



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:25 AM UTC

PDB ID : 4GON / pdb_00004gon
Title : Crystal Structure of E. coli DNA Adenine Methyltransferase in Complex with Indole Aza-SAM
Authors : Harmer, J.E.; Roach, P.L.
Deposited on : 2012-08-20
Resolution : 2.72 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)
Xtriage (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

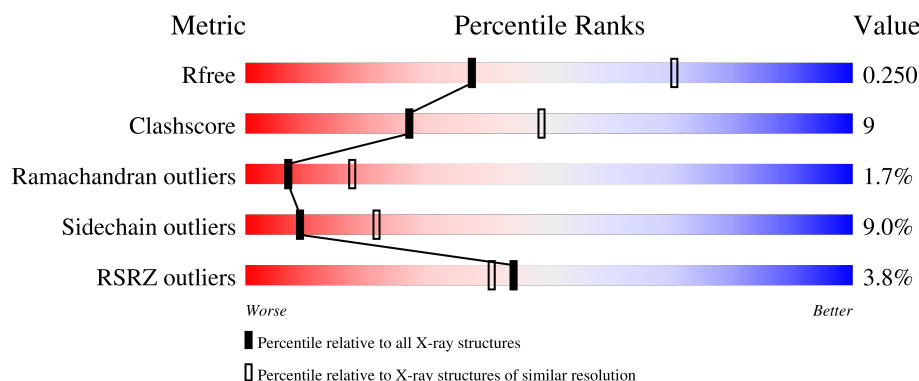
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	D	278	3% 66% 18% • 13%
1	E	278	4% 69% 14% 5% 12%
1	F	278	4% 64% 19% • 12%

2 Entry composition [i](#)

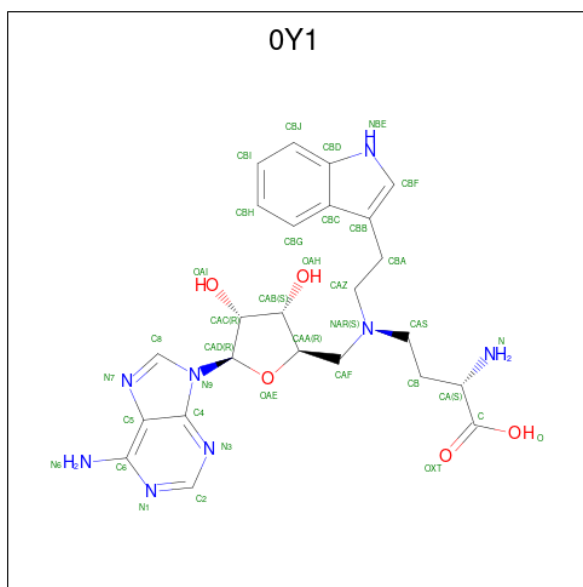
There are 3 unique types of molecules in this entry. The entry contains 6180 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA adenine methylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	243	Total	C	N	O	S	0	0	0
			2008	1300	338	362	8			
1	E	244	Total	C	N	O	S	0	0	0
			2016	1307	339	362	8			
1	F	244	Total	C	N	O	S	3	0	0
			2015	1305	339	363	8			

- Molecule 2 is 5'-{[(3S)-3-amino-3-carboxypropyl][2-(1H-indol-3-yl)ethyl]amino}-5'-deoxyadenosine (CCD ID: 0Y1) (formula: C₂₄H₃₀N₈O₅).



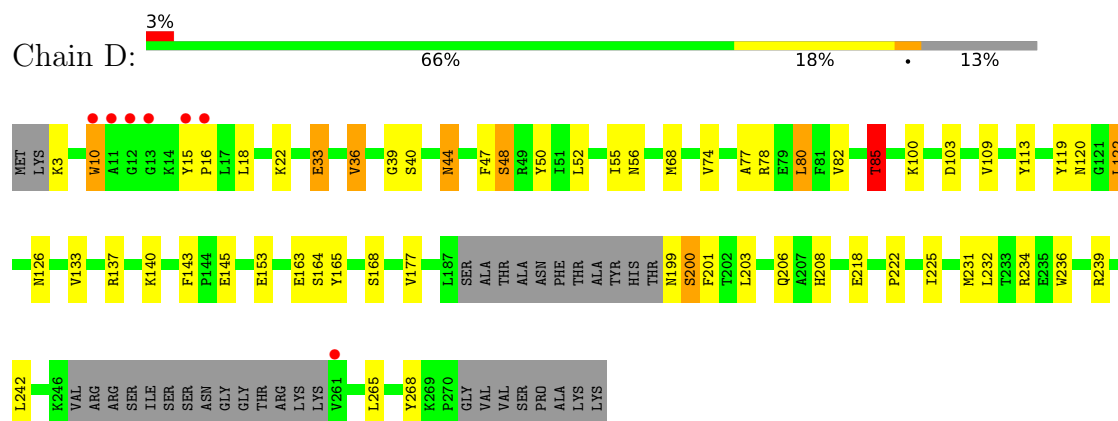
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	11	Total 11	O 11	0	0
3	E	7	Total 7	O 7	0	0
3	F	12	Total 12	O 12	0	0

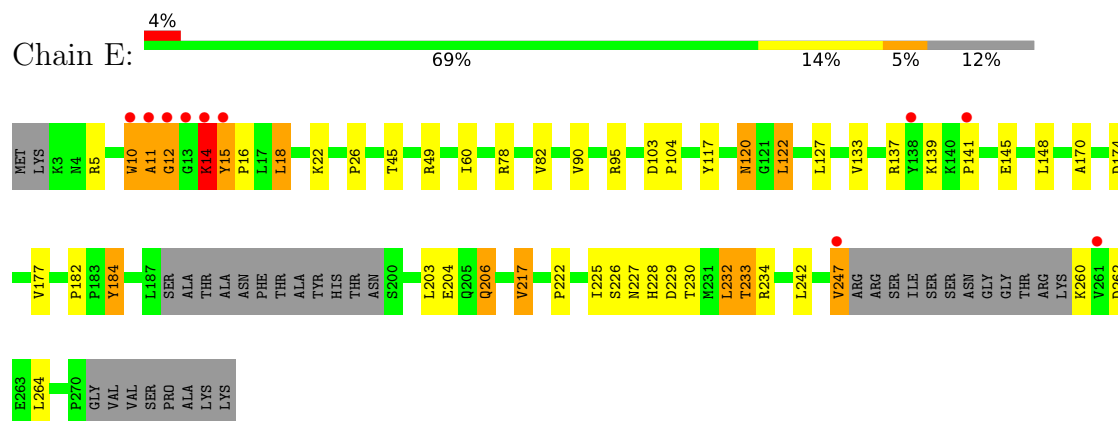
3 Residue-property plots [i](#)

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.

