



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 09:25 PM EDT

PDB ID : 8CXX
Title : CamA Adenine Methyltransferase Complexed to Cognate Substrate DNA and Compound 6
Authors : Horton, J.R.; Zhou, J.; Cheng, X.
Deposited on : 2022-05-22
Resolution : 2.34 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 : 2.36
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) : 2.36

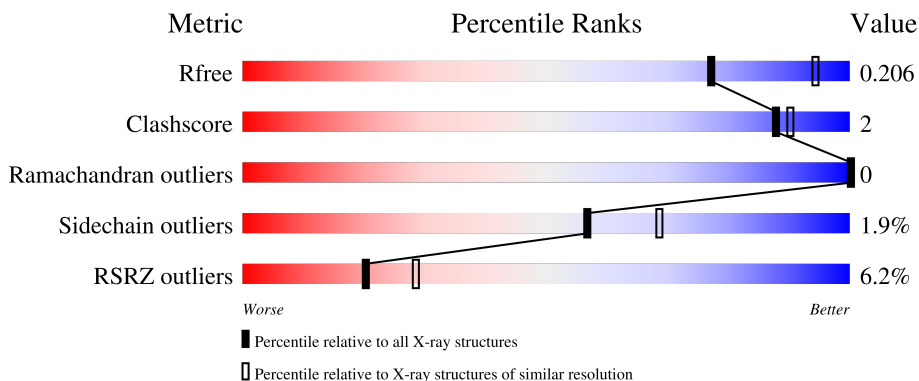
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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.



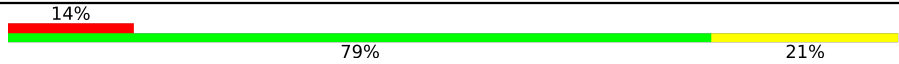

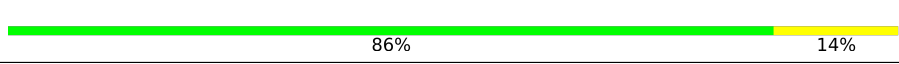
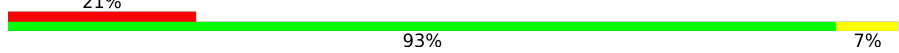
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	578	 2% 89% 5% • 6%
1	B	578	 3% 89% 6% • 5%
1	C	578	 12% 87% 6% • 7%
2	D	14	 7% 86% 14%
2	F	14	 93% 7%

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Mol	Chain	Length	Quality of chain
2	H	14	 14% 79% 21%
3	E	14	 14% 86% 14%
3	G	14	 86% 14%
3	I	14	 21% 93% 7%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15834 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 4537	C 2952	N 728	O 840	S 17	0	1	0
1	B	550	Total 4566	C 2975	N 731	O 843	S 17	0	1	0
1	C	540	Total 4361	C 2835	N 698	O 811	S 17	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q183J3
B	0	HIS	-	expression tag	UNP Q183J3
C	0	HIS	-	expression tag	UNP Q183J3

- Molecule 2 is a DNA chain called DNA Strand 1.

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

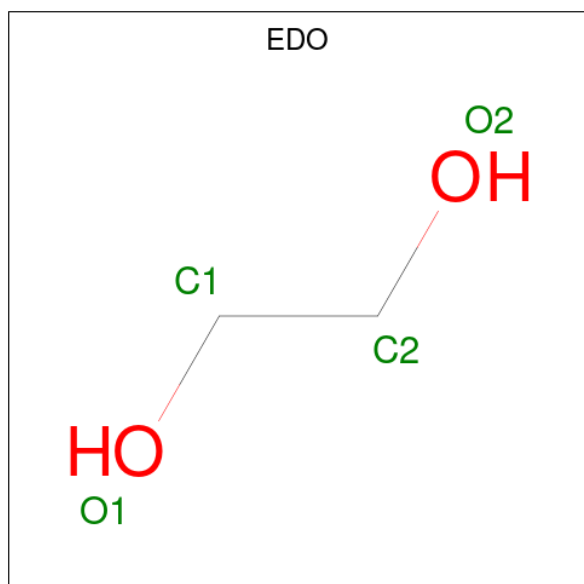
- Molecule 3 is a DNA chain called DNA Strand 2.

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



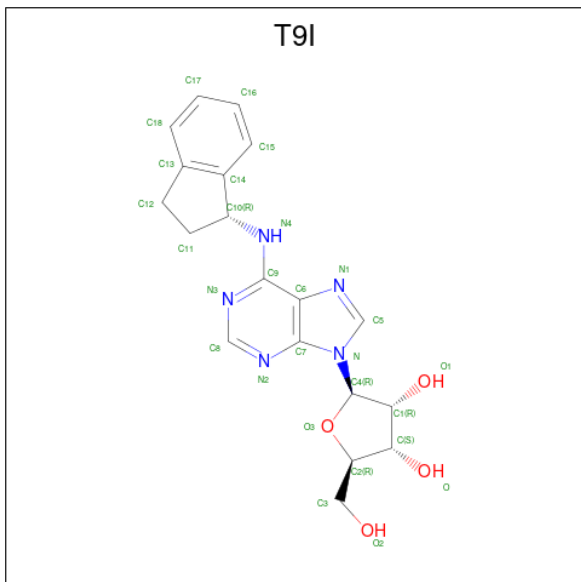
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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

