



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 9, 2023 – 06:11 PM EST

PDB ID : 8CXZ
Title : CamA Adenine Methyltransferase Complexed to Cognate Substrate DNA and Inhibitor N6-(3-Phenylpropyl)adenosine (Compound 14)
Authors : Zhou, J.; Horton, J.R.; Cheng, X.
Deposited on : 2022-05-22
Resolution : 2.35 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

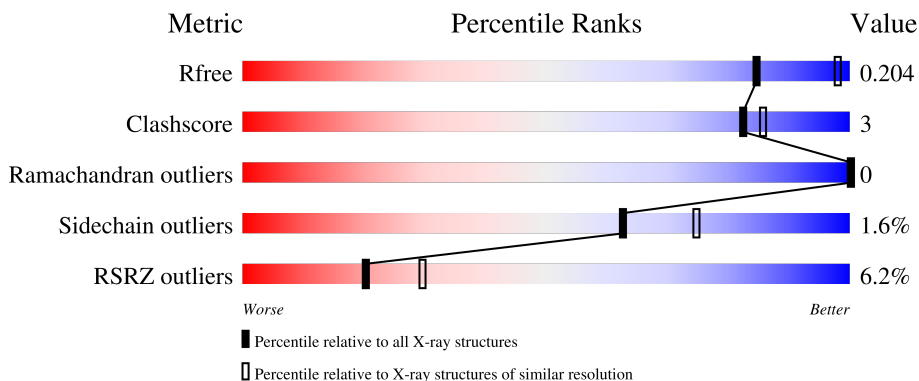
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	577	 2% 88% 6% 5%
1	B	577	 2% 88% 7% 5%
1	C	577	 12% 85% 8% 6%
2	E	14	 14% 64% 36%
2	G	14	 86% 14%

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Mol	Chain	Length	Quality of chain
2	I	14	
3	D	14	
3	F	14	
3	H	14	

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	EDO	B	603	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16061 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 Site-specific DNA-methyltransferase (adenine-specific).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	546	Total 4523	C 2942	N 723	O 841	S 17	0	0	0
1	B	550	Total 4556	C 2965	N 730	O 844	S 17	0	0	0
1	C	540	Total 4345	C 2824	N 694	O 810	S 17	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*GP*GP*GP*AP*CP*TP*TP*TP*TP*TP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	14	Total 287	C 139	N 50	O 85	P 13	0	0	0
2	G	14	Total 287	C 139	N 50	O 85	P 13	0	0	0
2	I	14	Total 287	C 139	N 50	O 85	P 13	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*TP*GP*GP*GP*AP*CP*TP*TP*TP*TP*TP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	Total 281	C 136	N 53	O 79	P 13	0	0	0
3	F	14	Total 281	C 136	N 53	O 79	P 13	0	0	0
3	H	14	Total 281	C 136	N 53	O 79	P 13	0	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



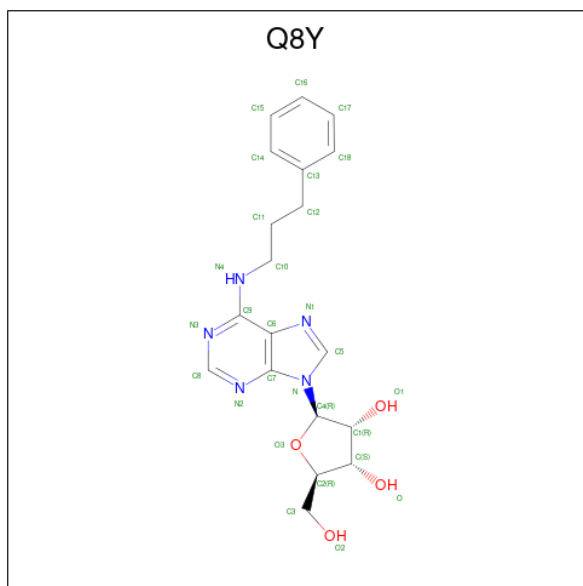
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total K 2 2	0	0
5	B	3	Total K 3 3	0	0
5	C	2	Total K 2 2	0	0

- Molecule 6 is N-(3-phenylpropyl)adenosine (three-letter code: Q8Y) (formula: C₁₉H₂₃N₅O₄)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
6	A	1	Total	C	N	O	0	0
			28	19	5	4		
6	B	1	Total	C	N	O	0	0
			28	19	5	4		
6	C	1	Total	C	N	O	0	0
			28	19	5	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	254	Total	O	0	0
			254	254		
7	B	261	Total	O	0	0
			261	261		
7	C	132	Total	O	0	0
			132	132		
7	E	32	Total	O	0	0
			32	32		
7	D	31	Total	O	0	0
			31	31		
7	F	33	Total	O	0	0
			33	33		
7	G	33	Total	O	0	0
			33	33		
7	H	19	Total	O	0	0
			19	19		

