



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:19 AM UTC

PDB ID : 9C3T / pdb_00009c3t
Title : Crystal structure of DNA N6-Adenine Methyltransferase M.BceJIV from Burkholderia cenocepacia in complex with duplex DNA substrate containing GTAAAC as recognition sequence
Authors : Kottur, J.; Quintana-Feliciano, R.; Aggarwal, A.K.
Deposited on : 2024-06-02
Resolution : 2.37 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

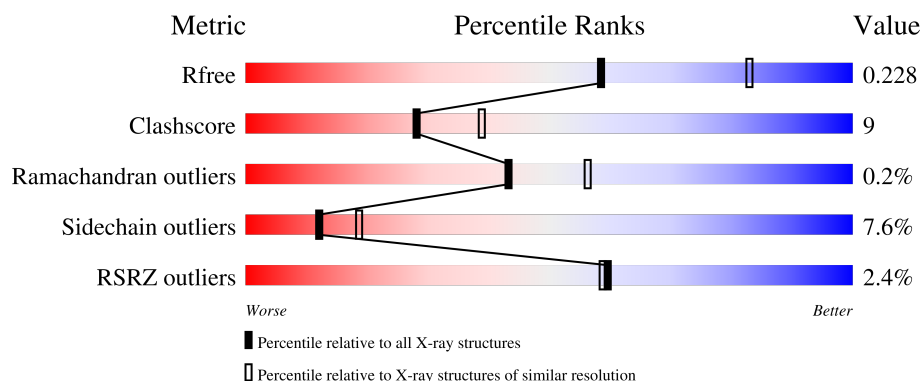
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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.



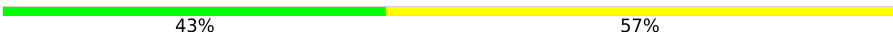
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	283	0% 66% 20% • 12%
1	B	283	72% 15% • 12%
1	C	283	4% 60% 25% • 12%
1	D	283	5% 61% 23% • 14%

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Mol	Chain	Length	Quality of chain
2	E	14	 71% 29%
2	G	14	 79% 21%
2	I	14	 64% 36%
2	K	14	 64% 36%
3	F	14	 50% 50%
3	H	14	 79% 21%
3	J	14	 71% 29%
3	L	14	 43% 57%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10491 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 Methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1978	1262	343	363	10			
1	B	249	Total	C	N	O	S	0	0	0
			1989	1267	347	365	10			
1	C	250	Total	C	N	O	S	0	0	0
			1913	1218	333	352	10			
1	D	244	Total	C	N	O	S	0	0	0
			1888	1206	329	343	10			

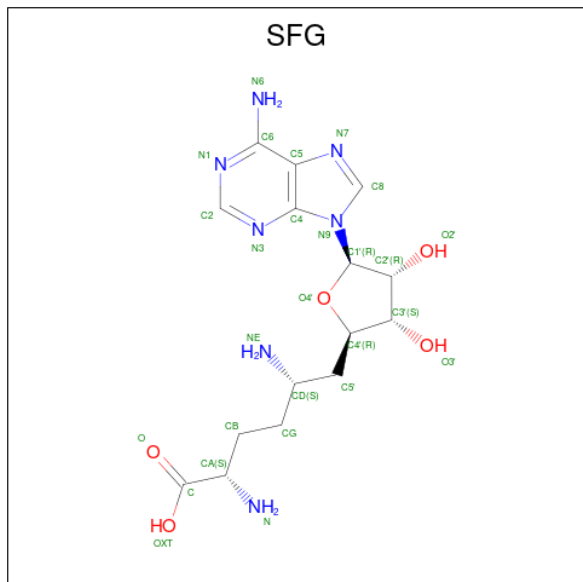
- Molecule 2 is a DNA chain called DNA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			283	137	52	81	13			
2	G	14	Total	C	N	O	P	0	0	0
			282	137	52	80	13			
2	I	14	Total	C	N	O	P	0	0	0
			283	137	52	81	13			
2	K	14	Total	C	N	O	P	0	0	0
			282	137	52	80	13			

