



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:29 PM UTC

PDB ID : 6K0W / pdb_00006k0w
Title : DNA methyltransferase in complex with sinefungin
Authors : Narayanan, N.; Nair, D.T.
Deposited on : 2019-05-07
Resolution : 2.65 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

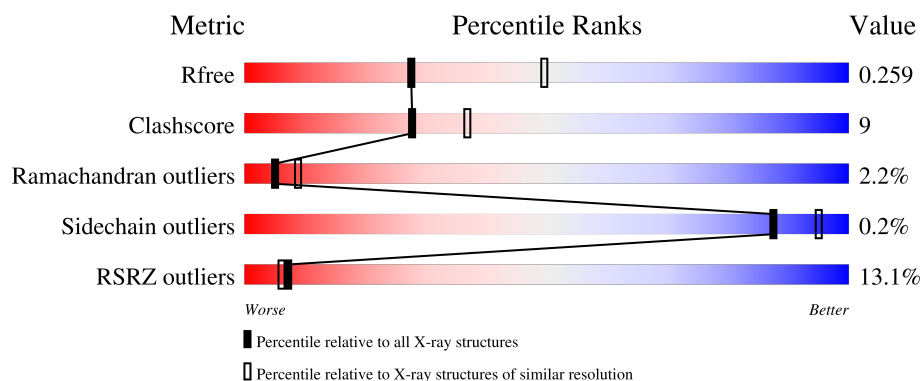
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	618	11% 71% 14% 15%
1	B	618	13% 63% 17% 19%
1	C	618	8% 56% 14% 30%
1	D	618	8% 58% 12% 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14455 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 Adenine specific DNA methyltransferase (Mod).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	499	Total	C	N	O	S	0	0	0
			3779	2408	618	734	19			
1	A	528	Total	C	N	O	S	0	0	0
			3987	2535	664	769	19			
1	C	433	Total	C	N	O	S	0	0	0
			3251	2067	535	634	15			
1	D	435	Total	C	N	O	S	0	0	0
			3239	2047	535	640	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP O25315
B	-18	GLY	-	expression tag	UNP O25315
B	-17	SER	-	expression tag	UNP O25315
B	-16	SER	-	expression tag	UNP O25315
B	-15	HIS	-	expression tag	UNP O25315
B	-14	HIS	-	expression tag	UNP O25315
B	-13	HIS	-	expression tag	UNP O25315
B	-12	HIS	-	expression tag	UNP O25315
B	-11	HIS	-	expression tag	UNP O25315
B	-10	HIS	-	expression tag	UNP O25315
B	-9	SER	-	expression tag	UNP O25315
B	-8	SER	-	expression tag	UNP O25315
B	-7	GLY	-	expression tag	UNP O25315
B	-6	LEU	-	expression tag	UNP O25315
B	-5	VAL	-	expression tag	UNP O25315
B	-4	PRO	-	expression tag	UNP O25315
B	-3	ARG	-	expression tag	UNP O25315
B	-2	GLY	-	expression tag	UNP O25315
B	-1	SER	-	expression tag	UNP O25315
B	0	HIS	-	expression tag	UNP O25315
A	-19	MET	-	initiating methionine	UNP O25315

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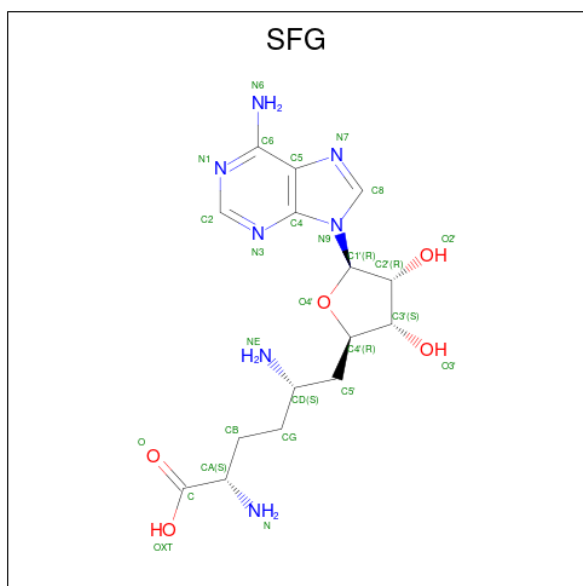
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O25315
A	-17	SER	-	expression tag	UNP O25315
A	-16	SER	-	expression tag	UNP O25315
A	-15	HIS	-	expression tag	UNP O25315
A	-14	HIS	-	expression tag	UNP O25315
A	-13	HIS	-	expression tag	UNP O25315
A	-12	HIS	-	expression tag	UNP O25315
A	-11	HIS	-	expression tag	UNP O25315
A	-10	HIS	-	expression tag	UNP O25315
A	-9	SER	-	expression tag	UNP O25315
A	-8	SER	-	expression tag	UNP O25315
A	-7	GLY	-	expression tag	UNP O25315
A	-6	LEU	-	expression tag	UNP O25315
A	-5	VAL	-	expression tag	UNP O25315
A	-4	PRO	-	expression tag	UNP O25315
A	-3	ARG	-	expression tag	UNP O25315
A	-2	GLY	-	expression tag	UNP O25315
A	-1	SER	-	expression tag	UNP O25315
A	0	HIS	-	expression tag	UNP O25315
C	-19	MET	-	initiating methionine	UNP O25315
C	-18	GLY	-	expression tag	UNP O25315
C	-17	SER	-	expression tag	UNP O25315
C	-16	SER	-	expression tag	UNP O25315
C	-15	HIS	-	expression tag	UNP O25315
C	-14	HIS	-	expression tag	UNP O25315
C	-13	HIS	-	expression tag	UNP O25315
C	-12	HIS	-	expression tag	UNP O25315
C	-11	HIS	-	expression tag	UNP O25315
C	-10	HIS	-	expression tag	UNP O25315
C	-9	SER	-	expression tag	UNP O25315
C	-8	SER	-	expression tag	UNP O25315
C	-7	GLY	-	expression tag	UNP O25315
C	-6	LEU	-	expression tag	UNP O25315
C	-5	VAL	-	expression tag	UNP O25315
C	-4	PRO	-	expression tag	UNP O25315
C	-3	ARG	-	expression tag	UNP O25315
C	-2	GLY	-	expression tag	UNP O25315
C	-1	SER	-	expression tag	UNP O25315
C	0	HIS	-	expression tag	UNP O25315
D	-19	MET	-	initiating methionine	UNP O25315
D	-18	GLY	-	expression tag	UNP O25315
D	-17	SER	-	expression tag	UNP O25315

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP O25315
D	-15	HIS	-	expression tag	UNP O25315
D	-14	HIS	-	expression tag	UNP O25315
D	-13	HIS	-	expression tag	UNP O25315
D	-12	HIS	-	expression tag	UNP O25315
D	-11	HIS	-	expression tag	UNP O25315
D	-10	HIS	-	expression tag	UNP O25315
D	-9	SER	-	expression tag	UNP O25315
D	-8	SER	-	expression tag	UNP O25315
D	-7	GLY	-	expression tag	UNP O25315
D	-6	LEU	-	expression tag	UNP O25315
D	-5	VAL	-	expression tag	UNP O25315
D	-4	PRO	-	expression tag	UNP O25315
D	-3	ARG	-	expression tag	UNP O25315
D	-2	GLY	-	expression tag	UNP O25315
D	-1	SER	-	expression tag	UNP O25315
D	0	HIS	-	expression tag	UNP O25315

- Molecule 2 is SINEFUNGIN (CCD ID: SFG) (formula: C₁₅H₂₃N₇O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			27	15	7	5		
2	A	1	Total	C	N	O	0	0
			27	15	7	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			27	15	7	5		
2	D	1	Total	C	N	O	0	0
			27	15	7	5		

