBK	-2.15	105.29	107.69
3	B	7001	240	CAL-CAP-CBD	2.04	122.98	120.80

There are no chirality outliers.

All (15) 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	OAE-CAZ-NBK-CBA
3	B	7001	240	OAE-CAZ-NBK-CBA
3	A	5001	240	FAH-CBL-OAX-CBC
3	A	5001	240	FAG-CBL-OAX-CBC
3	A	5001	240	FAI-CBL-OAX-CBC
3	A	5001	240	CBG-CAU-CBE-CBF
3	A	5001	240	OAF-CAY-CBJ-OAW
3	A	5001	240	CAR-CBC-OAX-CBL
3	A	5001	240	CAT-CBC-OAX-CBL
3	B	7001	240	CBG-CAU-CBE-CBF

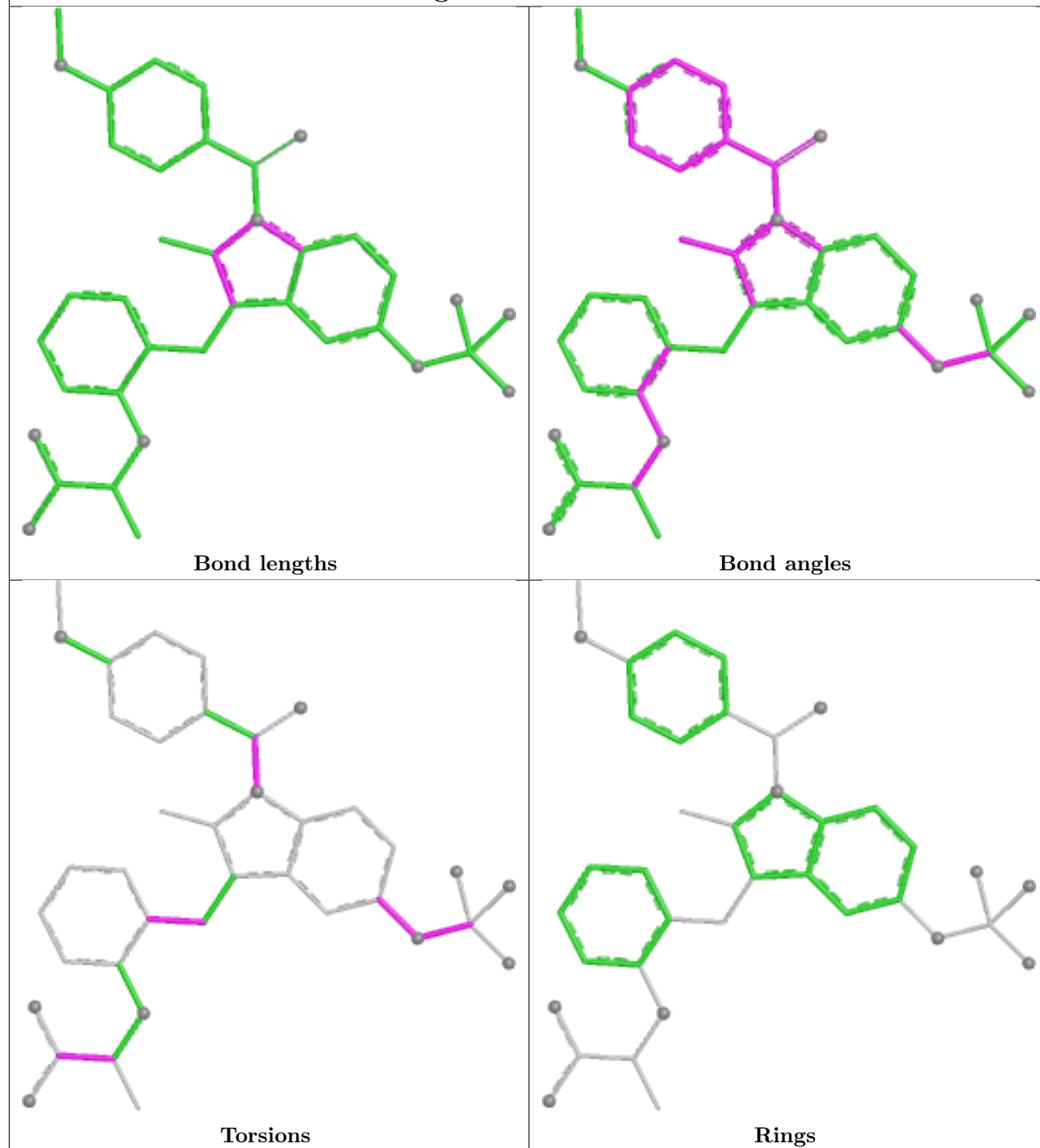
There are no ring outliers.

