



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:38 AM UTC

PDB ID : 4EA0 / pdb_00004ea0
Title : Crystal structure of dehydrosqualene synthase (Crtm) from *S. aureus* complexed with diphosphate and quinuclidine BPH-651
Authors : Lin, F.-Y.; Liu, Y.-L.; Oldfield, E.
Deposited on : 2012-03-21
Resolution : 2.12 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)
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

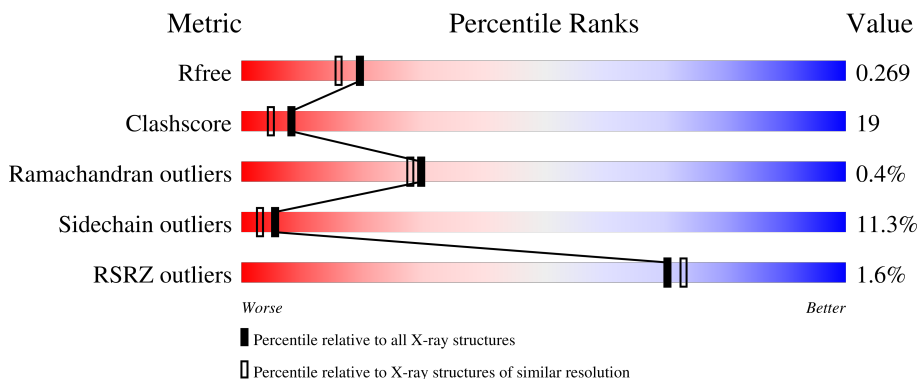
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	287	
1	B	287	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TLA	A	305	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5046 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.

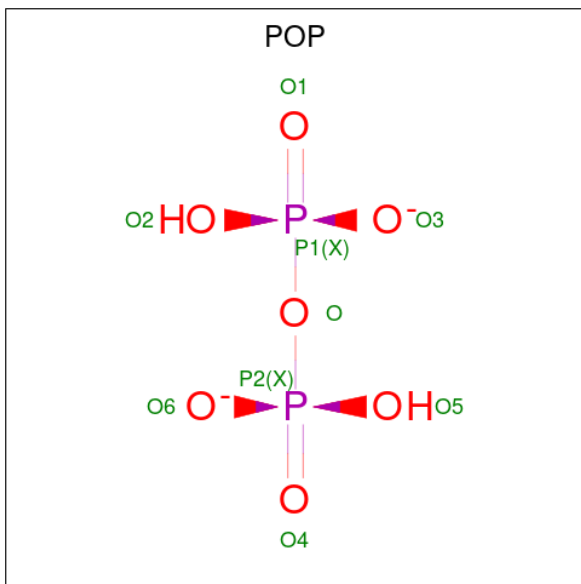
- Molecule 1 is a protein called Dehydrosqualene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	Total 2392	C 1536	N 400	O 444	S 12	0	0	0
1	B	284	Total 2392	C 1536	N 400	O 444	S 12	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

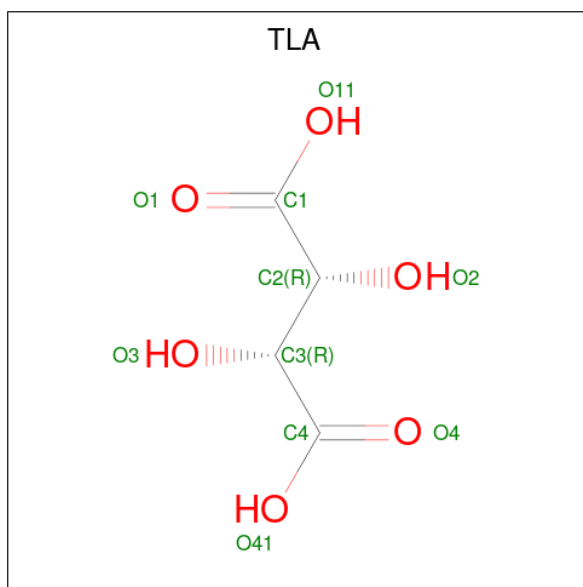
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Mg 3	0	0
2	B	3	Total 3	Mg 3	0	0

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



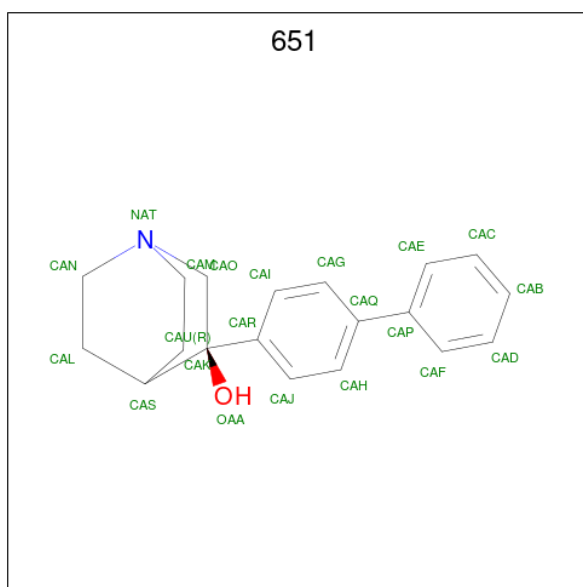
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is (3R)-3-biphenyl-4-yl-1-azabicyclo[2.2.2]octan-3-ol (CCD ID: 651) (formula: C₁₉H₂₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	19	1	1		
5	B	1	Total	C	N	O	0	0
			21	19	1	1		