- Molecule 3 is a DNA chain called DNA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			285	138	51	83	13			
3	H	14	Total	C	N	O	P	0	0	0
			284	138	51	82	13			
3	J	14	Total	C	N	O	P	0	0	0
			285	138	51	83	13			
3	L	14	Total	C	N	O	P	0	0	0
			285	138	51	83	13			

- Molecule 4 is SINEFUNGIN (CCD ID: SFG) (formula: $C_{15}H_{23}N_7O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	97	Total	O	0	0
			97	97		
5	C	36	Total	O	0	0
			36	36		
5	D	40	Total	O	0	0
			40	40		
5	E	12	Total	O	0	0
			12	12		
5	F	19	Total	O	0	0
			19	19		

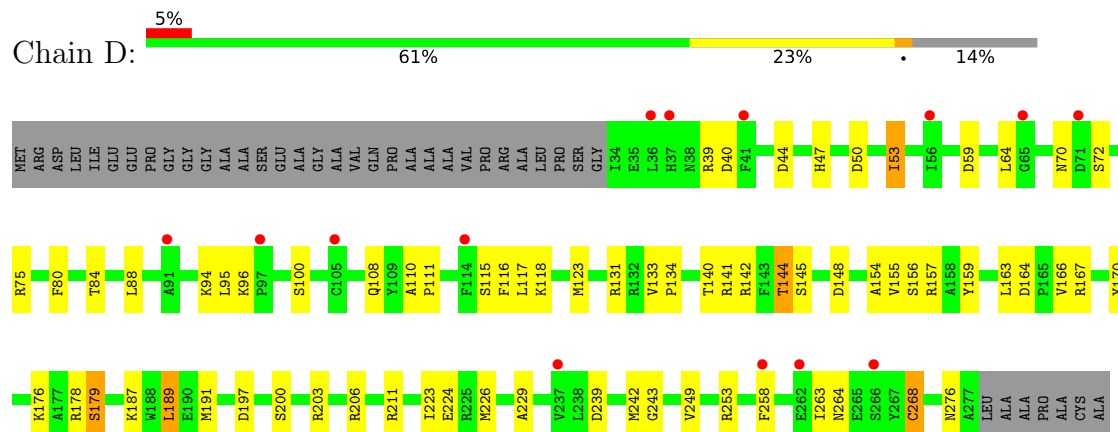
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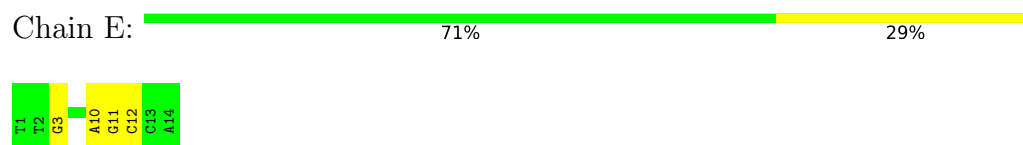
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	15	Total 15	O 15	0	0
5	H	21	Total 21	O 21	0	0
5	I	7	Total 7	O 7	0	0
5	J	12	Total 12	O 12	0	0
5	K	3	Total 3	O 3	0	0
5	L	10	Total 10	O 10	0	0