- Molecule 6 is N-[(1R)-2,3-dihydro-1H-inden-1-yl]adenosine (three-letter code: T9I) (formula: C₁₉H₂₁N₅O₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	146	Total O 146 146	0	0

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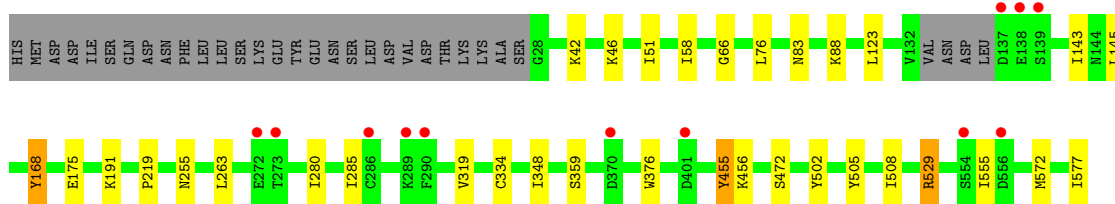
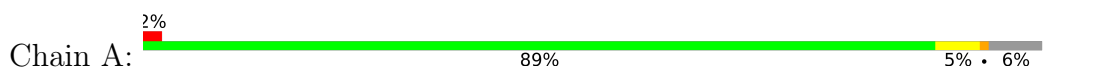
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	165	Total 165	O 165	0	0
7	C	94	Total 94	O 94	0	0
7	D	29	Total 29	O 29	0	0
7	E	19	Total 19	O 19	0	0
7	F	25	Total 25	O 25	0	0
7	G	15	Total 15	O 15	0	0
7	H	16	Total 16	O 16	0	0
7	I	14	Total 14	O 14	0	0

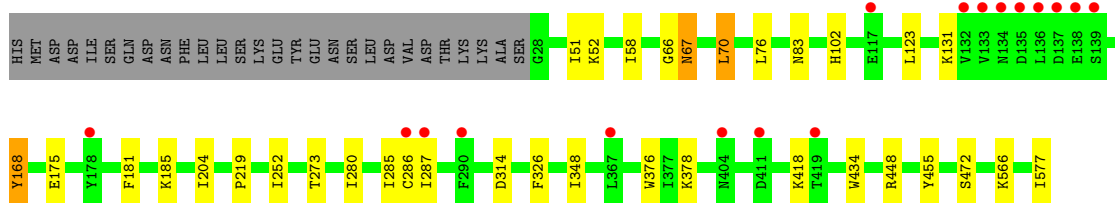
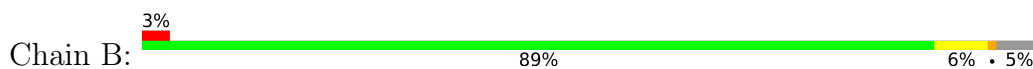
3 Residue-property plots [i](#)

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.

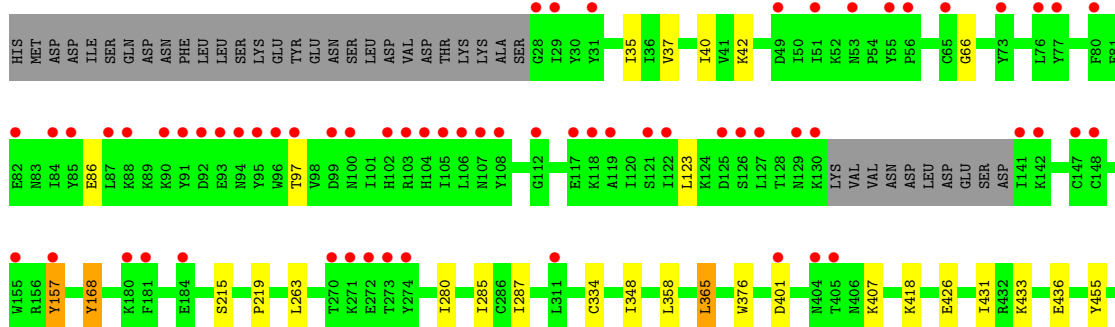
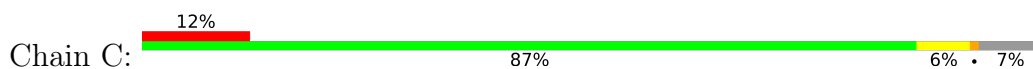
- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)



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

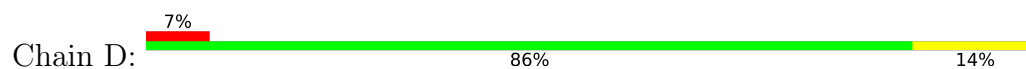


- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)





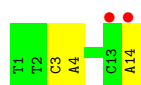
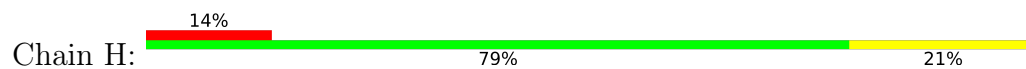
- Molecule 2: DNA Strand 1



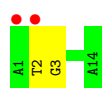
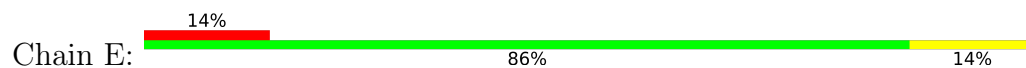
- Molecule 2: DNA Strand 1