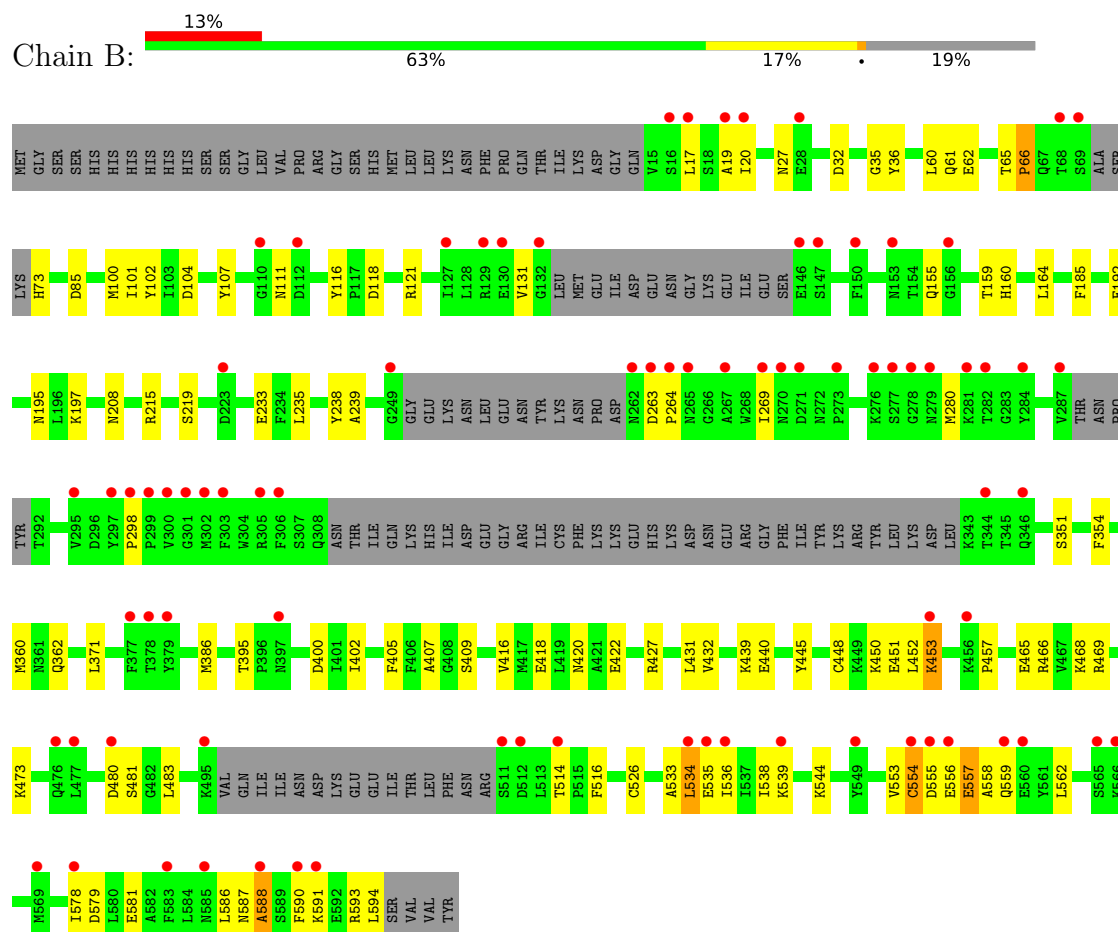
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	19	Total	O	0	0
			19	19		
3	A	28	Total	O	0	0
			28	28		
3	C	31	Total	O	0	0
			31	31		
3	D	13	Total	O	0	0
			13	13		

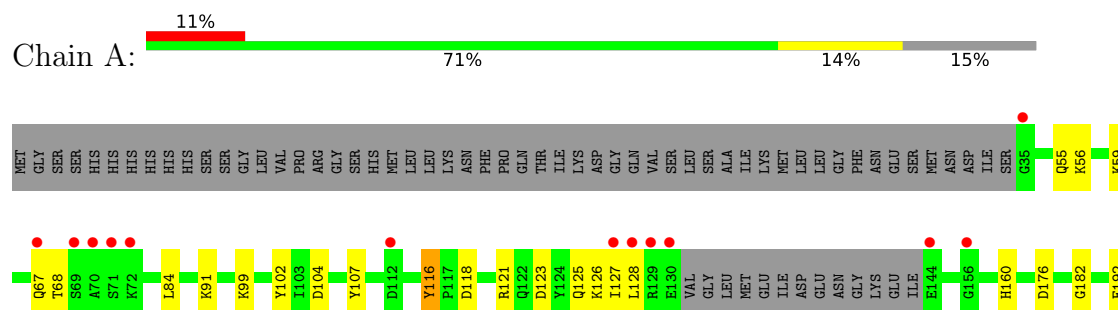
3 Residue-property plots

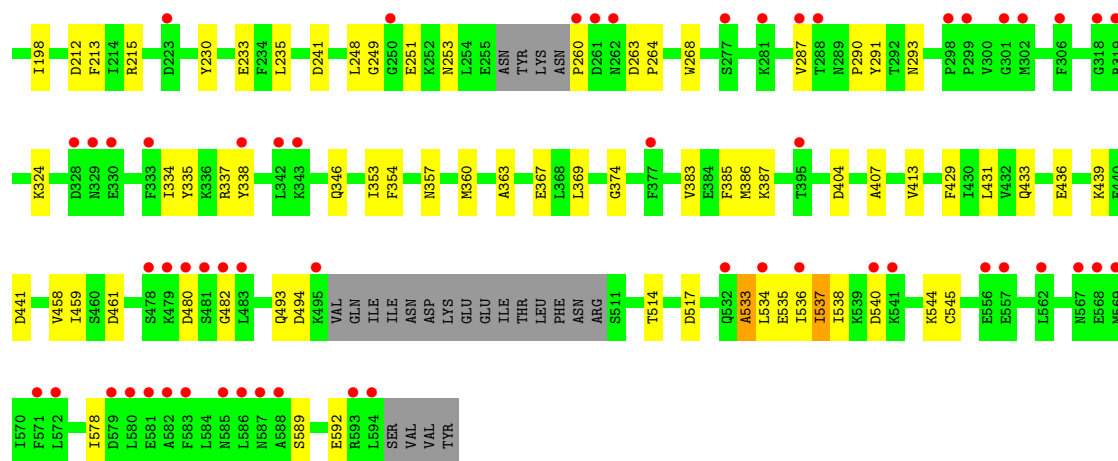
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Adenine specific DNA methyltransferase (Mod)

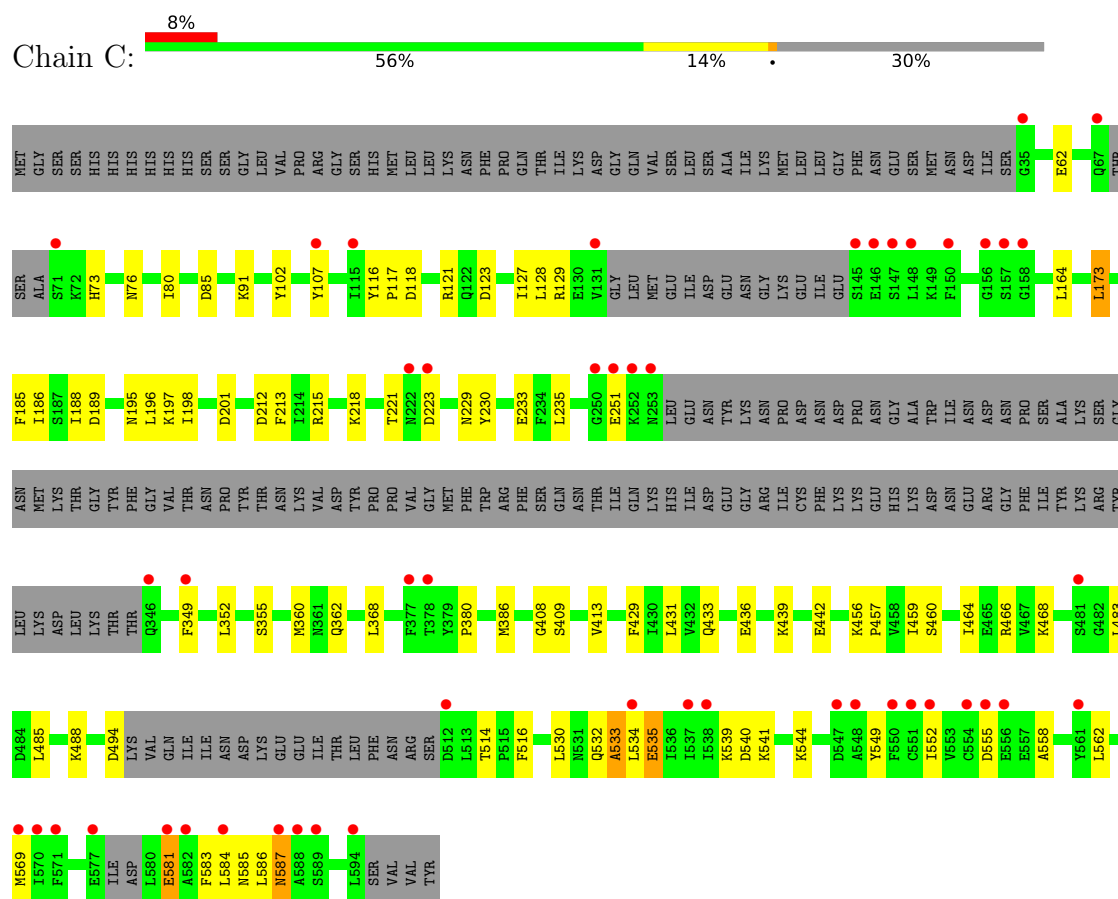


- Molecule 1: Adenine specific DNA methyltransferase (Mod)