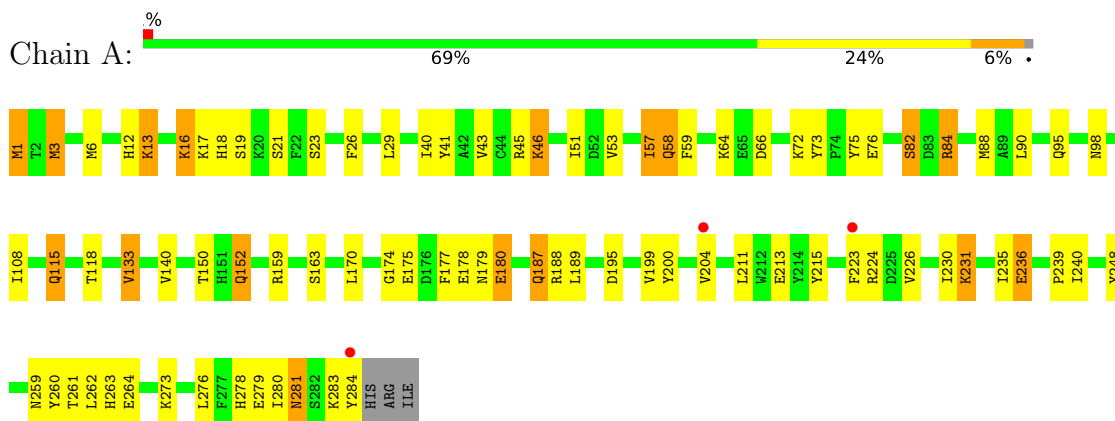
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	103	Total	O	0	0
			103	103		
6	B	83	Total	O	0	0
			83	83		

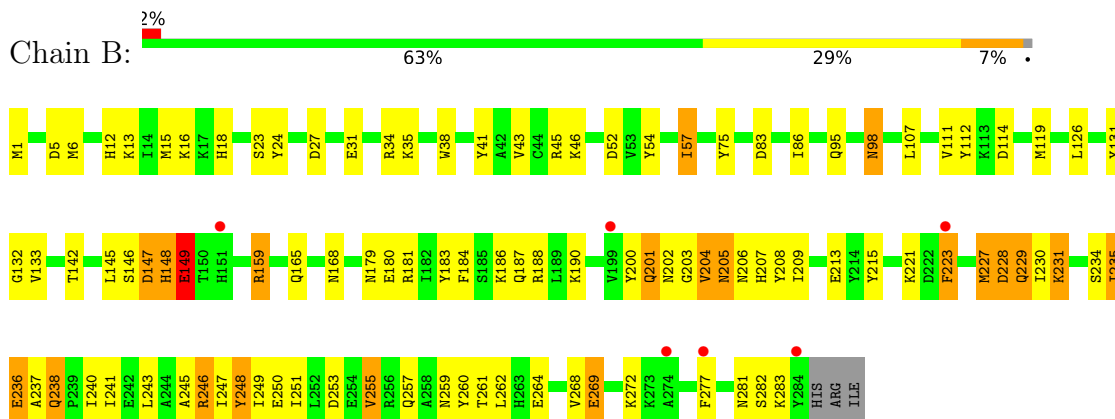
3 Residue-property plots [i](#)

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: Dehydrosqualene synthase



- Molecule 1: Dehydrosqualene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.32Å 80.32Å 180.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.46 – 2.12 32.46 – 2.12	Depositor EDS
% Data completeness (in resolution range)	94.2 (32.46-2.12) 94.2 (32.46-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.12Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.222 , 0.278 0.220 , 0.269	Depositor DCC
R_{free} test set	1856 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtrriage
Anisotropy	0.169	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5046	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0119e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, POP, 651, TLA

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	1/2448 (0.0%)	0.68	0/3301
1	B	0.63	0/2448	0.71	1/3301 (0.0%)
All	All	0.59	1/4896 (0.0%)	0.70	1/6602 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	VAL	C-O	-6.21	1.18	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	GLY	N-CA-C	8.17	119.72	111.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	TYR	Sidechain