CYS
ALA

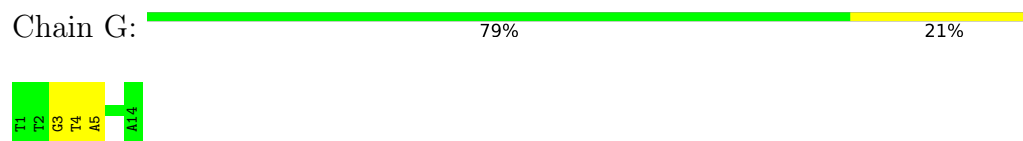
- Molecule 1: Methyltransferase



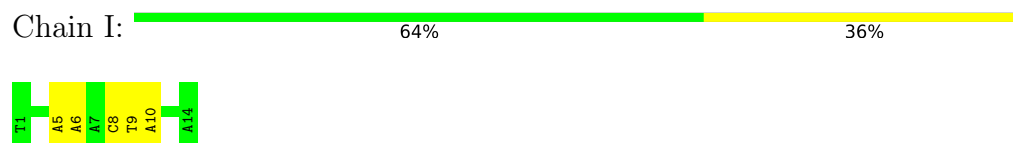
- Molecule 2: DNA1



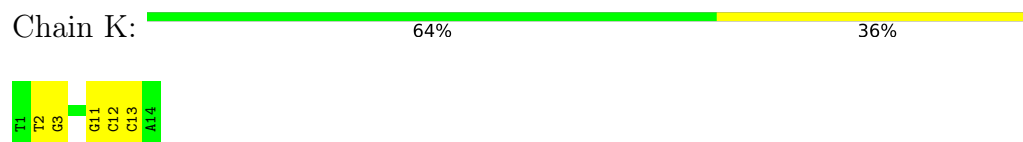
- Molecule 2: DNA1



- Molecule 2: DNA1

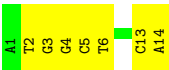


- Molecule 2: DNA1

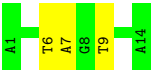
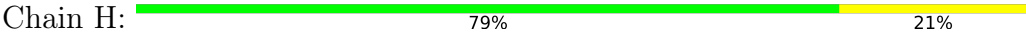


- Molecule 3: DNA2





● Molecule 3: DNA2



● Molecule 3: DNA2



● Molecule 3: DNA2



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	137.73Å 137.73Å 167.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.76 – 2.37 32.76 – 2.37	Depositor EDS
% Data completeness (in resolution range)	61.8 (32.76-2.37) 61.7 (32.76-2.37)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.36Å)	Xtriage
Refinement program	PHENIX (1.20rc3_4406: ???)	Depositor
R, R_{free}	0.181 , 0.235 0.193 , 0.228	Depositor DCC
R_{free} test set	1950 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for -h,k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10491	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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	0.76	0/2034	1.06	5/2764 (0.2%)
1	B	0.61	0/2045	0.86	1/2778 (0.0%)
1	C	0.72	0/1966	1.02	0/2681
1	D	0.54	0/1943	0.77	3/2645 (0.1%)
2	E	0.35	0/317	0.64	0/487
2	G	0.32	0/316	0.63	0/485
2	I	0.39	0/317	0.65	0/487
2	K	0.37	0/316	0.65	0/485
3	F	0.36	0/319	0.77	0/491
3	H	0.36	0/318	0.76	0/490
3	J	0.31	0/319	0.65	0/491
3	L	0.37	0/319	0.67	0/491
All	All	0.60	0/10529	0.88	9/14775 (0.1%)

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	A	0	3
1	B	0	3
1	C	0	2
1	D	0	2
All	All	0	10