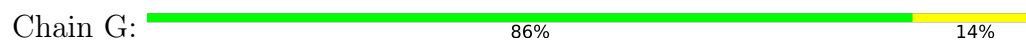
- Molecule 2: DNA Strand 1



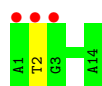
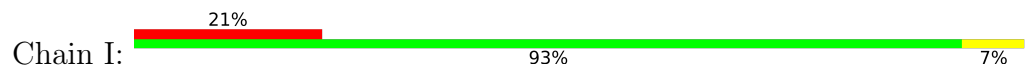
- Molecule 3: DNA Strand 2



- Molecule 3: DNA Strand 2



- Molecule 3: DNA Strand 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.76Å 161.47Å 230.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.29 – 2.34 44.29 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.2 (44.29-2.34) 96.3 (44.29-2.34)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.181 , 0.208 0.180 , 0.206	Depositor DCC
R_{free} test set	2000 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtrriage
Anisotropy	0.380	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15834	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 2.75% 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: T9I, K, 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	0.28	0/4633	0.49	0/6233
1	B	0.28	0/4664	0.49	0/6276
1	C	0.26	0/4450	0.47	0/6003
2	D	0.59	0/315	0.87	0/483
2	F	0.59	0/315	0.85	0/483
2	H	0.54	0/315	0.82	0/483
3	E	0.63	0/321	1.00	0/495
3	G	0.71	0/321	1.04	0/495
3	I	0.65	0/321	1.01	0/495
All	All	0.34	0/15655	0.57	0/21446

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	4537	0	4518	16	0
1	B	4566	0	4551	19	0
1	C	4361	0	4235	17	0
2	D	281	0	159	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	281	0	159	1	0
2	H	281	0	159	2	0
3	E	287	0	162	1	0
3	G	287	0	162	1	0
3	I	287	0	162	1	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
5	A	24	0	35	0	0
5	B	20	0	30	2	0
5	C	4	0	6	1	0
5	F	4	0	6	1	0
6	A	28	0	0	0	0
6	B	28	0	0	0	0
6	C	28	0	0	0	0
7	A	146	0	0	1	0
7	B	165	0	0	1	0
7	C	94	0	0	0	0
7	D	29	0	0	0	0
7	E	19	0	0	0	0
7	F	25	0	0	0	0
7	G	15	0	0	0	0
7	H	16	0	0	0	0
7	I	14	0	0	0	0
All	All	15834	0	14344	58	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 2.

All (58) 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:334:CYS:O	1:A:529:ARG:NH1	2.23	0.72
2:H:14:DA:H61	3:I:2:DT:H3	1.35	0.71
1:A:66:GLY:HA3	1:A:123:LEU:HD13	1.77	0.67
1:C:334:CYS:O	1:C:529:ARG:NH1	2.29	0.65
1:C:280:ILE:HD11	1:C:285:ILE:HG12	1.78	0.64
1:B:51:ILE:HD11	1:B:83:ASN:HB3	1.85	0.59
1:A:255:ASN:ND2	7:A:704:HOH:O	2.37	0.57
1:A:319:VAL:HG11	1:A:508:ILE:HG23	1.85	0.57
1:B:66:GLY:HA3	1:B:123:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:DA:H1'	3:G:2:DT:H5''	1.86	0.56
1:C:66:GLY:HA3	1:C:123:LEU:HD13	1.87	0.56
1:B:58:ILE:HD13	1:B:76:LEU:HD11	1.89	0.54
2:D:13:DC:H2''	2:D:14:DA:C8	2.42	0.54
1:B:168:TYR:CE1	1:B:219:PRO:HD3	2.43	0.54
3:E:2:DT:H2''	3:E:3:DG:C8	2.43	0.53
1:B:566:LYS:HG3	5:B:1007:EDO:H12	1.91	0.53
1:B:252:ILE:HD12	1:B:287:ILE:HD12	1.91	0.52
1:A:572:MET:HG2	1:A:577:ILE:HG13	1.92	0.52
1:C:168:TYR:CE1	1:C:219:PRO:HD3	2.45	0.51
1:A:280:ILE:HD11	1:A:285:ILE:HG12	1.93	0.50
1:B:67:ASN:OD1	1:B:67:ASN:N	2.43	0.49
1:B:204:ILE:HD11	5:B:1008:EDO:H12	1.94	0.49
1:A:168:TYR:CE1	1:A:219:PRO:HD3	2.48	0.49
1:C:35:ILE:HD11	1:C:287:ILE:HG13	1.95	0.49
1:A:51:ILE:HD11	1:A:83:ASN:HB3	1.95	0.48
1:A:58:ILE:HD13	1:A:76:LEU:HD11	1.94	0.48
1:C:496:ILE:HD11	1:C:530:ILE:HD12	1.96	0.47
1:B:280:ILE:HD11	1:B:285:ILE:HG12	1.96	0.47
1:C:376:TRP:CZ2	1:C:472:SER:HB2	2.50	0.47
1:C:86:GLU:OE1	1:C:86:GLU:N	2.48	0.47
1:C:40:ILE:HG23	1:C:215:SER:HB3	1.97	0.46
1:A:455:TYR:CZ	1:A:456:LYS:HD2	2.50	0.46
1:B:181:PHE:CE1	1:B:185:LYS:HG3	2.51	0.46
1:C:426:GLU:HG3	1:C:431:ILE:HD11	1.98	0.46
1:C:433:LYS:HB2	1:C:436:GLU:HG3	1.98	0.46
2:F:3:DC:O3'	5:F:101:EDO:H21	2.15	0.45
1:A:143:ILE:HG22	1:A:145:LEU:HG	1.98	0.45
1:A:348:ILE:O	1:A:472:SER:HA	2.16	0.45
2:H:3:DC:H2'	2:H:4:DA:C8	2.52	0.45
1:A:376:TRP:CZ2	1:A:472:SER:HB2	2.52	0.45
1:C:348:ILE:O	1:C:472:SER:HA	2.17	0.45
1:B:348:ILE:O	1:B:472:SER:HA	2.18	0.44
1:B:376:TRP:CZ2	1:B:472:SER:HB2	2.53	0.44
1:B:326:PHE:CE2	1:B:577:ILE:HD12	2.53	0.44
1:C:418:LYS:HD2	5:C:603:EDO:H22	1.99	0.43
1:C:358:LEU:HD12	1:C:365:LEU:HD13	2.01	0.43
1:B:418:LYS:HE2	1:B:434:TRP:CE2	2.54	0.43
1:B:448:ARG:HD3	7:B:1140:HOH:O	2.18	0.43
1:C:157:TYR:CD1	1:C:157:TYR:N	2.86	0.43
1:A:191:LYS:HE3	1:A:191:LYS:HB2	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:HE3	1:B:52:LYS:HB2	1.75	0.42
1:B:70:LEU:HD12	1:B:70:LEU:HA	1.85	0.41
1:C:464:ILE:HG13	1:C:494:VAL:HG11	2.00	0.41
1:B:102:HIS:CD2	1:B:131:LYS:HB2	2.56	0.41
1:C:502:TYR:HA	1:C:505:TYR:HB3	2.02	0.41
1:A:42:LYS:HG2	1:A:46:LYS:HB3	2.03	0.40
1:A:502:TYR:HA	1:A:505:TYR:HB3	2.03	0.40
1:B:378:LYS:HB3	1:B:378:LYS:HE3	1.89	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	543/578 (94%)	526 (97%)	17 (3%)	0	100	100
1	B	549/578 (95%)	535 (97%)	14 (3%)	0	100	100
1	C	536/578 (93%)	520 (97%)	16 (3%)	0	100	100
All	All	1628/1734 (94%)	1581 (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	498/548 (91%)	490 (98%)	8 (2%)	62	74
1	B	500/548 (91%)	492 (98%)	8 (2%)	62	74
1	C	463/548 (84%)	451 (97%)	12 (3%)	46	56
All	All	1461/1644 (89%)	1433 (98%)	28 (2%)	57	68

