



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 01:33 PM BST

PDB ID : 1Y5X  
Title : tRNA-guanine Transglycosylase (TGT) in complex with 6-Amino-4-[2-(4-methoxyphenyl)ethyl]-1,7-dihydro-8H-imidazo[4,5-g]quinazolin-8-one  
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Deposited on : 2004-12-03  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

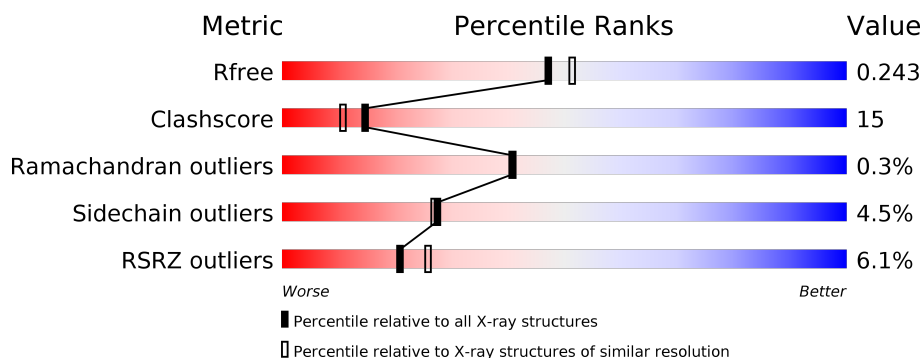
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>• 5%</div> </div> </div>
1	D	385	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>• 9%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5863 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.

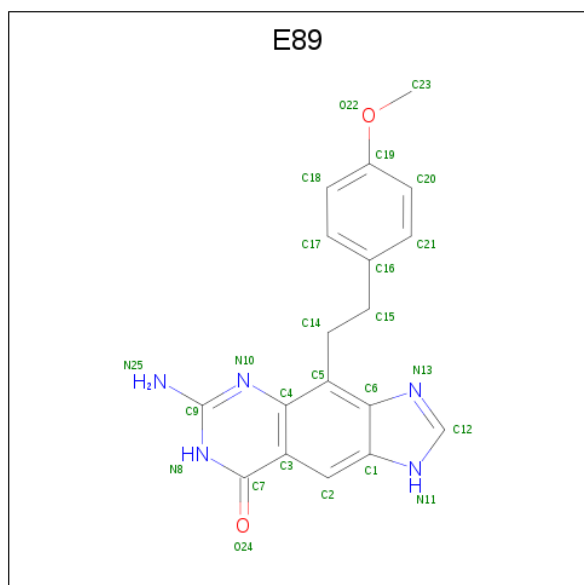
- Molecule 1 is a protein called Queuine tRNA-ribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2847	1785	512	529	21			
1	D	352	Total	C	N	O	S	0	0	0
			2721	1707	487	506	21			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 6-AMINO-4-[2-(4-METHOXYPHENYL)ETHYL]-1,7-DIHYDRO-8H-IMIDAZO[4,5-G]QUINAZOLIN-8-ONE (three-letter code: E89) (formula: C<sub>18</sub>H<sub>17</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	18	5	2		
3	D	1	Total	C	N	O	0	0
			25	18	5	2		

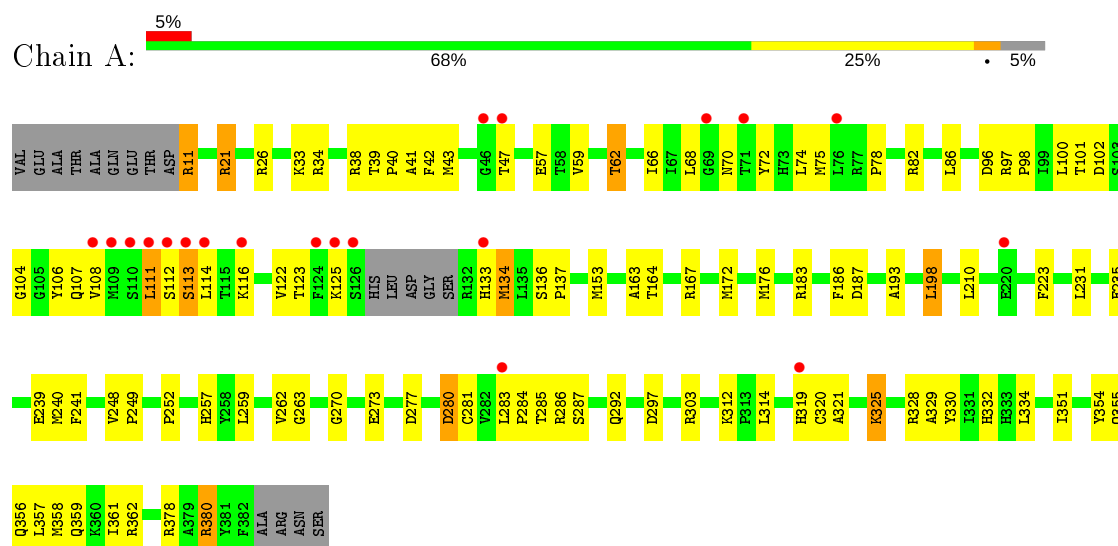
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	D	107	Total	O	0	0
			107	107		

