Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2021 – 12:07 PM EDT

PDB ID	:	7MSA
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)

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	:	2.23.1
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)	:	2.23.1

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 2.24 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.
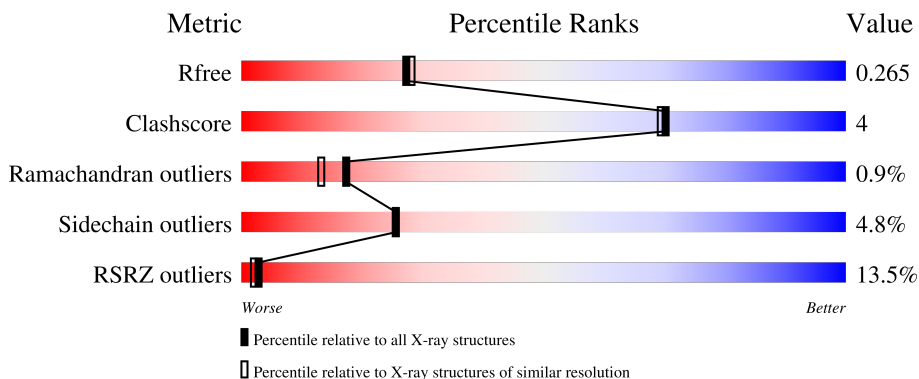
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 >=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 <=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	14% / 66% / 13% / • / 20%
1	B	280	9% / 70% / 11% / 19%
1	C	280	12% / 72% / 8% / 20%
1	D	280	8% / 74% / 9% / 16%

2 Entry composition ⓘ

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
1	D	234	Total 1800	C 1153	N 303	O 327	S 17	0	0	0
1	A	225	Total 1684	C 1071	N 289	O 307	S 17	0	1	0
1	C	225	Total 1744	C 1118	N 300	O 308	S 18	0	1	0
1	B	228	Total 1767	C 1136	N 301	O 314	S 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

(three-letter code: G9J) (formula: $C_{22}H_{17}IO_3$).
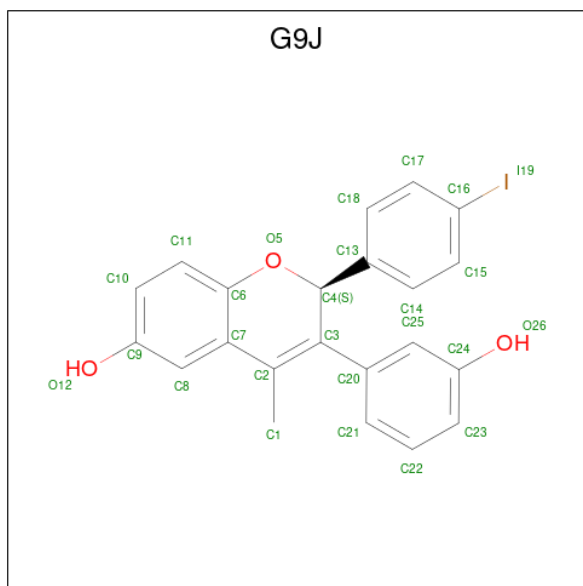
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total 26	C 22	I 1	O 3	0	0
2	B	1	Total 26	C 22	I 1	O 3	0	0

- Molecule 3 is 3-[(1R,3R)-1-(2,6-difluoro-4-{[1-(3-fluoropropyl)azetidin-3-yl]amino}phenyl)-3 -methyl-1,3,4,9-tetrahydro-2H-pyrido[3,4-b]indol-2-yl]-2,2-difluoropropan-1-ol (three-letter code: ZNM) (formula: $C_{27}H_{31}F_5N_4O$) (labeled as "Ligand of Interest" by depositor).
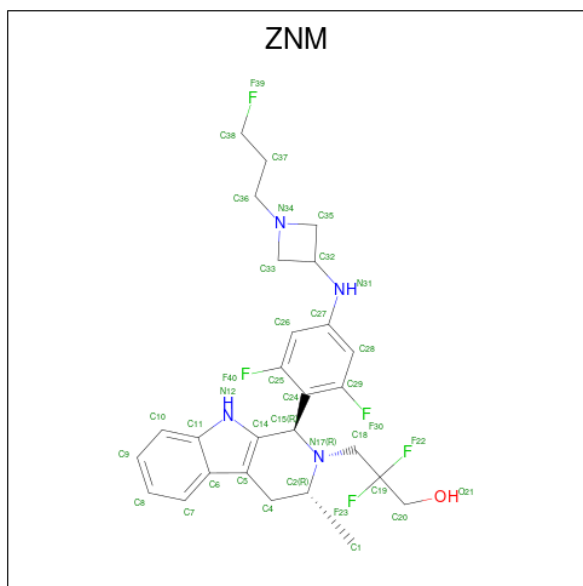
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 37	C 27	F 5	N 4	O 1	0	0
3	C	1	Total 37	C 27	F 5	N 4	O 1	0	0