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	A	168	TYR
1	A	175	GLU
1	A	263	LEU
1	A	359	SER
1	A	455	TYR
1	A	529	ARG
1	A	555	ILE
1	B	67	ASN
1	B	70	LEU
1	B	168	TYR
1	B	175	GLU
1	B	273	THR
1	B	286	CYS
1	B	314	ASP
1	B	455	TYR
1	C	37	VAL
1	C	42	LYS
1	C	97	THR
1	C	157	TYR
1	C	168	TYR
1	C	263	LEU
1	C	365	LEU
1	C	401	ASP
1	C	407	LYS
1	C	455	TYR
1	C	534	ASN
1	C	555	ILE

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 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 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	$\# Z > 2$
5	EDO	A	606	-	3,3,3	0.50	0	2,2,2	0.25	0
5	EDO	B	1004	4	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	B	1005	-	3,3,3	0.46	0	2,2,2	0.50	0
5	EDO	B	1007	-	3,3,3	0.51	0	2,2,2	0.23	0
5	EDO	C	603	-	3,3,3	0.47	0	2,2,2	0.39	0
5	EDO	A	608	-	3,3,3	0.48	0	2,2,2	0.36	0
5	EDO	A	603	4	3,3,3	0.47	0	2,2,2	0.28	0
5	EDO	F	101	-	3,3,3	0.56	0	2,2,2	0.26	0
6	T9I	C	604	-	27,32,32	0.53	0	29,47,47	0.74	1 (3%)
6	T9I	B	1009	-	27,32,32	0.54	0	29,47,47	0.74	1 (3%)
5	EDO	A	605	-	3,3,3	0.51	0	2,2,2	0.27	0
5	EDO	B	1008	-	3,3,3	0.46	0	2,2,2	0.44	0
5	EDO	A	607	-	3,3,3	0.50	0	2,2,2	0.37	0
5	EDO	B	1006	-	3,3,3	0.52	0	2,2,2	0.20	0
6	T9I	A	609	-	27,32,32	0.56	0	29,47,47	0.86	2 (6%)
5	EDO	A	604	-	3,3,3	0.55	0	2,2,2	0.16	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
5	EDO	A	606	-	-	0/1/1/1	-
5	EDO	B	1004	4	-	0/1/1/1	-
5	EDO	B	1005	-	-	0/1/1/1	-
5	EDO	B	1007	-	-	1/1/1/1	-
5	EDO	C	603	-	-	0/1/1/1	-
5	EDO	A	608	-	-	0/1/1/1	-
5	EDO	A	603	4	-	0/1/1/1	-
5	EDO	F	101	-	-	1/1/1/1	-
6	T9I	C	604	-	-	2/6/35/35	0/5/5/5
6	T9I	B	1009	-	-	2/6/35/35	0/5/5/5
5	EDO	A	605	-	-	1/1/1/1	-
5	EDO	B	1008	-	-	0/1/1/1	-
5	EDO	A	607	-	-	0/1/1/1	-
5	EDO	B	1006	-	-	0/1/1/1	-
6	T9I	A	609	-	-	2/6/35/35	0/5/5/5
5	EDO	A	604	-	-	0/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	604	T9I	C8-N3-C9	2.61	118.83	116.59
6	A	609	T9I	C12-C11-C10	-2.60	101.37	105.54
6	A	609	T9I	C8-N3-C9	2.33	118.58	116.59
6	B	1009	T9I	C8-N3-C9	2.08	118.38	116.59