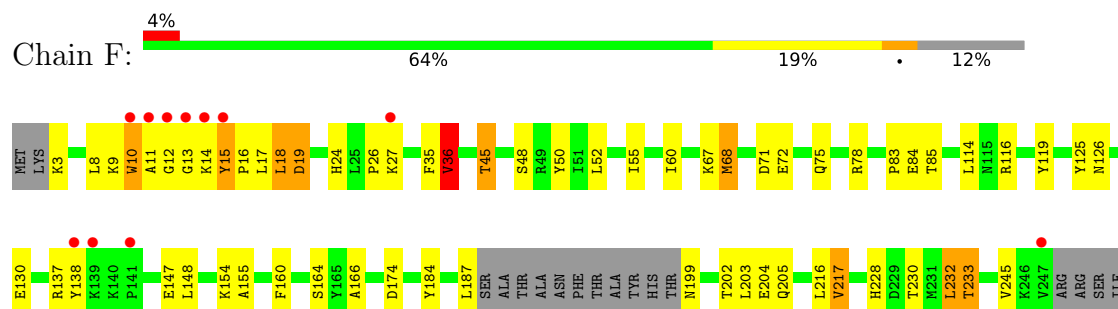
• Molecule 1: DNA adenine methylase



• Molecule 1: DNA adenine methylase



• Molecule 1: DNA adenine methylase



SER	SER	ASN	GLY	GLY	THR	ARG	LYS	LYS	V261	D262	P270	GLY	VAL	VAL	SER	PRO	ALA	LYS	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.31Å 161.31Å 95.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.04 – 2.72 30.04 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.04-2.72) 99.1 (30.04-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.258 0.203 , 0.250	Depositor DCC
R_{free} test set	1934 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6180	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0Y1

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	D	1.22	3/2063 (0.1%)	1.27	17/2794 (0.6%)
1	E	1.18	3/2071 (0.1%)	1.17	8/2804 (0.3%)
1	F	1.17	1/2070 (0.0%)	1.15	4/2804 (0.1%)
All	All	1.19	7/6204 (0.1%)	1.20	29/8402 (0.3%)

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	E	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	182	PRO	CA-C	-6.81	1.45	1.52
1	E	170	ALA	CA-CB	-6.07	1.42	1.53
1	D	137	ARG	CA-C	5.61	1.60	1.53
1	F	166	ALA	CA-CB	-5.32	1.45	1.53
1	D	48	SER	CA-C	5.18	1.59	1.52
1	E	14	LYS	CA-C	5.09	1.59	1.53
1	D	133	VAL	CA-CB	5.04	1.60	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	VAL	CB-CA-C	-9.44	99.67	112.04
1	D	140	LYS	CA-C-N	-9.33	111.17	120.31
1	D	140	LYS	C-N-CA	-9.33	111.17	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	VAL	CA-C-N	-9.14	110.41	119.64
1	D	82	VAL	C-N-CA	-9.14	110.41	119.64
1	D	153	GLU	N-CA-C	-8.02	102.12	111.03
1	F	217	VAL	CB-CA-C	-7.65	99.86	112.26
1	D	201	PHE	N-CA-C	-7.06	97.22	108.73
1	F	60	ILE	N-CA-C	-6.29	104.15	111.00
1	D	163	GLU	CB-CA-C	-6.08	100.21	109.99
1	E	217	VAL	CB-CA-C	-5.87	104.46	111.97
1	E	184	TYR	N-CA-C	5.81	118.44	110.24
1	E	95	ARG	N-CA-C	-5.74	105.10	111.36
1	E	217	VAL	N-CA-CB	5.69	117.20	110.55
1	D	44	ASN	N-CA-C	5.61	119.33	111.30
1	F	36	VAL	CB-CA-C	-5.60	102.10	111.29
1	F	12	GLY	N-CA-C	-5.52	104.86	112.25
1	D	36	VAL	N-CA-CB	5.35	117.16	110.47
1	D	137	ARG	N-CA-C	5.30	118.50	111.30
1	D	10	TRP	N-CA-C	5.28	118.07	107.41
1	D	85	THR	N-CA-C	-5.28	106.79	114.12
1	E	12	GLY	N-CA-C	-5.24	106.44	112.83
1	D	33	GLU	CA-C-N	-5.23	114.36	119.64
1	D	33	GLU	C-N-CA	-5.23	114.36	119.64
1	E	133	VAL	N-CA-C	5.15	113.81	109.02
1	D	168	SER	N-CA-C	-5.14	105.76	111.36
1	D	103	ASP	CB-CA-C	5.07	115.19	110.17
1	E	82	VAL	CA-C-N	-5.06	114.84	120.45
1	E	82	VAL	C-N-CA	-5.06	114.84	120.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	11	ALA	Peptide

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	D	2008	0	1944	45	0
1	E	2016	0	1960	30	0
1	F	2015	0	1953	36	0
2	D	37	0	29	12	0
2	E	37	0	29	1	0
2	F	37	0	27	1	0
3	D	11	0	0	0	0
3	E	7	0	0	0	0
3	F	12	0	0	0	0
All	All	6180	0	5942	111	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 9.