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

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.
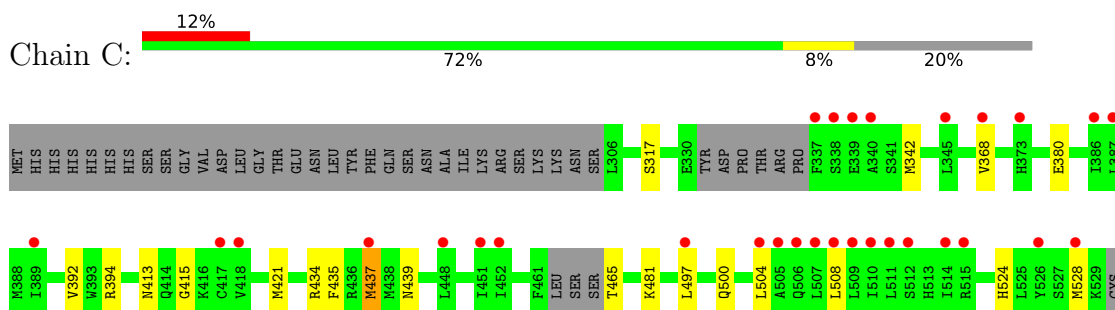
- Molecule 1: Estrogen receptor
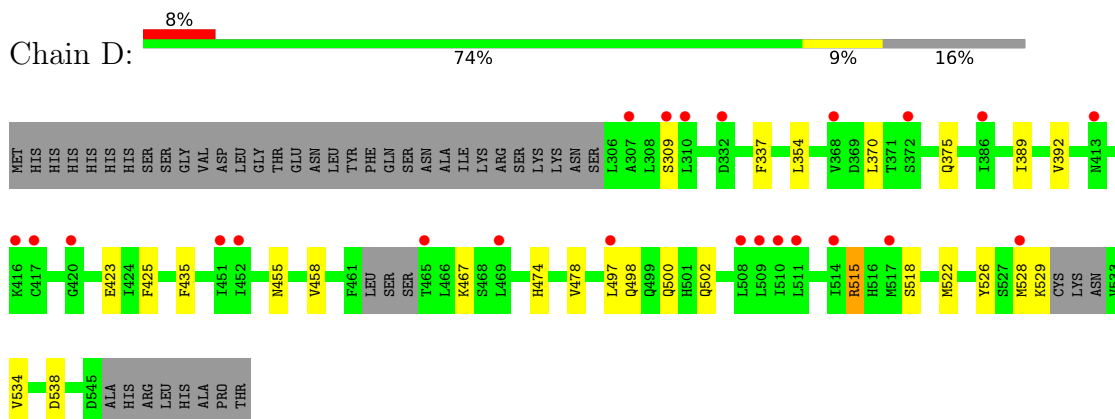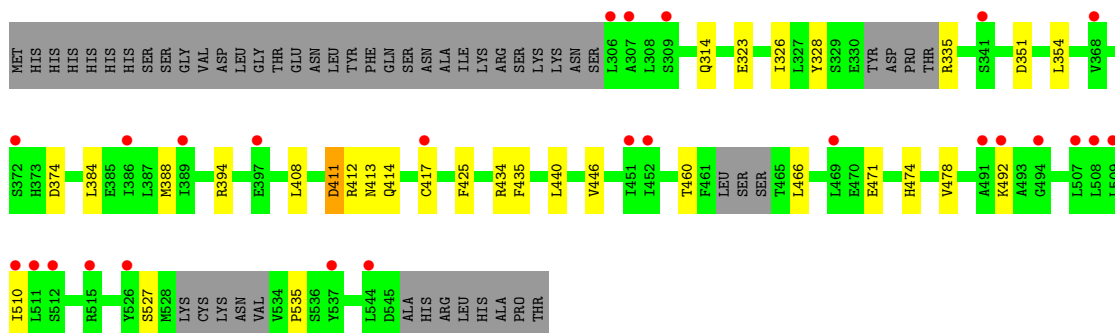

- Molecule 1: Estrogen receptor

- Molecule 1: Estrogen receptor

• Molecule 1: Estrogen receptor

Chain B:
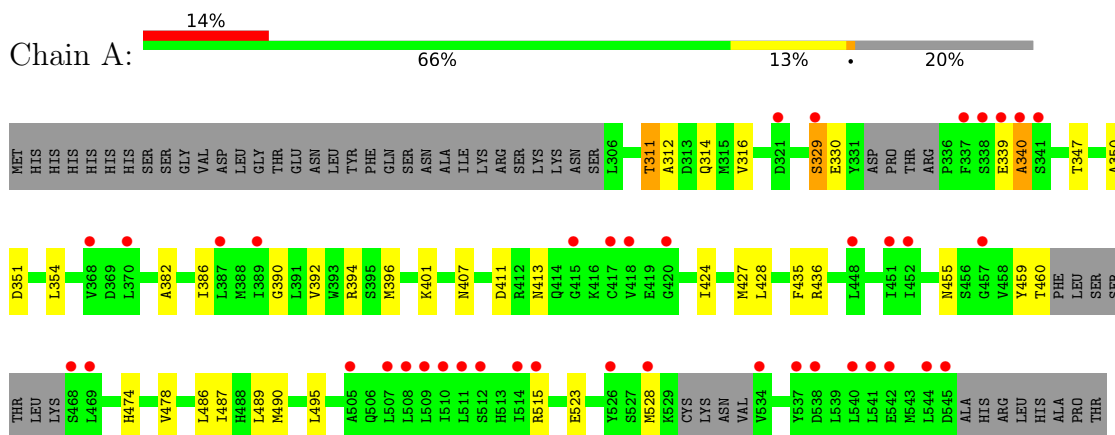
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.08Å　58.94Å　93.55Å 86.43°　75.08°　63.25°	Depositor
Resolution (Å)	33.22　–　2.24 33.22　–　2.18	Depositor EDS
% Data completeness (in resolution range)	81.7 (33.22-2.24) 88.7 (33.22-2.18)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.194　,　0.246 0.212　,　0.265	Depositor DCC
R_{free} test set	2274 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.5	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	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^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: G9J, ZNM

