



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:42 PM UTC

PDB ID : 7MSA / pdb\_00007msa  
Title : GDC-9545 in complex with estrogen receptor alpha  
Authors : Kiefer, J.R.; Vinogradova, M.; Liang, J.; Zbieg, J.R.; Wang, X.; Ortwine, D.F.  
Deposited on : 2021-05-10  
Resolution : 2.24 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>.

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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)  
Xtrriage (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

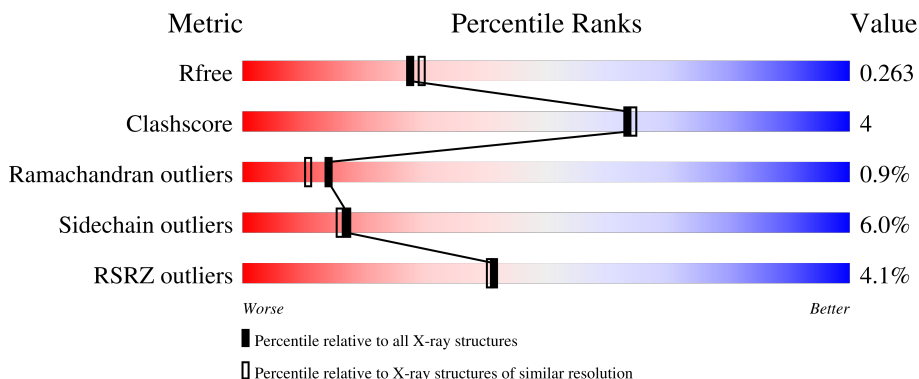
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	280	5% (Poor fit) 64% (0 outliers) 14% (1 outlier) 17% (2 outliers) 20% (Not modelled)
1	B	280	2% (Poor fit) 69% (0 outliers) 11% (1 outlier) 18% (2 outliers) 19% (Not modelled)
1	C	280	4% (Poor fit) 70% (0 outliers) 9% (1 outlier) 21% (2 outliers) 20% (Not modelled)
1	D	280	2% (Poor fit) 74% (0 outliers) 10% (1 outlier) 16% (2 outliers) 16% (Not modelled)

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7214 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	234	1800	1153	303	327	17	0	0	0
1	A	225	1684	1071	289	307	17	0	1	0
1	C	225	1744	1118	300	308	18	0	1	0
1	B	228	1767	1136	301	314	16	0	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	274	MET	-	expression tag	UNP P03372
D	275	HIS	-	expression tag	UNP P03372
D	276	HIS	-	expression tag	UNP P03372
D	277	HIS	-	expression tag	UNP P03372
D	278	HIS	-	expression tag	UNP P03372
D	279	HIS	-	expression tag	UNP P03372
D	280	HIS	-	expression tag	UNP P03372
D	281	SER	-	expression tag	UNP P03372
D	282	SER	-	expression tag	UNP P03372
D	283	GLY	-	expression tag	UNP P03372
D	284	VAL	-	expression tag	UNP P03372
D	285	ASP	-	expression tag	UNP P03372
D	286	LEU	-	expression tag	UNP P03372
D	287	GLY	-	expression tag	UNP P03372
D	288	THR	-	expression tag	UNP P03372
D	289	GLU	-	expression tag	UNP P03372
D	290	ASN	-	expression tag	UNP P03372
D	291	LEU	-	expression tag	UNP P03372
D	292	TYR	-	expression tag	UNP P03372
D	293	PHE	-	expression tag	UNP P03372
D	294	GLN	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
D	295	SER	-	expression tag	UNP P03372
D	296	ASN	-	expression tag	UNP P03372
D	297	ALA	-	expression tag	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372
A	274	MET	-	expression tag	UNP P03372
A	275	HIS	-	expression tag	UNP P03372
A	276	HIS	-	expression tag	UNP P03372
A	277	HIS	-	expression tag	UNP P03372
A	278	HIS	-	expression tag	UNP P03372
A	279	HIS	-	expression tag	UNP P03372
A	280	HIS	-	expression tag	UNP P03372
A	281	SER	-	expression tag	UNP P03372
A	282	SER	-	expression tag	UNP P03372
A	283	GLY	-	expression tag	UNP P03372
A	284	VAL	-	expression tag	UNP P03372
A	285	ASP	-	expression tag	UNP P03372
A	286	LEU	-	expression tag	UNP P03372
A	287	GLY	-	expression tag	UNP P03372
A	288	THR	-	expression tag	UNP P03372
A	289	GLU	-	expression tag	UNP P03372
A	290	ASN	-	expression tag	UNP P03372
A	291	LEU	-	expression tag	UNP P03372
A	292	TYR	-	expression tag	UNP P03372
A	293	PHE	-	expression tag	UNP P03372
A	294	GLN	-	expression tag	UNP P03372
A	295	SER	-	expression tag	UNP P03372
A	296	ASN	-	expression tag	UNP P03372
A	297	ALA	-	expression tag	UNP P03372
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
C	274	MET	-	expression tag	UNP P03372
C	275	HIS	-	expression tag	UNP P03372
C	276	HIS	-	expression tag	UNP P03372
C	277	HIS	-	expression tag	UNP P03372
C	278	HIS	-	expression tag	UNP P03372
C	279	HIS	-	expression tag	UNP P03372
C	280	HIS	-	expression tag	UNP P03372
C	281	SER	-	expression tag	UNP P03372
C	282	SER	-	expression tag	UNP P03372
C	283	GLY	-	expression tag	UNP P03372
C	284	VAL	-	expression tag	UNP P03372