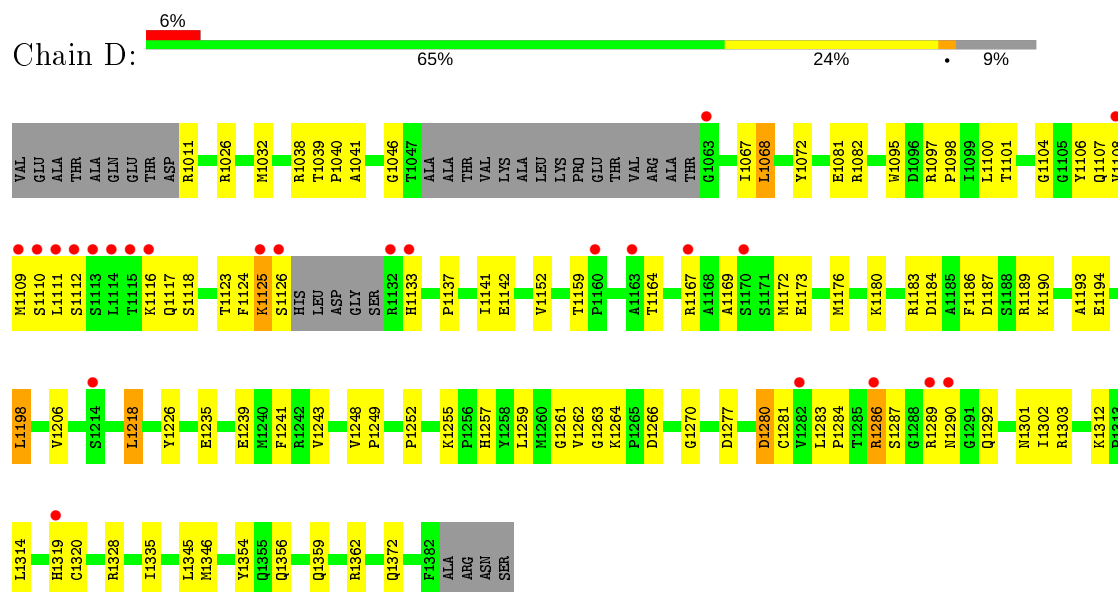
### 3 Residue-property plots

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: Queuine tRNA-ribosyltransferase



#### • Molecule 1: Queuine tRNA-ribosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.11Å 64.21Å 88.08Å 90.00° 95.11° 90.00°	Depositor
Resolution (Å)	19.84 – 2.10 19.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.7 (19.84-2.10) 90.5 (19.84-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.09Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.221 , 0.255 0.212 , 0.243	Depositor DCC
$R_{free}$ test set	2128 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.84 % 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 4.0911e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, E89

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	0.32	0/2906	0.57	0/3915
1	D	0.34	0/2779	0.57	0/3743
All	All	0.33	0/5685	0.57	0/7658

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2847	0	2784	95	0
1	D	2721	0	2625	74	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	25	0	17	1	0
3	D	25	0	17	1	0
4	A	136	0	0	5	0
4	D	107	0	0	0	0
All	All	5863	0	5443	169	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 15.