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	0.71	0/1710	0.82	0/2316
1	B	0.68	0/1798	0.77	0/2435
1	C	0.69	0/1771	0.79	0/2391
1	D	0.67	0/1832	0.77	0/2485
All	All	0.69	0/7111	0.79	0/9627

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

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1684	0	1629	21	0
1	B	1767	0	1765	12	0
1	C	1744	0	1765	6	0
1	D	1800	0	1781	12	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	51	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 (51) 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:487:ILE:HA	1:A:490:MET:HE3	1.69	0.71
1:A:459:TYR:O	1:A:460:THR:HG23	1.96	0.65
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:490:MET:HB3	1:A:495:LEU:HD22	1.99	0.45
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:A:455:ASN:CG	1:A:455:ASN:O	2.56	0.43
1:A:339:GLU:O	1:A:340:ALA:CB	2.68	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
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
1:B:411:ASP:OD1	1:B:411:ASP:C	2.59	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	217/280 (78%)	205 (94%)	10 (5%)	2 (1%)	17	13
1	B	220/280 (79%)	210 (96%)	7 (3%)	3 (1%)	11	6
1	C	218/280 (78%)	213 (98%)	3 (1%)	2 (1%)	17	13
1	D	228/280 (81%)	224 (98%)	3 (1%)	1 (0%)	34	35
All	All	883/1120 (79%)	852 (96%)	23 (3%)	8 (1%)	17	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ALA
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 ⓘ

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%)	165 (95%)	8 (5%)	27	28
1	B	190/252 (75%)	182 (96%)	8 (4%)	30	32
1	C	188/252 (75%)	176 (94%)	12 (6%)	17	14
1	D	194/252 (77%)	186 (96%)	8 (4%)	30	33
All	All	745/1008 (74%)	709 (95%)	36 (5%)	25	25

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	309	SER
1	D	337	PHE
1	D	354	LEU

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Mol	Chain	Res	Type
1	D	423	GLU
1	D	425	PHE
1	D	515	ARG
1	D	534	VAL
1	D	538	ASP
1	A	311	THR
1	A	401	LYS
1	A	411	ASP
1	A	413	ASN
1	A	427	MET
1	A	515	ARG
1	A	523	GLU
1	A	528	MET
1	C	317	SER
1	C	342	MET
1	C	368	VAL
1	C	380	GLU
1	C	394	ARG
1	C	413	ASN
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	411	ASP
1	B	412	ARG
1	B	425	PHE
1	B	434	ARG
1	B	492	LYS
1	B	527	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	439	ASN
1	A	439	ASN
1	A	506	GLN
1	A	516	HIS
1	A	519	ASN

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Mol	Chain	Res	Type
1	C	499	GLN
1	B	314	GLN
1	B	413	ASN
1	B	513	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	$\#|Z| > 2$
2	G9J	D	601	-	29,29,29	0.66	1 (3%)	38,42,42	1.23	5 (13%)
3	ZNM	C	601	-	35,41,41	1.06	1 (2%)	39,61,61	0.64	1 (2%)
2	G9J	B	601	-	29,29,29	0.66	0	38,42,42	1.24	3 (7%)
3	ZNM	A	601	-	35,41,41	0.94	1 (2%)	39,61,61	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G9J	D	601	-	-	0/8/24/24	0/4/4/4
3	ZNM	C	601	-	-	5/16/44/44	0/5/5/5
2	G9J	B	601	-	-	0/8/24/24	0/4/4/4
3	ZNM	A	601	-	-	2/16/44/44	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ZNM	C24-C15	-5.01	1.49	1.53
3	A	601	ZNM	C24-C15	-4.11	1.50	1.53
2	D	601	G9J	C7-C2	2.00	1.49	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	G9J	C6-C7-C2	-3.71	116.44	119.43
2	D	601	G9J	O5-C4-C13	-3.68	104.02	109.53
2	B	601	G9J	C21-C20-C3	-3.23	116.73	120.91
2	D	601	G9J	C1-C2-C3	-2.45	121.24	124.49
3	C	601	ZNM	C19-C18-N17	2.43	118.52	111.50
2	D	601	G9J	C18-C13-C14	2.35	121.22	118.29
2	B	601	G9J	C1-C2-C3	-2.27	121.49	124.49
2	D	601	G9J	C6-O5-C4	2.11	122.25	116.63
2	D	601	G9J	C6-C7-C2	-2.06	117.77	119.43