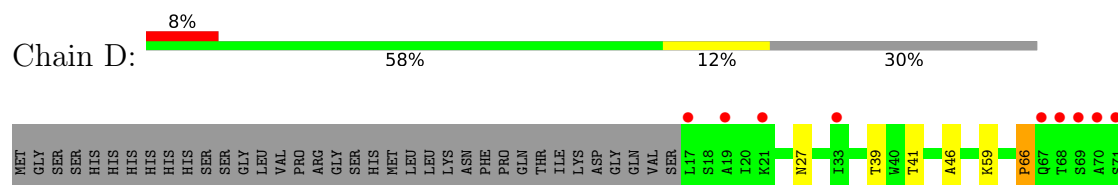


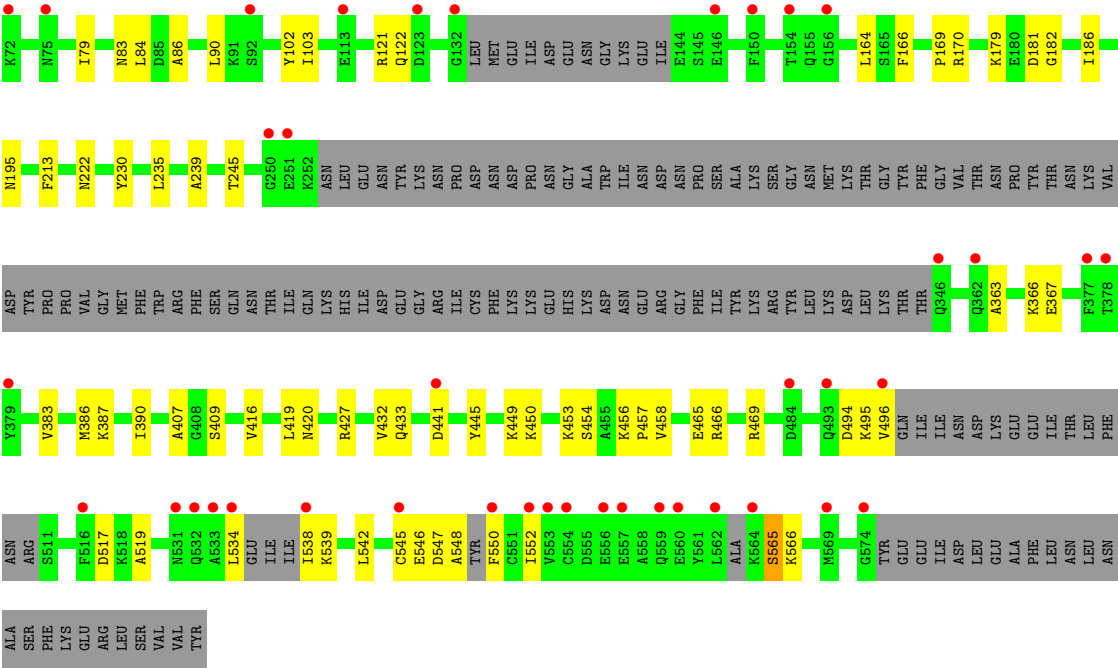


• Molecule 1: Adenine specific DNA methyltransferase (Mod)



• Molecule 1: Adenine specific DNA methyltransferase (Mod)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.81Å 88.48Å 163.33Å 90.00° 96.50° 90.00°	Depositor
Resolution (Å)	50.50 – 2.65 50.50 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.50-2.65) 91.6 (50.50-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.206 , 0.258 0.211 , 0.259	Depositor DCC
R_{free} test set	5095 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14455	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: SFG

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	0.34	0/4062	0.58	3/5497 (0.1%)
1	B	0.36	0/3844	0.63	3/5192 (0.1%)
1	C	0.35	0/3304	0.58	0/4464
1	D	0.32	0/3288	0.54	1/4438 (0.0%)
All	All	0.35	0/14498	0.59	7/19591 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	PRO	N-CA-CB	13.78	110.38	103.22
1	B	66	PRO	N-CA-CB	8.51	112.19	103.25
1	B	264	PRO	N-CA-CB	7.67	110.84	102.72
1	A	260	PRO	N-CA-CB	6.96	110.66	103.00
1	A	290	PRO	N-CA-CB	6.65	109.89	103.51
1	D	66	PRO	N-CA-CB	6.38	109.95	103.25
1	A	264	PRO	N-CA-CB	6.19	110.09	103.52

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	535	GLU	Peptide
1	C	581	GLU	Peptide