All (169) 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:164:THR:HG23	1:A:167:ARG:HH21	1.22	1.01
1:D:1116:LYS:HB3	1:D:1123:THR:HB	1.39	1.00
1:A:111:LEU:HD23	1:A:111:LEU:H	1.37	0.88
1:D:1335:ILE:HD11	1:D:1346:MET:HG3	1.54	0.87
1:D:1112:SER:HA	1:D:1126:SER:HB2	1.61	0.81
1:D:1263:GLY:HA3	1:D:1281:CYS:HB2	1.63	0.80
1:A:164:THR:HG23	1:A:167:ARG:NH2	1.96	0.79
1:A:62:THR:HG21	1:A:351:ILE:HG22	1.65	0.79
1:D:1068:LEU:HD21	1:D:1280:ASP:HB2	1.66	0.78
1:D:1319:HIS:H	1:D:1356:GLN:HE22	1.33	0.76
1:A:319:HIS:H	1:A:356:GLN:HE22	1.32	0.76
1:A:321:ALA:O	1:A:325:LYS:HD3	1.85	0.75
1:D:1263:GLY:HA3	1:D:1281:CYS:CB	2.15	0.75
1:D:1301:ASN:HD21	1:D:1303:ARG:HB2	1.53	0.73
1:D:1287:SER:HB3	1:D:1292:GLN:HB3	1.71	0.72
1:D:1281:CYS:SG	1:D:1283:LEU:HD23	2.30	0.69
1:A:47:THR:O	1:A:70:ASN:HB3	1.92	0.69
1:A:68:LEU:HD22	1:A:280:ASP:HB2	1.74	0.69
1:D:1108:VAL:O	1:D:1112:SER:HB3	1.95	0.66
1:A:62:THR:HG21	1:A:351:ILE:CG2	2.25	0.66
1:A:263:GLY:HA3	1:A:281:CYS:CB	2.26	0.65
1:A:78:PRO:HB2	1:A:82:ARG:HD2	1.78	0.64
1:A:62:THR:HG23	1:A:355:GLN:HG3	1.80	0.64
1:D:1169:ALA:O	1:D:1173:GLU:HG3	1.98	0.63
1:D:1302:ILE:HG21	1:D:1335:ILE:HD12	1.81	0.62
1:D:1263:GLY:HA3	1:D:1281:CYS:SG	2.39	0.61
1:A:359:GLN:NE2	1:A:362:ARG:HH21	1.97	0.60
1:A:357:LEU:O	1:A:361:ILE:HG12	2.00	0.60
1:A:21:ARG:HH11	1:A:21:ARG:HB3	1.67	0.59
1:D:1183:ARG:HD2	1:D:1187:ASP:OD2	2.02	0.59
1:A:68:LEU:CD1	1:A:100:LEU:HD22	2.33	0.58
1:D:1335:ILE:HD11	1:D:1346:MET:CG	2.32	0.58
1:A:108:VAL:O	1:A:112:SER:HB2	2.04	0.58
1:D:1125:LYS:H	1:D:1125:LYS:HD3	1.69	0.58
1:A:11:ARG:HD3	1:A:33:LYS:O	2.04	0.58
1:A:68:LEU:HD11	1:A:100:LEU:HD22	1.86	0.57
1:A:38:ARG:O	1:A:41:ALA:HB2	2.04	0.57
1:D:1106:TYR:O	1:D:1109:MET:HG2	2.04	0.57
1:A:263:GLY:HA3	1:A:281:CYS:SG	2.44	0.57
1:A:59:VAL:O	1:A:62:THR:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HB3	1:A:123:THR:HB	1.87	0.56
1:D:1301:ASN:ND2	1:D:1303:ARG:HB2	2.20	0.56
1:A:106:TYR:HD2	1:A:107:GLN:NE2	2.04	0.56
1:A:39:THR:HA	1:A:40:PRO:C	2.24	0.56
1:A:330:TYR:CE2	1:A:334:LEU:HD11	2.42	0.55
1:A:82:ARG:O	1:A:86:LEU:HD23	2.07	0.55
1:A:319:HIS:H	1:A:356:GLN:NE2	2.04	0.55
1:D:1286:ARG:HG3	1:D:1286:ARG:HH11	1.72	0.55
1:D:1011:ARG:HD2	1:D:1032:MET:O	2.07	0.54
1:A:231:LEU:HD13	1:A:240:MET:HG3	1.90	0.54
1:A:273:GLU:OE1	1:A:378:ARG:NH2	2.35	0.54
1:A:287:SER:HB3	1:A:292:GLN:HB3	1.90	0.53
1:A:111:LEU:CD2	1:A:111:LEU:H	2.17	0.53
1:A:70:ASN:O	1:A:74:LEU:HG	2.07	0.53
1:D:1252:PRO:O	1:D:1257:HIS:HE1	1.91	0.53
1:D:1359:GLN:NE2	1:D:1362:ARG:HH21	2.06	0.53
1:D:1226:TYR:HE1	1:D:1255:LYS:HG3	1.74	0.53
1:D:1100:LEU:C	1:D:1100:LEU:HD23	2.29	0.53
1:A:102:ASP:HB2	3:A:500:E89:H17	1.90	0.52
1:A:113:SER:HB2	1:A:125:LYS:HD3	1.91	0.52
1:D:1039:THR:HA	1:D:1040:PRO:C	2.28	0.52
1:D:1180:LYS:HE3	1:D:1184:ASP:OD2	2.09	0.52
1:A:186:PHE:CD2	1:A:198:LEU:HG	2.44	0.52
1:A:297:ASP:OD1	1:A:380:ARG:HD3	2.10	0.52
1:D:1100:LEU:HD23	1:D:1101:THR:N	2.25	0.52
1:A:68:LEU:HD22	1:A:280:ASP:CB	2.40	0.51
1:A:263:GLY:HA3	1:A:281:CYS:HB2	1.91	0.51
1:D:1302:ILE:CG2	1:D:1335:ILE:HD12	2.40	0.51
1:A:116:LYS:HD3	1:A:116:LYS:C	2.30	0.51
1:D:1239:GLU:HA	1:D:1239:GLU:OE2	2.10	0.51
1:A:11:ARG:NH1	1:A:11:ARG:HB3	2.25	0.51
1:D:1290:ASN:N	1:D:1290:ASN:HD22	2.08	0.51
1:A:172:MET:O	1:A:176:MET:HG2	2.11	0.51
1:D:1172:MET:O	1:D:1176:MET:HG2	2.11	0.51
1:D:1259:LEU:HD21	1:D:1262:VAL:HG21	1.92	0.51
1:A:40:PRO:HA	1:A:277:ASP:O	2.10	0.50
1:A:100:LEU:HD23	1:A:101:THR:N	2.26	0.50
1:A:359:GLN:HE22	1:A:362:ARG:HH21	1.59	0.50
1:A:164:THR:H	1:A:167:ARG:NH2	2.09	0.50
1:D:1176:MET:SD	1:D:1218:LEU:HD13	2.52	0.50
1:A:43:MET:HG2	1:A:66:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1038:ARG:O	1:D:1041:ALA:HB2	2.12	0.49
1:D:1112:SER:OG	1:D:1124:PHE:HB2	2.12	0.49
1:A:312:LYS:O	1:A:328:ARG:HG3	2.13	0.49
1:D:1261:GLY:HA3	3:D:1500:E89:C12	2.42	0.49
1:A:113:SER:HB2	1:A:125:LYS:CD	2.42	0.49
1:A:183:ARG:HD2	1:A:187:ASP:OD2	2.13	0.49
1:A:252:PRO:O	1:A:257:HIS:HE1	1.96	0.49
1:D:1312:LYS:O	1:D:1328:ARG:HG3	2.12	0.49