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	609	T9I	C6-C9-N4-C10
6	A	609	T9I	N3-C9-N4-C10
6	B	1009	T9I	C6-C9-N4-C10
6	B	1009	T9I	N3-C9-N4-C10
6	C	604	T9I	C6-C9-N4-C10
6	C	604	T9I	N3-C9-N4-C10
5	B	1007	EDO	O1-C1-C2-O2

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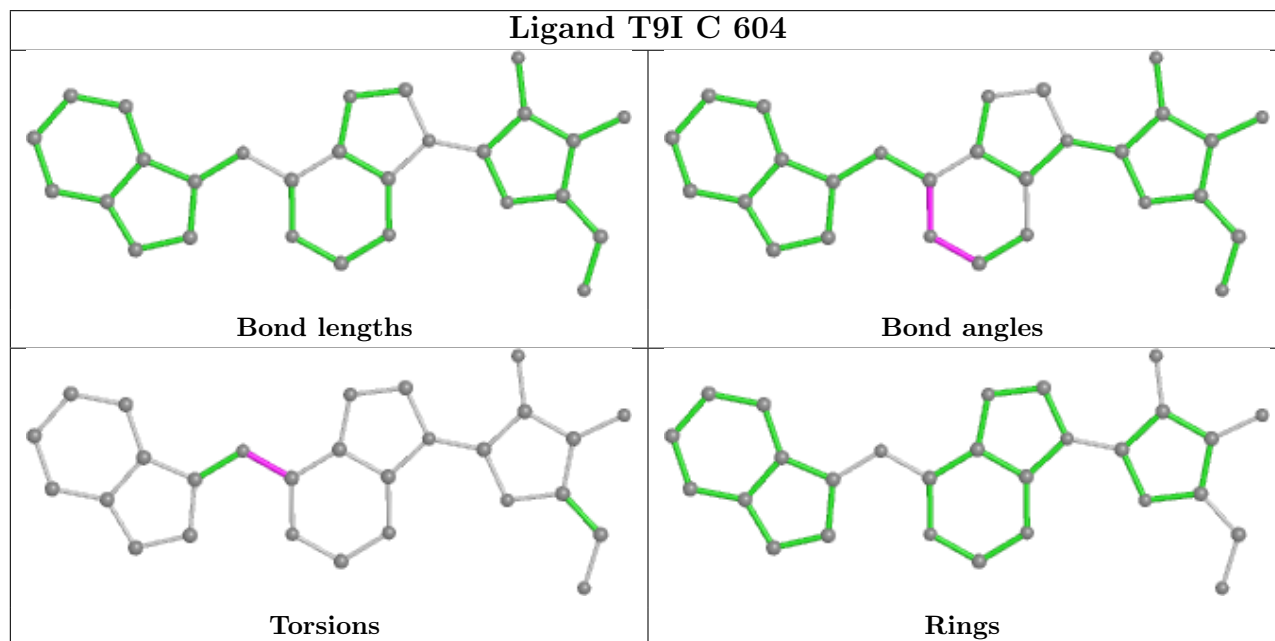
Mol	Chain	Res	Type	Atoms
5	F	101	EDO	O1-C1-C2-O2
5	A	605	EDO	O1-C1-C2-O2