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	2392	0	2321	65	0
1	B	2392	0	2321	109	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	9	0	0	3	0
3	B	9	0	0	2	0
4	A	10	0	4	3	0
5	A	21	0	21	7	0
5	B	21	0	21	3	0
6	A	103	0	0	10	1
6	B	83	0	0	4	1
All	All	5046	0	4688	184	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (184) 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:B:235:ILE:H	1:B:235:ILE:CD1	1.35	1.32
1:A:66:ASP:OD1	1:A:82:SER:HB2	1.36	1.25
1:B:235:ILE:HD13	1:B:235:ILE:N	1.48	1.17
1:B:205:ASN:OD1	1:B:207:HIS:N	1.78	1.15
1:B:227:MET:HE3	1:B:227:MET:HA	1.21	1.11
1:B:1:MET:HE3	1:B:6:MET:HG2	1.25	1.10
1:A:3:MET:HE3	1:A:6:MET:HE1	1.09	1.08
1:B:235:ILE:CD1	1:B:235:ILE:N	2.05	1.03
1:A:3:MET:CE	1:A:6:MET:HE1	1.87	1.03
1:A:3:MET:HA	1:A:6:MET:HE3	1.34	1.02
1:A:19:SER:HA	4:A:305:TLA:H3	1.03	1.02
1:B:227:MET:HA	1:B:227:MET:CE	1.90	1.00
1:B:234:SER:O	1:B:238:GLN:NE2	1.97	0.97
1:A:19:SER:CA	4:A:305:TLA:H3	1.92	0.97
1:B:223:PHE:CE1	1:B:249:ILE:HD11	2.00	0.95
1:A:3:MET:HE3	1:A:6:MET:CE	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ARG:CG	1:B:159:ARG:HH11	1.81	0.94
1:B:159:ARG:HB2	1:B:159:ARG:NH1	1.83	0.94
5:A:306:651:HAKA	6:A:501:HOH:O	1.66	0.93
1:B:148:HIS:H	1:B:148:HIS:CD2	1.85	0.92
1:A:66:ASP:OD1	1:A:82:SER:CB	2.17	0.92
1:A:19:SER:HA	4:A:305:TLA:C3	1.98	0.92
1:B:159:ARG:HH11	1:B:159:ARG:HG3	1.33	0.91
1:B:251:ILE:O	1:B:255:VAL:HG23	1.71	0.90
5:A:306:651:CAK	6:A:501:HOH:O	2.22	0.87
1:A:3:MET:CE	1:A:6:MET:CE	2.54	0.84
1:B:1:MET:CE	1:B:6:MET:HG2	2.08	0.84
1:B:1:MET:HE3	1:B:6:MET:CG	2.08	0.83
1:B:148:HIS:CD2	1:B:148:HIS:N	2.44	0.82
1:B:205:ASN:OD1	1:B:206:ASN:N	2.12	0.82
1:B:234:SER:C	1:B:238:GLN:HE22	1.87	0.82
1:A:3:MET:HA	1:A:6:MET:CE	2.08	0.82
1:B:223:PHE:CD1	1:B:249:ILE:HD11	2.17	0.80
1:B:235:ILE:H	1:B:235:ILE:HD13	0.65	0.79
1:A:195:ASP:O	1:A:199:VAL:HG23	1.83	0.79
1:B:253:ASP:O	1:B:257:GLN:HG3	1.85	0.76
5:A:306:651:OAA	5:A:306:651:HAN	1.86	0.76
1:B:205:ASN:OD1	1:B:205:ASN:C	2.30	0.75
1:B:159:ARG:NH1	1:B:159:ARG:CB	2.50	0.74
1:A:213:GLU:O	6:A:463:HOH:O	2.07	0.72
5:B:305:651:HAN	5:B:305:651:OAA	1.88	0.72
1:B:227:MET:HE3	1:B:227:MET:CA	2.11	0.71
1:B:1:MET:N	6:B:465:HOH:O	2.24	0.71
1:B:148:HIS:H	1:B:148:HIS:HD2	1.37	0.70
1:B:159:ARG:HH11	1:B:159:ARG:CB	2.04	0.69
1:B:148:HIS:N	1:B:148:HIS:HD2	1.89	0.69
1:B:251:ILE:O	1:B:255:VAL:CG2	2.40	0.69
5:A:306:651:OAA	5:A:306:651:CAN	2.30	0.69
1:A:1:MET:N	6:A:453:HOH:O	2.24	0.68
1:A:204:VAL:HG23	1:A:204:VAL:O	1.94	0.66
1:A:200:TYR:CE1	1:A:263:HIS:CE1	2.84	0.65
1:B:228:ASP:O	1:B:231:LYS:NZ	2.30	0.65
5:B:305:651:OAA	5:B:305:651:CAN	2.39	0.63
1:A:12:HIS:CD2	1:A:16:LYS:HD3	2.34	0.63
1:B:248:TYR:O	1:B:251:ILE:HB	2.00	0.61
1:A:224:ARG:NH2	6:A:474:HOH:O	2.20	0.61
1:A:235:ILE:H	1:A:235:ILE:HD12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:VAL:HG11	1:B:260:TYR:HB2	1.83	0.60
1:B:235:ILE:N	1:B:235:ILE:HD12	2.08	0.60
1:B:230:ILE:HG13	1:B:230:ILE:O	2.01	0.60
1:A:276:LEU:O	1:A:280:ILE:HG12	2.01	0.60
1:B:184:PHE:CD1	1:B:215:TYR:CE2	2.90	0.60
1:B:159:ARG:HH11	1:B:159:ARG:HB2	1.61	0.59
1:B:236:GLU:H	1:B:236:GLU:CD	2.03	0.58
1:A:3:MET:HE2	1:A:6:MET:CE	2.34	0.58
1:B:1:MET:HG3	1:B:5:ASP:HB2	1.86	0.57
1:B:148:HIS:O	1:B:149:GLU:C	2.46	0.57
1:A:17:LYS:O	1:A:17:LYS:HD2	2.05	0.56
1:A:13:LYS:HA	1:A:16:LYS:HE2	1.88	0.56
1:A:51:ILE:HD12	1:A:115:GLN:HG3	1.88	0.55
1:B:204:VAL:HG12	1:B:208:TYR:CD2	2.41	0.55
1:A:73:TYR:HB3	1:A:76:GLU:HG2	1.87	0.55
1:A:235:ILE:HD12	1:A:235:ILE:N	2.22	0.55
1:B:227:MET:O	1:B:230:ILE:HG22	2.07	0.55
1:B:52:ASP:HB2	6:B:482:HOH:O	2.06	0.55
1:B:223:PHE:CZ	1:B:249:ILE:HD11	2.42	0.55
1:A:3:MET:HE2	1:A:6:MET:HE3	1.89	0.54
1:A:236:GLU:H	1:A:236:GLU:CD	2.15	0.54
1:A:84:ARG:O	1:A:88:MET:HG2	2.08	0.53
1:B:45:ARG:HH22	3:B:304:POP:P2	2.30	0.53
1:B:237:ALA:HB1	1:B:241:ILE:HD12	1.91	0.53
1:B:234:SER:C	1:B:238:GLN:NE2	2.54	0.53
1:B:246:ARG:HA	1:B:249:ILE:HD12	1.91	0.53
1:B:238:GLN:HE21	1:B:238:GLN:H	1.58	0.52
1:B:245:ALA:O	1:B:249:ILE:HG13	2.09	0.52
1:B:268:VAL:HG12	1:B:272:LYS:HB3	1.90	0.52
1:B:223:PHE:CE1	1:B:249:ILE:CD1	2.84	0.52
1:A:204:VAL:O	1:A:204:VAL:CG2	2.57	0.52
1:B:236:GLU:OE2	1:B:236:GLU:N	2.23	0.51