All (111) 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:F:18:LEU:O	1:F:19:ASP:HB2	1.50	1.04
1:F:230:THR:HG22	1:F:232:LEU:H	1.29	0.96
1:E:247:VAL:HB	1:E:260:LYS:NZ	1.82	0.94
1:D:119:TYR:O	1:D:122:LEU:HD23	1.70	0.92
1:F:228:HIS:O	1:F:233:THR:HG21	1.76	0.85
1:D:80:LEU:O	1:D:85:THR:HG21	1.77	0.84
1:F:18:LEU:O	1:F:19:ASP:CB	2.27	0.79
1:F:230:THR:HG22	1:F:232:LEU:N	1.97	0.78
1:D:120:ASN:HB2	1:D:122:LEU:HD21	1.65	0.77
1:F:10:TRP:O	1:F:10:TRP:HE3	1.68	0.77
1:E:247:VAL:HB	1:E:260:LYS:HZ1	1.47	0.76
1:D:10:TRP:CB	2:D:301:OY1:H5	2.01	0.73
1:E:247:VAL:HB	1:E:260:LYS:HZ2	1.53	0.73
1:E:228:HIS:O	1:E:233:THR:HG21	1.88	0.73
1:F:10:TRP:O	1:F:10:TRP:CE3	2.42	0.72
1:E:177:VAL:HG22	1:E:222:PRO:HG2	1.73	0.70
1:F:202:THR:H	1:F:205:GLN:HE21	1.39	0.70
1:E:10:TRP:CZ3	1:E:14:LYS:HB3	2.26	0.69
1:E:15:TYR:N	1:E:16:PRO:HD2	2.06	0.69
1:D:119:TYR:O	1:D:122:LEU:CD2	2.40	0.68
1:E:233:THR:CG2	1:E:264:LEU:HD22	2.24	0.67
1:D:10:TRP:HB3	2:D:301:OY1:H5	1.58	0.67
1:D:165:TYR:HH	1:D:208:HIS:HD1	1.42	0.65
1:E:206:GLN:HE21	1:E:227:ASN:HD21	1.45	0.64
1:F:14:LYS:O	1:F:15:TYR:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:TYR:CE1	1:F:137:ARG:NH2	2.67	0.63
1:D:10:TRP:CB	2:D:301:OY1:NBE	2.62	0.62
1:D:234:ARG:HH12	1:E:137:ARG:HD3	1.63	0.62
1:E:15:TYR:N	1:E:16:PRO:CD	2.62	0.62
1:D:122:LEU:N	1:D:122:LEU:HD22	2.16	0.61
1:D:10:TRP:HB2	2:D:301:OY1:CBF	2.32	0.60
1:E:78:ARG:NH1	1:E:145:GLU:OE2	2.34	0.60
1:F:45:THR:HG23	1:F:50:TYR:OH	2.02	0.59
1:F:45:THR:O	1:F:154:LYS:NZ	2.36	0.59
1:F:15:TYR:N	1:F:16:PRO:HD3	2.17	0.59
2:D:301:OY1:H7	2:D:301:OY1:H24	1.84	0.59
1:D:78:ARG:HH12	1:D:145:GLU:CD	2.10	0.58
1:F:3:LYS:HB3	1:F:15:TYR:OH	2.04	0.58
1:F:202:THR:H	1:F:205:GLN:NE2	2.01	0.58
1:D:10:TRP:HB3	2:D:301:OY1:NBE	2.19	0.57
1:F:24:HIS:O	1:F:26:PRO:HD3	2.03	0.57
1:D:10:TRP:HB2	2:D:301:OY1:H6	1.88	0.56
1:E:18:LEU:O	1:E:22:LYS:HG3	2.06	0.55
1:D:55:ILE:HG12	2:D:301:OY1:C5	2.37	0.55
1:D:10:TRP:HA	2:D:301:OY1:H5	1.71	0.54
1:E:10:TRP:CH2	1:E:14:LYS:HB3	2.43	0.54
1:F:67:LYS:HG3	1:F:155:ALA:HB1	1.89	0.54
1:D:120:ASN:HB2	1:D:122:LEU:CD2	2.35	0.54
1:D:15:TYR:N	1:D:16:PRO:HD3	2.23	0.53
1:F:68:MET:HA	1:F:68:MET:HE2	1.90	0.53
1:D:22:LYS:NZ	1:D:44:ASN:O	2.40	0.52
1:F:35:PHE:O	1:F:36:VAL:C	2.51	0.52
1:D:78:ARG:NH1	1:D:145:GLU:OE1	2.43	0.52
1:E:229:ASP:OD2	1:E:234:ARG:NH2	2.44	0.51
1:D:10:TRP:CA	2:D:301:OY1:H5	2.24	0.51
1:D:78:ARG:NH1	1:D:145:GLU:CD	2.69	0.50
1:D:239:ARG:HH11	1:D:239:ARG:HG2	1.76	0.50
1:F:125:TYR:HA	1:F:130:GLU:O	2.11	0.50
1:D:77:ALA:HA	1:D:109:VAL:HG13	1.93	0.50
1:D:177:VAL:HG22	1:D:222:PRO:HG2	1.95	0.49
1:E:14:LYS:C	1:E:16:PRO:HD2	2.36	0.49
1:F:119:TYR:CZ	1:F:137:ARG:NH2	2.80	0.49
1:D:78:ARG:HB2	1:D:143:PHE:CE2	2.48	0.49
1:F:75:GLN:OE1	1:F:78:ARG:NH2	2.46	0.49
1:E:233:THR:HG22	1:E:264:LEU:HD22	1.95	0.48
1:E:230:THR:O	1:E:234:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:THR:HG23	1:D:113:TYR:HE1	1.80	0.47
1:D:199:ASN:CG	1:D:200:SER:H	2.22	0.47
1:D:231:MET:HE2	1:E:122:LEU:HD23	1.96	0.47
1:F:126:ASN:OD1	1:F:126:ASN:C	2.57	0.47
1:D:39:GLY:O	1:D:40:SER:C	2.57	0.46
1:F:14:LYS:C	1:F:16:PRO:HD3	2.40	0.46
1:D:122:LEU:CD2	1:D:122:LEU:N	2.78	0.46
2:E:301:OY1:H15	2:E:301:OY1:H10	1.41	0.46
1:F:230:THR:HB	1:F:233:THR:HB	1.96	0.46
2:D:301:OY1:H7	2:D:301:OY1:CAB	2.46	0.46
1:D:122:LEU:CD2	1:D:122:LEU:H	2.29	0.45
1:F:184:TYR:N	2:F:301:OY1:O	2.37	0.45
1:E:10:TRP:C	1:E:12:GLY:N	2.74	0.45
1:E:117:TYR:CZ	1:E:141:PRO:HG2	2.52	0.45
1:D:122:LEU:HD22	1:D:122:LEU:H	1.83	0.44
1:F:261:VAL:HB	1:F:262:ASP:H	1.59	0.44
1:F:71:ASP:O	1:F:72:GLU:C	2.59	0.44
1:D:55:ILE:HG12	2:D:301:OY1:C4	2.48	0.44
1:D:56:ASN:OD1	1:D:56:ASN:C	2.61	0.43
1:E:10:TRP:CD1	1:E:10:TRP:N	2.86	0.43
1:F:45:THR:CG2	1:F:50:TYR:OH	2.65	0.43
1:D:80:LEU:HD22	1:D:109:VAL:HG12	1.99	0.43
1:D:33:GLU:HB2	1:D:52:LEU:HD23	1.99	0.43
1:F:16:PRO:HD2	1:F:17:LEU:HD23	2.01	0.43
1:D:80:LEU:CD2	1:D:109:VAL:HG12	2.48	0.43
1:D:15:TYR:HB3	1:D:18:LEU:HD12	2.00	0.42
1:E:120:ASN:HB2	1:E:122:LEU:HD22	2.00	0.42
1:D:126:ASN:OD1	1:D:126:ASN:C	2.62	0.42
1:E:225:ILE:HG22	1:E:226:SER:N	2.34	0.42
1:E:230:THR:OG1	1:E:233:THR:HB	2.20	0.42
1:D:100:LYS:HZ3	1:D:100:LYS:HG3	1.75	0.42
1:F:52:LEU:O	1:F:160:PHE:HA	2.20	0.42
1:F:83:PRO:O	1:F:85:THR:N	2.52	0.42
1:E:232:LEU:HD12	1:E:232:LEU:HA	1.65	0.42
1:F:10:TRP:CE3	1:F:10:TRP:C	2.98	0.41
1:E:10:TRP:C	1:E:12:GLY:H	2.28	0.41
1:F:3:LYS:CB	1:F:15:TYR:OH	2.67	0.41
1:D:242:LEU:O	1:E:137:ARG:NH1	2.53	0.41
1:D:225:ILE:HD12	1:D:268:TYR:HE2	1.86	0.41
1:D:47:PHE:HB2	1:D:50:TYR:CZ	2.55	0.41
1:E:103:ASP:O	1:E:104:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:LYS:HD3	1:F:116:ARG:HD3	2.03	0.41
1:E:14:LYS:HD2	1:E:184:TYR:OH	2.21	0.41
1:F:147:GLU:H	1:F:147:GLU:CD	2.29	0.40
1:D:206:GLN:HB3	1:D:236:TRP:CZ3	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	D	237/278 (85%)	221 (93%)	15 (6%)	1 (0%)	30	52
1	E	238/278 (86%)	220 (92%)	13 (6%)	5 (2%)	5	13
1	F	238/278 (86%)	214 (90%)	18 (8%)	6 (2%)	4	10
All	All	713/834 (86%)	655 (92%)	46 (6%)	12 (2%)	7	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	200	SER
1	F	15	TYR
1	F	19	ASP
1	E	262	ASP
1	F	13	GLY
1	F	84	GLU
1	F	11	ALA
1	E	11	ALA
1	E	139	LYS
1	F	138	TYR
1	E	26	PRO
1	E	15	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	211/239 (88%)	198 (94%)	13 (6%)	16	38
1	E	212/239 (89%)	191 (90%)	21 (10%)	7	18
1	F	212/239 (89%)	189 (89%)	23 (11%)	6	15
All	All	635/717 (89%)	578 (91%)	57 (9%)	9	21