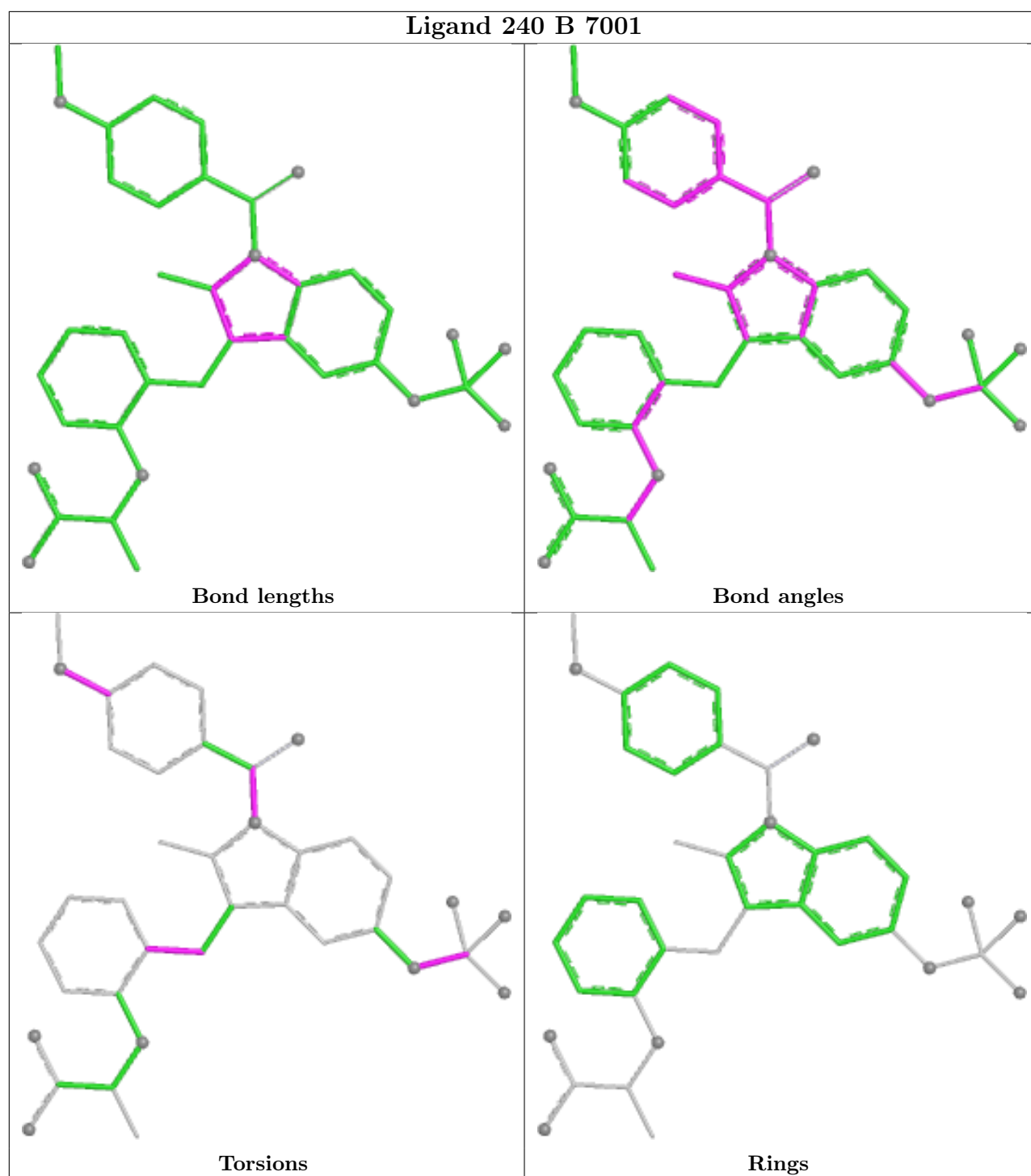
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5001	240	7	0
3	B	7001	240	6	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