1:A:123:THR:HA	1:A:133:HIS:O	2.14	0.48
1:A:104:GLY:O	1:A:108:VAL:HG23	2.14	0.48
1:A:97:ARG:HB3	1:A:98:PRO:CD	2.43	0.48
1:A:263:GLY:O	1:A:354:TYR:CE2	2.66	0.48
1:A:285:THR:HG23	1:A:286:ARG:N	2.28	0.48
1:A:72:TYR:O	1:A:75:MET:HG2	2.14	0.48
1:D:1164:THR:HG23	1:D:1167:ARG:HD3	1.96	0.47
1:D:1183:ARG:HD3	1:D:1183:ARG:O	2.14	0.47
1:A:319:HIS:HD2	1:A:356:GLN:HE21	1.61	0.47
1:A:113:SER:C	1:A:114:LEU:HD22	2.35	0.47
1:A:47:THR:HA	1:A:70:ASN:HB2	1.97	0.47
1:D:1111:LEU:C	1:D:1111:LEU:HD13	2.35	0.47
1:D:1116:LYS:CB	1:D:1123:THR:HB	2.28	0.46
1:A:62:THR:CG2	1:A:351:ILE:HG22	2.41	0.46
1:D:1283:LEU:HB2	1:D:1284:PRO:HD3	1.97	0.46
1:D:1040:PRO:HA	1:D:1277:ASP:O	2.15	0.46
1:A:354:TYR:O	1:A:358:MET:HG2	2.15	0.46
1:A:164:THR:HG23	1:A:167:ARG:HE	1.81	0.46
1:A:82:ARG:O	1:A:86:LEU:CD2	2.64	0.46
1:D:1319:HIS:H	1:D:1356:GLN:NE2	2.09	0.46
1:A:122:VAL:N	1:A:134:MET:HE1	2.31	0.45
1:A:42:PHE:CZ	1:A:284:PRO:HG2	2.52	0.45
1:A:57:GLU:HG2	4:A:2044:HOH:O	2.17	0.45
1:A:107:GLN:O	1:A:111:LEU:HD23	2.16	0.45
1:A:34:ARG:NH1	4:A:2186:HOH:O	2.48	0.45
1:A:78:PRO:HB3	4:A:2223:HOH:O	2.17	0.45
1:D:1284:PRO:HG3	1:D:1354:TYR:CE1	2.52	0.45
1:A:183:ARG:HD3	1:A:183:ARG:O	2.17	0.45
1:A:186:PHE:CE1	1:A:193:ALA:HA	2.52	0.45
1:D:1172:MET:SD	1:D:1172:MET:C	2.95	0.45
1:D:1117:GLN:O	1:D:1118:SER:HB3	2.17	0.44
1:A:113:SER:HB2	1:A:125:LYS:CG	2.48	0.44
1:D:1125:LYS:HD3	1:D:1125:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1112:SER:HA	1:D:1126:SER:CB	2.42	0.44
1:A:259:LEU:HD21	1:A:262:VAL:HG21	2.00	0.44
1:A:96:ASP:HB2	4:A:2186:HOH:O	2.18	0.44
1:D:1248:VAL:HB	1:D:1249:PRO:HD3	2.00	0.43
1:A:101:THR:O	1:A:153:MET:HG2	2.18	0.43
1:D:1206:VAL:HG12	1:D:1243:VAL:HG21	1.99	0.43
1:A:319:HIS:CD2	1:A:356:GLN:HE21	2.36	0.43
1:A:11:ARG:HH11	1:A:11:ARG:CB	2.31	0.43
1:D:1104:GLY:O	1:D:1108:VAL:HG23	2.18	0.43
1:D:1235:GLU:OE1	1:D:1235:GLU:N	2.39	0.43
1:A:283:LEU:HB2	1:A:284:PRO:HD3	2.00	0.43
1:A:285:THR:HG23	1:A:286:ARG:H	1.83	0.43
1:D:1284:PRO:HG3	1:D:1354:TYR:CZ	2.54	0.43
1:D:1046:GLY:HA3	1:D:1067:ILE:HD12	2.01	0.43
1:D:1072:TYR:HE1	1:D:1108:VAL:HG22	1.83	0.43
1:A:241:PHE:CZ	1:A:270:GLY:HA3	2.54	0.43
1:D:1290:ASN:N	1:D:1290:ASN:ND2	2.67	0.43
1:A:136:SER:HB2	1:A:137:PRO:CD	2.49	0.42
1:D:1072:TYR:HB2	1:D:1107:GLN:HB2	2.00	0.42
1:D:1190:LYS:O	1:D:1194:GLU:HG3	2.20	0.42
1:A:183:ARG:HH21	1:A:223:PHE:HA	1.84	0.42
1:D:1137:PRO:O	1:D:1141:ILE:HG12	2.19	0.42
1:D:1241:PHE:CZ	1:D:1270:GLY:HA3	2.54	0.42
1:D:1264:LYS:HG2	1:D:1266:ASP:OD1	2.20	0.42
1:D:1097:ARG:HB3	1:D:1098:PRO:CD	2.49	0.42
1:D:1124:PHE:O	1:D:1133:HIS:N	2.46	0.42
1:D:1072:TYR:OH	1:D:1111:LEU:HD12	2.19	0.42
1:A:359:GLN:NE2	1:A:362:ARG:NH2	2.66	0.42
1:A:248:VAL:HB	1:A:249:PRO:HD3	2.02	0.42
1:A:62:THR:HG23	1:A:355:GLN:CG	2.48	0.42
1:A:164:THR:CG2	1:A:167:ARG:HE	2.32	0.41
1:A:66:ILE:HG13	1:A:98:PRO:O	2.20	0.41
1:D:1072:TYR:CE1	1:D:1108:VAL:HA	2.55	0.41
1:D:1186:PHE:CE1	1:D:1193:ALA:HA	2.55	0.41
1:D:1142:GLU:HB2	1:D:1189:ARG:NH2	2.36	0.41
1:D:1372:GLN:HA	1:D:1372:GLN:NE2	2.34	0.41
1:A:183:ARG:CD	1:A:187:ASP:OD2	2.69	0.41
1:D:1095:TRP:CE2	1:D:1097:ARG:HB2	2.55	0.41
1:D:1289:ARG:C	1:D:1290:ASN:HD22	2.24	0.41
1:A:329:ALA:O	1:A:332:HIS:HB3	2.21	0.41
1:A:97:ARG:HB3	1:A:98:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HD2	4:A:2226:HOH:O	2.21	0.41
1:A:163:ALA:HA	1:A:167:ARG:NH2	2.36	0.40
1:D:1072:TYR:HB2	1:D:1107:GLN:CB	2.51	0.40
1:A:239:GLU:HA	1:A:239:GLU:OE2	2.21	0.40
1:A:235:GLU:CD	1:A:235:GLU:H	2.25	0.40
1:D:1152:VAL:O	1:D:1198:LEU:HD23	2.21	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	363/385 (94%)	349 (96%)	13 (4%)	1 (0%)	41	41
1	D	346/385 (90%)	330 (95%)	15 (4%)	1 (0%)	41	41
All	All	709/770 (92%)	679 (96%)	28 (4%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	D	1110	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	296/314 (94%)	283 (96%)	13 (4%)	28	28
1	D	281/314 (90%)	268 (95%)	13 (5%)	27	26
All	All	577/628 (92%)	551 (96%)	26 (4%)	27	27