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	LYS
1	D	36	VAL
1	D	48	SER
1	D	68	MET
1	D	74	VAL
1	D	80	LEU
1	D	85	THR
1	D	122	LEU
1	D	164	SER
1	D	203	LEU
1	D	218	GLU
1	D	232	LEU
1	D	265	LEU
1	E	5	ARG
1	E	10	TRP
1	E	14	LYS
1	E	18	LEU
1	E	45	THR
1	E	49	ARG
1	E	60	ILE
1	E	90	VAL
1	E	120	ASN
1	E	122	LEU
1	E	127	LEU
1	E	148	LEU
1	E	174	ASP

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Mol	Chain	Res	Type
1	E	203	LEU
1	E	204	GLU
1	E	206	GLN
1	E	217	VAL
1	E	232	LEU
1	E	233	THR
1	E	242	LEU
1	E	247	VAL
1	F	8	LEU
1	F	10	TRP
1	F	18	LEU
1	F	27	LYS
1	F	36	VAL
1	F	45	THR
1	F	48	SER
1	F	55	ILE
1	F	68	MET
1	F	114	LEU
1	F	148	LEU
1	F	164	SER
1	F	174	ASP
1	F	187	LEU
1	F	199	ASN
1	F	203	LEU
1	F	204	GLU
1	F	216	LEU
1	F	217	VAL
1	F	232	LEU
1	F	233	THR
1	F	245	VAL
1	F	261	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	24	HIS
1	D	64	ASN
1	D	120	ASN
1	D	199	ASN
1	D	238	GLN
1	E	93	GLN
1	E	102	GLN