5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	254/274 (92%)	-0.07	6 (2%) 59 56	6, 17, 27, 35	11 (4%)
2	B	253/274 (92%)	0.32	20 (7%) 18 16	8, 22, 38, 40	4 (1%)
All	All	507/548 (92%)	0.12	26 (5%) 33 30	6, 19, 37, 40	15 (2%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	ASP	5.3
2	B	243	ASP	4.0
2	B	475	ASP	3.9
2	B	456	ILE	2.8
2	B	446	VAL	2.7
2	B	227	PRO	2.7
2	B	263	LYS	2.6
2	B	277	VAL	2.5
2	B	260	ASP	2.5
2	B	278	ALA	2.4
2	B	450	VAL	2.4
1	A	281	ILE	2.3
2	B	468	LEU	2.3
2	B	242	THR	2.3
2	B	466	HIS	2.3
2	B	279	ILE	2.3
2	B	241	THR	2.2
2	B	448	GLU	2.2
2	B	244	LYS	2.2
1	A	242	THR	2.2
1	A	440	THR	2.1
2	B	250	TYR	2.1
1	A	207	GLU	2.1
2	B	210	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	455	VAL	2.1
1	A	426	PRO	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CME	A	285[A]	10/11	0.81	0.13	21,23,23,23	7
1	CME	A	285[B]	10/11	0.81	0.13	22,23,26,27	7

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

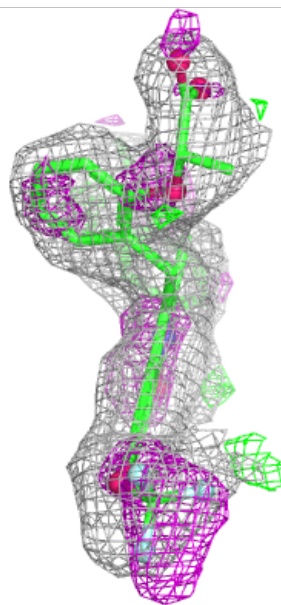
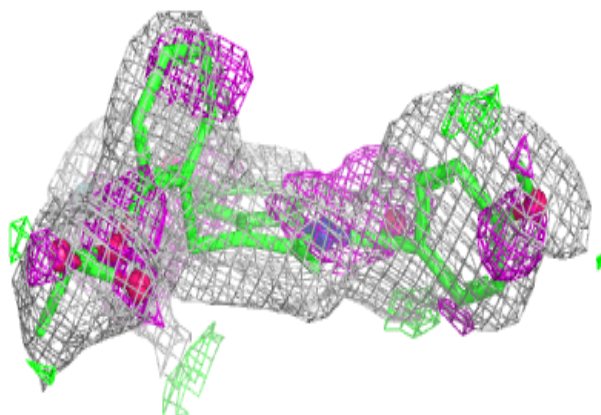
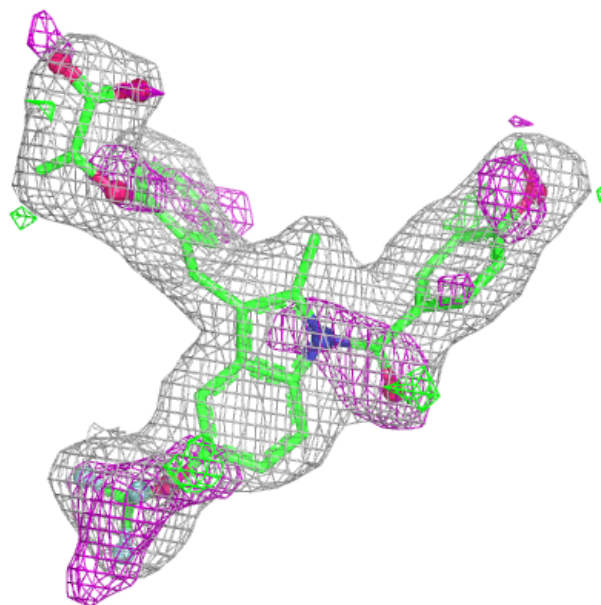
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	240	B	7001	38/38	0.76	0.12	38,41,46,47	0
3	240	A	5001	38/38	0.87	0.09	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.