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	21	ARG
1	A	26	ARG
1	A	62	THR
1	A	111	LEU
1	A	134	MET
1	A	198	LEU
1	A	210	LEU
1	A	280	ASP
1	A	314	LEU
1	A	320	CYS
1	A	325	LYS
1	A	380	ARG
1	D	1026	ARG
1	D	1068	LEU
1	D	1081	GLU
1	D	1082	ARG
1	D	1125	LYS
1	D	1159	THR
1	D	1198	LEU
1	D	1218	LEU
1	D	1280	ASP
1	D	1286	ARG
1	D	1314	LEU
1	D	1320	CYS
1	D	1345	LEU

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

Mol	Chain	Res	Type
1	A	192	GLN
1	A	202	GLN
1	A	237	GLN
1	A	257	HIS

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Mol	Chain	Res	Type
1	A	319	HIS
1	A	356	GLN
1	A	359	GLN
1	A	372	GLN
1	D	1202	GLN
1	D	1237	GLN
1	D	1257	HIS
1	D	1290	ASN
1	D	1301	ASN
1	D	1319	HIS
1	D	1356	GLN
1	D	1359	GLN
1	D	1372	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	E89	D	1500	-	25,28,28	1.60	5 (20%)	28,40,40	2.80	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	E89	A	500	-	25,28,28	1.64	7 (28%)	28,40,40	2.80	8 (28%)

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	E89	D	1500	-	-	0/7/7/7	0/4/4/4
3	E89	A	500	-	-	2/7/7/7	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1500	E89	C7-N8	3.32	1.38	1.33
3	A	500	E89	C7-N8	3.12	1.38	1.33
3	D	1500	E89	C20-C19	2.95	1.44	1.38
3	A	500	E89	C20-C19	2.79	1.44	1.38
3	A	500	E89	C17-C18	2.60	1.43	1.38
3	A	500	E89	O22-C19	2.33	1.42	1.37
3	D	1500	E89	C17-C18	2.29	1.42	1.38
3	A	500	E89	C18-C19	2.23	1.43	1.38
3	D	1500	E89	O22-C19	2.18	1.42	1.37
3	A	500	E89	C2-C3	2.15	1.43	1.39
3	D	1500	E89	C18-C19	2.05	1.42	1.38
3	A	500	E89	C3-C4	2.04	1.45	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1500	E89	C3-C7-N8	-9.95	117.46	124.40
3	A	500	E89	C3-C7-N8	-9.92	117.49	124.40
3	D	1500	E89	C7-C3-C4	-5.88	115.55	119.98
3	A	500	E89	C7-C3-C4	-5.78	115.63	119.98
3	A	500	E89	C3-C2-C1	-3.92	114.34	121.67
3	D	1500	E89	C3-C2-C1	-3.89	114.39	121.67
3	A	500	E89	N10-C9-N8	-3.79	122.17	127.22
3	D	1500	E89	N10-C9-N8	-3.68	122.32	127.22
3	D	1500	E89	C9-N10-C4	3.61	124.11	116.16
3	A	500	E89	C7-N8-C9	3.58	121.61	115.93
3	A	500	E89	C9-N10-C4	3.56	124.00	116.16
3	D	1500	E89	C7-N8-C9	3.37	121.28	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	E89	C3-C4-N10	-3.07	119.10	123.33
3	D	1500	E89	C3-C4-N10	-2.94	119.27	123.33
3	D	1500	E89	C15-C14-C5	-2.15	110.16	112.81
3	A	500	E89	C1-C6-N13	-2.06	103.57	107.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	E89	C18-C19-O22-C23
3	A	500	E89	C20-C19-O22-C23

There are no ring outliers.