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Mol	Chain	Res	Type
1	E	150	HIS
1	E	206	GLN
1	E	238	GLN
1	F	205	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	0Y1	F	301	-	40,41,41	2.64	17 (42%)	54,59,59	2.49	20 (37%)
2	0Y1	E	301	-	40,41,41	2.15	11 (27%)	54,59,59	2.56	20 (37%)
2	0Y1	D	301	-	40,41,41	1.78	6 (15%)	54,59,59	2.32	15 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0Y1	F	301	-	-	5/22/38/38	0/5/5/5
2	0Y1	E	301	-	-	10/22/38/38	0/5/5/5
2	0Y1	D	301	-	-	7/22/38/38	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	0Y1	CBC-CBB	-8.95	1.29	1.44
2	E	301	0Y1	CBC-CBB	-7.55	1.31	1.44
2	D	301	0Y1	CBC-CBB	-6.12	1.34	1.44
2	F	301	0Y1	CBC-CBD	-4.99	1.35	1.41
2	D	301	0Y1	C6-N6	4.92	1.46	1.34
2	E	301	0Y1	C6-N6	4.71	1.46	1.34
2	F	301	0Y1	C5-N7	-4.54	1.30	1.39
2	F	301	0Y1	C8-N9	-4.35	1.30	1.37
2	E	301	0Y1	CBD-NBE	4.20	1.44	1.37
2	D	301	0Y1	CBC-CBD	-4.00	1.36	1.41
2	F	301	0Y1	C6-N6	3.83	1.44	1.34
2	E	301	0Y1	CBC-CBD	-3.67	1.36	1.41
2	F	301	0Y1	C4-N9	-3.38	1.30	1.37
2	E	301	0Y1	CB-CA	-3.24	1.46	1.53
2	F	301	0Y1	OAH-CAB	-3.23	1.35	1.43
2	F	301	0Y1	CAC-CAB	-3.15	1.44	1.53
2	F	301	0Y1	CAB-CAA	-3.00	1.45	1.53
2	E	301	0Y1	CBF-NBE	2.99	1.42	1.37
2	F	301	0Y1	OAI-CAC	-2.98	1.35	1.43
2	F	301	0Y1	CB-CA	-2.95	1.46	1.53
2	D	301	0Y1	CBF-NBE	2.88	1.41	1.37
2	E	301	0Y1	CAC-CAB	-2.60	1.46	1.53
2	E	301	0Y1	CAF-CAA	-2.46	1.44	1.51
2	E	301	0Y1	C5-N7	-2.40	1.34	1.39
2	F	301	0Y1	C6-N1	-2.32	1.29	1.35
2	F	301	0Y1	CAF-CAA	-2.27	1.44	1.51
2	F	301	0Y1	CAC-CAD	-2.26	1.46	1.53
2	F	301	0Y1	C4-N3	-2.12	1.30	1.34
2	F	301	0Y1	C5-C4	-2.12	1.35	1.39
2	E	301	0Y1	OAI-CAC	-2.11	1.37	1.43
2	E	301	0Y1	OXT-C	2.10	1.28	1.22
2	D	301	0Y1	CAC-CAB	-2.04	1.47	1.53
2	F	301	0Y1	CBF-NBE	2.03	1.40	1.37
2	D	301	0Y1	OXT-C	2.01	1.28	1.22

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	0Y1	CBD-NBE-CBF	-8.35	101.65	109.08
2	D	301	0Y1	CAZ-CBA-CBB	7.09	125.56	112.58
2	E	301	0Y1	CBD-NBE-CBF	-7.07	102.78	109.08
2	D	301	0Y1	N1-C2-N3	-6.04	119.44	128.58
2	E	301	0Y1	CBC-CBB-CBF	5.83	112.12	106.16
2	D	301	0Y1	C5-C4-N3	-5.65	118.93	126.72
2	F	301	0Y1	C5-C4-N3	-5.18	119.58	126.72
2	F	301	0Y1	CAZ-CBA-CBB	5.13	121.96	112.58
2	E	301	0Y1	N9-C8-N7	-5.07	106.74	113.94
2	F	301	0Y1	N1-C2-N3	-5.05	120.94	128.58
2	E	301	0Y1	N1-C2-N3	-5.05	120.94	128.58
2	D	301	0Y1	CBD-NBE-CBF	-4.73	104.86	109.08
2	D	301	0Y1	N3-C4-N9	4.54	134.89	127.17
2	D	301	0Y1	C2-N3-C4	4.46	122.73	111.83
2	E	301	0Y1	C5-C4-N3	-4.37	120.70	126.72
2	E	301	0Y1	CAS-NAR-CAF	-4.35	101.76	111.89
2	E	301	0Y1	C5-N7-C8	4.33	110.26	103.45
2	E	301	0Y1	C4-N9-C8	4.11	110.05	105.74
2	D	301	0Y1	CBC-CBB-CBF	4.02	110.27	106.16
2	F	301	0Y1	CBC-CBD-NBE	3.90	110.77	107.52
2	F	301	0Y1	C4-C5-N7	-3.81	106.22	110.58
2	E	301	0Y1	N3-C4-N9	3.78	133.60	127.17
2	F	301	0Y1	N9-C8-N7	-3.75	108.61	113.94
2	F	301	0Y1	C2-N3-C4	3.68	120.82	111.83
2	F	301	0Y1	CBC-CBB-CBF	3.68	109.92	106.16
2	E	301	0Y1	CBC-CBD-NBE	3.67	110.58	107.52
2	F	301	0Y1	C5-N7-C8	3.45	108.86	103.45
2	E	301	0Y1	C2-N3-C4	3.33	119.95	111.83
2	D	301	0Y1	N9-C8-N7	-3.29	109.27	113.94
2	E	301	0Y1	CBJ-CBD-CBC	-3.23	119.06	122.19
2	F	301	0Y1	CAS-NAR-CAZ	-3.12	104.00	111.44
2	F	301	0Y1	N3-C4-N9	3.01	132.29	127.17
2	E	301	0Y1	CAZ-CBA-CBB	2.94	117.95	112.58
2	E	301	0Y1	CAA-OAE-CAD	-2.92	103.01	109.47
2	E	301	0Y1	C4-C5-N7	-2.92	107.25	110.58
2	E	301	0Y1	C4-N9-CAD	-2.89	119.87	126.63
2	F	301	0Y1	C4-N9-CAD	-2.86	119.95	126.63
2	D	301	0Y1	C4-N9-C8	2.84	108.72	105.74
2	D	301	0Y1	C5-N7-C8	2.84	107.91	103.45
2	F	301	0Y1	CAC-CAB-CAA	2.73	107.89	102.61
2	E	301	0Y1	CBB-CBF-NBE	-2.57	107.48	110.31
2	E	301	0Y1	CB-CA-N	-2.57	103.42	110.12
2	D	301	0Y1	CBB-CBF-NBE	-2.53	107.53	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	0Y1	O-C-OXT	-2.40	118.64	124.08
2	E	301	0Y1	OAE-CAD-N9	2.36	112.62	108.09
2	D	301	0Y1	C4-C5-N7	-2.33	107.92	110.58
2	F	301	0Y1	CBJ-CBD-CBC	-2.31	119.95	122.19
2	F	301	0Y1	C4-N9-C8	2.31	108.16	105.74
2	F	301	0Y1	CAC-CAD-N9	2.23	118.84	113.30
2	D	301	0Y1	CB-CAS-NAR	2.21	119.50	113.69
2	F	301	0Y1	OAE-CAA-CAF	-2.20	105.29	108.88
2	F	301	0Y1	CAD-N9-C8	2.15	131.86	127.09
2	E	301	0Y1	OAE-CAA-CAB	2.14	109.39	105.15
2	F	301	0Y1	C5-C4-N9	2.12	108.12	105.81
2	D	301	0Y1	CAS-NAR-CAF	2.06	116.69	111.89