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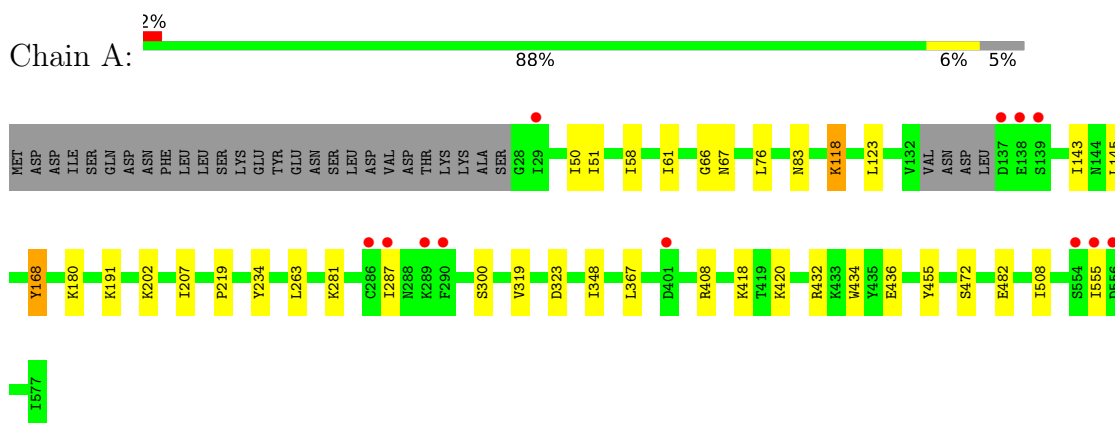
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	15	Total	O	0	0
			15	15		

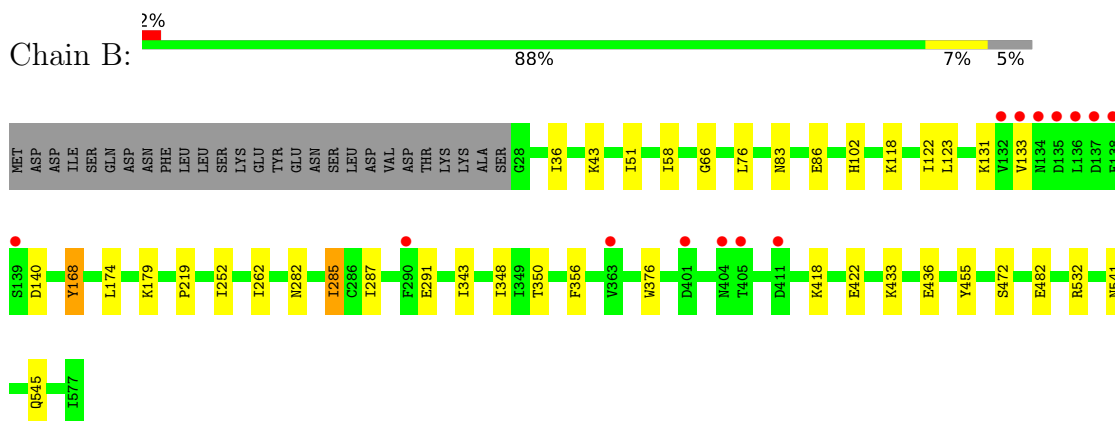
3 Residue-property plots [i](#)

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.

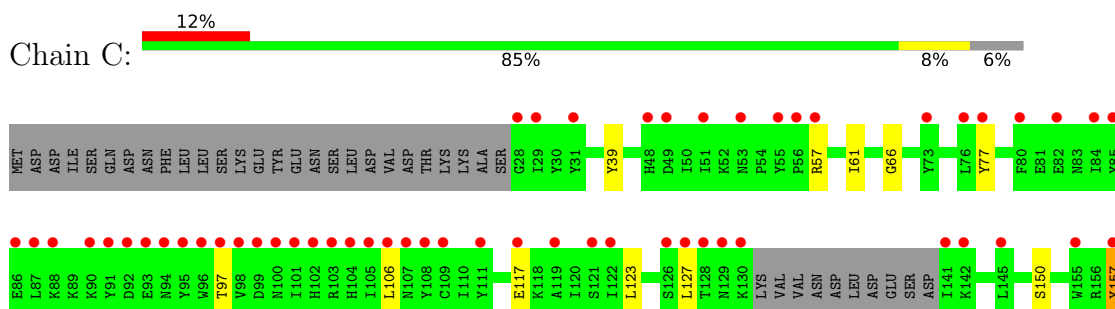
- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)

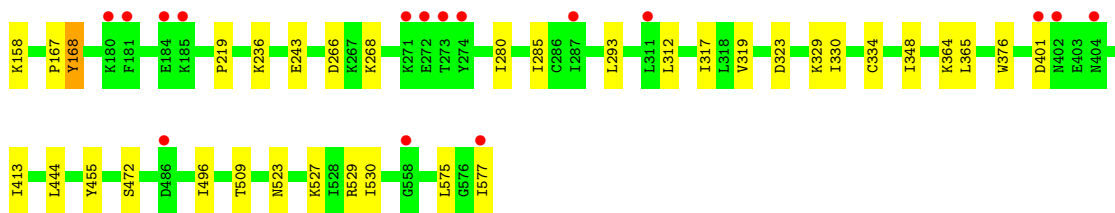


- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)

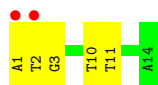


- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)





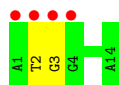
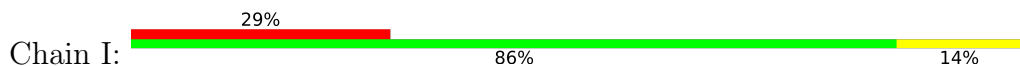
- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*GP*AP*CP*TP*TP*TP*TP*TP*GP*A)-3')



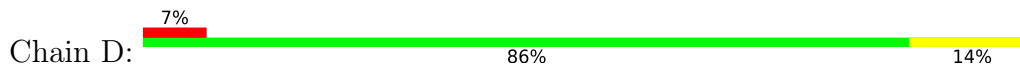
- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*GP*AP*CP*TP*TP*TP*TP*TP*GP*A)-3')