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	HIS	N-CA-C	-6.83	104.94	113.28
1	D	197	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	198	VAL	N-CA-CB	5.82	119.21	111.64
1	A	97	PRO	N-CA-CB	-5.64	97.32	103.25
1	A	251	CYS	N-CA-C	-5.47	106.74	113.41
1	B	140	THR	N-CA-C	-5.23	104.93	113.19
1	A	104	PHE	CA-CB-CG	5.02	118.82	113.80
1	A	69	GLY	N-CA-C	-5.02	108.33	115.30
1	D	148	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ARG	Sidechain
1	A	206	ARG	Sidechain
1	A	274	ARG	Sidechain
1	B	141	ARG	Sidechain
1	B	253	ARG	Sidechain
1	B	75	ARG	Sidechain
1	C	131	ARG	Sidechain
1	C	142	ARG	Sidechain
1	D	141	ARG	Sidechain
1	D	142	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1978	0	1908	29	0
1	B	1989	0	1918	25	0
1	C	1913	0	1780	49	0
1	D	1888	0	1757	42	0
2	E	283	0	160	5	0
2	G	282	0	158	2	0
2	I	283	0	160	3	0
2	K	282	0	158	4	0
3	F	285	0	161	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	284	0	158	2	0
3	J	285	0	161	5	0
3	L	285	0	161	6	0
4	A	27	0	22	2	0
4	B	27	0	21	4	0
4	C	27	0	22	3	0
4	D	27	0	21	7	0
5	A	74	0	0	0	0
5	B	97	0	0	1	0
5	C	36	0	0	0	0
5	D	40	0	0	0	0
5	E	12	0	0	1	0
5	F	19	0	0	0	0
5	G	15	0	0	0	0
5	H	21	0	0	0	0
5	I	7	0	0	0	0
5	J	12	0	0	0	0
5	K	3	0	0	0	0
5	L	10	0	0	0	0
All	All	10491	0	8726	164	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 (164) 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:223:ILE:HA	1:C:226:MET:HE2	1.73	0.70
1:A:223:ILE:HA	1:A:226:MET:HE2	1.76	0.67
1:D:59:ASP:OD2	4:D:301:SFG:N	2.28	0.67
1:C:55:LEU:HD21	1:C:57:VAL:HG23	1.77	0.66
3:F:2:DT:H2''	3:F:3:DG:H5''	1.77	0.65
2:K:12:DC:H2''	2:K:13:DC:H5'	1.79	0.65
3:L:5:DC:H2'	3:L:6:DT:C6	2.31	0.64
1:A:180:ARG:NH2	2:G:3:DG:O6	2.30	0.63
1:C:214:HIS:CE1	4:C:301:SFG:HB1	2.33	0.63
1:C:228:LEU:HD21	1:C:254:GLN:HG3	1.81	0.62
1:D:224:GLU:CD	1:D:253:ARG:HH21	2.08	0.61
1:D:166:VAL:HG21	1:D:229:ALA:HB2	1.83	0.60
1:D:167:ARG:NH2	3:J:9:DT:OP1	2.30	0.60
1:A:88:LEU:HD22	1:A:117:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:6:DT:H2'	3:L:7:DA:C8	2.38	0.59
1:D:133:VAL:HG11	1:D:203:ARG:HH21	1.68	0.58
1:A:164:ASP:HA	1:A:167:ARG:HD2	1.85	0.58
1:C:56:ILE:HG13	1:C:95:LEU:HD13	1.86	0.58
1:C:249:VAL:HG11	1:C:274:ARG:HB3	1.86	0.57
1:C:95:LEU:HG	1:C:99:GLY:HA3	1.87	0.57
1:C:196:LYS:HE3	1:D:134:PRO:HG3	1.87	0.56
1:A:166:VAL:HG11	1:A:229:ALA:HB2	1.88	0.55
1:D:75:ARG:HB3	1:D:80:PHE:HB2	1.88	0.55
1:B:214:HIS:CE1	4:B:301:SFG:HB1	2.41	0.55
1:A:134:PRO:HB3	1:B:196:LYS:HD3	1.87	0.55
1:B:96:LYS:HB2	1:B:97:PRO:HD2	1.87	0.55
1:C:56:ILE:HB	1:C:101:MET:HG3	1.88	0.55
2:E:10:DA:H2''	2:E:11:DG:C8	2.41	0.55
1:B:206:ARG:HA	1:B:211:ARG:HG2	1.88	0.54
1:C:249:VAL:O	1:C:253:ARG:HG2	2.08	0.54
2:K:11:DG:H2'	2:K:12:DC:C6	2.43	0.54
1:C:36:LEU:HB3	1:C:242:MET:HE1	1.90	0.54
1:D:187:LYS:HD3	1:D:191:MET:SD	2.48	0.54
1:A:61:PRO:HG3	1:A:72:SER:HB2	1.89	0.53
1:A:249:VAL:O	1:A:253:ARG:HG2	2.08	0.53
1:B:54:ASP:OD1	1:B:96:LYS:HD2	2.09	0.53
2:I:5:DA:H2''	2:I:6:DA:C8	2.44	0.53
3:J:6:DT:H2'	3:J:7:DA:C8	2.43	0.53