There are no chirality outliers.

All (22) torsion outliers are listed below:

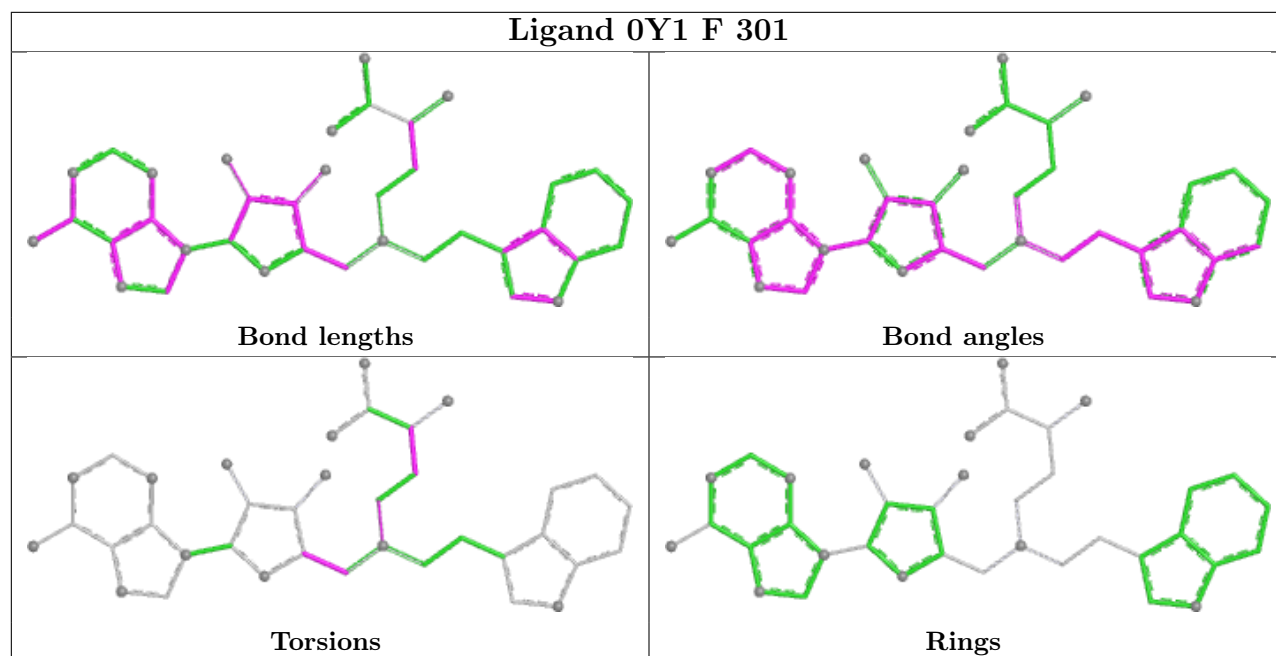
Mol	Chain	Res	Type	Atoms
2	D	301	0Y1	NAR-CAZ-CBA-CBB
2	D	301	0Y1	NAR-CAS-CB-CA
2	D	301	0Y1	C-CA-CB-CAS
2	D	301	0Y1	N-CA-CB-CAS
2	D	301	0Y1	OAE-CAA-CAF-NAR
2	D	301	0Y1	CAB-CAA-CAF-NAR
2	E	301	0Y1	OAE-CAA-CAF-NAR
2	E	301	0Y1	CAB-CAA-CAF-NAR
2	F	301	0Y1	N-CA-CB-CAS
2	F	301	0Y1	OAE-CAA-CAF-NAR
2	F	301	0Y1	CAB-CAA-CAF-NAR
2	F	301	0Y1	CB-CAS-NAR-CAZ
2	E	301	0Y1	CB-CAS-NAR-CAZ
2	D	301	0Y1	O-C-CA-N
2	E	301	0Y1	C-CA-CB-CAS
2	E	301	0Y1	OXT-C-CA-CB
2	E	301	0Y1	CAA-CAF-NAR-CAZ
2	E	301	0Y1	NAR-CAZ-CBA-CBB
2	F	301	0Y1	CB-CAS-NAR-CAF
2	E	301	0Y1	O-C-CA-CB
2	E	301	0Y1	CAC-CAD-N9-C8
2	E	301	0Y1	OAE-CAD-N9-C8