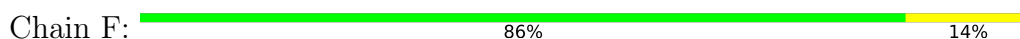
- Molecule 2: DNA (5'-D(*AP*TP*GP*GP*GP*AP*CP*TP*TP*TP*TP*TP*GP*A)-3')



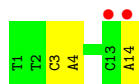
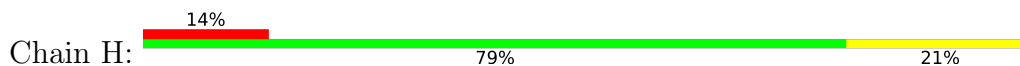
- Molecule 3: DNA (5'-D(*AP*TP*GP*GP*GP*AP*CP*TP*TP*TP*TP*TP*GP*A)-3')



- Molecule 3: DNA (5'-D(*AP*TP*GP*GP*GP*AP*CP*TP*TP*TP*TP*TP*GP*A)-3')



- Molecule 3: DNA (5'-D(*AP*TP*GP*GP*GP*AP*CP*TP*TP*TP*TP*TP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 161.43Å 229.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.89 – 2.35 45.89 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.89-2.35) 99.1 (45.89-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.174 , 0.204 0.173 , 0.204	Depositor DCC
R_{free} test set	1999 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtrriage
Anisotropy	0.475	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16061	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, Q8Y, EDO

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	0.26	0/4616	0.47	0/6212
1	B	0.26	0/4650	0.47	0/6257
1	C	0.25	0/4433	0.45	0/5983
2	E	0.58	0/321	0.99	0/495
2	G	0.62	0/321	1.03	0/495
2	I	0.58	0/321	1.00	0/495
3	D	0.54	0/315	0.87	0/483
3	F	0.51	0/315	0.85	0/483
3	H	0.47	0/315	0.82	0/483
All	All	0.31	0/15607	0.55	0/21386

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 [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	4523	0	4485	21	0
1	B	4556	0	4539	20	0
1	C	4345	0	4207	24	0
2	E	287	0	162	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	287	0	162	2	0
2	I	287	0	162	2	0
3	D	281	0	159	1	0
3	F	281	0	159	1	0
3	H	281	0	159	2	0
4	A	4	0	6	0	0
4	B	24	0	35	1	0
4	F	4	0	6	0	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	2	0	0	0	0
6	A	28	0	0	0	0
6	B	28	0	0	0	0
6	C	28	0	0	1	0
7	A	254	0	0	0	0
7	B	261	0	0	1	0
7	C	132	0	0	1	0
7	D	31	0	0	0	0
7	E	32	0	0	0	0
7	F	33	0	0	0	0
7	G	33	0	0	0	0
7	H	19	0	0	0	0
7	I	15	0	0	0	0
All	All	16061	0	14241	74	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 3.