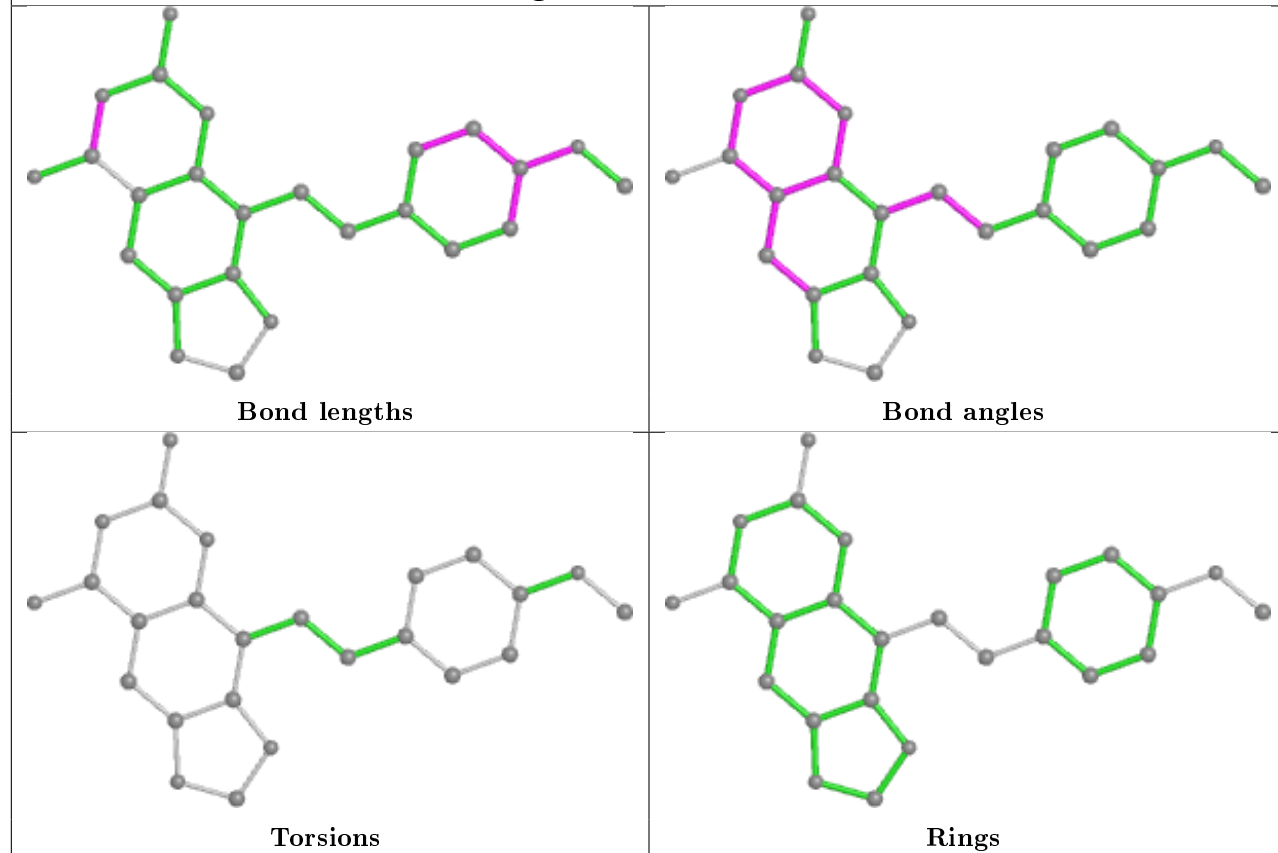
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1500	E89	1	0
3	A	500	E89	1	0

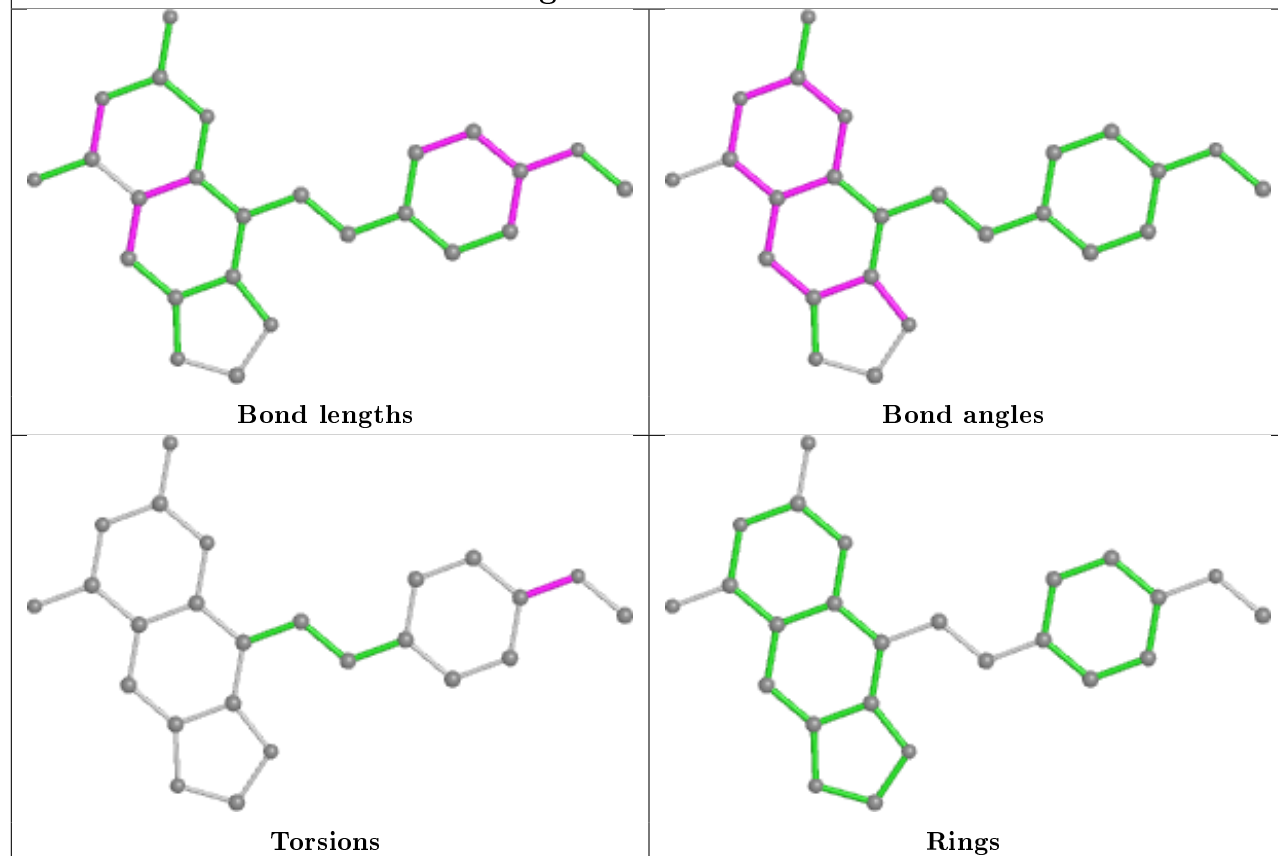
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand E89 D 1500