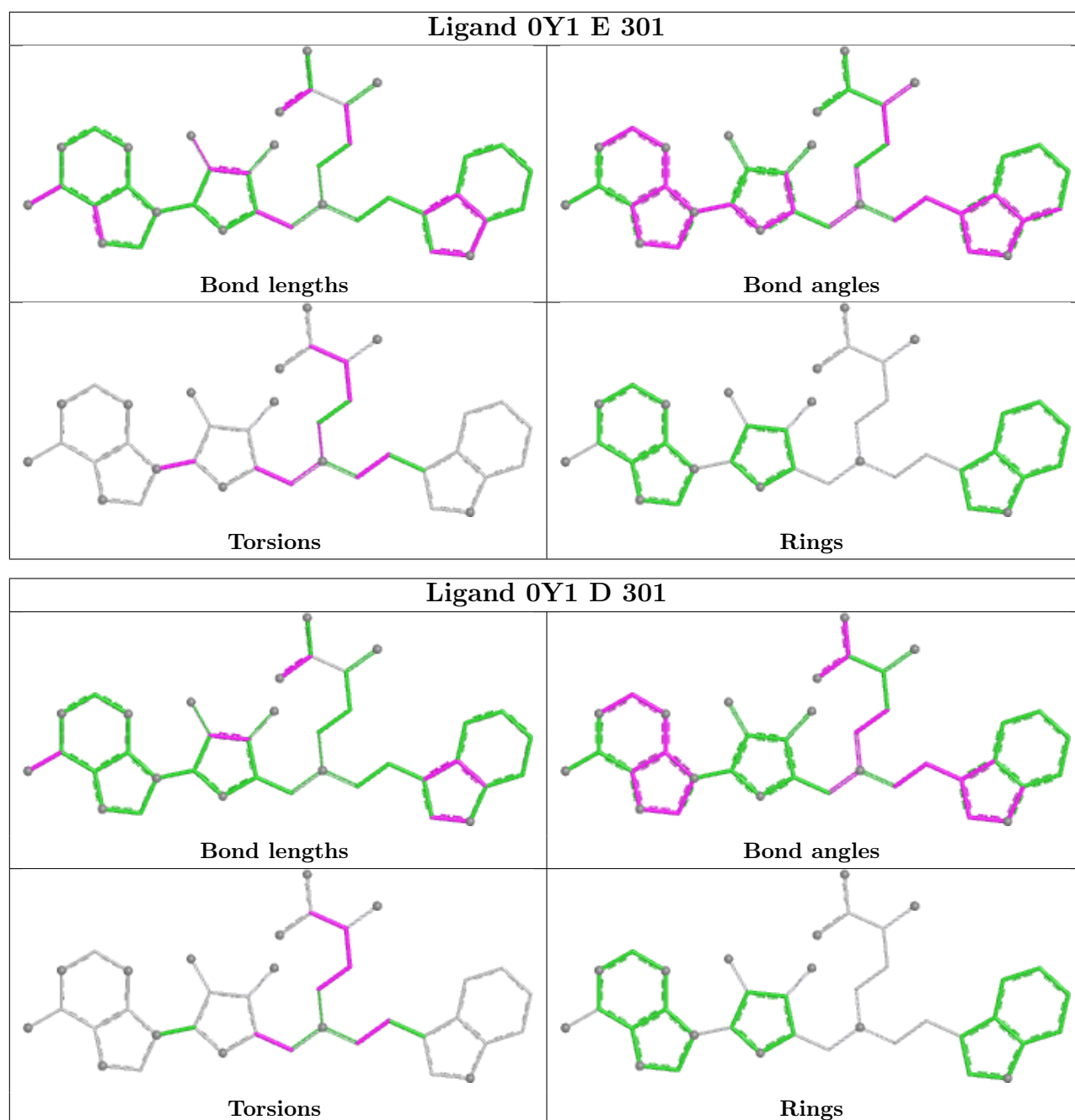
There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	0Y1	1	0
2	E	301	0Y1	1	0
2	D	301	0Y1	12	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	D	243/278 (87%)	-0.20	7 (2%) 53 50	34, 48, 76, 102	0
1	E	244/278 (87%)	-0.02	10 (4%) 41 38	35, 54, 88, 108	0
1	F	244/278 (87%)	-0.08	11 (4%) 38 35	36, 52, 81, 110	1 (0%)
All	All	731/834 (87%)	-0.10	28 (3%) 44 40	34, 52, 83, 110	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	11	ALA	5.4
1	D	10	TRP	5.3
1	F	14	LYS	4.8
1	F	13	GLY	4.7
1	D	15	TYR	4.5
1	E	14	LYS	4.4
1	F	15	TYR	4.0
1	D	12	GLY	4.0
1	E	247	VAL	4.0
1	E	12	GLY	3.8
1	E	15	TYR	3.8
1	F	138	TYR	3.7
1	E	13	GLY	3.7
1	F	247	VAL	3.7
1	F	10	TRP	3.6
1	E	261	VAL	3.4
1	E	138	TYR	3.3
1	E	10	TRP	3.0
1	E	141	PRO	2.9
1	D	13	GLY	2.6
1	E	11	ALA	2.5
1	D	16	PRO	2.3
1	F	12	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	261	VAL	2.2
1	F	141	PRO	2.1
1	F	139	LYS	2.0
1	F	11	ALA	2.0
1	F	27	LYS	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](#)