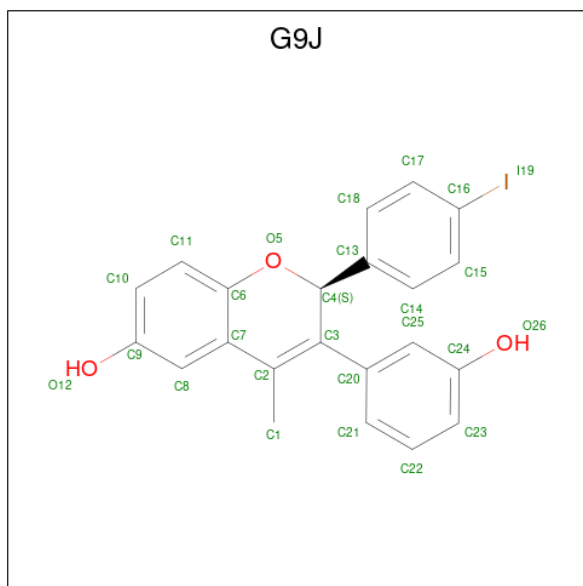
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Chain	Residue	Modelled	Actual	Comment	Reference
C	285	ASP	-	expression tag	UNP P03372
C	286	LEU	-	expression tag	UNP P03372
C	287	GLY	-	expression tag	UNP P03372
C	288	THR	-	expression tag	UNP P03372
C	289	GLU	-	expression tag	UNP P03372
C	290	ASN	-	expression tag	UNP P03372
C	291	LEU	-	expression tag	UNP P03372
C	292	TYR	-	expression tag	UNP P03372
C	293	PHE	-	expression tag	UNP P03372
C	294	GLN	-	expression tag	UNP P03372
C	295	SER	-	expression tag	UNP P03372
C	296	ASN	-	expression tag	UNP P03372
C	297	ALA	-	expression tag	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
B	274	MET	-	expression tag	UNP P03372
B	275	HIS	-	expression tag	UNP P03372
B	276	HIS	-	expression tag	UNP P03372
B	277	HIS	-	expression tag	UNP P03372
B	278	HIS	-	expression tag	UNP P03372
B	279	HIS	-	expression tag	UNP P03372
B	280	HIS	-	expression tag	UNP P03372
B	281	SER	-	expression tag	UNP P03372
B	282	SER	-	expression tag	UNP P03372
B	283	GLY	-	expression tag	UNP P03372
B	284	VAL	-	expression tag	UNP P03372
B	285	ASP	-	expression tag	UNP P03372
B	286	LEU	-	expression tag	UNP P03372
B	287	GLY	-	expression tag	UNP P03372
B	288	THR	-	expression tag	UNP P03372
B	289	GLU	-	expression tag	UNP P03372
B	290	ASN	-	expression tag	UNP P03372
B	291	LEU	-	expression tag	UNP P03372
B	292	TYR	-	expression tag	UNP P03372
B	293	PHE	-	expression tag	UNP P03372
B	294	GLN	-	expression tag	UNP P03372
B	295	SER	-	expression tag	UNP P03372
B	296	ASN	-	expression tag	UNP P03372
B	297	ALA	-	expression tag	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372

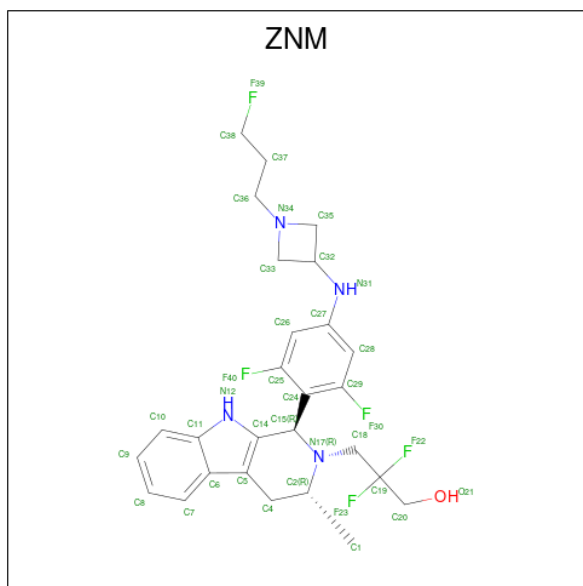
- Molecule 2 is (2S)-3-(3-hydroxyphenyl)-2-(4-iodophenyl)-4-methyl-2H-1-benzopyran-6-ol

(CCD ID: G9J) (formula: C<sub>22</sub>H<sub>17</sub>IO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	D	1	Total	C	I	O	0	0
			26	22	1	3		
2	B	1	Total	C	I	O	0	0
			26	22	1	3		

- Molecule 3 is 3-[(1R,3R)-1-(2,6-difluoro-4-{[1-(3-fluoropropyl)azetid-3-yl]amino}phenyl)-3-methyl-1,3,4,9-tetrahydro-2H-pyrido[3,4-b]indol-2-yl]-2,2-difluoropropan-1-ol (CCD ID: ZNM) (formula: C<sub>27</sub>H<sub>31</sub>F<sub>5</sub>N<sub>4</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			37	27	5	4	1		
3	C	1	Total	C	F	N	O	0	0
			37	27	5	4	1		

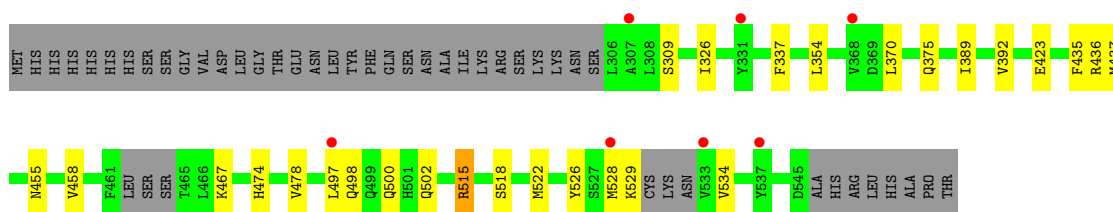
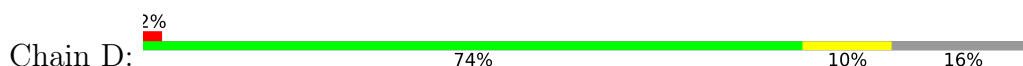
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	19	Total	O	0	2
			21	21		
4	A	27	Total	O	0	0
			27	27		
4	C	22	Total	O	0	1
			23	23		
4	B	22	Total	O	0	0
			22	22		

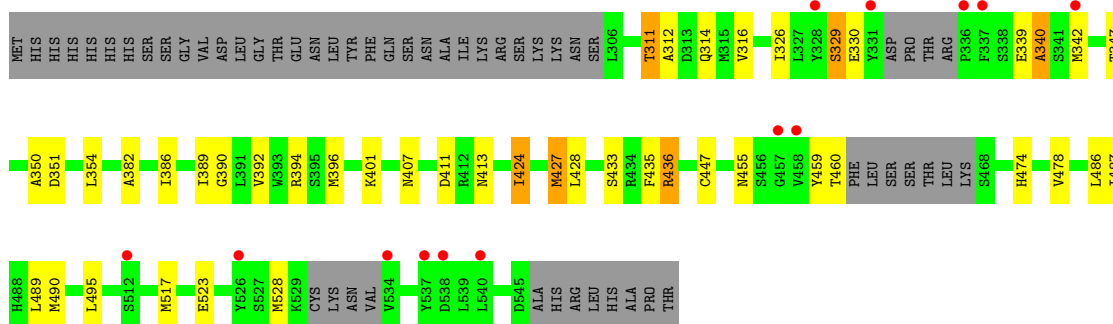
### 3 Residue-property plots [i](#)

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.