2:K:2:DT:H2'	2:K:3:DG:C8	2.44	0.52
3:L:13:DC:H2'	3:L:14:DA:C8	2.45	0.52
1:A:212:VAL:HG11	1:A:274:ARG:HD3	1.91	0.52
1:D:179:SER:HA	1:D:189:LEU:HD11	1.91	0.52
2:K:12:DC:H2'	2:K:13:DC:C6	2.44	0.52
1:A:147:HIS:NE2	1:B:126:GLU:OE1	2.39	0.52
1:C:236:ARG:HG3	1:C:257:ASP:HB3	1.92	0.52
1:C:262:GLU:HB3	1:C:268:CYS:SG	2.50	0.52
1:D:39:ARG:NH1	1:D:44:ASP:OD2	2.42	0.52
1:D:88:LEU:CD1	1:D:117:LEU:HD11	2.40	0.51
1:B:241:PHE:HB3	4:B:301:SFG:O4'	2.09	0.51
1:C:275:VAL:HA	1:C:278:LEU:HD12	1.93	0.51
1:A:142:ARG:HD2	2:E:10:DA:OP1	2.10	0.51
1:D:115:SER:HA	1:D:118:LYS:HG3	1.92	0.51
1:B:164:ASP:N	1:B:165:PRO:HD2	2.26	0.50
1:C:84:THR:HA	1:C:87:TRP:CD1	2.46	0.50
1:C:269:ALA:O	1:C:272:HIS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:6:DT:H4'	3:J:7:DA:OP1	2.11	0.50
1:D:206:ARG:HA	1:D:211:ARG:HG2	1.94	0.49
1:B:84:THR:HA	1:B:87:TRP:CD1	2.47	0.49
1:C:224:GLU:O	1:C:228:LEU:HG	2.12	0.49
1:C:206:ARG:NH1	1:C:211:ARG:HE	2.11	0.49
3:L:3:DG:H2''	3:L:4:DG:H8	1.77	0.49
3:F:5:DC:H2'	3:F:6:DT:C6	2.48	0.49
1:C:34:ILE:HG23	1:C:258:PHE:HB3	1.95	0.48
1:A:142:ARG:HH21	1:B:124:VAL:HA	1.79	0.48
2:I:9:DT:H2''	2:I:10:DA:C8	2.48	0.48
1:D:239:ASP:HB2	1:D:258:PHE:CE1	2.49	0.48
1:A:241:PHE:HB3	4:A:301:SFG:O4'	2.14	0.47
1:B:249:VAL:HG12	1:B:253:ARG:HD3	1.95	0.47
3:L:3:DG:H2''	3:L:4:DG:C8	2.50	0.47
1:C:78:ASP:HA	1:C:81:LEU:HD12	1.96	0.47
4:D:301:SFG:HB1	4:D:301:SFG:H5'2	1.54	0.47
3:F:3:DG:H2''	3:F:4:DG:C8	2.49	0.47
1:D:263:ILE:HG13	4:D:301:SFG:C2	2.45	0.47
3:H:6:DT:H2'	3:H:7:DA:C8	2.50	0.47
1:C:129:TRP:HB2	1:C:150:ILE:HD11	1.97	0.47
1:A:84:THR:HA	1:A:87:TRP:CD1	2.50	0.46
1:D:88:LEU:HD12	1:D:117:LEU:HD11	1.97	0.46
1:D:163:LEU:HG	1:D:167:ARG:HG2	1.97	0.46
1:B:88:LEU:HD22	1:B:117:LEU:HD21	1.97	0.46
1:C:194:ASN:OD1	1:D:144:THR:N	2.33	0.46
1:D:223:ILE:HA	1:D:226:MET:HE2	1.96	0.46
2:E:11:DG:N2	3:F:6:DT:O2	2.48	0.46
1:C:85:ARG:HA	1:C:88:LEU:HD12	1.98	0.46
1:D:50:ASP:HA	1:D:94:LYS:HA	1.96	0.46
1:D:40:ASP:OD1	4:D:301:SFG:N6	2.47	0.46
1:C:131:ARG:O	1:C:133:VAL:N	2.44	0.46
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.85	0.46
1:A:214:HIS:CE1	4:A:301:SFG:HB1	2.51	0.45
1:A:160:TYR:CG	1:A:232:PRO:HG3	2.51	0.45
1:C:206:ARG:HA	1:C:206:ARG:HD3	1.81	0.45
4:C:301:SFG:H4'	4:C:301:SFG:HG2	1.81	0.45
1:A:34:ILE:HG21	1:A:275:VAL:HG11	1.98	0.45
1:A:131:ARG:O	1:A:133:VAL:N	2.41	0.45
1:B:68:TYR:O	1:B:264:ASN:ND2	2.42	0.45
1:C:70:ASN:HB2	1:C:71:ASP:H	1.52	0.45
2:E:3:DG:OP2	5:E:101:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:PHE:CG	1:C:240:PRO:HB3	2.51	0.45
1:C:53:ILE:HD13	1:C:236:ARG:HB3	1.98	0.45
1:D:84:THR:O	1:D:88:LEU:HD23	2.17	0.45
1:D:239:ASP:HB2	1:D:258:PHE:HE1	1.82	0.44
1:C:269:ALA:O	1:C:270:ILE:C	2.60	0.44
1:A:92:ILE:N	1:A:93:PRO:HD2	2.32	0.44
1:C:57:VAL:HG22	1:C:226:MET:HE3	1.99	0.44
3:J:5:DC:H2'	3:J:6:DT:C6	2.52	0.44
1:D:239:ASP:HB3	1:D:242:MET:HB3	1.99	0.44
1:A:206:ARG:HA	1:A:211:ARG:HG2	2.00	0.44
1:C:87:TRP:HA	1:C:90:LEU:HG	1.99	0.44
1:C:245:GLY:O	1:C:249:VAL:HG13	2.17	0.44