There are no chirality outliers.
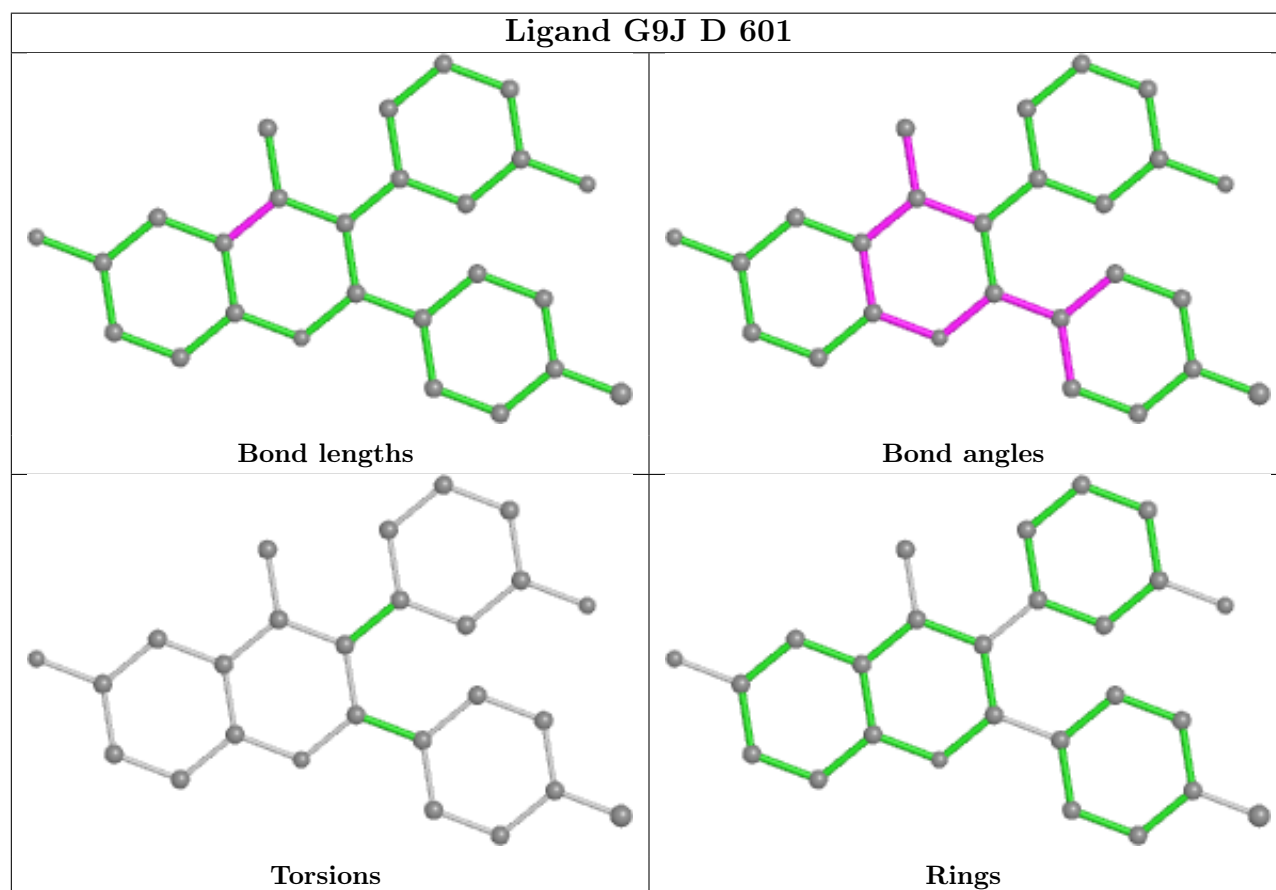
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	ZNM	C36-C37-C38-F39
3	A	601	ZNM	C26-C27-N31-C32
3	C	601	ZNM	C26-C27-N31-C32
3	A	601	ZNM	C28-C27-N31-C32
3	C	601	ZNM	C28-C27-N31-C32
3	C	601	ZNM	N34-C36-C37-C38
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 then 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 G9J D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ZNM C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand G9J B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ZNM A 601