1:B:243:LEU:O	1:B:247:ILE:HG13	2.12	0.50
1:A:75:TYR:CE1	1:A:95:GLN:HG2	2.47	0.50
1:B:186:LYS:O	1:B:187:GLN:C	2.55	0.50
1:B:43:VAL:CG2	1:B:86:ILE:CG2	2.90	0.50
1:B:148:HIS:O	1:B:149:GLU:O	2.30	0.50
1:A:239:PRO:HD3	1:A:284:TYR:CE2	2.47	0.50
1:B:236:GLU:O	1:B:240:ILE:HD12	2.12	0.50
1:B:75:TYR:CE1	1:B:95:GLN:HG2	2.47	0.50
1:A:189:LEU:HD23	1:A:211:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASN:O	1:A:284:TYR:O	2.30	0.49
1:B:159:ARG:CG	1:B:159:ARG:NH1	2.50	0.49
1:B:179:ASN:O	1:B:180:GLU:HB2	2.11	0.49
1:B:227:MET:HE1	1:B:230:ILE:HD13	1.94	0.49
1:A:18:HIS:CB	1:A:45:ARG:HD3	2.42	0.49
1:B:159:ARG:NH1	1:B:159:ARG:HG3	2.14	0.49
1:A:57:ILE:C	1:A:57:ILE:HD13	2.38	0.49
1:A:187:GLN:OE1	1:A:188:ARG:CZ	2.61	0.49
1:B:18:HIS:CB	1:B:45:ARG:HD3	2.43	0.48
3:A:304:POP:O	5:A:306:651:CAM	2.62	0.48
1:B:12:HIS:HB2	1:B:38:TRP:CE3	2.48	0.48
1:B:83:ASP:CG	1:B:86:ILE:HD12	2.37	0.48
3:A:304:POP:O3	6:A:503:HOH:O	2.18	0.48
1:B:41:TYR:C	1:B:41:TYR:CD1	2.93	0.47
1:B:200:TYR:HA	1:B:262:LEU:HD22	1.97	0.47
1:B:1:MET:HG3	1:B:5:ASP:CB	2.44	0.47
1:B:213:GLU:OE2	1:B:260:TYR:OH	2.23	0.47
1:B:119:MET:HE2	1:B:119:MET:HB3	1.83	0.47
1:A:170:LEU:HD21	1:A:215:TYR:HB2	1.96	0.46
1:B:201:GLN:HG3	1:B:202:ASN:OD1	2.15	0.46
1:A:235:ILE:H	1:A:235:ILE:CD1	2.28	0.46
1:A:46:LYS:NZ	1:A:59:PHE:HZ	2.14	0.46
5:A:306:651:HAK	6:A:501:HOH:O	2.01	0.46
1:A:261:THR:HG21	1:A:264:GLU:HG3	1.96	0.46
1:B:107:LEU:HA	1:B:132:GLY:O	2.15	0.46
1:B:43:VAL:HG22	1:B:86:ILE:CG2	2.46	0.46
1:B:15:MET:HA	1:B:41:TYR:CE1	2.50	0.46
1:B:52:ASP:CB	6:B:482:HOH:O	2.64	0.46
1:B:229:GLN:HA	1:B:231:LYS:NZ	2.31	0.46
1:B:223:PHE:CZ	1:B:249:ILE:CD1	2.99	0.45
1:B:126:LEU:HD13	1:B:183:TYR:O	2.16	0.45
1:B:43:VAL:HG22	1:B:86:ILE:HG22	1.99	0.45
1:B:24:TYR:CD2	1:B:24:TYR:C	2.93	0.45
1:B:209:ILE:O	1:B:213:GLU:HG2	2.16	0.45
1:B:237:ALA:O	1:B:238:GLN:C	2.59	0.45
1:A:3:MET:CE	1:A:6:MET:HE3	2.44	0.45
1:A:16:LYS:HB2	1:A:16:LYS:HE3	1.60	0.45
1:A:177:PHE:O	1:A:180:GLU:N	2.34	0.45
1:B:98:ASN:C	1:B:98:ASN:ND2	2.75	0.45
1:B:43:VAL:HG23	1:B:86:ILE:CG2	2.47	0.45
1:B:205:ASN:HD21	1:B:207:HIS:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLU:O	1:B:35:LYS:HG3	2.16	0.44
1:A:21:SER:HA	1:A:273:LYS:HE2	1.99	0.44
1:B:46:LYS:NZ	6:B:469:HOH:O	2.50	0.44
1:A:236:GLU:O	1:A:240:ILE:HD13	2.17	0.44
1:B:146:SER:HA	1:B:234:SER:HB3	2.00	0.44
1:A:231:LYS:HD3	1:A:231:LYS:HA	1.52	0.44
1:A:260:TYR:O	1:A:262:LEU:HD12	2.17	0.44
1:B:188:ARG:HA	1:B:188:ARG:HD3	1.80	0.44
1:B:269:GLU:H	1:B:269:GLU:HG3	1.66	0.44
1:A:43:VAL:HG21	1:A:90:LEU:HD22	1.99	0.44
1:A:64:LYS:HB2	1:A:108:ILE:HD13	1.99	0.44
1:A:150:THR:OG1	1:A:152:GLN:HG2	2.17	0.44
1:B:165:GLN:O	1:B:168:ASN:HB3	2.18	0.44
1:B:248:TYR:HA	1:B:251:ILE:HD12	1.99	0.43
1:B:16:LYS:HG3	1:B:23:SER:OG	2.18	0.43
1:A:174:GLY:O	1:A:178:GLU:HG3	2.18	0.43
1:B:111:VAL:O	1:B:114:ASP:HB2	2.18	0.43
1:B:145:LEU:O	1:B:146:SER:OG	2.32	0.43
1:A:98:ASN:OD1	1:A:98:ASN:C	2.61	0.43
1:B:246:ARG:NH1	1:B:250:GLU:OE1	2.45	0.43
1:B:184:PHE:CE1	1:B:215:TYR:CD2	3.06	0.43
1:A:53:VAL:HG21	1:B:54:TYR:OH	2.19	0.42
1:B:268:VAL:CG1	1:B:272:LYS:HB3	2.48	0.42
3:A:304:POP:O	5:A:306:651:HAMA	2.19	0.42
1:A:259:ASN:OD1	6:A:497:HOH:O	2.21	0.42
1:B:46:LYS:HG3	1:B:86:ILE:HD13	2.02	0.42
1:B:231:LYS:H	1:B:231:LYS:HG3	1.57	0.42
1:A:278:HIS:O	1:A:279:GLU:C	2.63	0.42
3:B:304:POP:O	5:B:305:651:CAM	2.68	0.41
1:A:159:ARG:HG2	1:A:226:VAL:CG2	2.51	0.41
1:A:177:PHE:C	1:A:179:ASN:N	2.78	0.41
1:B:237:ALA:HB1	1:B:241:ILE:CD1	2.50	0.41
1:A:26:PHE:HD1	1:A:29:LEU:HD11	1.86	0.41
1:B:57:ILE:HG13	1:B:112:TYR:HE1	1.86	0.41
1:B:145:LEU:C	1:B:146:SER:OG	2.64	0.41
1:A:40:ILE:HD13	1:A:140:VAL:HG12	2.03	0.41
1:A:13:LYS:HE3	6:A:478:HOH:O	2.20	0.40
1:A:46:LYS:HD2	1:A:46:LYS:HA	1.72	0.40
1:B:159:ARG:CB	1:B:159:ARG:CZ	2.98	0.40
1:A:41:TYR:CD1	1:A:41:TYR:C	2.98	0.40
1:A:46:LYS:HZ3	1:A:59:PHE:HZ	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ASP:O	1:B:34:ARG:NH1	2.55	0.40
1:B:243:LEU:HD22	1:B:277:PHE:CD2	2.56	0.40
1:B:147:ASP:OD1	1:B:147:ASP:N	2.53	0.40
1:A:58:GLN:HB2	6:A:484:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:459:HOH:O	6:B:448:HOH:O[4_545]	2.07	0.13