1:D:131:ARG:O	1:D:133:VAL:N	2.42	0.44
1:D:154:ALA:HB1	1:D:159:TYR:HB3	2.00	0.44
4:B:301:SFG:HG2	4:B:301:SFG:H4'	1.87	0.44
1:C:111:PRO:HG2	1:D:123:MET:HE1	2.00	0.44
1:A:38:ASN:ND2	1:A:262:GLU:O	2.46	0.43
1:A:232:PRO:HA	1:A:233:PRO:HD3	1.89	0.43
1:D:131:ARG:C	1:D:133:VAL:H	2.25	0.43
4:D:301:SFG:H8	4:D:301:SFG:H2'	1.80	0.43
1:C:170:TYR:OH	3:L:10:DT:H3'	2.18	0.43
1:C:166:VAL:HG13	1:C:228:LEU:HB2	2.00	0.43
1:D:110:ALA:O	1:D:111:PRO:C	2.61	0.43
1:B:133:VAL:HB	1:B:203:ARG:HG2	2.01	0.43
1:A:48:LEU:HA	1:A:49:PRO:HD3	1.81	0.43
1:B:30:LEU:N	5:B:412:HOH:O	2.51	0.43
1:C:218:LYS:HA	1:C:219:PRO:HD3	1.90	0.43
1:A:167:ARG:NH2	3:H:9:DT:OP1	2.43	0.43
3:F:13:DC:H2'	3:F:14:DA:C8	2.54	0.43
1:D:70:ASN:OD1	1:D:72:SER:N	2.48	0.42
1:C:55:LEU:HD12	1:C:230:SER:HB2	2.01	0.42
2:G:4:DT:H2''	2:G:5:DA:C8	2.53	0.42
1:B:104:PHE:CZ	1:B:226:MET:HE1	2.54	0.42
1:C:61:PRO:HG2	1:C:72:SER:HB2	2.02	0.42
1:D:53:ILE:O	1:D:95:LEU:HD23	2.19	0.42
1:D:110:ALA:N	1:D:111:PRO:HD2	2.33	0.42
1:B:212:VAL:HG11	1:B:274:ARG:HD2	2.01	0.42
1:C:212:VAL:HG11	1:C:274:ARG:HD2	2.01	0.42
1:D:131:ARG:NH2	1:D:145:SER:OG	2.53	0.42
1:A:142:ARG:NH2	1:B:124:VAL:HA	2.34	0.41
1:B:243:GLY:HA3	4:B:301:SFG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:6:DT:H2''	3:J:7:DA:O5'	2.20	0.41
1:A:237:VAL:HG22	1:A:258:PHE:HD1	1.85	0.41
1:C:108:GLN:NE2	2:I:8:DC:O2	2.54	0.41
1:D:170:TYR:CE1	1:D:178:ARG:HG3	2.56	0.41
2:E:11:DG:H2''	2:E:12:DC:H5''	2.02	0.41
1:D:116:PHE:CD2	1:D:117:LEU:HD22	2.55	0.41
1:D:164:ASP:HA	1:D:167:ARG:HD2	2.00	0.41
1:B:204:LEU:HG	1:B:219:PRO:HG3	2.03	0.41
1:C:118:LYS:NZ	1:D:108:GLN:O	2.54	0.41
1:D:59:ASP:HB3	4:D:301:SFG:HN2	1.86	0.41
1:A:197:ASP:OD2	1:B:145:SER:HA	2.20	0.41
1:C:263:ILE:HG13	4:C:301:SFG:C4	2.50	0.41
1:A:143:PHE:CD1	1:B:195:PRO:HG2	2.56	0.41
1:C:46:ALA:O	1:C:48:LEU:N	2.45	0.41
1:C:127:ILE:HB	1:C:150:ILE:HB	2.03	0.41
1:D:116:PHE:HD2	1:D:117:LEU:HD22	1.86	0.41
1:B:188:TRP:HA	1:B:192:GLY:O	2.21	0.40
1:B:191:MET:HE2	1:B:191:MET:HB3	1.85	0.40
1:C:218:LYS:HZ2	1:C:218:LYS:HG2	1.78	0.40
1:C:273:GLU:N	1:C:273:GLU:OE1	2.54	0.40
1:D:224:GLU:OE1	1:D:253:ARG:NE	2.48	0.40
1:C:101:MET:HE3	1:C:103:ILE:HB	2.03	0.40
1:D:243:GLY:HA3	4:D:301:SFG:HB2	2.03	0.40
1:C:66:LYS:H	1:C:73:ASP:HB3	1.86	0.40
1:A:227:VAL:CG1	1:A:256:ARG:HD2	2.51	0.40
1:C:194:ASN:O	1:C:196:LYS:HG3	2.20	0.40
1:D:264:ASN:O	1:D:268:CYS:SG	2.79	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	247/283 (87%)	232 (94%)	14 (6%)	1 (0%)	30	40
1	B	247/283 (87%)	238 (96%)	9 (4%)	0	100	100
1	C	248/283 (88%)	226 (91%)	21 (8%)	1 (0%)	30	40
1	D	101/283 (36%)	95 (94%)	6 (6%)	0	100	100
All	All	843/1132 (74%)	791 (94%)	50 (6%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	47	HIS
1	A	31	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	209/231 (90%)	190 (91%)	19 (9%)	9	13
1	B	210/231 (91%)	200 (95%)	10 (5%)	23	37
1	C	189/231 (82%)	174 (92%)	15 (8%)	11	17
1	D	186/231 (80%)	170 (91%)	16 (9%)	10	14
All	All	794/924 (86%)	734 (92%)	60 (8%)	12	19