Bond lengths

Bond angles

Torsions

Rings
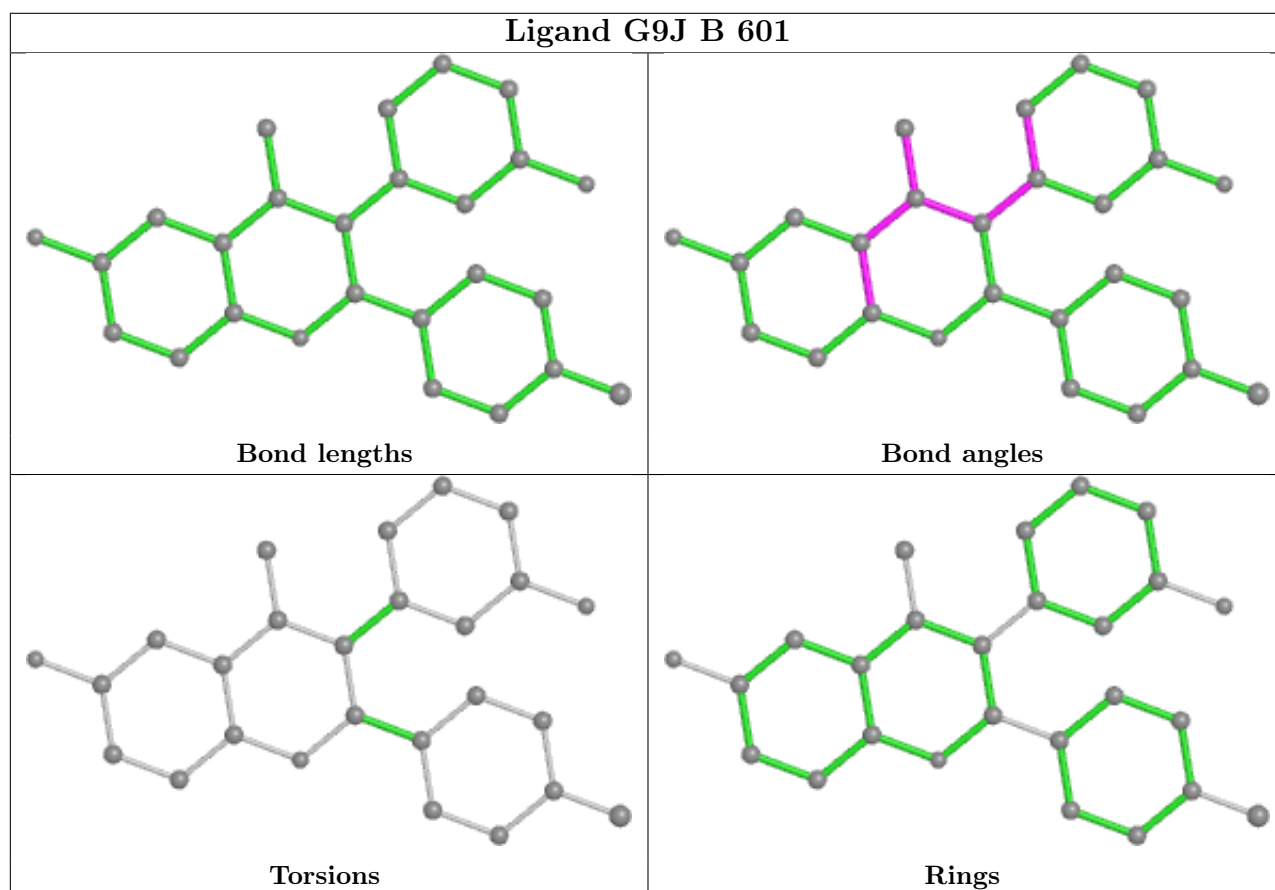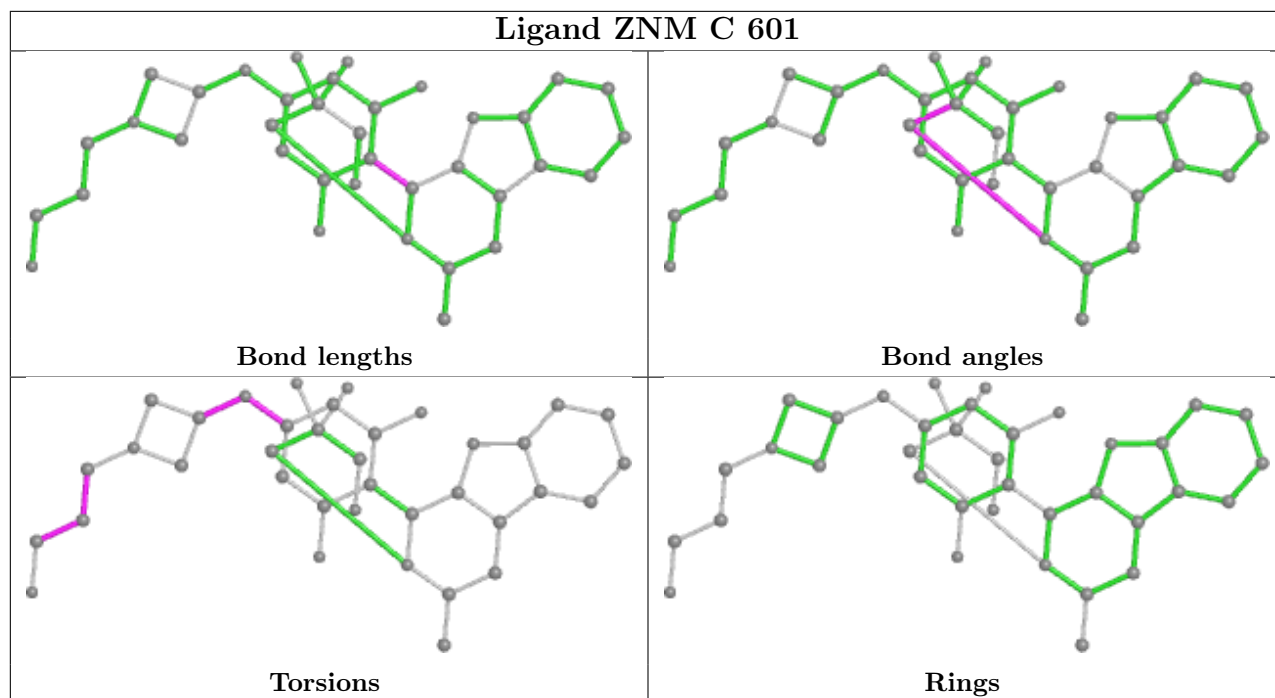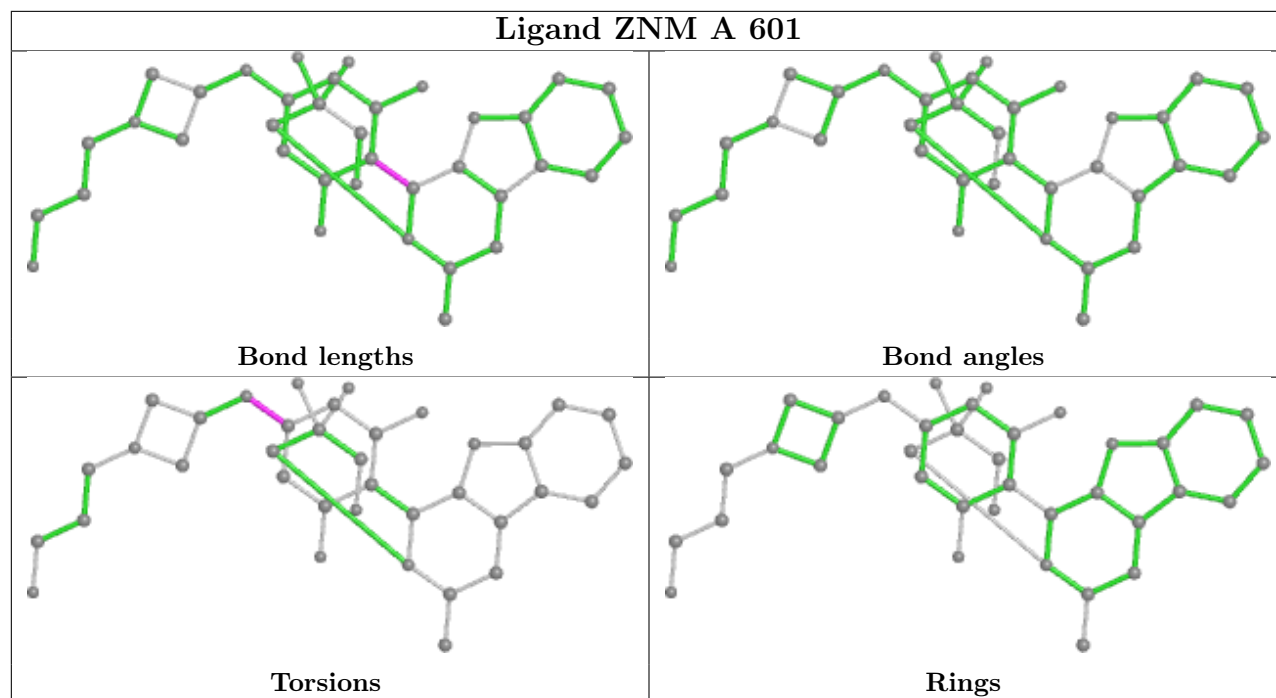
5.7 Other polymers (i)