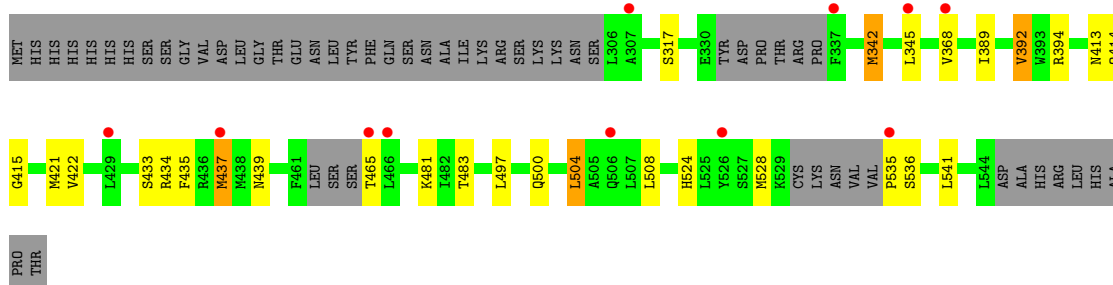
- Molecule 1: Estrogen receptor



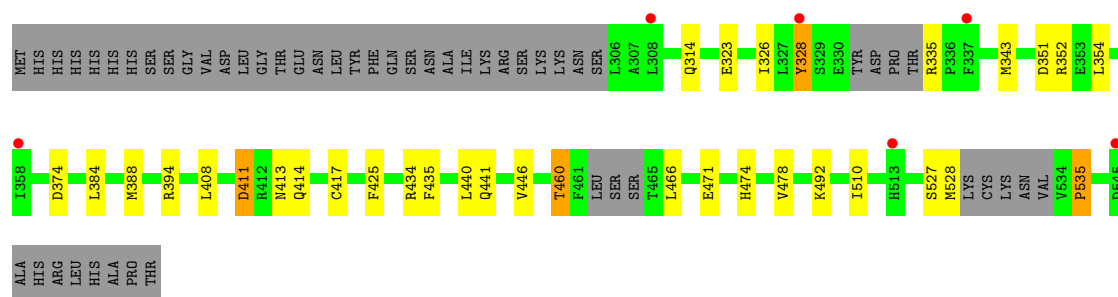
- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.08Å 58.94Å 93.55Å 86.43° 75.08° 63.25°	Depositor
Resolution (Å)	33.22 – 2.24 33.22 – 2.24	Depositor EDS
% Data completeness (in resolution range)	81.7 (33.22-2.24) 94.3 (33.22-2.24)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.194 , 0.246 0.210 , 0.263	Depositor DCC
$R_{free}$ test set	2274 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.098 for h,h-k,h-l	Xtriage
Reported twinning fraction	0.890 for H, K, L 0.110 for H, H-K, H-L	Depositor
Outliers	0 of 45098 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.21% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZNM, G9J

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.07	0/1710	1.61	4/2316 (0.2%)
1	B	1.03	1/1798 (0.1%)	1.55	2/2435 (0.1%)
1	C	1.04	0/1771	1.55	3/2391 (0.1%)
1	D	1.01	0/1832	1.55	2/2485 (0.1%)
All	All	1.04	1/7111 (0.0%)	1.56	11/9627 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	TYR	C-N	6.89	1.43	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	GLN	CA-C-N	5.59	126.30	120.03
1	B	441	GLN	C-N-CA	5.59	126.30	120.03
1	A	447	CYS	CA-C-N	5.50	127.65	120.28
1	A	447	CYS	C-N-CA	5.50	127.65	120.28
1	C	483	THR	CA-CB-OG1	-5.41	101.48	109.60
1	A	436	ARG	CA-C-N	5.18	127.74	120.28
1	A	436	ARG	C-N-CA	5.18	127.74	120.28
1	D	436	ARG	CA-C-N	5.13	127.40	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	436	ARG	C-N-CA	5.13	127.40	120.38
1	C	504	LEU	CA-C-N	5.04	127.00	120.44
1	C	504	LEU	C-N-CA	5.04	127.00	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	328	TYR	Mainchain

## 5.2 Too-close contacts [i](#)

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	1684	0	1629	23	0
1	B	1767	0	1765	13	0
1	C	1744	0	1765	7	0
1	D	1800	0	1781	13	0
2	B	26	0	0	0	0
2	D	26	0	0	0	0
3	A	37	0	0	0	0
3	C	37	0	0	1	0
4	A	27	0	0	0	0
4	B	22	0	0	0	0
4	C	23	0	0	0	0
4	D	21	0	0	2	0
All	All	7214	0	6940	56	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 4.