All (74) 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:C:280:ILE:HD11	1:C:285:ILE:HG12	1.74	0.69
3:H:14:DA:H61	2:I:2:DT:H3	1.44	0.65
1:C:329:LYS:HE2	1:C:577:ILE:HG22	1.78	0.64
1:C:334:CYS:O	1:C:529:ARG:NH1	2.31	0.63
1:A:61:ILE:HD11	1:A:207:ILE:HD11	1.81	0.62
1:A:319:VAL:HG11	1:A:508:ILE:HG23	1.81	0.62
1:C:57:ARG:NH1	1:C:158:LYS:O	2.33	0.61
1:B:282:ASN:HB3	1:B:285:ILE:HD12	1.83	0.59
1:B:51:ILE:HD11	1:B:83:ASN:HB3	1.85	0.59
1:C:66:GLY:HA3	1:C:123:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LYS:NZ	1:B:422:GLU:OE2	2.32	0.58
1:B:343:ILE:HA	4:B:602:EDO:H21	1.86	0.56
1:B:58:ILE:HD13	1:B:76:LEU:HD11	1.87	0.55
1:A:66:GLY:HA3	1:A:123:LEU:HD13	1.89	0.55
1:B:66:GLY:HA3	1:B:123:LEU:HD13	1.89	0.55
1:A:482:GLU:HG3	1:B:482:GLU:HG2	1.88	0.54
3:D:13:DC:H2''	3:D:14:DA:C8	2.43	0.54
2:G:1:DA:H2''	2:G:2:DT:H5''	1.89	0.54
1:A:168:TYR:CE1	1:A:219:PRO:HD3	2.44	0.53
1:C:364:LYS:HE2	1:C:413:ILE:HG12	1.91	0.53
1:B:168:TYR:CE1	1:B:219:PRO:HD3	2.44	0.53
1:A:367:LEU:HD22	1:A:408:ARG:HG2	1.90	0.52
1:B:43:LYS:NZ	7:B:701:HOH:O	2.32	0.52
1:C:61:ILE:HG23	1:C:150:SER:HB3	1.91	0.52
2:E:2:DT:H2''	2:E:3:DG:C8	2.45	0.51
1:C:168:TYR:CE1	1:C:219:PRO:HD3	2.44	0.51
1:C:317:ILE:HD12	1:C:509:THR:HG22	1.94	0.50
1:C:57:ARG:HH22	1:C:157:TYR:HB2	1.77	0.50
1:B:252:ILE:HD12	1:B:287:ILE:HD12	1.94	0.49
1:C:529:ARG:NH2	7:C:705:HOH:O	2.44	0.49
1:B:102:HIS:CD2	1:B:131:LYS:HB2	2.49	0.48
1:B:433:LYS:HB2	1:B:436:GLU:HG2	1.95	0.47
1:A:319:VAL:HB	1:A:323:ASP:HB2	1.97	0.47
1:A:432:ARG:HG3	1:A:436:GLU:HB2	1.96	0.47
1:B:36:ILE:HD11	1:B:287:ILE:HD11	1.98	0.46
1:A:143:ILE:HG22	1:A:145:LEU:HG	1.97	0.46
2:E:1:DA:H2''	2:E:2:DT:H5''	1.98	0.45
1:A:118:LYS:HE3	1:A:118:LYS:H	1.82	0.45
1:A:51:ILE:HD11	1:A:83:ASN:HB3	1.99	0.45
1:A:348:ILE:O	1:A:472:SER:HA	2.17	0.44
1:B:118:LYS:HE3	1:B:122:ILE:HD11	1.98	0.44
1:C:39:TYR:OH	1:C:243:GLU:OE2	2.33	0.44
2:E:10:DT:H2''	2:E:11:DT:H72	1.99	0.44
1:C:496:ILE:HD11	1:C:530:ILE:HD12	1.99	0.44
1:C:376:TRP:CZ2	1:C:472:SER:HB2	2.53	0.44
1:B:348:ILE:O	1:B:472:SER:HA	2.18	0.44
1:A:202:LYS:HD2	1:A:234:TYR:CZ	2.53	0.43
1:C:348:ILE:O	1:C:472:SER:HA	2.18	0.43
1:B:174:LEU:HB3	1:B:179:LYS:HE2	2.00	0.43
1:C:319:VAL:HB	1:C:323:ASP:HB2	1.99	0.43
1:A:420:LYS:HA	1:A:420:LYS:HD2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ILE:HG12	1:C:575:LEU:HD13	2.01	0.43
1:C:39:TYR:CG	1:C:293:LEU:HD23	2.54	0.42
1:C:106:LEU:HD21	1:C:127:LEU:HB3	2.01	0.42
2:I:2:DT:H2''	2:I:3:DG:C8	2.54	0.42
2:G:1:DA:C2'	2:G:2:DT:H5''	2.49	0.42
1:C:266:ASP:HB2	1:C:268:LYS:HG3	2.01	0.42
1:B:541:ASN:O	1:B:545:GLN:HG3	2.20	0.42
1:C:236:LYS:HE2	1:C:312:LEU:HB2	2.02	0.42
1:A:191:LYS:HE3	1:A:191:LYS:HB2	1.67	0.42
1:A:418:LYS:HG3	1:A:434:TRP:CE3	2.54	0.42
1:A:287:ILE:HA	1:A:287:ILE:HD12	1.80	0.41
1:C:523:ASN:O	1:C:527:LYS:HE2	2.19	0.41
1:C:57:ARG:NH2	1:C:157:TYR:HB2	2.35	0.41
1:A:281:LYS:HD2	1:A:300:SER:O	2.21	0.41
1:B:350:THR:HB	1:B:356:PHE:CD2	2.56	0.41
1:B:36:ILE:HD12	1:B:262:ILE:HD11	2.03	0.41
3:H:3:DC:H2'	3:H:4:DA:C8	2.56	0.40
1:A:58:ILE:HD13	1:A:76:LEU:HD11	2.02	0.40
1:B:376:TRP:CZ2	1:B:472:SER:HB2	2.56	0.40
1:C:167:PRO:HG3	6:C:603:Q8Y:C5	2.50	0.40
1:A:50:ILE:HD12	1:A:50:ILE:HA	1.98	0.40
1:A:180:LYS:HE3	1:A:180:LYS:HB3	1.99	0.40
3:F:13:DC:H2''	3:F:14:DA:C8	2.56	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	542/577 (94%)	526 (97%)	16 (3%)	0	100 100
1	B	548/577 (95%)	533 (97%)	15 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	536/577 (93%)	520 (97%)	16 (3%)	0	100	100
All	All	1626/1731 (94%)	1579 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	495/547 (90%)	489 (99%)	6 (1%)	71	82
1	B	500/547 (91%)	492 (98%)	8 (2%)	62	75
1	C	460/547 (84%)	451 (98%)	9 (2%)	55	66
All	All	1455/1641 (89%)	1432 (98%)	23 (2%)	62	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	118	LYS
1	A	168	TYR
1	A	263	LEU
1	A	455	TYR
1	A	555	ILE
1	B	86	GLU
1	B	133	VAL
1	B	140	ASP
1	B	168	TYR
1	B	285	ILE
1	B	291	GLU
1	B	455	TYR
1	B	532	ARG
1	C	77	TYR
1	C	97	THR
1	C	117	GLU