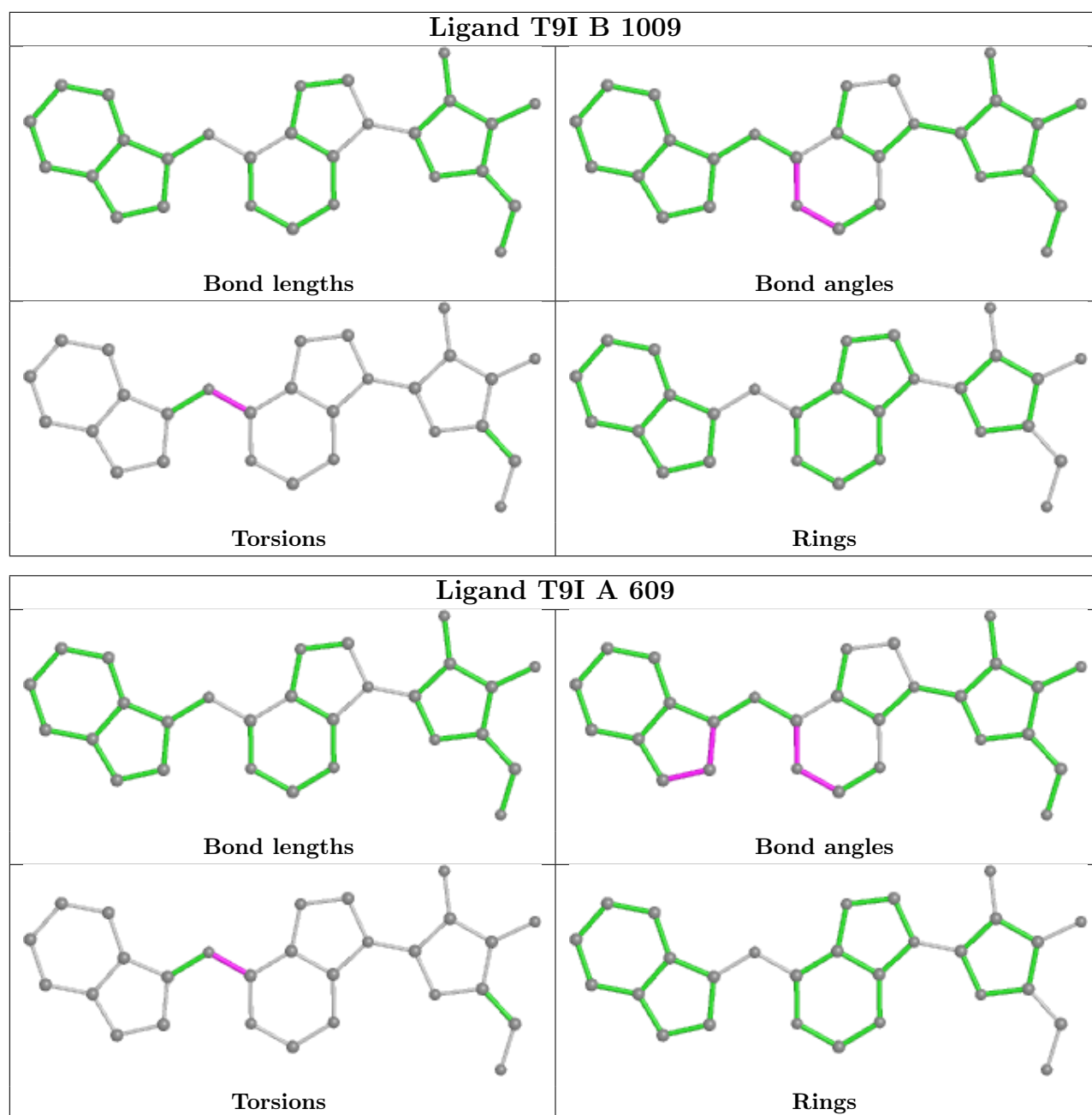
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1007	EDO	1	0
5	C	603	EDO	1	0
5	F	101	EDO	1	0
5	B	1008	EDO	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 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	546/578 (94%)	-0.06	12 (2%) 62 71	27, 45, 75, 109	0
1	B	550/578 (95%)	0.07	17 (3%) 49 59	27, 45, 74, 141	0
1	C	540/578 (93%)	0.35	69 (12%) 3 6	37, 58, 107, 133	0
2	D	14/14 (100%)	0.11	1 (7%) 16 23	32, 37, 109, 123	0
2	F	14/14 (100%)	-0.03	0 100 100	30, 35, 71, 74	0
2	H	14/14 (100%)	0.46	2 (14%) 2 4	40, 56, 127, 154	0
3	E	14/14 (100%)	0.43	2 (14%) 2 4	33, 38, 137, 155	0
3	G	14/14 (100%)	-0.36	0 100 100	33, 37, 64, 65	0
3	I	14/14 (100%)	0.71	3 (21%) 0 1	43, 52, 140, 170	0
All	All	1720/1818 (94%)	0.13	106 (6%) 20 28	27, 49, 96, 170	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	ASP	9.6
1	B	139	SER	7.2
1	C	96	TRP	6.7
1	B	136	LEU	6.4
2	H	14	DA	5.9
1	C	95	TYR	5.7
3	I	1	DA	5.7
1	C	87	LEU	5.7
1	C	103	ARG	5.3
3	E	1	DA	5.3
1	B	134	ASN	5.1
1	C	73	TYR	5.0
1	C	119	ALA	4.7
1	C	91	TYR	4.5
1	C	55	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	77	TYR	4.3
1	B	133	VAL	4.2
1	C	273	THR	4.2
1	B	290	PHE	4.1
1	B	137	ASP	4.0
1	C	108	TYR	4.0
1	B	138	GLU	4.0
1	A	290	PHE	3.9
1	C	401	ASP	3.9
1	C	102	HIS	3.9
1	C	85	TYR	3.8
3	I	2	DT	3.7
1	C	97	THR	3.7
1	A	286	CYS	3.6
1	C	141	ILE	3.6
1	B	404	ASN	3.5
1	C	558	GLY	3.5
1	C	31	TYR	3.5
1	C	76	LEU	3.4
1	C	107	ASN	3.4
1	C	88	LYS	3.4
1	C	92	ASP	3.3
1	C	271	LYS	3.3
1	A	137	ASP	3.3
1	C	84	ILE	3.3
1	C	129	ASN	3.2
1	B	132	VAL	3.2
1	C	100	ASN	3.2
1	C	404	ASN	3.2
1	B	287	ILE	3.2
3	E	2	DT	3.1
1	C	155	TRP	3.1
1	C	127	LEU	3.1
1	C	180	LYS	3.1
1	C	93	GLU	3.1
3	I	3	DG	3.0
1	C	80	PHE	3.0
1	C	94	ASN	3.0
1	A	139	SER	3.0
1	C	184	GLU	3.0
1	C	104	HIS	2.9
1	A	272	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	148	CYS	2.8
1	A	556	ASP	2.8
1	C	99	ASP	2.8
1	C	112	GLY	2.7
1	C	51	ILE	2.7
2	H	13	DC	2.7
1	B	117	GLU	2.7
1	C	555	ILE	2.7
1	C	311	LEU	2.7
1	C	90	LYS	2.7
1	C	557	LYS	2.7
1	C	121	SER	2.6
1	C	157	TYR	2.6
1	C	105	ILE	2.6
2	D	14	DA	2.6
1	B	286	CYS	2.6
1	C	270	THR	2.6
1	A	138	GLU	2.6
1	C	142	LYS	2.6
1	C	106	LEU	2.5
1	C	272	GLU	2.5
1	C	181	PHE	2.5
1	A	401	ASP	2.4
1	C	274	TYR	2.4
1	C	53	ASN	2.4
1	A	289	LYS	2.3
1	A	554	SER	2.4
1	C	125	ASP	2.3
1	B	178[A]	TYR	2.3
1	C	82	GLU	2.3
1	C	405	THR	2.3
1	C	147	CYS	2.3
1	C	122	ILE	2.3
1	B	367	LEU	2.3
1	C	65	CYS	2.3
1	C	118	LYS	2.3
1	C	29	ILE	2.3
1	C	56	PRO	2.2
1	B	419	THR	2.2
1	C	130	LYS	2.2
1	B	411	ASP	2.2
1	A	370	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	486	ASP	2.2
1	C	126	SER	2.2
1	C	28	GLY	2.1
1	C	554	SER	2.1
1	C	49	ASP	2.0
1	C	117	GLU	2.0
1	A	273	THR	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.