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, 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	225/280 (80%)	0.80	40 (17%)	1	1	49, 76, 125, 136	0
1	B	228/280 (81%)	0.60	26 (11%)	5	4	52, 77, 108, 137	0
1	C	225/280 (80%)	0.72	34 (15%)	2	1	50, 73, 109, 136	0
1	D	234/280 (83%)	0.54	23 (9%)	7	7	50, 76, 108, 125	0
All	All	912/1120 (81%)	0.66	123 (13%)	3	2	49, 76, 113, 137	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	LEU	5.9
1	A	338	SER	5.5
1	A	339	GLU	5.4
1	C	340	ALA	5.2
1	C	511	LEU	5.0
1	B	491	ALA	4.9
1	D	307	ALA	4.9
1	C	509	LEU	4.9
1	B	509	LEU	4.7
1	A	537	TYR	4.7
1	A	340	ALA	4.5
1	A	511	LEU	4.5
1	A	508	LEU	4.3
1	A	368	VAL	4.3
1	B	510	ILE	4.3
1	D	509	LEU	4.2
1	B	306	LEU	4.2
1	A	417	CYS	4.2
1	A	528	MET	4.1
1	B	511	LEU	4.1
1	D	469	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	338	SER	3.9
1	D	511	LEU	3.9
1	A	538	ASP	3.9
1	A	509	LEU	3.8
1	A	534	VAL	3.8
1	C	510	ILE	3.7
1	C	514	ILE	3.7
1	D	465	THR	3.6
1	D	508	LEU	3.6
1	A	544	LEU	3.6
1	C	508	LEU	3.6
1	C	339	GLU	3.4
1	B	417	CYS	3.4
1	A	370	LEU	3.4
1	A	452	ILE	3.4
1	C	345	LEU	3.4
1	C	505	ALA	3.4
1	B	452	ILE	3.4
1	C	515[A]	ARG	3.3
1	C	452	ILE	3.3
1	D	368	VAL	3.3
1	D	497	LEU	3.3
1	C	451	ILE	3.3
1	C	544	LEU	3.2
1	C	526	TYR	3.2