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Mol	Chain	Res	Type
1	C	157	TYR
1	C	168	TYR
1	C	365	LEU
1	C	401	ASP
1	C	444	LEU
1	C	455	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	$\# Z > 2$
4	EDO	B	603	-	3,3,3	0.49	0	2,2,2	0.24	0
6	Q8Y	A	904	-	27,31,31	0.58	0	28,43,43	0.71	1 (3%)
4	EDO	B	601	-	3,3,3	0.46	0	2,2,2	0.42	0
4	EDO	B	602	-	3,3,3	0.49	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	605	-	3,3,3	0.49	0	2,2,2	0.25	0
6	Q8Y	C	603	-	27,31,31	0.55	0	28,43,43	0.61	1 (3%)
4	EDO	A	901	-	3,3,3	0.50	0	2,2,2	0.19	0
4	EDO	F	101	-	3,3,3	0.48	0	2,2,2	0.30	0
6	Q8Y	B	610	-	27,31,31	0.56	0	28,43,43	0.60	1 (3%)
4	EDO	B	606	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	B	604	5	3,3,3	0.44	0	2,2,2	0.32	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
4	EDO	B	603	-	-	0/1/1/1	-
6	Q8Y	A	904	-	-	4/9/29/29	0/4/4/4
4	EDO	B	601	-	-	1/1/1/1	-
4	EDO	B	602	-	-	0/1/1/1	-
4	EDO	B	605	-	-	0/1/1/1	-
6	Q8Y	C	603	-	-	4/9/29/29	0/4/4/4
4	EDO	A	901	-	-	0/1/1/1	-
4	EDO	F	101	-	-	0/1/1/1	-
6	Q8Y	B	610	-	-	2/9/29/29	0/4/4/4
4	EDO	B	606	-	-	0/1/1/1	-
4	EDO	B	604	5	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	603	Q8Y	C8-N3-C9	2.20	118.47	116.59
6	B	610	Q8Y	C8-N3-C9	2.16	118.44	116.59
6	A	904	Q8Y	C8-N3-C9	2.13	118.42	116.59

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	904	Q8Y	C6-C9-N4-C10
6	A	904	Q8Y	N3-C9-N4-C10

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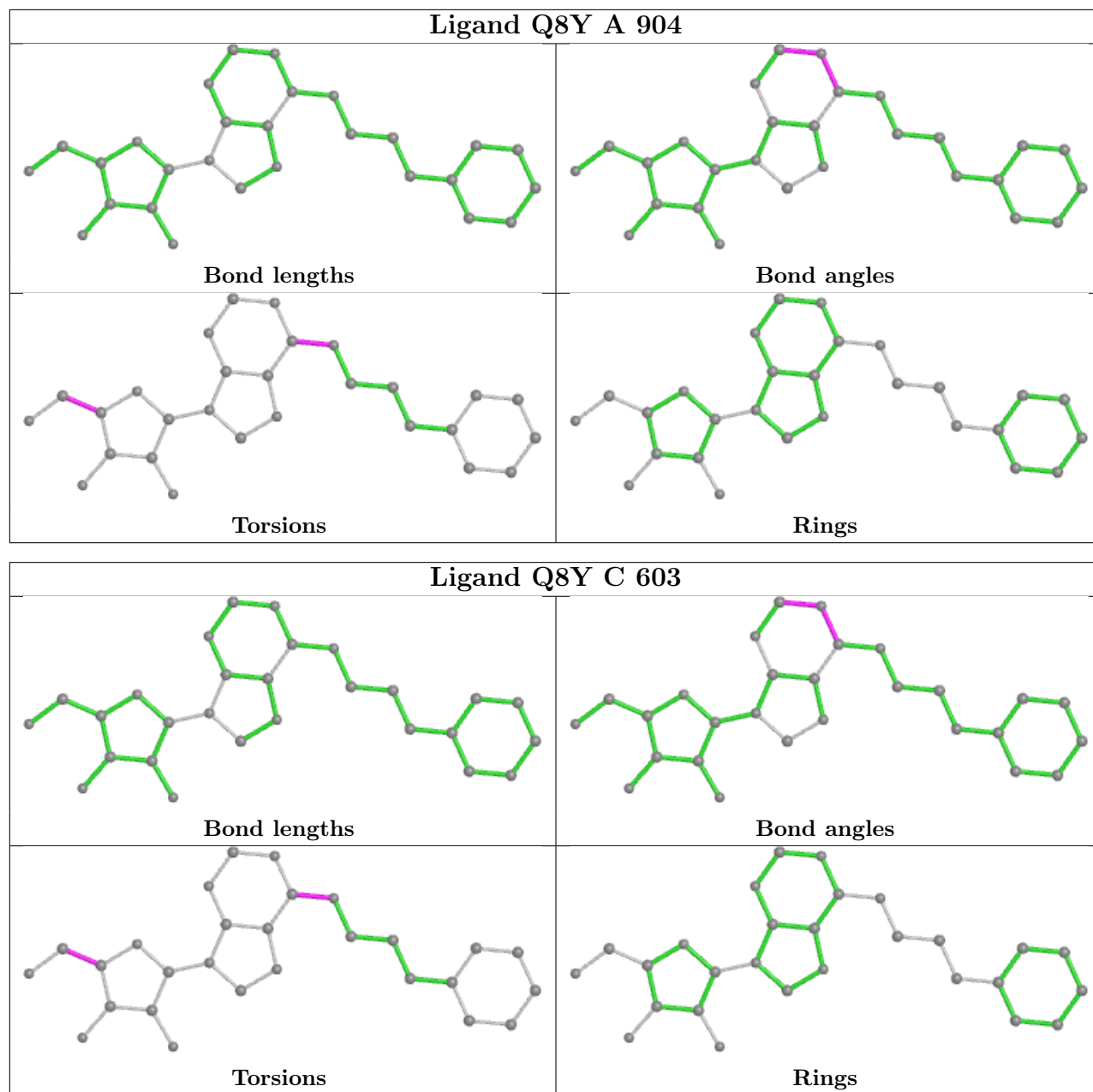
Mol	Chain	Res	Type	Atoms
6	B	610	Q8Y	C6-C9-N4-C10
6	B	610	Q8Y	N3-C9-N4-C10
6	C	603	Q8Y	C-C2-C3-O2
6	C	603	Q8Y	O3-C2-C3-O2
6	C	603	Q8Y	C6-C9-N4-C10
6	C	603	Q8Y	N3-C9-N4-C10
6	A	904	Q8Y	C-C2-C3-O2
6	A	904	Q8Y	O3-C2-C3-O2
4	B	601	EDO	O1-C1-C2-O2