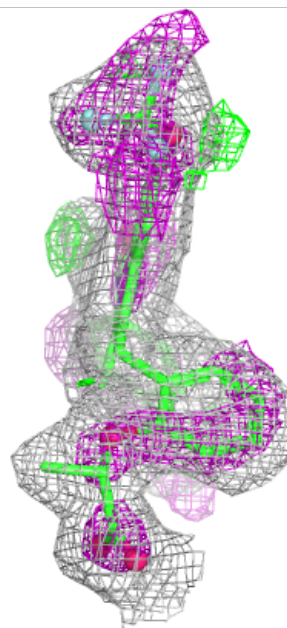
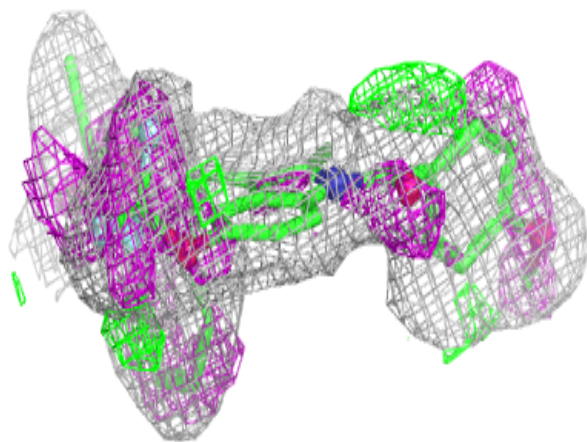
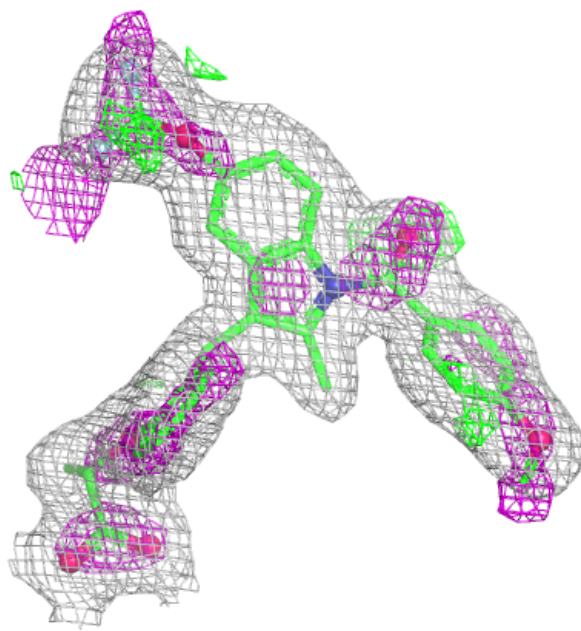
Electron density around 240 B 7001:

$2mF_o-DF_c$ (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.