All (56) 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:459:TYR:O	1:A:460:THR:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:GLN:O	1:D:502:GLN:HG3	1.97	0.64
1:D:370:LEU:O	1:D:375:GLN:NE2	2.30	0.60
1:B:374:ASP:OD2	1:B:471:GLU:OE1	2.21	0.57
1:B:474:HIS:O	1:B:478:VAL:HG23	2.05	0.57
1:B:384:LEU:O	1:B:388:MET:HG3	2.05	0.56
1:B:414:GLN:O	1:B:417:CYS:SG	2.63	0.56
1:D:474:HIS:O	1:D:478:VAL:HG23	2.09	0.53
1:A:487:ILE:HA	1:A:490:MET:HE3	1.91	0.52
1:A:392:VAL:HG12	1:A:435:PHE:CD2	2.46	0.51
1:D:518:SER:OG	4:D:706[B]:HOH:O	2.20	0.50
1:B:351:ASP:HA	1:B:354:LEU:HD12	1.94	0.50
1:A:351:ASP:HA	1:A:354:LEU:HD12	1.92	0.50
1:D:528:MET:O	1:D:529:LYS:CB	2.60	0.49
1:A:311:THR:HG23	1:A:314:GLN:H	1.76	0.49
1:A:390:GLY:O	1:A:394:ARG:HG3	2.12	0.49
1:A:455:ASN:CG	1:A:455:ASN:O	2.56	0.48
1:B:323:GLU:OE1	1:B:446:VAL:HG12	2.13	0.48
1:B:435:PHE:CE1	1:B:510:ILE:HG21	2.48	0.48
1:D:522:MET:O	1:D:526:TYR:HD2	1.97	0.48
1:B:326:ILE:HD12	1:B:394:ARG:HD3	1.97	0.47
1:D:392:VAL:HG23	1:D:435:PHE:CE2	2.51	0.46
1:B:435:PHE:CD1	1:B:440:LEU:HD22	2.51	0.46
1:A:487:ILE:HA	1:A:490:MET:CE	2.45	0.46
1:A:311:THR:OG1	1:A:312:ALA:N	2.49	0.46
1:C:434:ARG:HA	1:C:437:MET:HG2	1.98	0.45
1:C:342:MET:HE1	1:C:414:GLN:O	2.17	0.45
1:B:411:ASP:OD1	1:B:411:ASP:C	2.59	0.45
1:A:490:MET:HB3	1:A:495:LEU:HD22	1.99	0.45
1:A:427:MET:HE3	1:A:517:MET:HA	1.98	0.44
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.99	0.44
1:D:515:ARG:NH1	4:D:707:HOH:O	2.50	0.43
1:D:437:MET:HE2	1:D:437:MET:HB2	1.92	0.43
1:A:339:GLU:O	1:A:340:ALA:CB	2.68	0.42
1:B:343:MET:HE2	1:B:528:MET:HE3	2.01	0.42
1:D:497:LEU:O	1:D:500:GLN:HB2	2.20	0.42
1:A:329:SER:OG	1:A:330:GLU:N	2.48	0.42
1:C:415:GLY:O	1:C:421:MET:HB3	2.20	0.42
1:C:504:LEU:O	1:C:508:LEU:HG	2.20	0.42
1:D:389:ILE:HA	1:D:392:VAL:HG22	2.00	0.42
1:A:347:THR:O	1:A:350:ALA:HB3	2.20	0.42
1:C:392:VAL:CG1	1:C:435:PHE:CD2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ALA:O	1:A:386:ILE:HG13	2.20	0.41
1:D:522:MET:O	1:D:526:TYR:CD2	2.72	0.41
1:A:486:LEU:O	1:A:490:MET:HG3	2.20	0.41
1:B:411:ASP:OD1	1:B:413:ASN:N	2.51	0.41
1:A:329:SER:HB3	1:A:407:ASN:OD1	2.21	0.41
1:A:474:HIS:O	1:A:478:VAL:HG23	2.21	0.41
1:A:487:ILE:HD13	1:A:490:MET:CE	2.51	0.41
1:B:408:LEU:HD12	1:B:408:LEU:HA	1.95	0.41
1:D:455:ASN:O	1:D:458:VAL:HG12	2.21	0.41
1:A:350:ALA:O	1:A:354:LEU:HG	2.21	0.41
1:C:524:HIS:HD1	3:C:601:ZNM:C20	2.34	0.41
1:A:396:MET:O	1:A:436:ARG:NE	2.46	0.40
1:C:497:LEU:O	1:C:500:GLN:HB2	2.21	0.40
1:A:424:ILE:O	1:A:428:LEU:HG	2.22	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	217/280 (78%)	205 (94%)	10 (5%)	2 (1%)	14	11
1	B	220/280 (79%)	210 (96%)	7 (3%)	3 (1%)	9	5
1	C	218/280 (78%)	213 (98%)	3 (1%)	2 (1%)	14	11
1	D	228/280 (81%)	224 (98%)	3 (1%)	1 (0%)	30	30
All	All	883/1120 (79%)	852 (96%)	23 (3%)	8 (1%)	14	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ALA

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Mol	Chain	Res	Type
1	C	439	ASN
1	B	460	THR
1	B	466	LEU
1	D	467	LYS
1	A	329	SER
1	C	536	SER
1	B	535	PRO

### 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	173/252 (69%)	161 (93%)	12 (7%)	14	11
1	B	190/252 (75%)	180 (95%)	10 (5%)	20	20
1	C	188/252 (75%)	172 (92%)	16 (8%)	10	6
1	D	194/252 (77%)	187 (96%)	7 (4%)	31	36
All	All	745/1008 (74%)	700 (94%)	45 (6%)	17	16

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	309	SER
1	D	326	ILE
1	D	337	PHE
1	D	354	LEU
1	D	423	GLU
1	D	515	ARG
1	D	534	VAL
1	A	311	THR
1	A	326	ILE
1	A	342	MET
1	A	389	ILE
1	A	401	LYS
1	A	411	ASP
1	A	413	ASN

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Mol	Chain	Res	Type
1	A	424	ILE
1	A	427	MET
1	A	433	SER
1	A	523	GLU
1	A	528	MET
1	C	317	SER
1	C	342	MET
1	C	345	LEU
1	C	368	VAL
1	C	389	ILE
1	C	392	VAL
1	C	394	ARG
1	C	413	ASN
1	C	422	VAL
1	C	433	SER
1	C	437	MET
1	C	465	THR
1	C	481	LYS
1	C	528	MET
1	C	535	PRO
1	C	541	LEU
1	B	314	GLN
1	B	335	ARG
1	B	352	ARG
1	B	411	ASP
1	B	425	PHE
1	B	434	ARG
1	B	460	THR
1	B	492	LYS
1	B	527	SER
1	B	535	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	439	ASN
1	D	474	HIS
1	D	488	HIS
1	D	498	GLN
1	D	500	GLN
1	A	506	GLN
1	C	375	GLN

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Mol	Chain	Res	Type
1	C	474	HIS
1	C	476	HIS
1	C	499	GLN
1	C	516	HIS
1	C	519	ASN
1	B	314	GLN
1	B	413	ASN
1	B	501	HIS
1	B	513	HIS
1	B	519	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	ZNM	C	601	-	38,41,41	0.45	1 (2%)	51,61,61	0.70	1 (1%)
3	ZNM	A	601	-	38,41,41	0.40	0	51,61,61	0.59	1 (1%)
2	G9J	D	601	-	29,29,29	0.66	0	39,42,42	1.31	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	G9J	B	601	-	29,29,29	0.67	0	39,42,42	1.33	4 (10%)