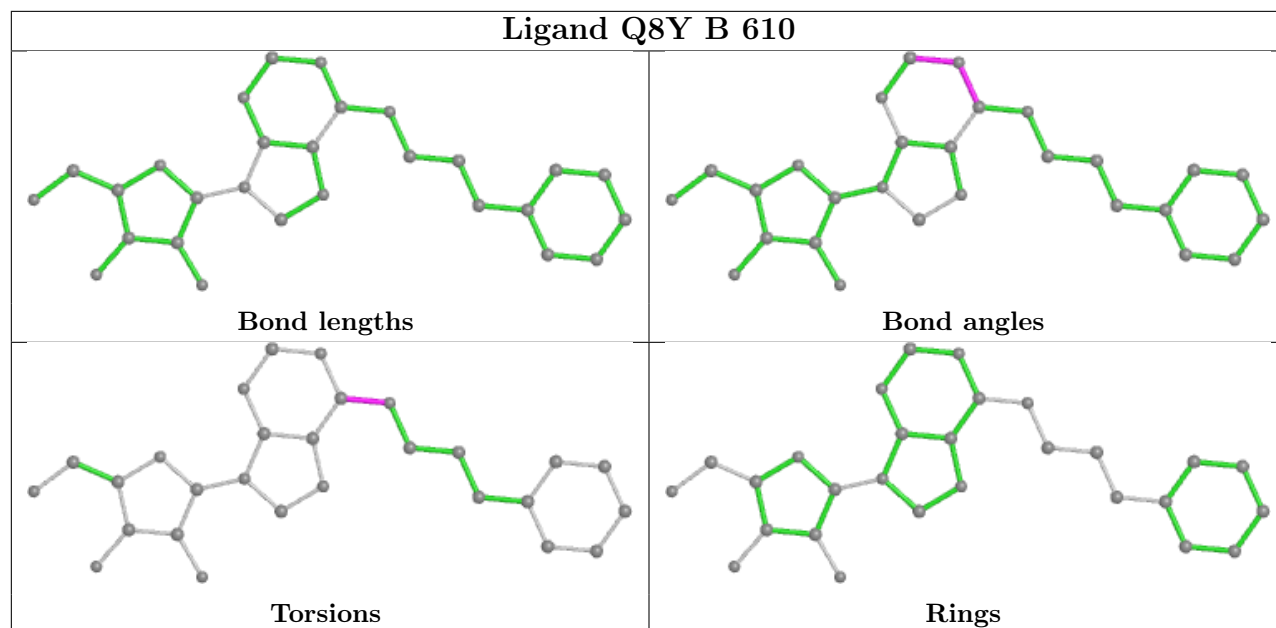
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	EDO	1	0
6	C	603	Q8Y	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, 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	546/577 (94%)	-0.12	12 (2%) 62 72	25, 44, 79, 131	0
1	B	550/577 (95%)	0.04	14 (2%) 57 67	26, 43, 74, 159	0
1	C	540/577 (93%)	0.40	71 (13%) 3 5	36, 61, 116, 145	0
2	E	14/14 (100%)	0.48	2 (14%) 2 4	34, 39, 154, 180	0
2	G	14/14 (100%)	-0.49	0 100 100	32, 36, 65, 66	0
2	I	14/14 (100%)	0.71	4 (28%) 0 0	43, 53, 156, 190	0
3	D	14/14 (100%)	0.12	1 (7%) 16 23	29, 36, 117, 136	0
3	F	14/14 (100%)	-0.11	0 100 100	29, 34, 72, 74	0
3	H	14/14 (100%)	0.50	2 (14%) 2 4	42, 58, 132, 158	0
All	All	1720/1815 (94%)	0.11	106 (6%) 20 29	25, 48, 105, 190	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	ASP	9.3
1	B	139	SER	7.4
1	C	87	LEU	6.7
1	C	55	TYR	6.5
3	H	14	DA	6.4
2	I	1	DA	6.1
1	B	136	LEU	6.1
2	E	1	DA	6.1
1	C	51	ILE	5.9
1	A	137	ASP	5.7
1	C	95	TYR	5.7
1	C	119	ALA	5.7
1	C	108	TYR	5.5
1	C	29	ILE	5.4
1	B	133	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	76	LEU	5.4
1	C	28	GLY	5.3
1	C	273	THR	5.1
1	C	80	PHE	5.1
1	C	97	THR	5.1
1	C	91	TYR	4.8
1	C	401	ASP	4.8
1	C	92	ASP	4.7
1	C	103	ARG	4.6
1	C	94	ASN	4.5
1	B	132	VAL	4.3
1	A	290	PHE	4.3
1	C	155	TRP	4.3
1	C	141	ILE	4.1
1	B	134	ASN	4.1
1	C	105	ILE	4.0
1	B	138	GLU	3.9
1	C	96	TRP	3.9
2	I	2	DT	3.8
1	C	99	ASP	3.7
1	C	107	ASN	3.7
1	C	85	TYR	3.7
1	B	290	PHE	3.6
1	C	157	TYR	3.6
1	C	73	TYR	3.6
1	C	404	ASN	3.4
2	I	3	DG	3.4
1	C	100	ASN	3.3
1	C	77	TYR	3.3
1	C	98	VAL	3.3
1	C	84	ILE	3.3
2	E	2	DT	3.2
1	C	181	PHE	3.2
1	C	272	GLU	3.1
1	C	102	HIS	3.0
1	A	554	SER	3.0
1	B	404	ASN	3.0
1	C	88	LYS	3.0
1	C	129	ASN	3.0
1	C	142	LYS	2.9
1	A	138	GLU	2.9
1	C	56	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	106	LEU	2.8
1	C	558	GLY	2.8
1	A	29	ILE	2.8
1	A	286	CYS	2.8
1	C	180	LYS	2.7
1	C	127	LEU	2.7
1	A	289	LYS	2.7
1	C	126	SER	2.7
1	B	405	THR	2.7
1	C	121	SER	2.6
1	C	122	ILE	2.6
1	C	104	HIS	2.6
1	C	93	GLU	2.6
1	C	117	GLU	2.6
1	B	401	ASP	2.6
1	C	287	ILE	2.6
3	H	13	DC	2.6
1	C	31	TYR	2.5
1	C	486	ASP	2.5
1	A	555	ILE	2.5
1	C	184	GLU	2.5
3	D	14	DA	2.4
1	C	90	LYS	2.4
1	C	48	HIS	2.4
1	C	311	LEU	2.4
1	B	363	VAL	2.4
1	A	556	ASP	2.4
1	C	271	LYS	2.4
1	A	401	ASP	2.3
1	C	185	LYS	2.3
1	A	287	ILE	2.3
1	C	274	TYR	2.3
1	C	101	ILE	2.3
1	B	411	ASP	2.3
1	C	130	LYS	2.3
1	C	49	ASP	2.2
1	C	128	THR	2.2
1	B	137	ASP	2.2
1	C	145	LEU	2.2
1	C	402	ASN	2.2
1	C	111	TYR	2.1
1	C	57	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	4	DG	2.1
1	C	86	GLU	2.1
1	A	139	SER	2.1
1	C	577	ILE	2.1
1	C	82	GLU	2.1
1	C	53	ASN	2.0
1	C	109	CYS	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 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, 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.