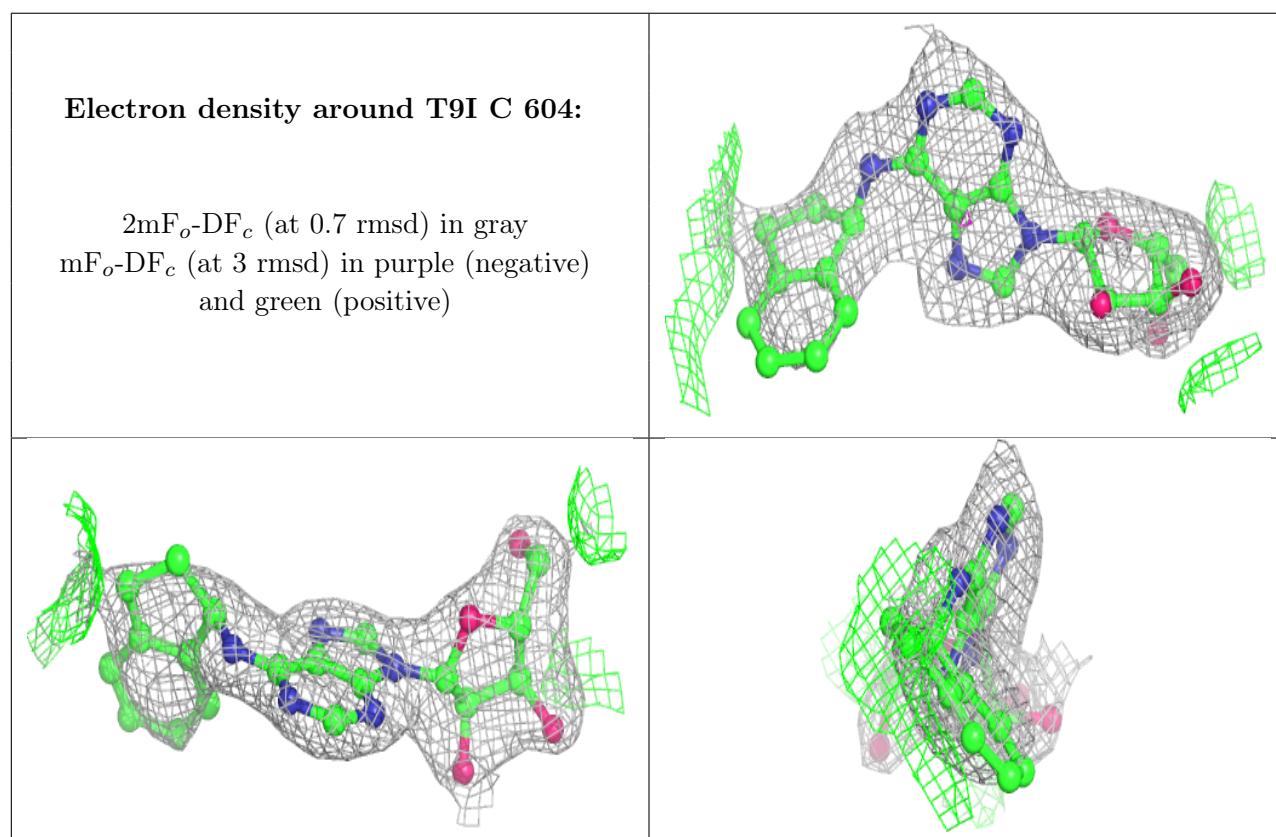
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	1007	4/4	0.75	0.39	59,60,61,66	0
5	EDO	A	607	4/4	0.76	0.22	62,63,68,72	0
5	EDO	A	604	4/4	0.81	0.20	55,57,57,57	0
5	EDO	B	1006	4/4	0.86	0.32	48,53,55,57	0
6	T9I	C	604	28/28	0.86	0.26	77,86,95,100	0
5	EDO	F	101	4/4	0.87	0.26	40,47,49,56	0
5	EDO	B	1004	4/4	0.87	0.27	52,55,59,65	0
5	EDO	C	603	4/4	0.88	0.32	56,58,62,66	0
5	EDO	A	605	4/4	0.89	0.17	47,51,54,59	0
4	K	B	1003	1/1	0.89	0.08	79,79,79,79	0
6	T9I	B	1009	28/28	0.90	0.19	44,52,63,64	0
6	T9I	A	609	28/28	0.90	0.20	55,61,67,69	0
5	EDO	A	603	4/4	0.91	0.17	55,57,60,62	0
5	EDO	B	1008	4/4	0.92	0.21	47,47,49,55	0
5	EDO	A	606	4/4	0.92	0.21	49,52,61,66	0
5	EDO	A	608	4/4	0.93	0.19	55,56,60,61	0