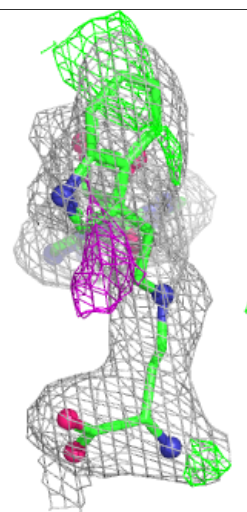
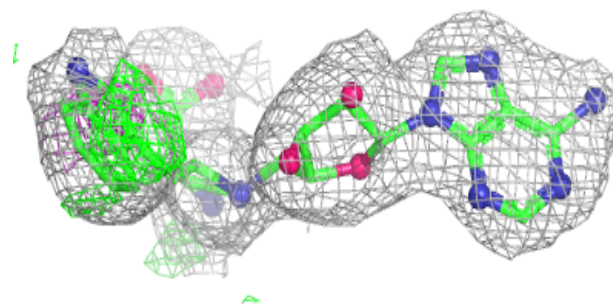
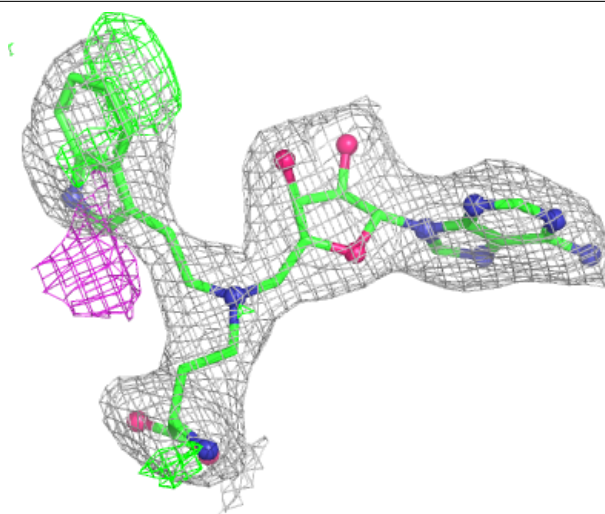
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	0Y1	F	301	37/37	0.91	0.11	39,55,73,73	0
2	0Y1	E	301	37/37	0.93	0.12	48,64,83,84	0
2	0Y1	D	301	37/37	0.93	0.11	63,70,81,83	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.

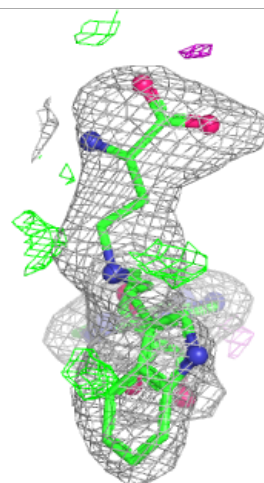
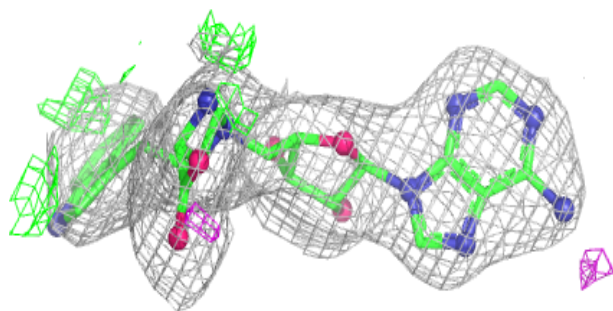
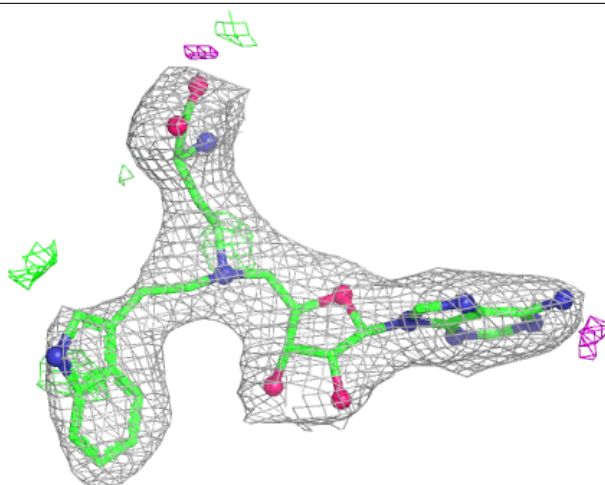
Electron density around 0Y1 F 301:

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



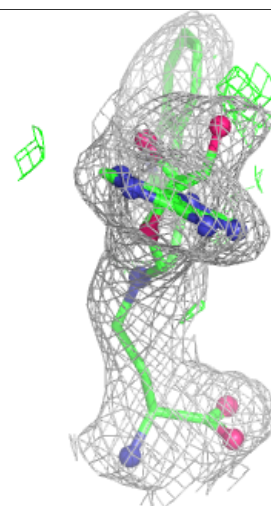
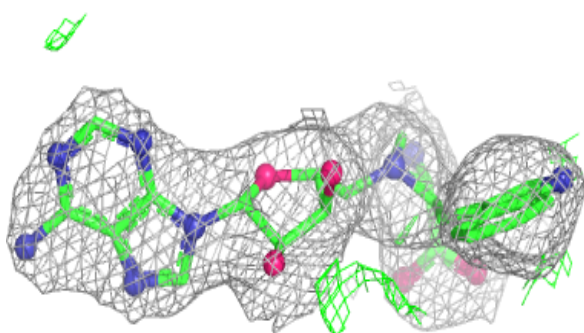
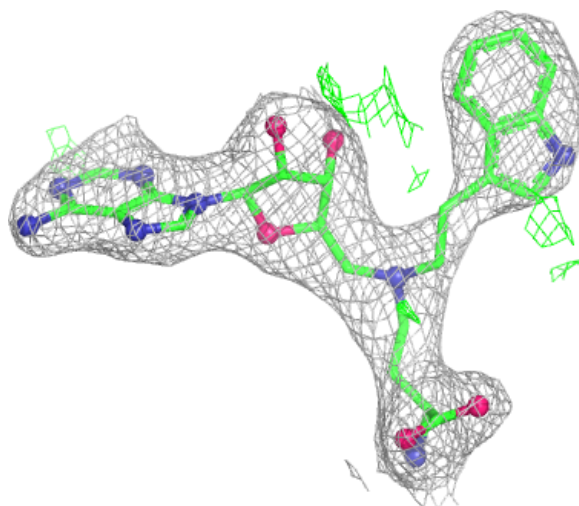
Electron density around 0Y1 E 301:

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



Electron density around 0Y1 D 301:

$2mF_o-DF_c$ (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.