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	48	LEU
1	A	52	SER
1	A	66	LYS
1	A	70	ASN
1	A	100	SER
1	A	131	ARG
1	A	132	ARG
1	A	140	THR

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Mol	Chain	Res	Type
1	A	141	ARG
1	A	144	THR
1	A	200	SER
1	A	206	ARG
1	A	224	GLU
1	A	237	VAL
1	A	256	ARG
1	A	259	VAL
1	A	266	SER
1	A	268	CYS
1	B	44	ASP
1	B	53	ILE
1	B	76	SER
1	B	85	ARG
1	B	100	SER
1	B	140	THR
1	B	156	SER
1	B	191	MET
1	B	200	SER
1	B	224	GLU
1	C	66	LYS
1	C	70	ASN
1	C	72	SER
1	C	90	LEU
1	C	93	PRO
1	C	106	THR
1	C	132	ARG
1	C	146	VAL
1	C	156	SER
1	C	173	ASP
1	C	175	LYS
1	C	197	ASP
1	C	218	LYS
1	C	263	ILE
1	C	266	SER
1	D	53	ILE
1	D	64	LEU
1	D	96	LYS
1	D	100	SER
1	D	140	THR
1	D	144	THR
1	D	155	VAL

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Mol	Chain	Res	Type
1	D	156	SER
1	D	157	ARG
1	D	176	LYS
1	D	179	SER
1	D	189	LEU
1	D	200	SER
1	D	249	VAL
1	D	268	CYS
1	D	276	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	C	38	ASN
1	C	254	GLN
1	D	108	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](#)