## Ligand E89 A 500



## 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	367/385 (95%)	0.32	20 (5%) 25 31	18, 30, 52, 84	0
1	D	352/385 (91%)	0.29	24 (6%) 17 21	16, 29, 57, 85	0
All	All	719/770 (93%)	0.30	44 (6%) 21 26	16, 29, 57, 85	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1114	LEU	12.6
1	A	114	LEU	8.6
1	A	113	SER	7.2
1	A	110	SER	5.9
1	A	109	MET	5.9
1	D	1111	LEU	4.9
1	D	1112	SER	4.8
1	D	1113	SER	4.8
1	D	1126	SER	4.3
1	D	1282	VAL	3.5
1	D	1109	MET	3.4
1	A	125	LYS	3.4
1	D	1125	LYS	3.3
1	D	1108	VAL	3.2
1	D	1110	SER	3.2
1	A	126	SER	3.1
1	D	1063	GLY	3.1
1	D	1167	ARG	3.1
1	D	1319	HIS	3.1
1	D	1116	LYS	3.0
1	A	112	SER	2.9
1	D	1163	ALA	2.9
1	A	111	LEU	2.8
1	D	1289	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	1160	PRO	2.8
1	A	76	LEU	2.7
1	A	283	LEU	2.7
1	A	47	THR	2.6
1	D	1115	THR	2.5
1	A	319	HIS	2.5
1	D	1132	ARG	2.5
1	A	124	PHE	2.4
1	A	220	GLU	2.4
1	D	1214	SER	2.3
1	A	108	VAL	2.3
1	A	69	GLY	2.3
1	A	71	THR	2.3
1	A	46	GLY	2.3
1	D	1133	HIS	2.2
1	D	1290	ASN	2.2
1	D	1286	ARG	2.2
1	D	1170	SER	2.2
1	A	133	HIS	2.1
1	A	116	LYS	2.1

## 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 monosaccharides 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.