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	ZNM	C	601	-	-	5/16/44/44	0/5/5/5
3	ZNM	A	601	-	-	2/16/44/44	0/5/5/5
2	G9J	D	601	-	-	0/8/24/24	0/4/4/4
2	G9J	B	601	-	-	0/8/24/24	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ZNM	C24-C15	-2.15	1.49	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	G9J	C6-C7-C2	-3.90	116.44	119.38
2	D	601	G9J	O5-C4-C13	-3.74	104.02	109.33
2	B	601	G9J	C21-C20-C3	-3.22	116.73	120.91
3	C	601	ZNM	C19-C18-N17	2.73	118.52	111.62
2	B	601	G9J	C20-C3-C4	-2.70	112.67	116.18
2	D	601	G9J	C20-C3-C4	-2.70	112.68	116.18
2	D	601	G9J	C1-C2-C3	-2.54	121.24	124.43
2	D	601	G9J	C18-C13-C14	2.36	121.22	118.30
2	B	601	G9J	C1-C2-C3	-2.35	121.49	124.43
2	D	601	G9J	C6-O5-C4	2.25	122.25	116.58
2	D	601	G9J	C6-C7-C2	-2.13	117.77	119.38
3	A	601	ZNM	C19-C18-N17	2.01	116.70	111.62

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	ZNM	C36-C37-C38-F39
3	A	601	ZNM	C26-C27-N31-C32

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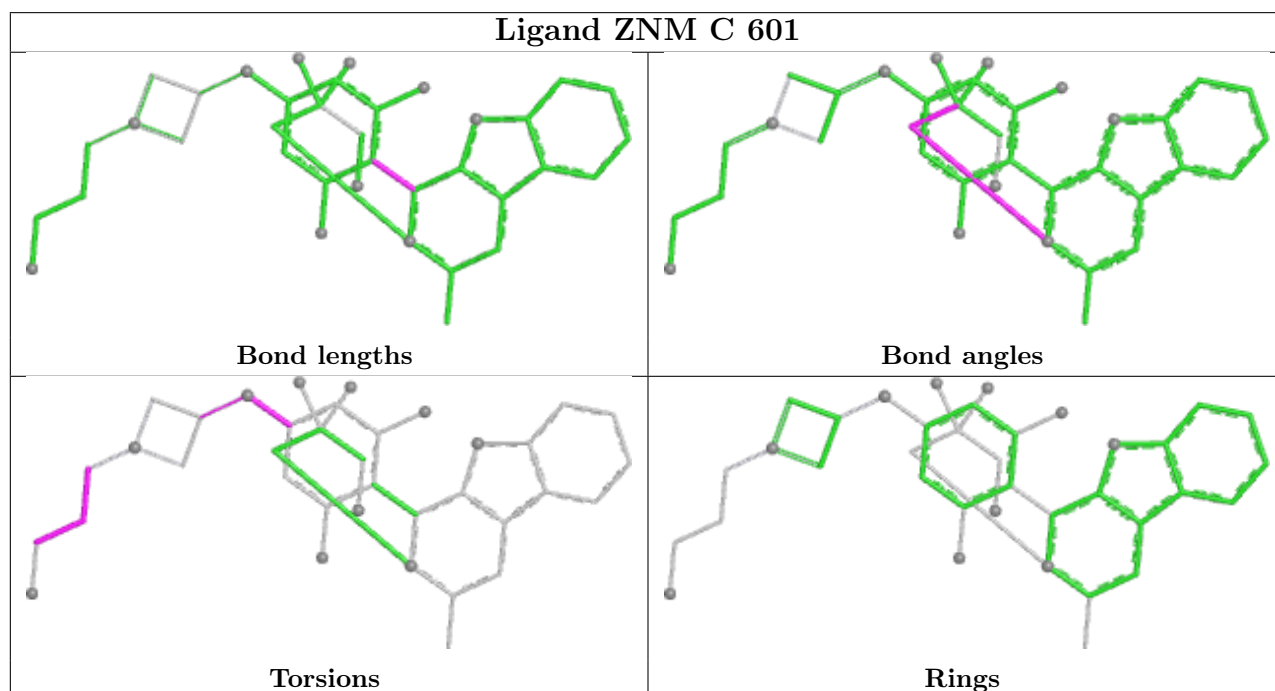
Mol	Chain	Res	Type	Atoms
3	C	601	ZNM	C26-C27-N31-C32
3	A	601	ZNM	C28-C27-N31-C32
3	C	601	ZNM	N34-C36-C37-C38
3	C	601	ZNM	C28-C27-N31-C32
3	C	601	ZNM	C33-C32-N31-C27

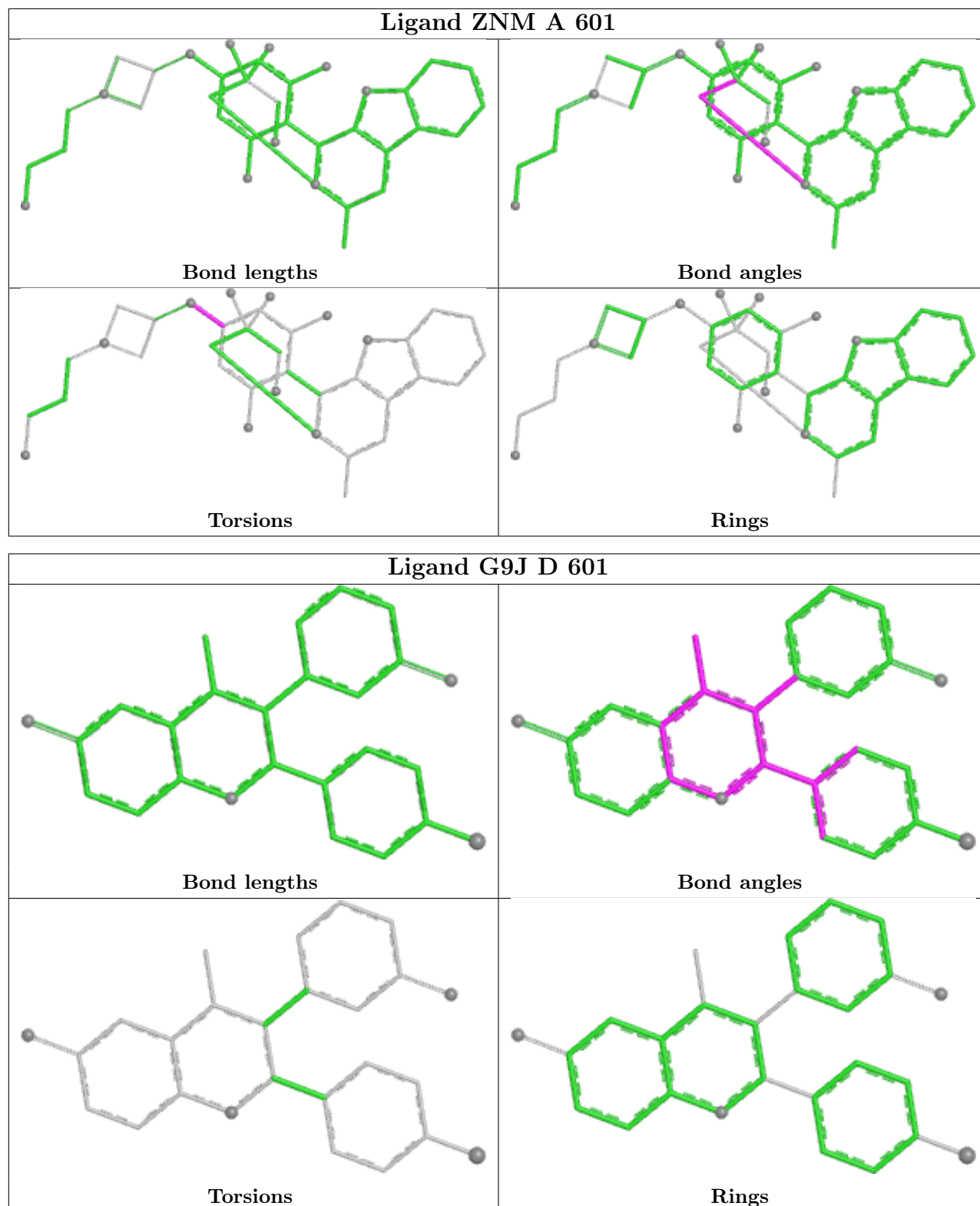
There are no ring outliers.