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	282/287 (98%)	271 (96%)	10 (4%)	1 (0%)	30	28
1	B	282/287 (98%)	261 (93%)	20 (7%)	1 (0%)	30	28
All	All	564/574 (98%)	532 (94%)	30 (5%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	GLU
1	A	82	SER

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	257/260 (99%)	232 (90%)	25 (10%)	8	5
1	B	257/260 (99%)	224 (87%)	33 (13%)	4	2
All	All	514/520 (99%)	456 (89%)	58 (11%)	5	3

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	MET
1	A	13	LYS
1	A	16	LYS
1	A	23	SER
1	A	46	LYS
1	A	57	ILE
1	A	58	GLN
1	A	72	LYS
1	A	84	ARG
1	A	115	GLN
1	A	118	THR
1	A	133	VAL
1	A	152	GLN
1	A	163	SER
1	A	175	GLU
1	A	180	GLU
1	A	187	GLN
1	A	223	PHE
1	A	230	ILE
1	A	231	LYS
1	A	236	GLU
1	A	248	TYR
1	A	281	ASN
1	A	283	LYS
1	B	13	LYS
1	B	57	ILE
1	B	98	ASN
1	B	133	VAL
1	B	142	THR
1	B	147	ASP
1	B	148	HIS
1	B	149	GLU

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Mol	Chain	Res	Type
1	B	159	ARG
1	B	181	ARG
1	B	190	LYS
1	B	201	GLN
1	B	204	VAL
1	B	205	ASN
1	B	221	LYS
1	B	223	PHE
1	B	227	MET
1	B	228	ASP
1	B	229	GLN
1	B	231	LYS
1	B	235	ILE
1	B	236	GLU
1	B	238	GLN
1	B	246	ARG
1	B	248	TYR
1	B	255	VAL
1	B	259	ASN
1	B	261	THR
1	B	264	GLU
1	B	269	GLU
1	B	281	ASN
1	B	282	SER
1	B	283	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	202	ASN
1	A	263	HIS
1	B	98	ASN
1	B	148	HIS
1	B	152	GLN
1	B	179	ASN
1	B	229	GLN
1	B	238	GLN
1	B	257	GLN
1	B	263	HIS
1	B	281	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](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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	POP	B	304	2	6,8,8	0.75	0	12,13,13	1.07	1 (8%)
3	POP	A	304	2	6,8,8	0.81	0	12,13,13	1.07	1 (8%)
5	651	B	305	-	23,24,24	1.67	3 (13%)	27,35,35	1.58	6 (22%)
4	TLA	A	305	-	9,9,9	1.49	2 (22%)	12,12,12	2.33	7 (58%)
5	651	A	306	-	23,24,24	1.75	5 (21%)	27,35,35	1.74	5 (18%)