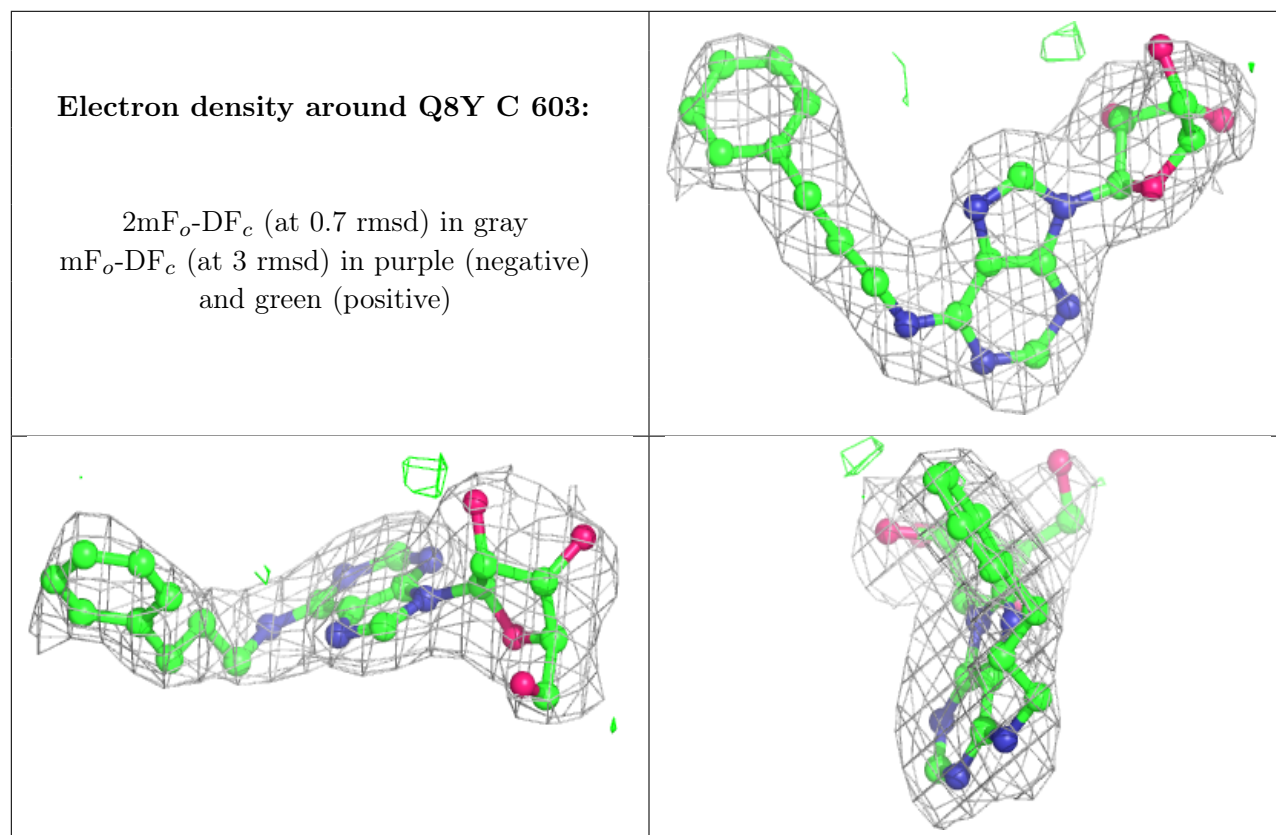
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	B	606	4/4	0.75	0.19	58,65,81,83	0
4	EDO	B	603	4/4	0.78	0.56	57,57,77,82	0
4	EDO	A	901	4/4	0.81	0.23	58,59,61,63	0
4	EDO	B	605	4/4	0.87	0.11	60,61,65,66	0
4	EDO	F	101	4/4	0.88	0.40	40,55,55,69	0
5	K	B	609	1/1	0.89	0.09	81,81,81,81	0
4	EDO	B	602	4/4	0.90	0.22	43,50,56,57	0
6	Q8Y	C	603	28/28	0.91	0.16	64,72,80,84	0
4	EDO	B	604	4/4	0.93	0.21	53,54,56,56	0
5	K	C	602	1/1	0.94	0.09	77,77,77,77	0
5	K	B	608	1/1	0.95	0.07	50,50,50,50	0
5	K	A	902	1/1	0.95	0.10	49,49,49,49	0
5	K	A	903	1/1	0.96	0.11	63,63,63,63	0
6	Q8Y	B	610	28/28	0.96	0.13	32,41,49,65	0
5	K	C	601	1/1	0.96	0.08	55,55,55,55	0
4	EDO	B	601	4/4	0.97	0.14	37,47,52,52	0