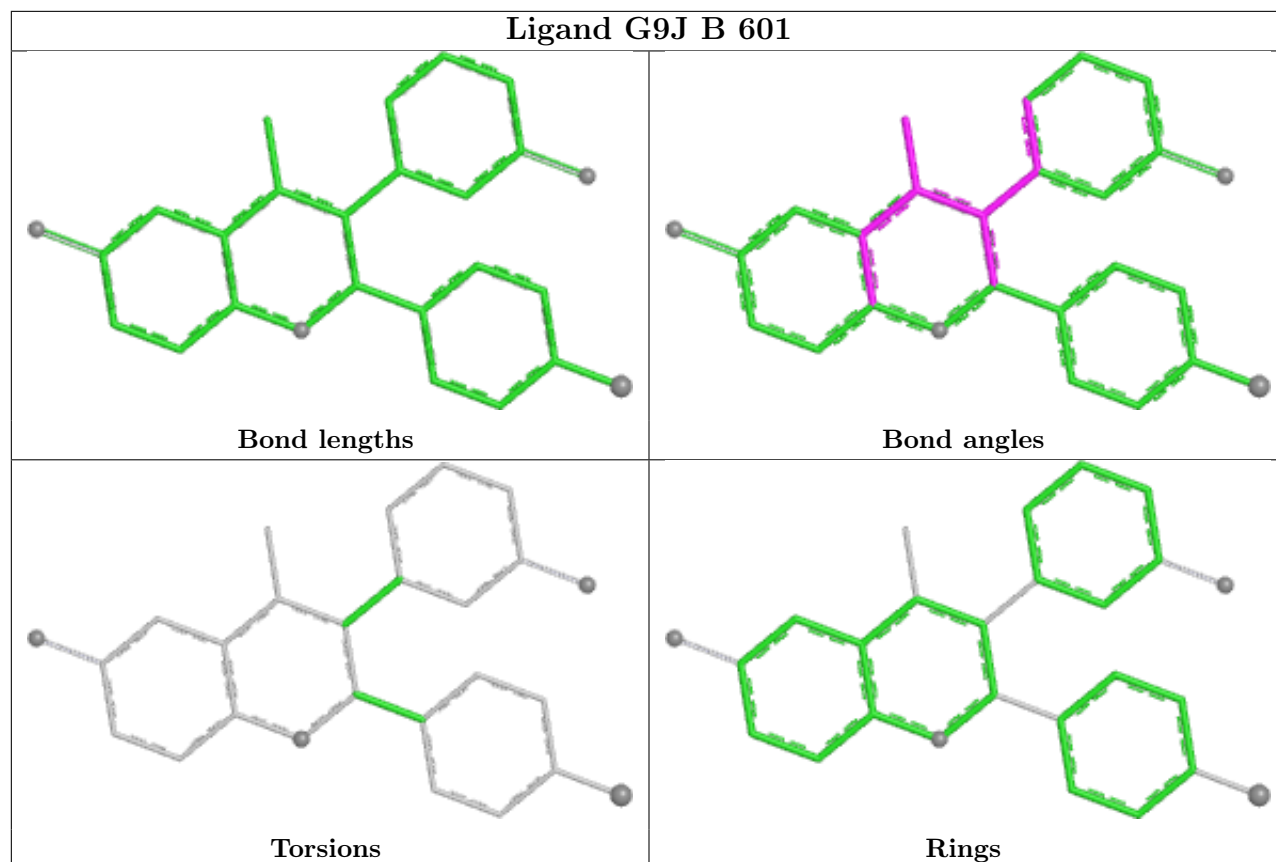
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	ZNM	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	225/280 (80%)	0.62	13 (5%) 29 27	49, 76, 125, 136	0
1	B	228/280 (81%)	0.48	6 (2%) 57 58	52, 77, 108, 137	0
1	C	225/280 (80%)	0.51	11 (4%) 35 33	28, 73, 109, 136	1 (0%)
1	D	234/280 (83%)	0.51	7 (2%) 52 52	50, 76, 108, 125	0
All	All	912/1120 (81%)	0.53	37 (4%) 41 41	28, 76, 113, 137	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	533	VAL	4.1
1	A	538	ASP	3.9
1	B	545	ASP	3.5
1	A	534	VAL	3.3
1	A	537	TYR	3.2
1	B	337	PHE	3.1
1	A	457	GLY	3.1
1	C	437	MET	2.9
1	B	328	TYR	2.9
1	C	535	PRO	2.8
1	C	337	PHE	2.8
1	A	336	PRO	2.8
1	C	429	LEU	2.7
1	C	526	TYR	2.7
1	D	331	TYR	2.6
1	A	540	LEU	2.6
1	A	526	TYR	2.6
1	D	497	LEU	2.5
1	D	528	MET	2.5
1	A	512	SER	2.5
1	B	513	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	337	PHE	2.5
1	C	368	VAL	2.5
1	C	307	ALA	2.5
1	C	465	THR	2.4
1	A	328	TYR	2.3
1	D	307	ALA	2.3
1	D	537	TYR	2.2
1	B	358	ILE	2.1
1	A	342	MET	2.1
1	A	331	TYR	2.1
1	C	466	LEU	2.1
1	C	506	GLN	2.1
1	A	458	VAL	2.1
1	B	308	LEU	2.1
1	D	368	VAL	2.0
1	C	345	LEU	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.