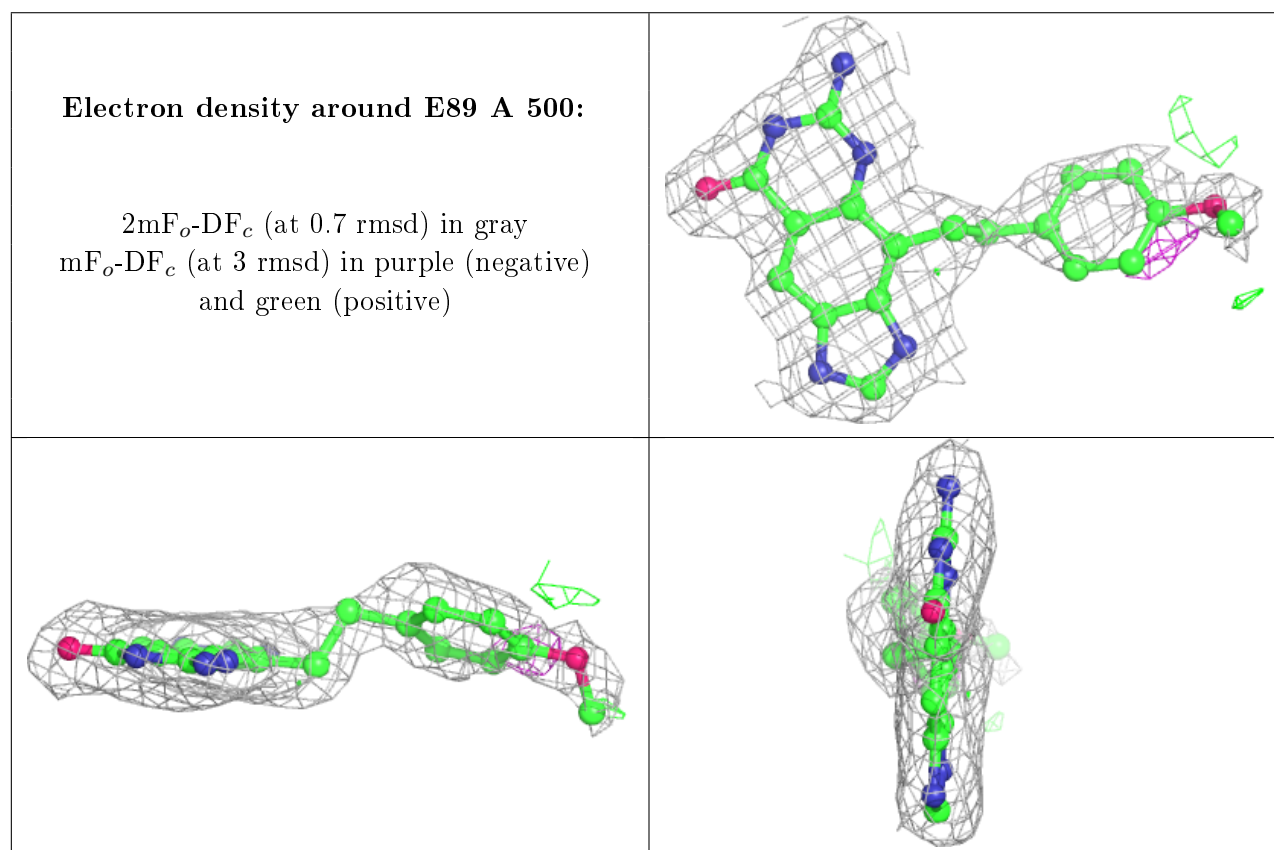
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	E89	A	500	25/25	0.85	0.17	34,40,57,58	0
3	E89	D	1500	25/25	0.93	0.12	27,30,33,34	0
2	ZN	D	1400	1/1	0.99	0.04	28,28,28,28	0

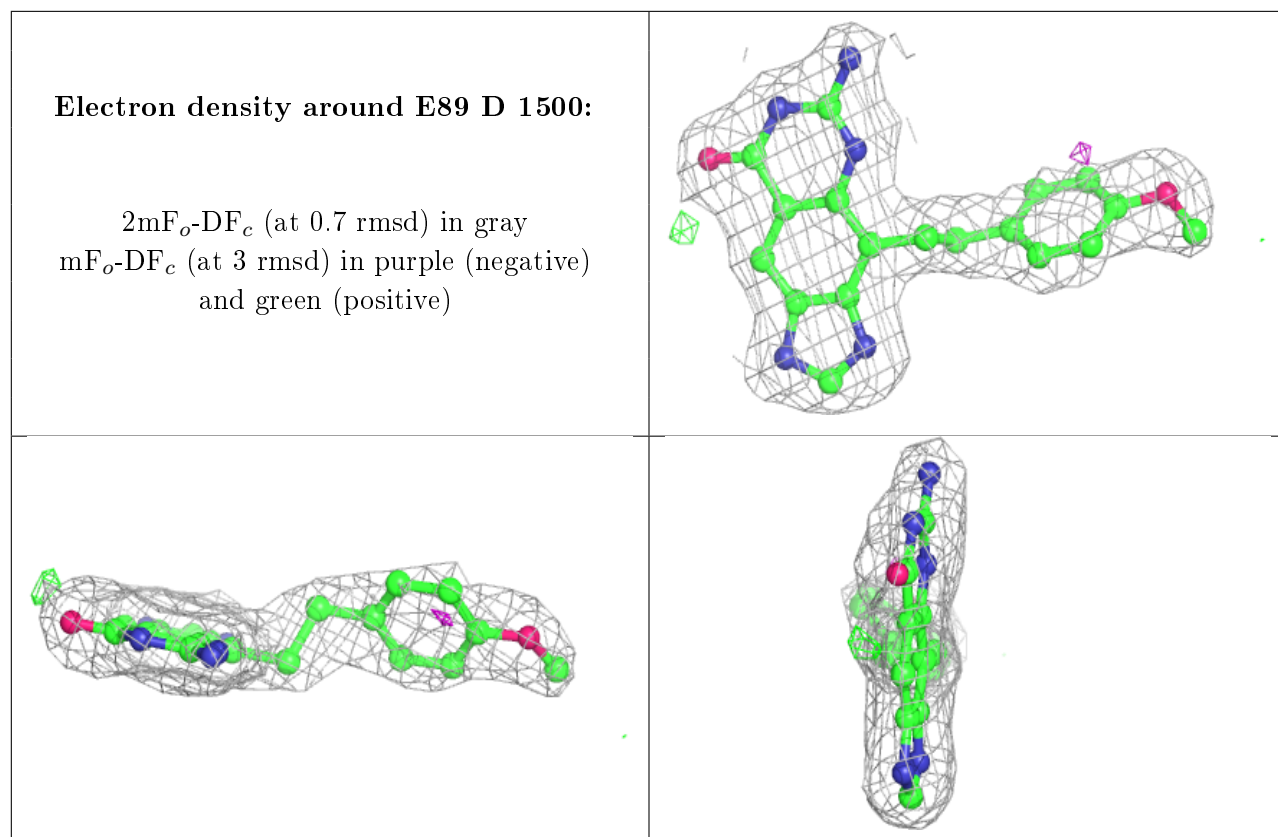
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	400	1/1	1.00	0.04	27,27,27,27	0

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.