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	3987	0	3682	53	0
1	B	3779	0	3513	72	0
1	C	3251	0	3014	74	0
1	D	3239	0	2976	57	0
2	A	27	0	21	1	0
2	B	27	0	21	2	0
2	C	27	0	21	2	0
2	D	27	0	21	0	0
3	A	28	0	0	0	0
3	B	19	0	0	0	0
3	C	31	0	0	0	0
3	D	13	0	0	0	0
All	All	14455	0	13269	248	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 (248) 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:213:PHE:CE2	1:C:349:PHE:CE1	2.10	1.40
1:C:413:VAL:CG2	1:C:431:LEU:HD11	1.67	1.25
1:C:213:PHE:CE2	1:C:349:PHE:CD1	2.37	1.12
1:C:413:VAL:HG21	1:C:431:LEU:CD1	1.81	1.10
1:C:213:PHE:HE2	1:C:349:PHE:CD1	1.68	1.09
1:C:413:VAL:HG21	1:C:431:LEU:HD11	1.13	1.08
1:C:107:TYR:CE1	1:C:188:ILE:HA	1.91	1.05
1:C:213:PHE:CD2	1:C:349:PHE:CE1	2.46	1.03
1:C:213:PHE:CE2	1:C:349:PHE:CZ	2.62	0.87
1:D:179:LYS:NZ	1:D:181:ASP:OD1	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ILE:HG22	1:B:539:LYS:HE2	1.61	0.82
1:D:519:ALA:HB2	1:D:552:ILE:HD11	1.61	0.81
1:C:413:VAL:HG23	1:C:431:LEU:HD11	1.62	0.81
1:B:155:GLN:O	1:B:159:THR:OG1	1.99	0.79
1:D:164:LEU:HD21	1:D:195:ASN:HB3	1.65	0.77
1:C:107:TYR:CE1	1:C:188:ILE:CA	2.67	0.77
1:D:179:LYS:NZ	1:D:181:ASP:OD2	2.17	0.77
1:D:179:LYS:NZ	1:D:181:ASP:CG	2.43	0.76
1:C:368:LEU:HD22	1:C:380:PRO:HG3	1.68	0.76
1:B:554:CYS:HB3	1:B:578:ILE:HD13	1.70	0.73
1:C:436:GLU:HB3	1:C:459:ILE:HD12	1.72	0.72
1:B:514:THR:HG22	1:B:516:PHE:H	1.55	0.72
1:D:179:LYS:CE	1:D:181:ASP:OD1	2.38	0.71
1:C:532:GLN:O	1:C:534:LEU:N	2.24	0.71
1:B:452:LEU:C	1:B:453:LYS:HD2	2.17	0.70
1:B:450:LYS:HE2	1:B:451:GLU:HG2	1.75	0.69
1:A:293:ASN:O	1:A:293:ASN:ND2	2.27	0.68
1:C:514:THR:HG22	1:C:516:PHE:H	1.59	0.68
1:B:555:ASP:O	1:B:557:GLU:N	2.27	0.67
1:D:179:LYS:HZ2	1:D:181:ASP:CG	2.01	0.66
1:D:538:ILE:N	1:D:542:LEU:O	2.29	0.66
1:B:558:ALA:O	1:B:562:LEU:N	2.18	0.65
1:C:483:LEU:HD12	1:C:485:LEU:HD21	1.78	0.65
1:C:558:ALA:O	1:C:562:LEU:N	2.29	0.65
1:C:62:GLU:OE2	1:C:468:LYS:NZ	2.29	0.65
1:C:456:LYS:NZ	1:C:457:PRO:O	2.31	0.64
1:A:534:LEU:HA	1:A:545:CYS:HB2	1.80	0.63
1:C:197:LYS:NZ	1:C:201:ASP:OD1	2.30	0.63
1:C:85:ASP:CG	1:C:121:ARG:HH22	2.07	0.63
1:C:514:THR:HG22	1:C:516:PHE:N	2.14	0.62
1:C:413:VAL:HG13	1:C:429:PHE:CE2	2.34	0.62
1:C:409:SER:OG	1:C:466:ARG:NH2	2.33	0.62
1:B:557:GLU:HG2	1:B:558:ALA:H	1.65	0.61
1:A:291:TYR:HD2	1:A:324:LYS:HA	1.66	0.61
1:C:533:ALA:C	1:C:535:GLU:H	2.09	0.61
1:C:581:GLU:OE2	1:C:583:PHE:CB	2.48	0.61
1:D:103:ILE:HG13	1:D:186:ILE:HG23	1.82	0.60
1:D:166:PHE:CD1	1:D:170:ARG:NH1	2.70	0.60
1:B:185:PHE:HB3	1:B:235:LEU:HD11	1.83	0.59
1:C:413:VAL:CG2	1:C:431:LEU:CD1	2.55	0.59
1:B:535:GLU:N	1:B:535:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LYS:HE2	1:D:181:ASP:OD1	2.03	0.58
1:C:583:PHE:C	1:C:585:ASN:H	2.11	0.58
1:D:121:ARG:NH1	1:D:122:GLN:OE1	2.37	0.58
1:B:32:ASP:O	1:D:41:THR:HG22	2.03	0.58
1:B:17:LEU:O	1:B:20:ILE:HG23	2.04	0.58
1:C:218:LYS:HA	1:C:360:MET:HE3	1.86	0.58
1:B:395:THR:HG22	1:B:400:ASP:OD2	2.04	0.58
1:D:179:LYS:HZ3	1:D:181:ASP:CG	2.12	0.58
1:C:352:LEU:O	1:C:355:SER:OG	2.20	0.58
1:D:83:ASN:OD1	1:D:170:ARG:HD3	2.04	0.57
1:A:55:GLN:N	1:A:55:GLN:OE1	2.38	0.57
1:D:456:LYS:HG2	1:D:458:VAL:HG13	1.87	0.57
1:C:544:LYS:HD2	1:C:549:TYR:CZ	2.39	0.57
1:C:530:LEU:HA	1:C:534:LEU:HD11	1.86	0.57
1:C:213:PHE:CZ	1:C:349:PHE:CZ	2.94	0.56
1:C:494:ASP:OD1	1:C:494:ASP:N	2.35	0.56
1:B:526:CYS:SG	1:B:594:LEU:HD11	2.45	0.56
1:B:85:ASP:OD1	1:B:121:ARG:NH2	2.38	0.55
1:B:100:MET:HE3	1:B:102:TYR:HB2	1.87	0.55
1:C:213:PHE:CD2	1:C:349:PHE:HE1	2.16	0.55
1:D:548:ALA:O	1:D:550:PHE:N	2.40	0.55
1:B:402:ILE:HD12	1:B:416:VAL:HG22	1.89	0.55
1:D:102:TYR:CG	1:D:386:MET:HE1	2.42	0.55
1:A:213:PHE:HB2	1:A:235:LEU:HB3	1.88	0.55
1:C:185:PHE:HB3	1:C:235:LEU:HD11	1.89	0.55
1:C:583:PHE:O	1:C:585:ASN:N	2.39	0.55
1:C:118:ASP:HA	1:C:121:ARG:HG3	1.89	0.54
1:B:164:LEU:HD21	1:B:195:ASN:HB3	1.89	0.54
1:D:534:LEU:HA	1:D:545:CYS:HB2	1.89	0.54
1:D:545:CYS:O	1:D:546:GLU:HG3	2.07	0.54
1:C:107:TYR:CE2	1:C:189:ASP:HB3	2.43	0.54
1:C:164:LEU:HD21	1:C:195:ASN:HB3	1.89	0.54
1:B:407:ALA:O	2:B:601:SFG:HA	2.08	0.54
1:D:407:ALA:HB3	1:D:433:GLN:HB2	1.89	0.53
1:D:179:LYS:HG3	1:D:181:ASP:OD1	2.07	0.53
1:A:514:THR:HG23	1:A:517:ASP:H	1.74	0.53
1:B:73:HIS:CD2	1:B:534:LEU:H	2.27	0.52
1:B:578:ILE:HD12	1:B:579:ASP:H	1.74	0.52
1:B:439:LYS:HG3	1:B:440:GLU:N	2.23	0.52
1:B:553:VAL:O	1:B:555:ASP:N	2.38	0.52
1:C:221:THR:HB	1:C:229:ASN:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:HIS:CD2	1:B:533:ALA:HA	2.45	0.52
1:C:413:VAL:HG21	1:C:431:LEU:HD13	1.84	0.52
1:B:351:SER:HB3	1:D:230:TYR:HA	1.92	0.52
1:C:213:PHE:CD2	1:C:349:PHE:CZ	2.96	0.52
1:A:121:ARG:NH1	1:A:123:ASP:OD2	2.44	0.51
1:B:481:SER:C	1:B:483:LEU:H	2.17	0.51
1:B:418:GLU:O	1:B:422:GLU:HG3	2.10	0.51
1:D:84:LEU:HB2	1:D:170:ARG:HE	1.75	0.51
1:D:456:LYS:O	1:D:456:LYS:HD3	2.10	0.51
1:B:533:ALA:O	1:B:535:GLU:N	2.44	0.51
1:A:334:ILE:HD12	1:A:335:TYR:H	1.76	0.50
1:B:554:CYS:HB3	1:B:578:ILE:CD1	2.40	0.50
1:D:465:GLU:O	1:D:469:ARG:HG3	2.12	0.50
1:B:100:MET:CE	1:B:102:TYR:HB2	2.42	0.50
1:A:514:THR:HG22	1:A:517:ASP:CG	2.37	0.50
1:D:390:ILE:HD13	1:D:416:VAL:HG12	1.94	0.49
1:B:420:ASN:HD21	1:B:427:ARG:N	2.10	0.49
1:A:59:LYS:HD2	1:A:493:GLN:OE1	2.12	0.49
1:A:433:GLN:HE22	2:A:701:SFG:H1'	1.77	0.49
1:D:84:LEU:HD23	1:D:121:ARG:CZ	2.43	0.49
1:A:383:VAL:HG12	1:A:387:LYS:HE2	1.94	0.49
1:C:102:TYR:CG	1:C:386:MET:HE1	2.48	0.48
1:D:84:LEU:HB2	1:D:170:ARG:NE	2.27	0.48
1:C:91:LYS:HD2	1:C:173:LEU:HD12	1.95	0.48
1:B:407:ALA:HB2	1:B:431:LEU:HG	1.96	0.48
1:C:409:SER:HG	1:C:466:ARG:NH2	2.11	0.48
1:B:17:LEU:CD2	1:B:19:ALA:HB3	2.44	0.48
1:A:537:ILE:C	1:A:538:ILE:HD13	2.38	0.48
1:D:445:TYR:CD2	1:D:457:PRO:HG2	2.49	0.48
1:D:59:LYS:HG3	1:D:517:ASP:OD2	2.14	0.48
1:A:514:THR:CG2	1:A:517:ASP:H	2.27	0.48
1:C:360:MET:HE2	1:C:362:GLN:OE1	2.13	0.48
1:C:439:LYS:N	1:C:442:GLU:OE1	2.38	0.48
1:B:450:LYS:CE	1:B:451:GLU:HG2	2.42	0.47
1:D:449:LYS:O	1:D:453:LYS:HA	2.13	0.47
1:D:409:SER:O	1:D:466:ARG:HD2	2.14	0.47
1:A:67:GLN:OE1	1:A:67:GLN:N	2.41	0.47
1:D:494:ASP:O	1:D:496:VAL:N	2.46	0.47
1:A:67:GLN:O	1:A:68:THR:HG22	2.13	0.47
1:A:84:LEU:HD23	1:A:121:ARG:CZ	2.45	0.47
1:D:387:LYS:HG2	1:D:419:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:GLU:HB3	1:A:459:ILE:HD12	1.97	0.47
1:B:107:TYR:N	1:B:107:TYR:CD1	2.83	0.47
1:A:212:ASP:OD1	1:C:230:TYR:OH	2.33	0.47
1:A:357:ASN:HB3	1:A:360:MET:HE2	1.97	0.47
1:C:516:PHE:HE1	1:C:535:GLU:CB	2.28	0.47
1:C:127:ILE:C	1:C:129:ARG:H	2.24	0.47
1:B:536:ILE:HD12	1:B:544:LYS:HD2	1.96	0.46
1:C:80:ILE:HG12	1:C:460:SER:HB2	1.98	0.46
1:C:409:SER:HB3	2:C:801:SFG:OXT	2.15	0.46
1:A:125:GLN:C	1:A:127:ILE:H	2.23	0.46
1:C:80:ILE:HD11	1:C:464:ILE:HD11	1.97	0.46
1:D:363:ALA:O	1:D:367:GLU:HG3	2.15	0.46
1:D:450:LYS:HD2	1:D:453:LYS:HZ2	1.81	0.46
1:B:60:LEU:HD23	1:B:61:GLN:N	2.30	0.46
1:A:407:ALA:HB3	1:A:433:GLN:HB2	1.97	0.46
1:C:409:SER:O	1:C:466:ARG:HD2	2.16	0.46
1:A:215:ARG:HD3	1:A:385:PHE:CE1	2.50	0.46
1:D:213:PHE:HB2	1:D:235:LEU:HB3	1.97	0.46
1:A:230:TYR:OH	1:C:212:ASP:OD1	2.33	0.45
1:C:539:LYS:C	1:C:541:LYS:H	2.24	0.45
1:D:545:CYS:HB3	1:D:550:PHE:HE2	1.81	0.45
1:B:62:GLU:OE2	1:B:468:LYS:NZ	2.43	0.45
1:D:449:LYS:HD2	1:D:454:SER:O	2.17	0.45
1:B:538:ILE:O	1:B:539:LYS:HG2	2.17	0.45
1:A:480:ASP:C	1:A:482:GLY:H	2.25	0.45
1:D:546:GLU:CD	1:D:547:ASP:H	2.24	0.45
1:C:213:PHE:CZ	1:C:349:PHE:CE2	3.05	0.45
1:D:420:ASN:HD21	1:D:427:ARG:N	2.15	0.45
1:B:17:LEU:HD21	1:B:19:ALA:HB3	1.98	0.45
1:B:100:MET:HG2	1:B:101:ILE:N	2.32	0.45
1:B:104:ASP:OD2	2:B:601:SFG:HB2	2.17	0.45
1:B:197:LYS:HD2	1:B:238:TYR:OH	2.17	0.45
1:A:102:TYR:CG	1:A:386:MET:HE1	2.52	0.45
1:C:121:ARG:HB3	1:C:123:ASP:OD1	2.17	0.45
1:C:569:MET:HB2	1:C:569:MET:HE3	1.83	0.44
1:D:239:ALA:HB1	1:D:245:THR:HG21	1.99	0.44
1:D:441:ASP:OD1	1:D:441:ASP:N	2.44	0.44
1:B:409:SER:O	1:B:466:ARG:HD2	2.17	0.44
1:A:407:ALA:CB	1:A:431:LEU:HD22	2.47	0.44
1:B:587:ASN:CG	1:B:588:ALA:N	2.76	0.44
1:C:456:LYS:HA	1:C:456:LYS:HD2	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:ALA:C	1:C:535:GLU:N	2.73	0.44
1:A:241:ASP:OD1	1:A:241:ASP:C	2.61	0.44
1:A:533:ALA:C	1:A:535:GLU:H	2.25	0.44
1:D:79:ILE:O	1:D:432:VAL:HA	2.17	0.44
1:B:36:TYR:HA	1:D:39:THR:O	2.18	0.44
1:B:579:ASP:OD2	1:B:581:GLU:HG2	2.18	0.44
1:A:102:TYR:OH	1:A:104:ASP:HB2	2.17	0.44
1:B:360:MET:HB3	1:B:362:GLN:OE1	2.18	0.43
1:C:586:LEU:O	1:C:587:ASN:C	2.61	0.43
1:C:107:TYR:CZ	1:C:188:ILE:CA	3.01	0.43
1:D:390:ILE:CD1	1:D:416:VAL:HG12	2.49	0.43
1:B:533:ALA:O	1:B:534:LEU:C	2.61	0.43
1:A:160:HIS:HD1	1:A:192:GLU:CD	2.25	0.43
1:A:215:ARG:HA	1:A:354:PHE:O	2.18	0.43
1:B:578:ILE:HD12	1:B:579:ASP:N	2.32	0.43
1:B:593:ARG:C	1:B:594:LEU:HD23	2.44	0.43
1:B:586:LEU:HD12	1:B:586:LEU:HA	1.88	0.43
1:A:458:VAL:O	1:A:461:ASP:HB2	2.19	0.43
1:B:27:ASN:OD1	1:D:27:ASN:ND2	2.52	0.43
1:A:107:TYR:N	1:A:107:TYR:CD1	2.86	0.43
1:A:198:ILE:HD12	1:C:198:ILE:HD13	2.01	0.43
1:A:251:GLU:OE1	1:A:253:ASN:N	2.52	0.43
1:A:439:LYS:HG2	1:A:441:ASP:H	1.84	0.43
1:B:448:CYS:HA	1:B:452:LEU:HB2	2.01	0.43
1:A:369:LEU:HD23	1:A:374:GLY:HA3	2.01	0.43
1:B:35:GLY:HA2	1:D:41:THR:CG2	2.49	0.43
1:B:215:ARG:HH21	1:B:233:GLU:CD	2.27	0.43
1:B:360:MET:HE2	1:B:362:GLN:NE2	2.34	0.43
1:A:160:HIS:ND1	1:A:192:GLU:OE2	2.47	0.43
1:D:367:GLU:OE1	1:D:383:VAL:HB	2.18	0.43
1:B:371:LEU:HD23	1:B:473:LYS:HE2	2.01	0.43
1:D:86:ALA:O	1:D:90:LEU:HD12	2.18	0.43
1:B:405:PHE:HA	1:B:432:VAL:HB	2.01	0.42
1:A:536:ILE:CB	1:A:544:LYS:HB3	2.48	0.42
1:C:213:PHE:CE2	1:C:349:PHE:CG	3.04	0.42
1:C:73:HIS:CE1	1:C:488:LYS:HE2	2.54	0.42
1:D:239:ALA:CB	1:D:245:THR:HG21	2.49	0.42
1:A:363:ALA:O	1:A:367:GLU:HG3	2.19	0.42
1:B:219:SER:N	1:B:360:MET:HE3	2.34	0.42
1:B:116:TYR:CZ	1:B:118:ASP:HB2	2.55	0.42
1:B:590:PHE:C	1:B:591:LYS:HD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:CYS:HB3	1:D:550:PHE:CE2	2.55	0.41
1:B:480:ASP:O	1:B:483:LEU:HB3	2.20	0.41
1:B:534:LEU:O	1:B:535:GLU:C	2.62	0.41
1:C:215:ARG:HH21	1:C:233:GLU:CD	2.27	0.41
1:D:366:LYS:HA	1:D:366:LYS:HD2	1.90	0.41
1:B:102:TYR:CG	1:B:386:MET:HE1	2.54	0.41
1:A:268:TRP:HB3	1:A:338:TYR:CD1	2.54	0.41
1:C:533:ALA:O	1:C:535:GLU:N	2.54	0.41
1:A:116:TYR:CZ	1:A:118:ASP:HB2	2.56	0.41
1:A:215:ARG:HH21	1:A:233:GLU:CD	2.28	0.41
1:C:408:GLY:N	1:C:433:GLN:OE1	2.52	0.41
1:B:445:TYR:CD2	1:B:457:PRO:HG2	2.56	0.41
1:B:557:GLU:C	1:B:559:GLN:N	2.78	0.41
1:A:91:LYS:HE3	1:A:176:ASP:OD2	2.21	0.41
1:A:118:ASP:HA	1:A:121:ARG:HG3	2.02	0.41
1:B:208:ASN:HB3	1:B:239:ALA:O	2.20	0.41
1:A:99:LYS:O	1:A:182:GLY:HA2	2.21	0.41
1:C:433:GLN:HE22	2:C:801:SFG:H1'	1.86	0.41
1:D:102:TYR:CD1	1:D:102:TYR:C	2.97	0.41
1:C:186:ILE:HG21	1:C:196:LEU:HD21	2.02	0.41
1:A:248:LEU:HD13	1:A:346:GLN:HB3	2.03	0.41
1:A:357:ASN:O	1:A:360:MET:HG3	2.21	0.41
1:C:76:ASN:HB3	1:C:429:PHE:CE1	2.56	0.41
1:A:413:VAL:HG22	1:A:429:PHE:CG	2.56	0.41
1:C:552:ILE:HD12	1:C:552:ILE:N	2.36	0.41
1:B:160:HIS:HD1	1:B:192:GLU:CD	2.28	0.40
1:B:215:ARG:HA	1:B:354:PHE:O	2.21	0.40
1:A:56:LYS:HE2	1:A:494:ASP:OD1	2.21	0.40
1:D:46:ALA:O	1:D:169:PRO:HG3	2.22	0.40
1:B:465:GLU:O	1:B:469:ARG:HG3	2.20	0.40
1:A:404:ASP:HB3	1:A:431:LEU:HD23	2.02	0.40
1:A:353:ILE:HD12	1:A:353:ILE:HA	1.86	0.40
1:D:179:LYS:O	1:D:182:GLY:N	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	520/618 (84%)	463 (89%)	44 (8%)	13 (2%)	4	7
1	B	485/618 (78%)	433 (89%)	40 (8%)	12 (2%)	4	7
1	C	421/618 (68%)	383 (91%)	28 (7%)	10 (2%)	4	7
1	D	421/618 (68%)	377 (90%)	38 (9%)	6 (1%)	9	14
All	All	1847/2472 (75%)	1656 (90%)	150 (8%)	41 (2%)	5	9