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	POP	B	304	2	-	0/6/6/6	-
3	POP	A	304	2	-	0/6/6/6	-
5	651	B	305	-	-	4/10/31/31	0/5/4/4
4	TLA	A	305	-	-	12/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	651	A	306	-	-	4/10/31/31	0/5/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	305	651	CAQ-CAP	-5.10	1.36	1.49
5	A	306	651	CAQ-CAP	-4.53	1.38	1.49
5	A	306	651	CAK-CAS	-3.42	1.44	1.53
5	B	305	651	CAK-CAS	-3.27	1.45	1.53
4	A	305	TLA	C3-C4	-3.21	1.48	1.52
5	B	305	651	CAO-CAU	-3.18	1.49	1.53
5	A	306	651	CAU-CAR	-2.85	1.49	1.52
5	A	306	651	CAO-CAU	-2.82	1.49	1.53
4	A	305	TLA	O11-C1	-2.16	1.23	1.30
5	A	306	651	CAO-NAT	-2.08	1.41	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	306	651	CAM-NAT-CAO	-6.10	100.36	109.46
4	A	305	TLA	O4-C4-C3	-3.98	111.02	121.62
4	A	305	TLA	O41-C4-C3	3.84	123.99	113.31
4	A	305	TLA	O11-C1-C2	3.17	122.12	113.31
5	A	306	651	CAF-CAP-CAQ	-3.14	115.84	121.25
5	B	305	651	CAM-CAK-CAS	-3.05	104.23	111.08
5	B	305	651	CAM-NAT-CAO	-2.90	105.14	109.46
5	B	305	651	CAE-CAP-CAQ	-2.72	116.55	121.25
5	A	306	651	CAM-CAK-CAS	-2.69	105.03	111.08
3	A	304	POP	O5-P2-O	2.68	113.61	104.64
5	B	305	651	CAF-CAP-CAQ	2.38	125.37	121.25
5	A	306	651	CAE-CAP-CAQ	2.38	125.36	121.25
3	B	304	POP	O5-P2-O	2.37	112.58	104.64
4	A	305	TLA	O2-C2-C3	-2.33	105.43	110.17
4	A	305	TLA	O3-C3-C4	2.32	115.64	110.69
5	A	306	651	CAJ-CAR-CAU	-2.18	117.88	121.07
5	B	305	651	CAC-CAE-CAP	2.18	123.02	120.54
5	B	305	651	CAL-CAN-NAT	-2.14	107.60	111.08
4	A	305	TLA	C2-C3-C4	-2.14	105.08	109.82
4	A	305	TLA	O11-C1-O1	-2.14	119.22	124.08

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	TLA	O2-C2-C3-O3
4	A	305	TLA	C1-C2-C3-O3
4	A	305	TLA	O2-C2-C3-C4
4	A	305	TLA	O1-C1-C2-O2
4	A	305	TLA	O11-C1-C2-O2
4	A	305	TLA	O3-C3-C4-O4
4	A	305	TLA	O3-C3-C4-O41
4	A	305	TLA	C2-C3-C4-O41
4	A	305	TLA	C1-C2-C3-C4
4	A	305	TLA	C2-C3-C4-O4
5	B	305	651	CAI-CAR-CAU-OAA
5	B	305	651	CAJ-CAR-CAU-OAA
4	A	305	TLA	O11-C1-C2-C3
5	B	305	651	CAI-CAR-CAU-CAS
5	A	306	651	CAI-CAR-CAU-OAA
5	A	306	651	CAJ-CAR-CAU-OAA
5	A	306	651	CAJ-CAR-CAU-CAS
5	B	305	651	CAJ-CAR-CAU-CAS
4	A	305	TLA	O1-C1-C2-C3
5	A	306	651	CAI-CAR-CAU-CAS