1	C	528	MET	3.2
1	D	413	ASN	3.2
1	B	512	SER	3.1
1	A	415	GLY	3.1
1	C	437	MET	3.1
1	B	469	LEU	3.0
1	A	514	ILE	3.0
1	C	417	CYS	3.0
1	D	309	SER	3.0
1	D	372	SER	3.0
1	C	389	ILE	3.0
1	D	417	CYS	3.0
1	B	508	LEU	3.0
1	C	368	VAL	2.9
1	A	469	LEU	2.9
1	D	420	GLY	2.9
1	D	510	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	332	ASP	2.9
1	A	545	ASP	2.9
1	B	492	LYS	2.9
1	A	542	GLU	2.9
1	A	341	SER	2.9
1	C	448	LEU	2.9
1	A	337	PHE	2.8
1	D	528	MET	2.8
1	B	386	ILE	2.8
1	C	387	LEU	2.8
1	A	389	ILE	2.7
1	A	321	ASP	2.7
1	D	514	ILE	2.7
1	A	468	SER	2.7
1	A	510	ILE	2.6
1	B	451	ILE	2.6
1	C	506	GLN	2.6
1	C	507	LEU	2.6
1	A	507	LEU	2.6
1	A	329	SER	2.6
1	D	386	ILE	2.6
1	A	451	ILE	2.5
1	A	540	LEU	2.5
1	B	397	GLU	2.5
1	B	341	SER	2.5
1	C	337	PHE	2.4
1	A	448	LEU	2.4
1	B	526	TYR	2.4
1	A	515	ARG	2.4
1	A	526	TYR	2.4
1	C	512	SER	2.3
1	B	494	GLY	2.3
1	D	452	ILE	2.3
1	B	309	SER	2.3
1	D	310	LEU	2.3
1	A	387	LEU	2.2
1	B	372	SER	2.2
1	D	451	ILE	2.2
1	C	541	LEU	2.2
1	A	512	SER	2.2
1	B	515	ARG	2.2
1	A	505	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	504	LEU	2.2
1	B	537	TYR	2.2
1	C	418	VAL	2.2
1	C	538	ASP	2.2
1	B	507	LEU	2.1
1	A	418	VAL	2.1
1	B	307	ALA	2.1
1	A	457	GLY	2.1
1	D	416	LYS	2.1
1	B	368	VAL	2.1