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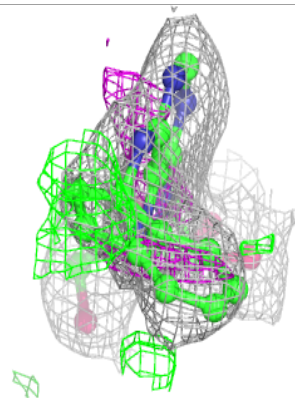
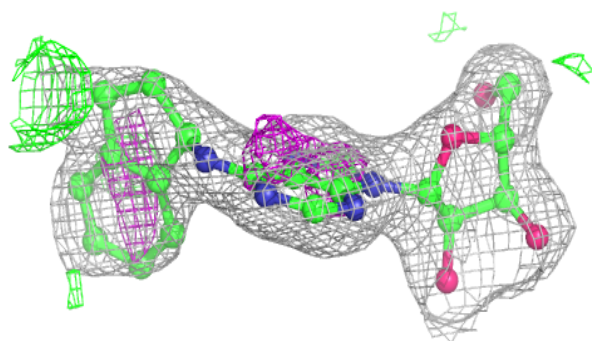
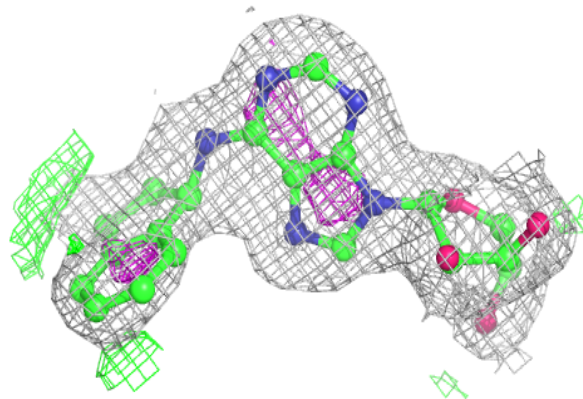
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	K	C	602	1/1	0.93	0.07	68,68,68,68	0
4	K	A	601	1/1	0.95	0.07	52,52,52,52	0
5	EDO	B	1005	4/4	0.95	0.14	41,43,45,50	0
4	K	A	602	1/1	0.96	0.09	61,61,61,61	0
4	K	C	601	1/1	0.98	0.11	60,60,60,60	0
4	K	B	1002	1/1	0.98	0.07	48,48,48,48	0
4	K	B	1001	1/1	0.98	0.08	54,54,54,54	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.

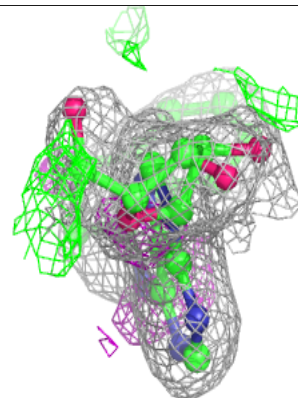
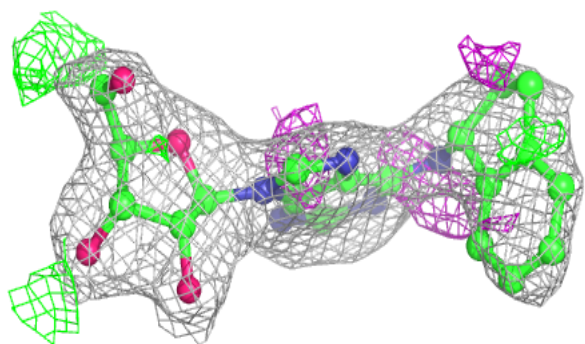
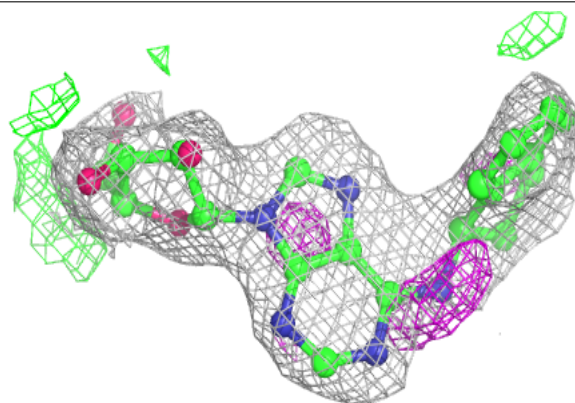


Electron density around T9I B 1009:

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

**Electron density around T9I A 609:**

$2mF_o-DF_c$ (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.