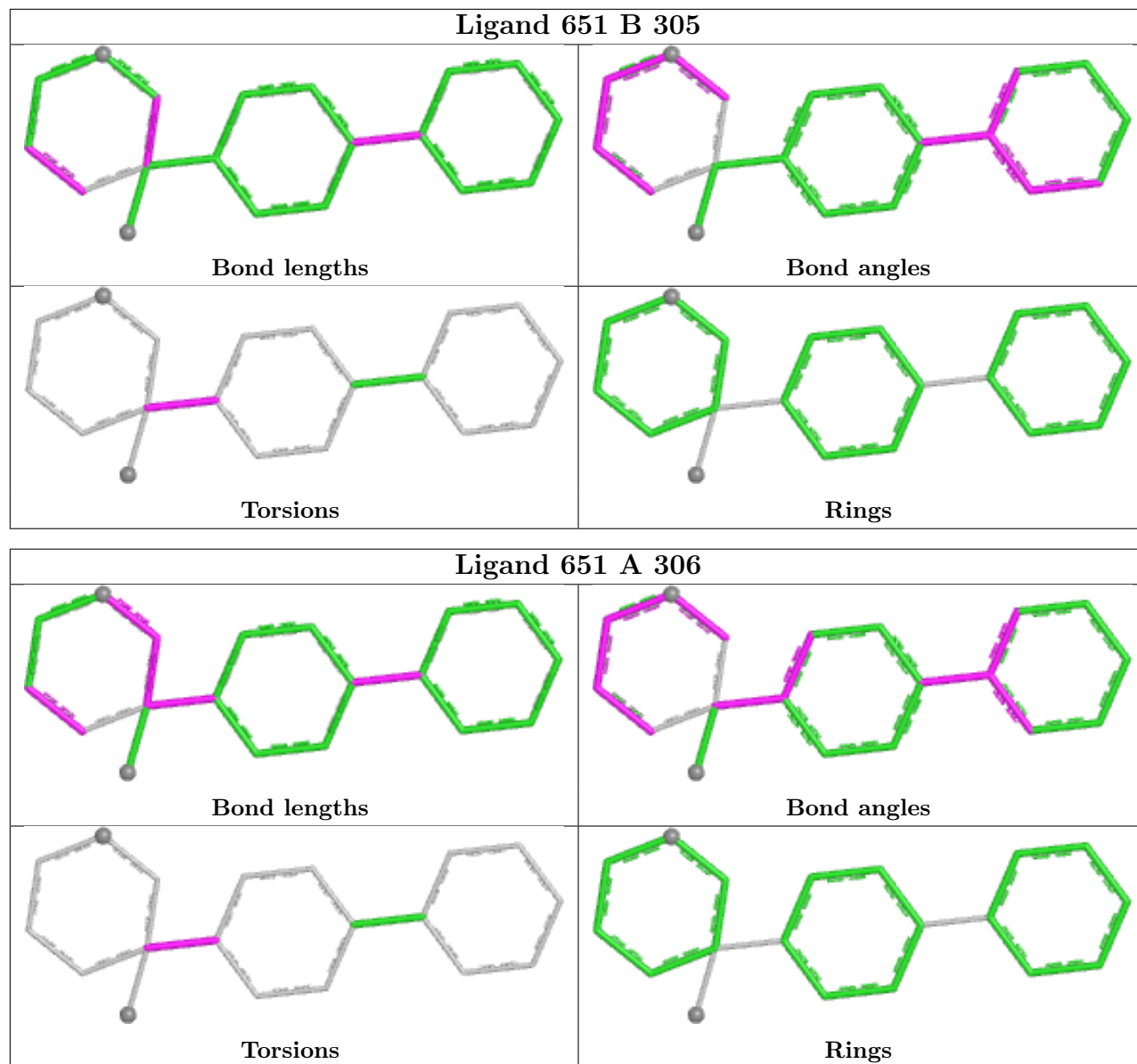
There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	304	POP	2	0
3	A	304	POP	3	0
5	B	305	651	3	0
4	A	305	TLA	3	0
5	A	306	651	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.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	284/287 (98%)	0.12	3 (1%) 78 80	24, 42, 64, 87	0
1	B	284/287 (98%)	0.27	6 (2%) 63 66	25, 48, 71, 104	0
All	All	568/574 (98%)	0.19	9 (1%) 70 73	24, 44, 69, 104	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	PHE	3.2
1	A	204	VAL	2.8
1	B	277	PHE	2.6
1	B	151	HIS	2.5
1	A	223	PHE	2.4
1	B	199	VAL	2.3
1	B	274	ALA	2.3
1	A	284	TYR	2.0
1	B	284	TYR	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.

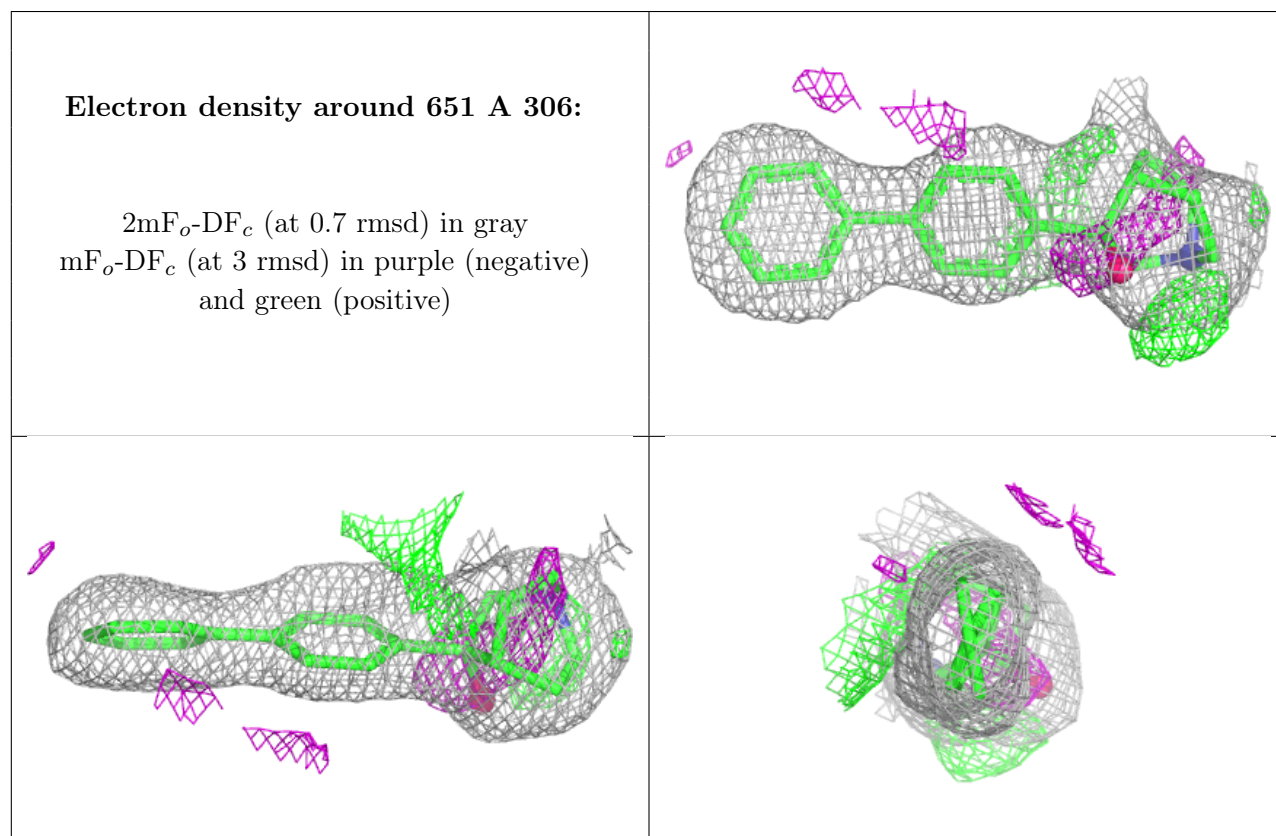
6.4 Ligands [i](#)