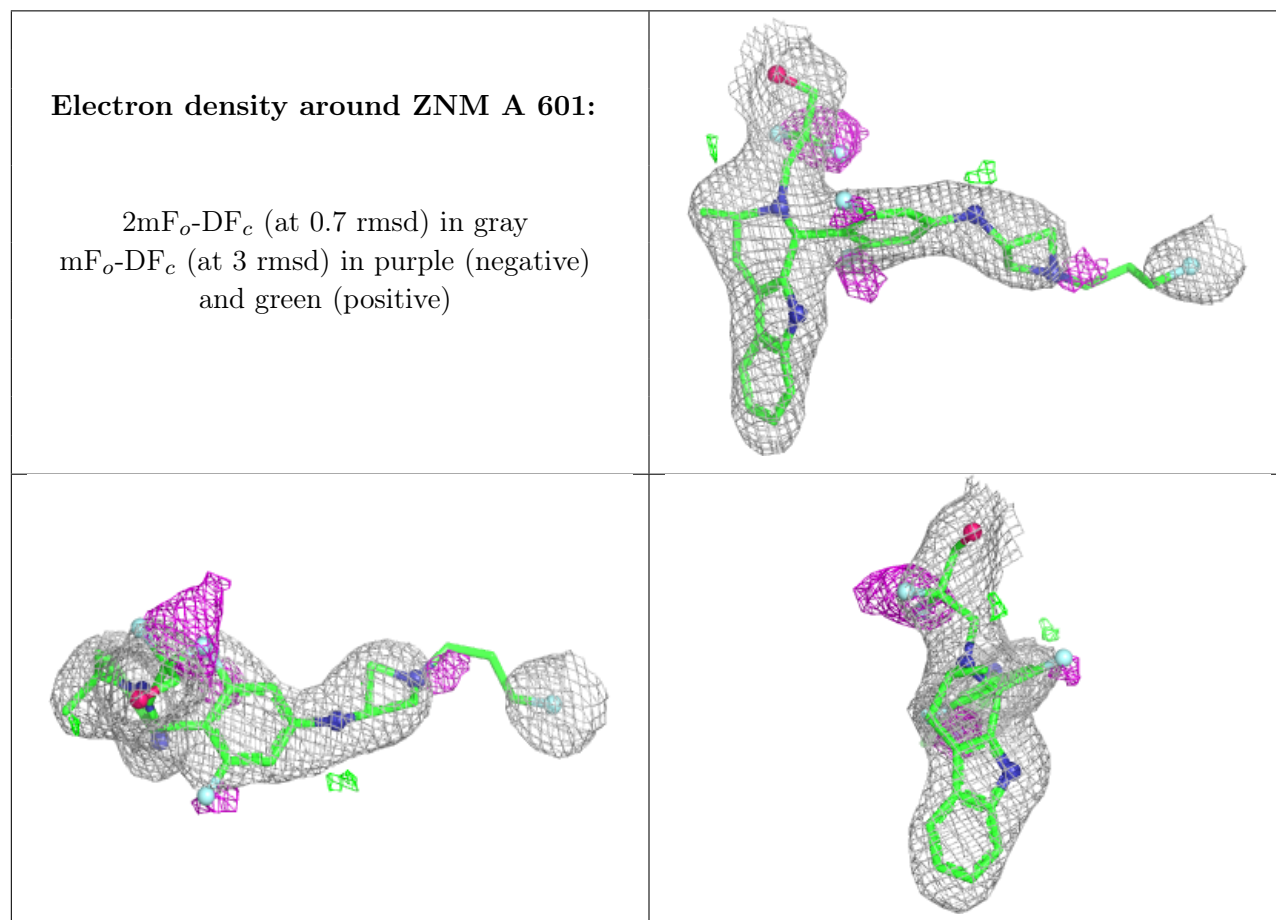
## 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
3	ZNM	A	601	37/37	0.84	0.14	62,71,90,91	0
3	ZNM	C	601	37/37	0.88	0.12	61,70,89,97	0
2	G9J	D	601	26/26	0.96	0.12	57,65,83,87	0
2	G9J	B	601	26/26	0.96	0.11	55,62,78,80	0

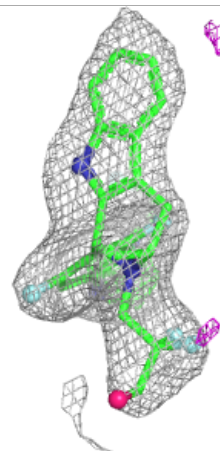
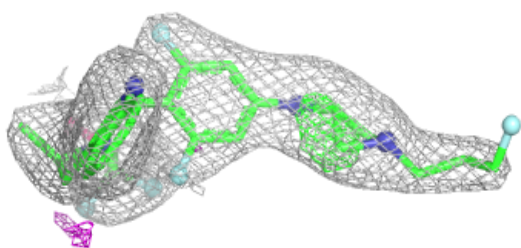
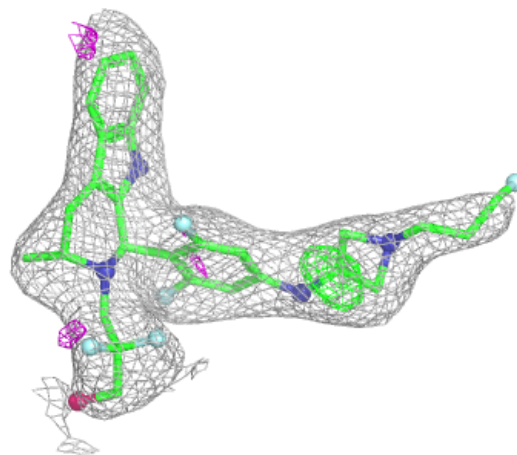
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