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	PRO
1	B	263	ASP
1	B	556	GLU
1	A	337	ARG
1	A	537	ILE
1	C	116	TYR
1	C	533	ALA
1	C	555	ASP
1	B	111	ASN
1	B	131	VAL
1	B	534	LEU
1	B	588	ALA
1	A	249	GLY
1	A	287	VAL
1	A	533	ALA
1	C	223	ASP
1	C	251	GLU
1	C	540	ASP
1	C	587	ASN
1	D	495	LYS
1	B	280	MET
1	B	554	CYS

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Mol	Chain	Res	Type
1	B	557	GLU
1	A	263	ASP
1	A	540	ASP
1	A	578	ILE
1	C	128	LEU
1	D	66	PRO
1	D	222	ASN
1	D	565	SER
1	A	126	LYS
1	A	589	SER
1	A	592	GLU
1	C	584	LEU
1	A	116	TYR
1	A	128	LEU
1	D	539	LYS
1	D	566	LYS
1	B	65	THR
1	B	269	ILE
1	C	117	PRO

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	A	392/549 (71%)	392 (100%)	0	100	100
1	B	376/549 (68%)	375 (100%)	1 (0%)	86	94
1	C	320/549 (58%)	319 (100%)	1 (0%)	86	94
1	D	319/549 (58%)	318 (100%)	1 (0%)	86	94
All	All	1407/2196 (64%)	1404 (100%)	3 (0%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	453	LYS
1	C	173	LEU

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Mol	Chain	Res	Type
1	D	565	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	GLN
1	B	191	ASN
1	A	195	ASN
1	A	362	GLN
1	C	397	ASN
1	D	27	ASN
1	D	47	ASN
1	D	73	HIS
1	D	191	ASN
1	D	370	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	SFG	C	801	-	28,29,29	2.98	9 (32%)	34,42,42	2.17	10 (29%)
2	SFG	D	901	-	28,29,29	3.03	10 (35%)	34,42,42	2.48	12 (35%)
2	SFG	B	601	-	28,29,29	2.99	11 (39%)	34,42,42	2.23	11 (32%)
2	SFG	A	701	-	28,29,29	3.05	10 (35%)	34,42,42	2.45	11 (32%)