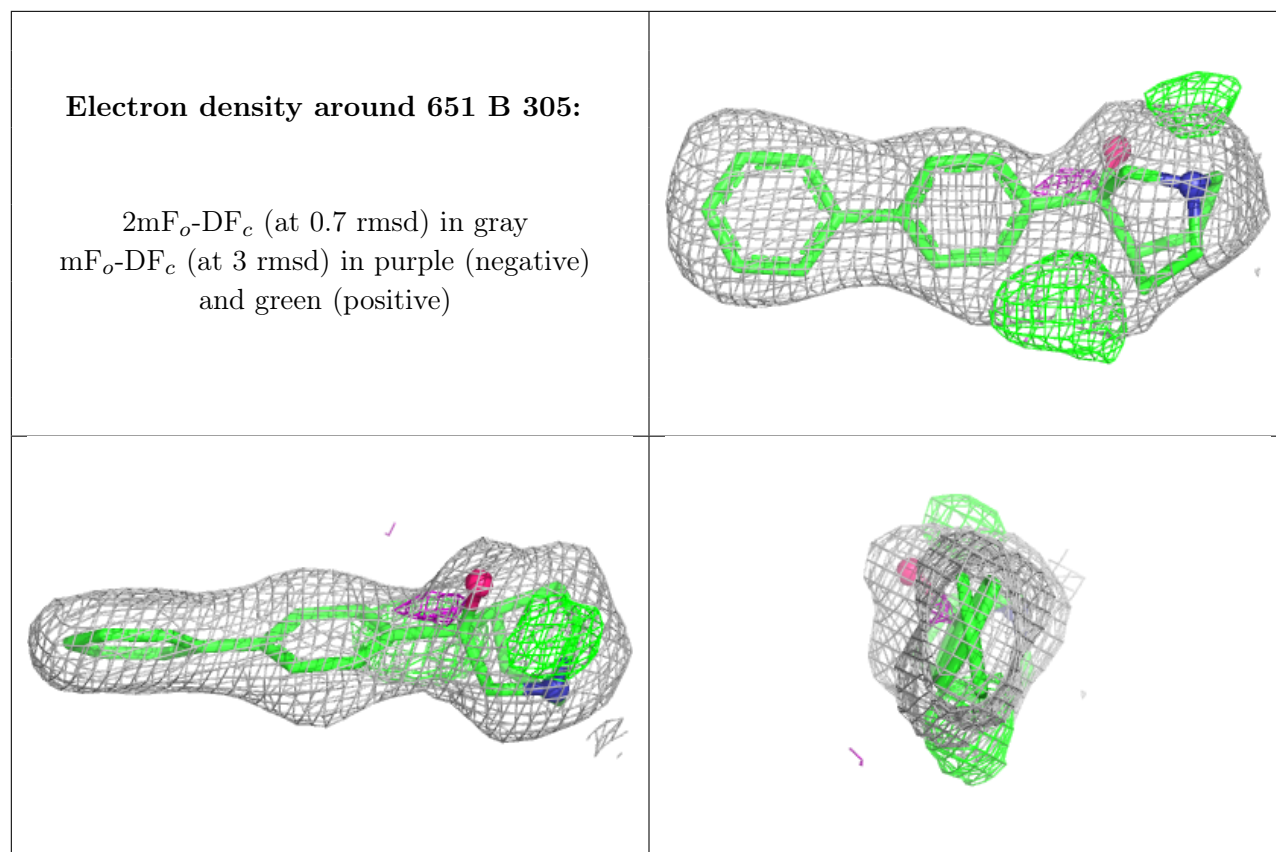
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
4	TLA	A	305	10/10	0.76	0.11	47,57,62,63	0
5	651	A	306	21/21	0.82	0.12	26,35,42,52	0
5	651	B	305	21/21	0.85	0.11	33,39,44,48	0
3	POP	B	304	9/9	0.98	0.06	26,31,35,37	0
2	MG	A	301	1/1	0.98	0.05	34,34,34,34	0
2	MG	A	302	1/1	0.98	0.04	23,23,23,23	0
3	POP	A	304	9/9	0.98	0.04	25,27,28,30	0
2	MG	B	303	1/1	0.99	0.02	37,37,37,37	0
2	MG	A	303	1/1	0.99	0.02	29,29,29,29	0
2	MG	B	301	1/1	0.99	0.02	29,29,29,29	0
2	MG	B	302	1/1	1.00	0.02	33,33,33,33	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.