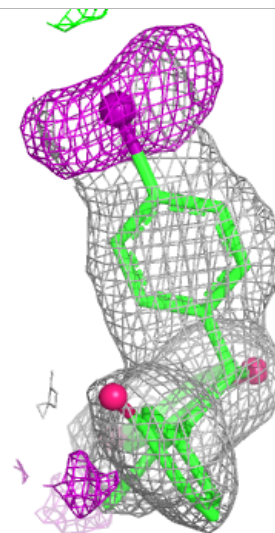
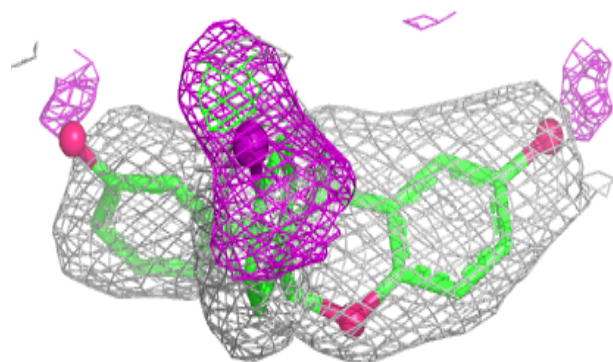
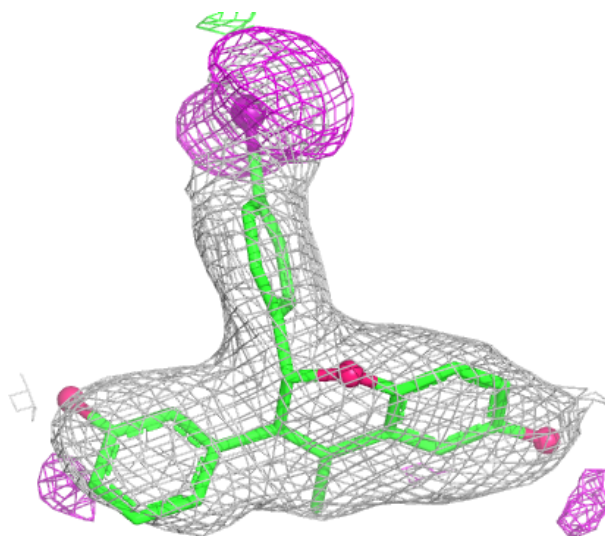
**Electron density around ZNM C 601:**

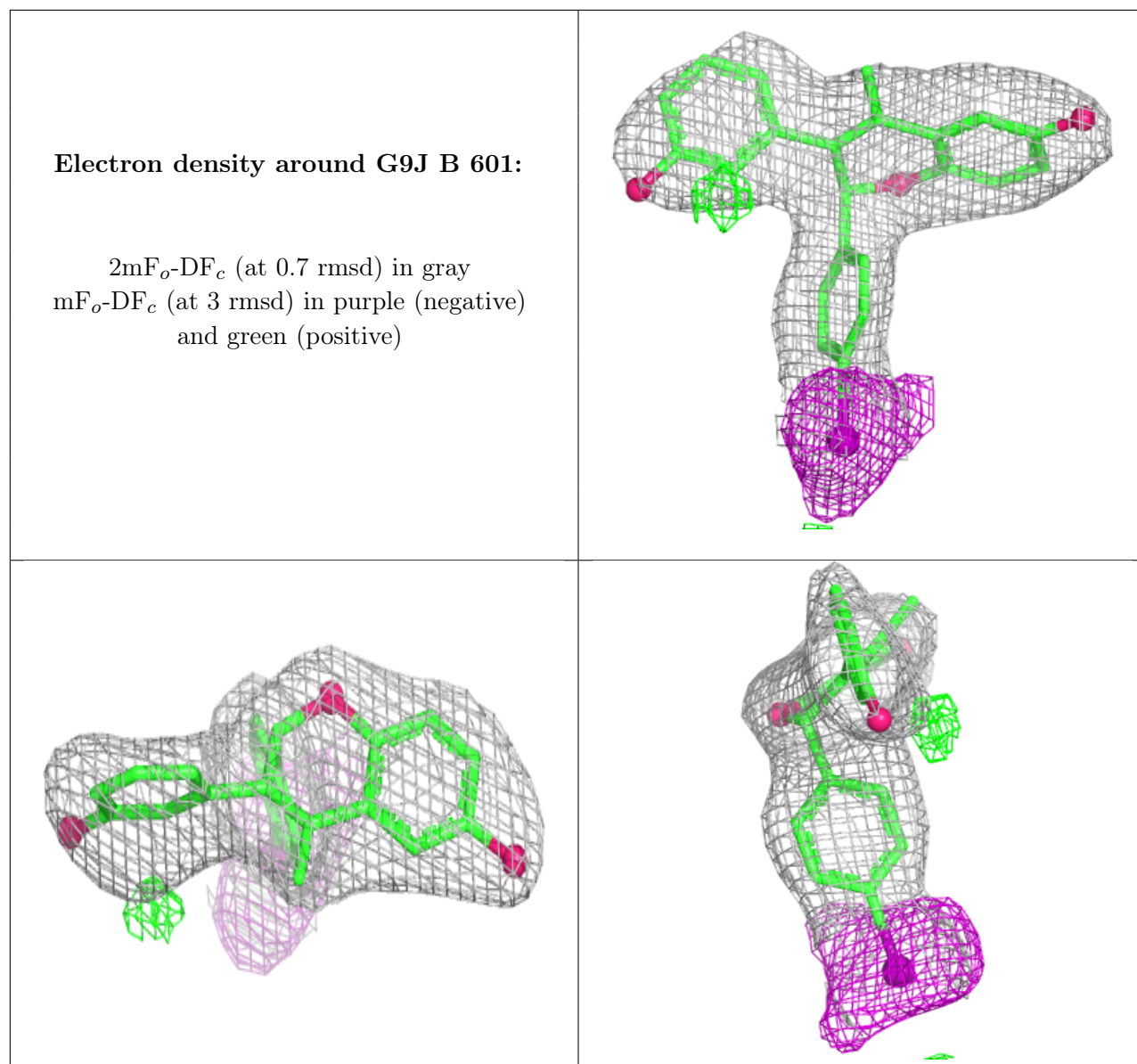
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around G9J D 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.