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	SFG	C	801	-	-	3/17/33/33	0/3/3/3
2	SFG	D	901	-	-	3/17/33/33	0/3/3/3
2	SFG	B	601	-	-	4/17/33/33	0/3/3/3
2	SFG	A	701	-	-	2/17/33/33	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	SFG	O4'-C1'	8.25	1.61	1.42
2	C	801	SFG	O4'-C1'	8.00	1.60	1.42
2	D	901	SFG	O4'-C1'	7.77	1.60	1.42
2	B	601	SFG	O4'-C1'	7.68	1.59	1.42
2	A	701	SFG	C2'-C1'	-7.03	1.31	1.53
2	D	901	SFG	C2'-C1'	-6.94	1.31	1.53
2	B	601	SFG	C2'-C1'	-6.70	1.32	1.53
2	C	801	SFG	C2'-C1'	-6.68	1.32	1.53
2	B	601	SFG	O4'-C4'	-6.42	1.30	1.45
2	A	701	SFG	O4'-C4'	-6.15	1.31	1.45
2	C	801	SFG	O4'-C4'	-6.13	1.31	1.45
2	D	901	SFG	O4'-C4'	-6.10	1.31	1.45
2	D	901	SFG	C6-N6	5.05	1.47	1.34
2	B	601	SFG	C6-N6	5.00	1.47	1.34
2	A	701	SFG	C6-N6	4.90	1.46	1.34
2	C	801	SFG	C6-N6	4.81	1.46	1.34
2	B	601	SFG	O2'-C2'	4.48	1.54	1.43
2	C	801	SFG	O2'-C2'	4.35	1.53	1.43
2	A	701	SFG	C5'-CD	4.24	1.60	1.53
2	D	901	SFG	O2'-C2'	4.10	1.53	1.43
2	D	901	SFG	C5'-CD	4.01	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	SFG	O2'-C2'	3.98	1.52	1.43
2	C	801	SFG	C5'-CD	3.94	1.59	1.53
2	B	601	SFG	C5'-CD	3.82	1.59	1.53
2	D	901	SFG	O3'-C3'	-2.85	1.35	1.43
2	A	701	SFG	CG-CD	-2.76	1.49	1.53
2	D	901	SFG	C5-C4	-2.75	1.34	1.39
2	D	901	SFG	C5'-C4'	2.72	1.57	1.52
2	B	601	SFG	O3'-C3'	-2.71	1.36	1.43
2	A	701	SFG	O3'-C3'	-2.69	1.36	1.43
2	C	801	SFG	O3'-C3'	-2.66	1.36	1.43
2	B	601	SFG	C5-C4	-2.62	1.34	1.39
2	A	701	SFG	C5'-C4'	2.50	1.57	1.52
2	D	901	SFG	C5-N7	-2.36	1.34	1.39
2	C	801	SFG	C5'-C4'	2.29	1.56	1.52
2	A	701	SFG	C5-C4	-2.10	1.35	1.39
2	C	801	SFG	C5-C4	-2.07	1.35	1.39
2	B	601	SFG	CD-NE	-2.07	1.40	1.46
2	B	601	SFG	C5-N7	-2.06	1.35	1.39
2	B	601	SFG	C5'-C4'	2.00	1.56	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	SFG	N3-C2-N1	-6.21	119.18	128.58
2	B	601	SFG	N3-C2-N1	-5.81	119.79	128.58
2	A	701	SFG	N3-C2-N1	-5.74	119.89	128.58
2	D	901	SFG	C5-C4-N3	-5.59	119.02	126.72
2	C	801	SFG	N3-C2-N1	-5.58	120.13	128.58
2	A	701	SFG	C5-C4-N3	-5.41	119.27	126.72
2	C	801	SFG	C5-C4-N3	-5.38	119.31	126.72
2	A	701	SFG	N6-C6-N1	-5.26	106.66	118.38
2	B	601	SFG	C5-C4-N3	-5.21	119.54	126.72
2	D	901	SFG	N6-C6-N1	-4.88	107.51	118.38
2	A	701	SFG	N9-C8-N7	-4.81	107.11	113.94
2	D	901	SFG	N9-C8-N7	-4.47	107.59	113.94
2	B	601	SFG	N9-C8-N7	-4.13	108.08	113.94
2	D	901	SFG	C2-N3-C4	4.13	121.91	111.83
2	C	801	SFG	N6-C6-N1	-3.91	109.67	118.38
2	A	701	SFG	C2-N3-C4	3.85	121.23	111.83
2	A	701	SFG	C5-C6-N6	3.77	132.62	123.29
2	B	601	SFG	N3-C4-N9	3.74	133.52	127.17
2	C	801	SFG	N9-C8-N7	-3.66	108.74	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	SFG	C2-N3-C4	3.66	120.76	111.83
2	C	801	SFG	C2-N3-C4	3.60	120.61	111.83
2	C	801	SFG	N3-C4-N9	3.54	133.18	127.17
2	B	601	SFG	N6-C6-N1	-3.53	110.51	118.38
2	A	701	SFG	C5-N7-C8	3.42	108.82	103.45
2	D	901	SFG	C5-C6-N6	3.29	131.43	123.29
2	D	901	SFG	N3-C4-N9	3.16	132.54	127.17
2	D	901	SFG	C5-N7-C8	3.15	108.39	103.45
2	B	601	SFG	O4'-C1'-N9	3.08	114.00	108.09
2	D	901	SFG	O4'-C1'-N9	2.91	113.67	108.09
2	A	701	SFG	N3-C4-N9	2.90	132.10	127.17
2	A	701	SFG	C4-C5-N7	-2.87	107.30	110.58
2	B	601	SFG	C4-N9-C8	2.78	108.65	105.74
2	D	901	SFG	C4-C5-N7	-2.70	107.50	110.58
2	A	701	SFG	C5-C4-N9	2.58	108.62	105.81
2	C	801	SFG	C5-C6-N6	2.42	129.28	123.29
2	D	901	SFG	C5-C4-N9	2.41	108.44	105.81
2	B	601	SFG	C5-N7-C8	2.29	107.05	103.45
2	A	701	SFG	C4-N9-C8	2.29	108.14	105.74
2	B	601	SFG	C5-C6-N6	2.21	128.77	123.29
2	D	901	SFG	C4-N9-C8	2.20	108.05	105.74
2	C	801	SFG	C6-C5-C4	2.11	120.06	117.18
2	C	801	SFG	C4-N9-C8	2.11	107.95	105.74
2	C	801	SFG	C5-N7-C8	2.10	106.75	103.45
2	B	601	SFG	C6-C5-C4	2.02	119.93	117.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

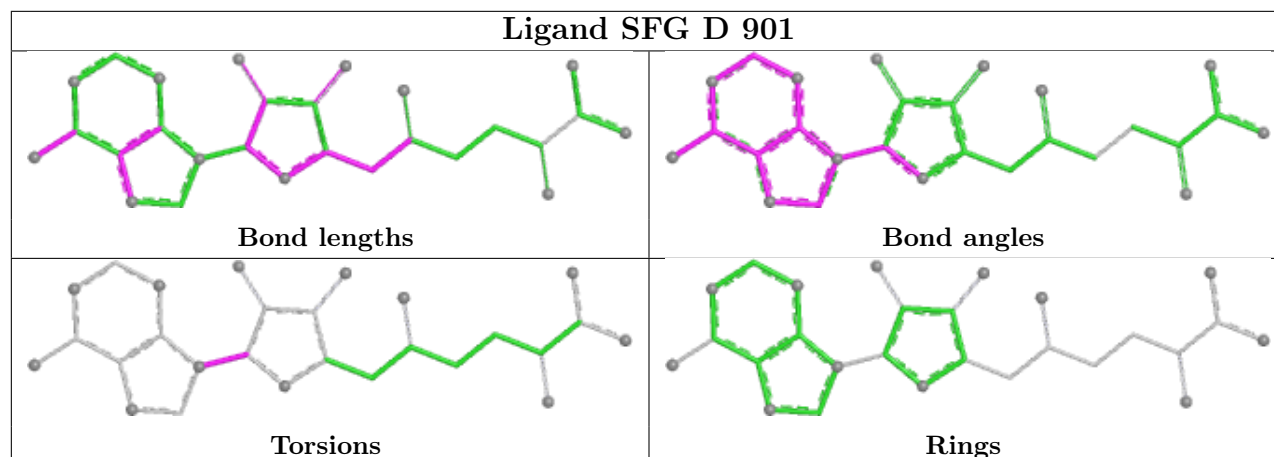
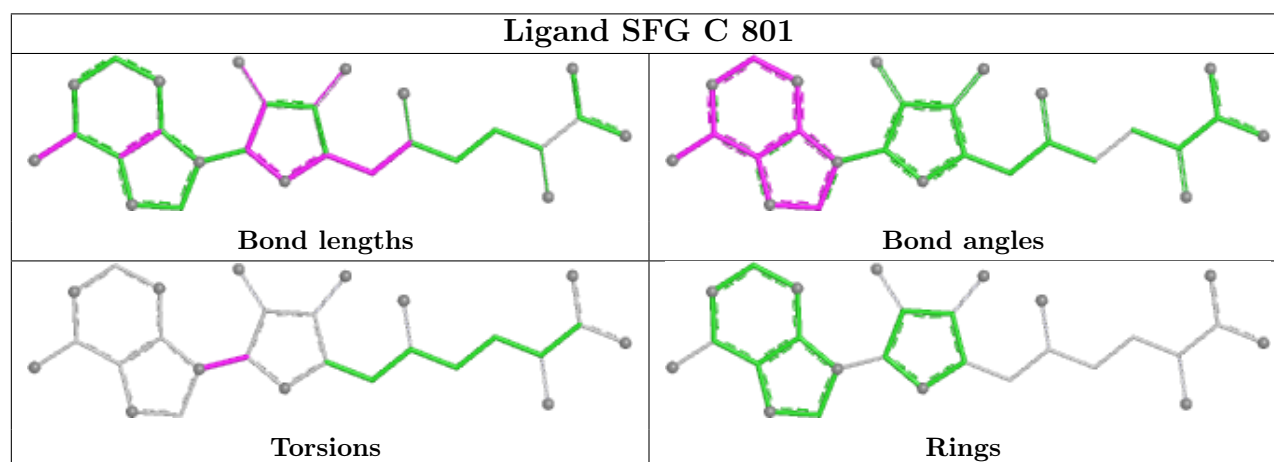
Mol	Chain	Res	Type	Atoms
2	D	901	SFG	C2'-C1'-N9-C8
2	B	601	SFG	C2'-C1'-N9-C8
2	A	701	SFG	C2'-C1'-N9-C8
2	C	801	SFG	C2'-C1'-N9-C8
2	B	601	SFG	O4'-C4'-C5'-CD
2	C	801	SFG	C2'-C1'-N9-C4
2	C	801	SFG	O4'-C1'-N9-C8
2	D	901	SFG	C2'-C1'-N9-C4
2	B	601	SFG	O4'-C1'-N9-C8
2	A	701	SFG	O4'-C1'-N9-C8
2	D	901	SFG	O4'-C1'-N9-C8
2	B	601	SFG	C3'-C4'-C5'-CD