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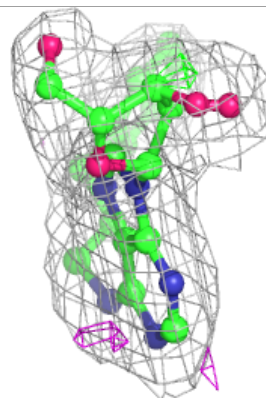
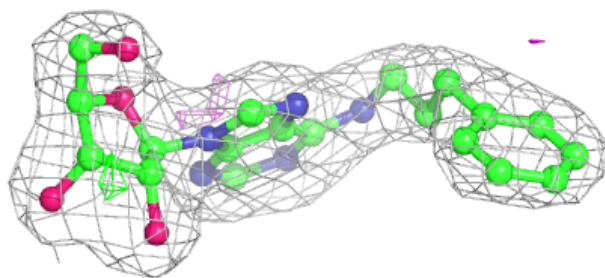
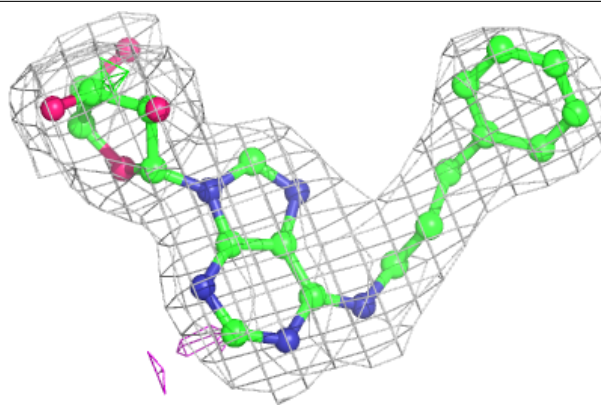
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	Q8Y	A	904	28/28	0.97	0.12	34,44,57,66	0
5	K	B	607	1/1	0.98	0.08	49,49,49,49	0

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.

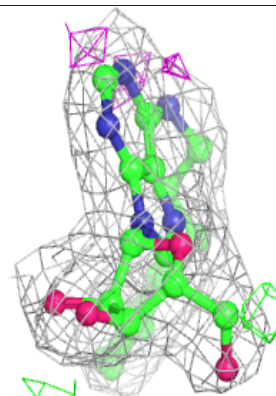
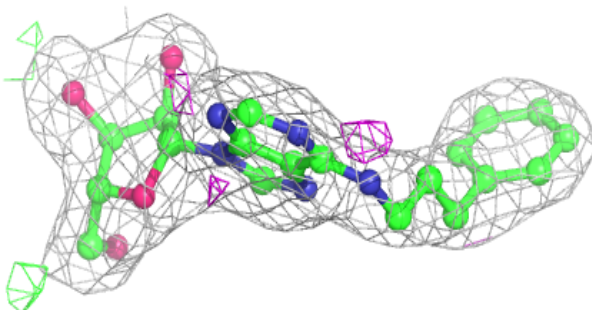
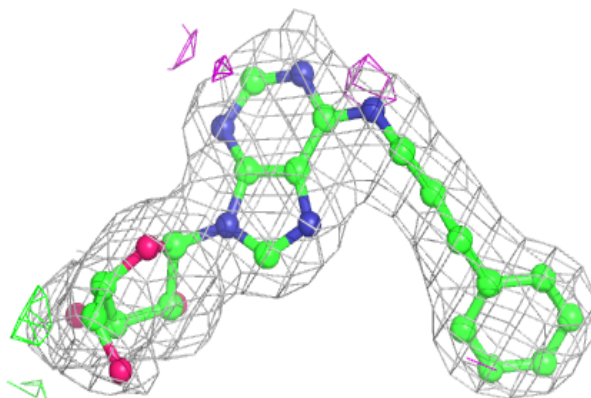


Electron density around Q8Y B 610:

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

**Electron density around Q8Y A 904:**

$2mF_o-DF_c$ (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.