1	C	536	SER	2.1
1	C	386	ILE	2.1
1	C	497	LEU	2.1
1	C	373	HIS	2.0
1	A	420	GLY	2.0
1	B	389	ILE	2.0
1	B	544	LEU	2.0
1	D	517	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	ZNM	A	601	37/37	0.85	0.19	62,71,90,91	0
3	ZNM	C	601	37/37	0.89	0.16	61,70,89,97	0
2	G9J	B	601	26/26	0.96	0.11	55,62,78,80	0
2	G9J	D	601	26/26	0.97	0.12	57,65,83,87	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.
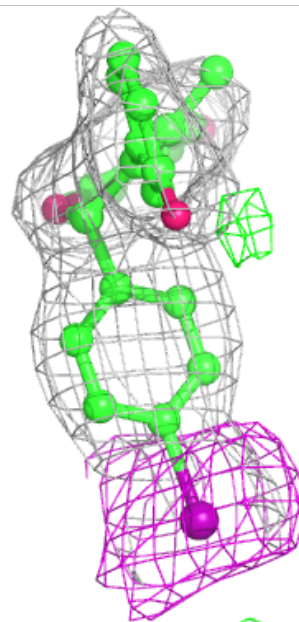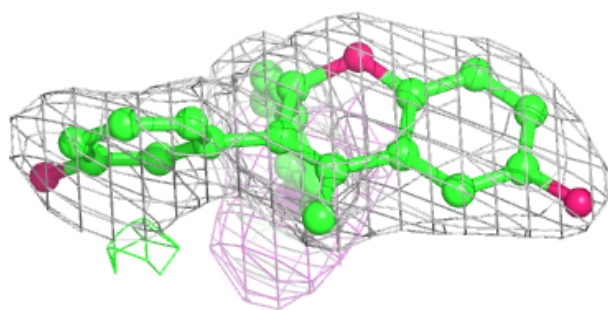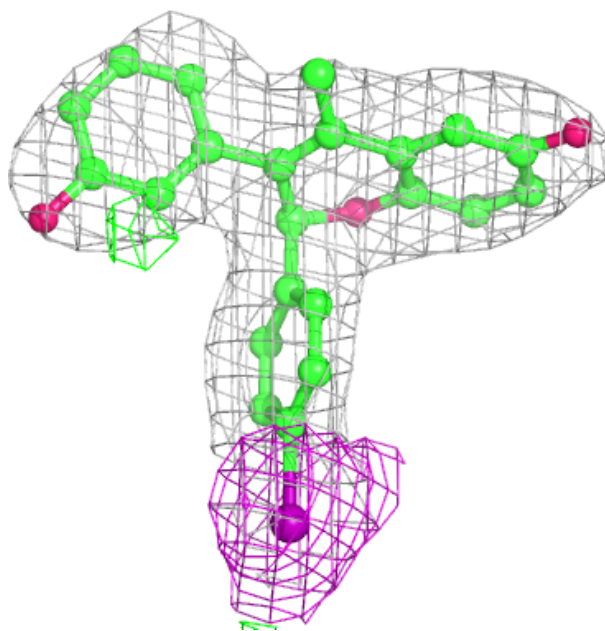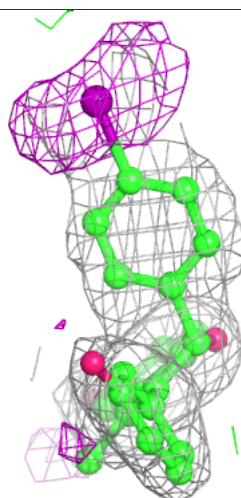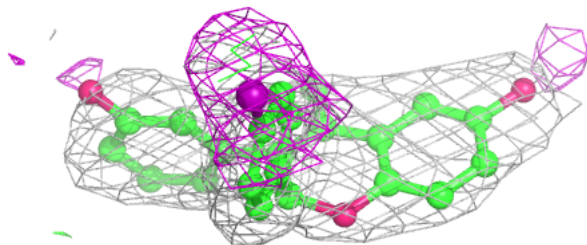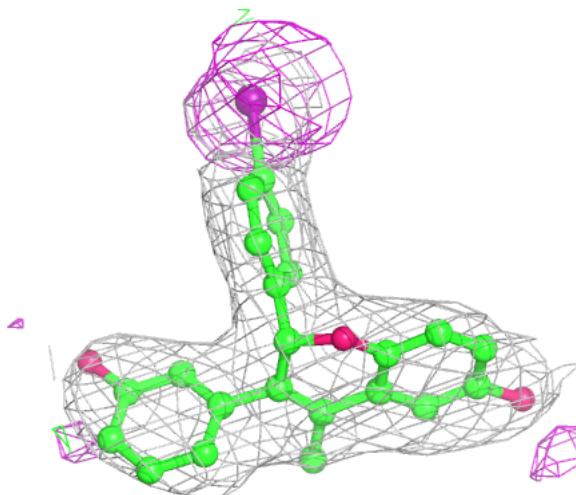
Electron density around ZNM A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
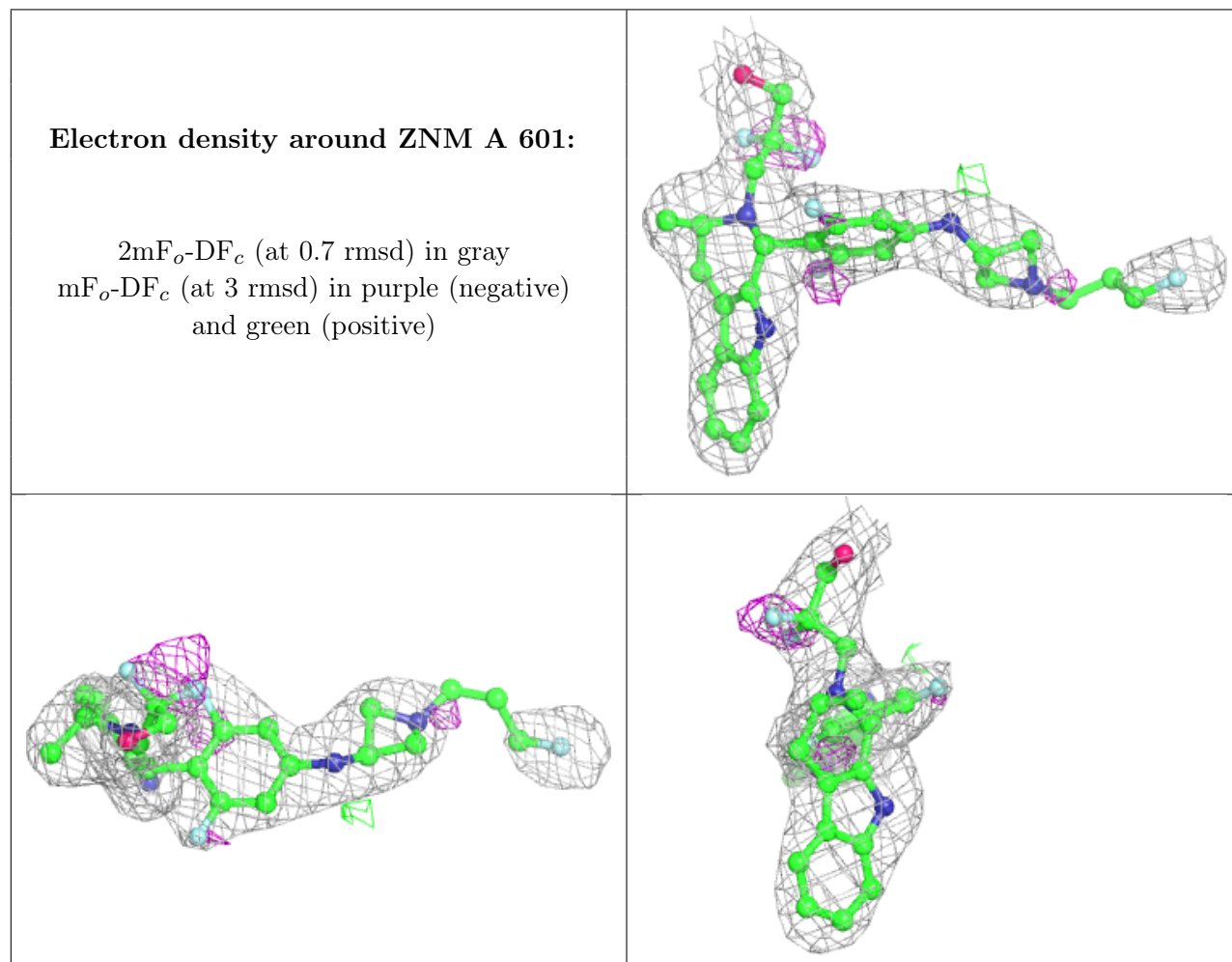
Electron density around ZNM C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
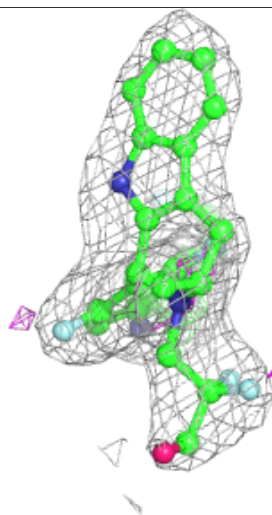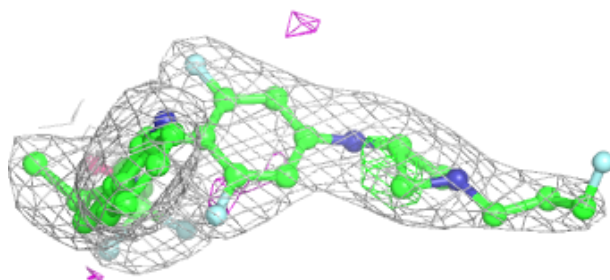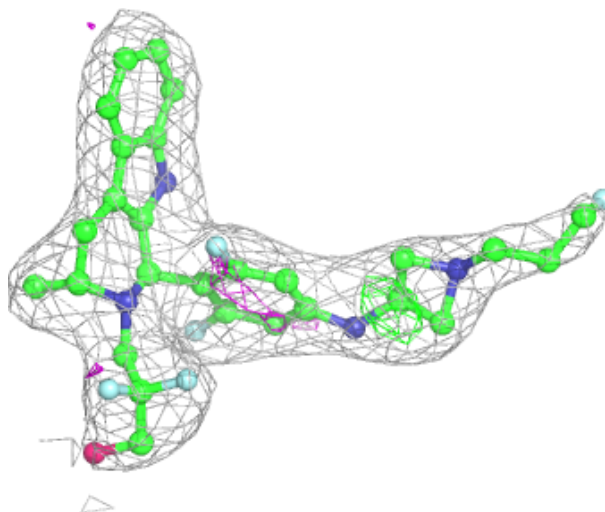
Electron density around G9J B 601:

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

Electron density around G9J D 601:

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

6.5 Other polymers (i)

There are no such residues in this entry.