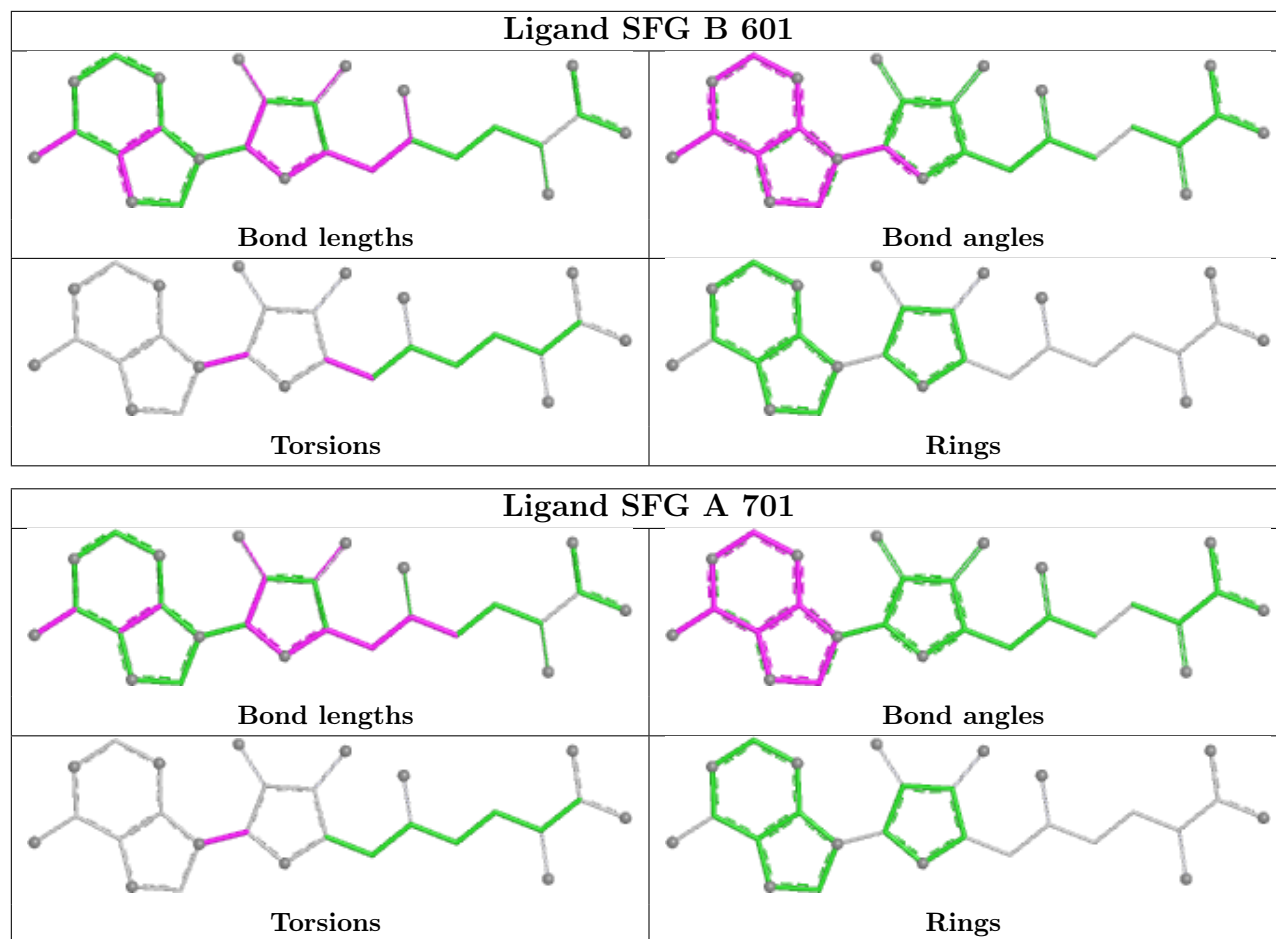
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	SFG	2	0
2	B	601	SFG	2	0
2	A	701	SFG	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	528/618 (85%)	0.59	69 (13%) 7 6	35, 81, 158, 191	0
1	B	499/618 (80%)	0.64	81 (16%) 4 3	42, 81, 152, 221	0
1	C	433/618 (70%)	0.47	49 (11%) 10 8	39, 73, 143, 195	0
1	D	435/618 (70%)	0.62	49 (11%) 10 8	40, 81, 160, 210	0
All	All	1895/2472 (76%)	0.58	248 (13%) 7 6	35, 79, 156, 221	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	577	GLU	6.9
1	B	132	GLY	6.3
1	A	586	LEU	6.0
1	A	534	LEU	6.0
1	C	534	LEU	5.6
1	B	69	SER	5.6
1	D	75	ASN	5.1
1	B	267	ALA	5.0
1	D	553	VAL	4.9
1	C	346	GLN	4.8
1	B	306	PHE	4.8
1	B	301	GLY	4.7
1	A	594	LEU	4.7
1	A	495	LYS	4.6
1	B	300	VAL	4.6
1	D	574	GLY	4.5
1	D	379	TYR	4.4
1	C	158	GLY	4.4
1	B	281	LYS	4.3
1	D	378	THR	4.3
1	A	579	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	146	GLU	4.2
1	C	146	GLU	4.2
1	A	582	ALA	4.2
1	C	253	ASN	4.2
1	A	342	LEU	4.1
1	D	554	CYS	4.1
1	C	512	ASP	4.1
1	B	287	VAL	4.1
1	D	71	SER	4.1
1	B	284	TYR	4.0
1	C	71	SER	4.0
1	B	249	GLY	3.9
1	B	583	PHE	3.9
1	D	531	ASN	3.8
1	B	554	CYS	3.8
1	C	378	THR	3.8
1	D	113	GLU	3.8
1	C	147	SER	3.8
1	B	377	PHE	3.8
1	A	478	SER	3.7
1	A	260	PRO	3.7
1	A	330	GLU	3.7
1	C	67	GLN	3.7
1	C	569	MET	3.7
1	A	301	GLY	3.6
1	D	132	GLY	3.6
1	A	129	ARG	3.6
1	C	107	TYR	3.6
1	A	130	GLU	3.6
1	B	588	ALA	3.6
1	A	329	ASN	3.5
1	B	556	GLU	3.5
1	A	536	ILE	3.4
1	D	67	GLN	3.4
1	B	20	ILE	3.4
1	D	69	SER	3.4
1	A	223	ASP	3.4
1	B	269	ILE	3.4
1	B	536	ILE	3.4
1	C	35	GLY	3.4
1	B	271	ASP	3.4
1	D	72	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	377	PHE	3.3
1	C	555	ASP	3.3
1	D	377	PHE	3.3
1	D	534	LEU	3.3
1	C	588	ALA	3.3
1	B	559	GLN	3.3
1	A	287	VAL	3.3
1	A	572	LEU	3.2
1	C	377	PHE	3.2
1	A	72	LYS	3.2
1	A	67	GLN	3.2
1	C	548	ALA	3.2
1	D	251	GLU	3.1
1	B	16	SER	3.1
1	C	589	SER	3.1
1	C	571	PHE	3.1
1	D	538	ILE	3.1
1	B	397	ASN	3.1
1	A	128	LEU	3.1
1	D	496	VAL	3.1
1	A	127	ILE	3.1
1	C	594	LEU	3.0
1	C	251	GLU	3.0
1	C	551	CYS	3.0
1	B	534	LEU	3.0
1	A	261	ASP	3.0
1	C	131	VAL	3.0
1	B	130	GLU	3.0
1	D	556	GLU	3.0
1	B	262	ASN	3.0
1	B	299	PRO	3.0
1	A	540	ASP	3.0
1	D	68	THR	3.0
1	A	250	GLY	3.0
1	A	532	GLN	2.9
1	C	554	CYS	2.9
1	A	112	ASP	2.9
1	B	511	SER	2.9
1	B	297	TYR	2.9
1	A	581	GLU	2.9
1	B	379	TYR	2.9
1	A	328	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	582	ALA	2.9
1	A	298	PRO	2.9
1	D	569	MET	2.9
1	A	277	SER	2.9
1	B	265	ASN	2.9
1	B	585	ASN	2.9
1	A	585	ASN	2.9
1	C	537	ILE	2.9
1	B	19	ALA	2.9
1	A	281	LYS	2.8
1	C	250	GLY	2.8
1	A	583	PHE	2.8
1	D	545	CYS	2.8
1	B	147	SER	2.8
1	C	148	LEU	2.8
1	C	538	ILE	2.8
1	D	33	ILE	2.8
1	A	262	ASN	2.7
1	B	344	THR	2.7
1	A	70	ALA	2.7
1	B	512	ASP	2.7
1	B	264	PRO	2.7
1	A	299	PRO	2.7
1	A	588	ALA	2.7
1	B	295	VAL	2.7
1	D	250	GLY	2.6
1	B	277	SER	2.6
1	D	154	THR	2.6
1	C	570	ILE	2.6
1	B	590	PHE	2.6
1	C	223	ASP	2.6
1	D	123	ASP	2.6
1	C	252	LYS	2.6
1	B	378	THR	2.6
1	B	480	ASP	2.6
1	D	484	ASP	2.6
1	A	482	GLY	2.6
1	C	584	LEU	2.5
1	B	591	LYS	2.5
1	C	349	PHE	2.5
1	A	480	ASP	2.5
1	A	580	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	110	GLY	2.5
1	B	156	GLY	2.5
1	D	150	PHE	2.5
1	A	302	MET	2.5
1	B	565	SER	2.5
1	B	453	LYS	2.5
1	C	145	SER	2.5
1	B	28	GLU	2.5
1	A	35	GLY	2.5
1	D	532	GLN	2.5
1	B	17	LEU	2.4
1	B	112	ASP	2.4
1	B	68	THR	2.4
1	C	222	ASN	2.4
1	B	278	GLY	2.4
1	D	550	PHE	2.4
1	D	562	LEU	2.4
1	B	346	GLN	2.4
1	B	270	ASN	2.4
1	A	144	GLU	2.4
1	C	547	ASP	2.4
1	D	441	ASP	2.4
1	A	569	MET	2.4
1	A	288	THR	2.3
1	A	479	LYS	2.3
1	A	481	SER	2.3
1	D	21	LYS	2.3
1	C	561	TYR	2.3
1	B	279	ASN	2.3
1	D	560	GLU	2.3
1	D	92	SER	2.3
1	B	150	PHE	2.3
1	D	17	LEU	2.3
1	B	127	ILE	2.3
1	B	514	THR	2.3
1	C	556	GLU	2.3
1	D	564	LYS	2.3
1	B	555	ASP	2.3
1	D	19	ALA	2.3
1	A	557	GLU	2.3
1	A	567	ASN	2.3
1	C	115	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	319	ARG	2.2
1	D	559	GLN	2.2
1	B	276	LYS	2.2
1	B	303	PHE	2.2
1	B	539	LYS	2.2
1	B	535	GLU	2.2
1	A	395	THR	2.2
1	A	541	LYS	2.2
1	D	552	ILE	2.2
1	B	282	THR	2.2
1	C	581	GLU	2.2
1	B	129	ARG	2.2
1	D	346	GLN	2.2
1	B	223	ASP	2.2
1	B	456	LYS	2.2
1	B	495	LYS	2.2
1	D	156	GLY	2.2
1	C	157	SER	2.2
1	D	557	GLU	2.2
1	B	153	ASN	2.2
1	B	273	PRO	2.2
1	B	263	ASP	2.2
1	A	69	SER	2.2
1	A	306	PHE	2.2
1	D	70	ALA	2.1
1	B	560	GLU	2.1
1	A	483	LEU	2.1
1	A	562	LEU	2.1
1	A	571	PHE	2.1
1	D	516	PHE	2.1
1	B	302	MET	2.1
1	A	338	TYR	2.1
1	A	156	GLY	2.1
1	C	156	GLY	2.1
1	C	552	ILE	2.1
1	C	150	PHE	2.1
1	A	556	GLU	2.1
1	D	533	ALA	2.1
1	B	569	MET	2.1
1	B	477	LEU	2.1
1	A	587	ASN	2.1
1	A	568	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	593	ARG	2.0
1	D	146	GLU	2.0
1	A	71	SER	2.0
1	B	566	LYS	2.0
1	A	343	LYS	2.0
1	C	587	ASN	2.0
1	B	578	ILE	2.0
1	B	305	ARG	2.0
1	A	333	PHE	2.0
1	C	550	PHE	2.0
1	C	481	SER	2.0
1	B	298	PRO	2.0
1	B	476	GLN	2.0
1	D	362	GLN	2.0
1	D	493	GLN	2.0
1	A	318	GLY	2.0
1	B	549	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

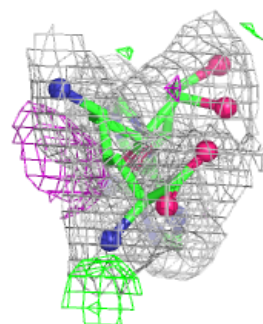
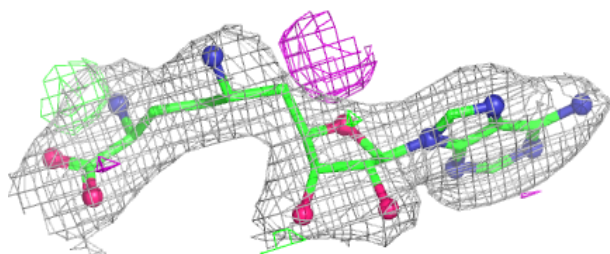
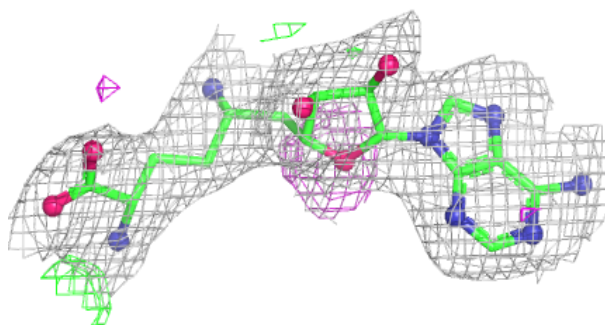
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SFG	B	601	27/27	0.94	0.09	40,47,61,64	0
2	SFG	D	901	27/27	0.94	0.10	46,58,67,71	0
2	SFG	C	801	27/27	0.95	0.08	43,51,62,68	0
2	SFG	A	701	27/27	0.95	0.08	34,46,57,62	0

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.

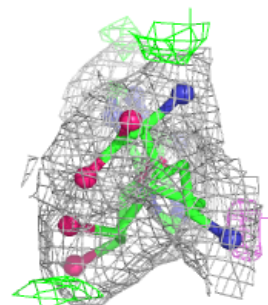
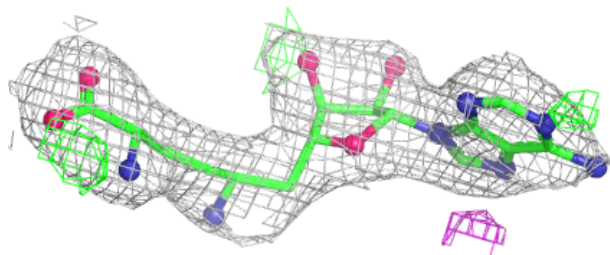
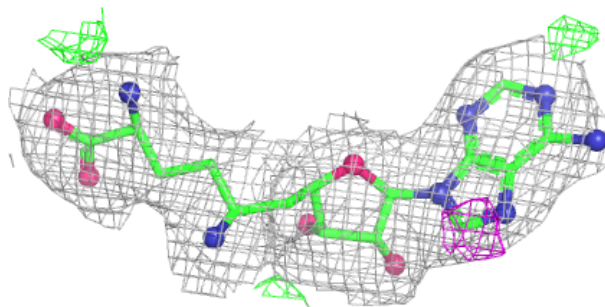
Electron density around SFG B 601:

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

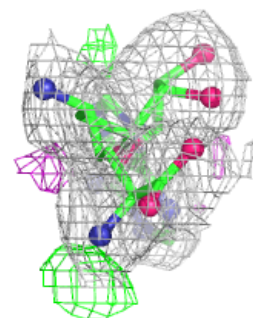
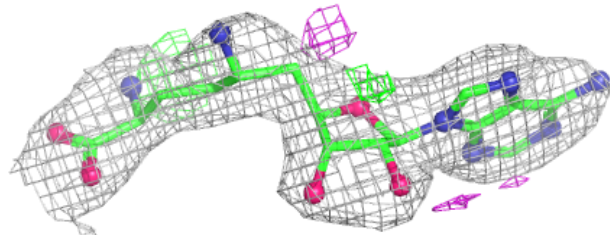
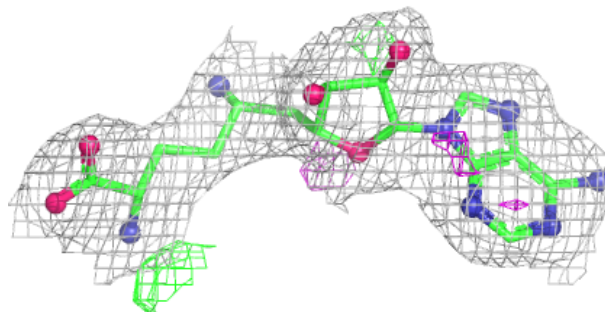


Electron density around SFG D 901:

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

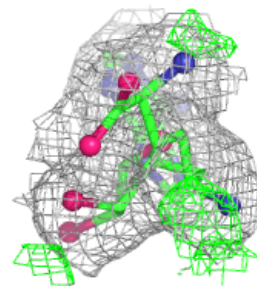
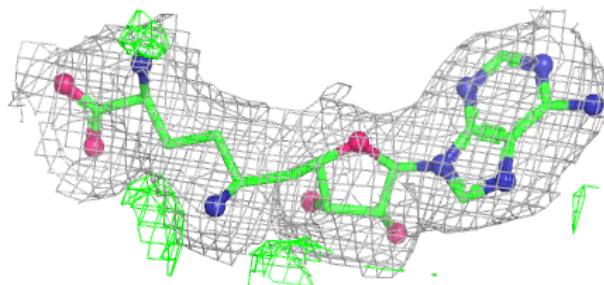
**Electron density around SFG C 801:**

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



Electron density around SFG A 701:

$2mF_o-DF_c$ (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.