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	$\# Z > 2$
4	SFG	A	301	-	28,29,29	0.62	1 (3%)	34,42,42	0.45	0
4	SFG	B	301	-	28,29,29	2.92	9 (32%)	34,42,42	2.23	11 (32%)
4	SFG	D	301	-	28,29,29	2.92	9 (32%)	34,42,42	2.24	11 (32%)
4	SFG	C	301	-	28,29,29	0.57	1 (3%)	34,42,42	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SFG	A	301	-	-	1/17/33/33	0/3/3/3
4	SFG	B	301	-	-	3/17/33/33	0/3/3/3
4	SFG	D	301	-	-	13/17/33/33	0/3/3/3
4	SFG	C	301	-	-	7/17/33/33	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	SFG	O4'-C1'	8.68	1.62	1.42
4	B	301	SFG	O4'-C1'	8.58	1.61	1.42
4	B	301	SFG	C2'-C1'	-7.20	1.30	1.53
4	D	301	SFG	C2'-C1'	-7.17	1.31	1.53
4	B	301	SFG	O4'-C4'	-6.36	1.30	1.45
4	D	301	SFG	O4'-C4'	-6.25	1.31	1.45
4	D	301	SFG	C6-N6	4.52	1.45	1.34
4	B	301	SFG	C6-N6	4.48	1.45	1.34
4	B	301	SFG	C5-C4	-2.93	1.33	1.39
4	D	301	SFG	C5-C4	-2.81	1.34	1.39
4	D	301	SFG	O3'-C3'	-2.78	1.36	1.43
4	D	301	SFG	O2'-C2'	2.77	1.49	1.43
4	B	301	SFG	O2'-C2'	2.75	1.49	1.43
4	B	301	SFG	O3'-C3'	-2.73	1.36	1.43
4	D	301	SFG	C5-N7	-2.54	1.34	1.39
4	A	301	SFG	OXT-C	-2.53	1.22	1.30
4	B	301	SFG	C5-N7	-2.52	1.34	1.39
4	C	301	SFG	OXT-C	-2.22	1.23	1.30
4	B	301	SFG	C8-N9	-2.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	SFG	C8-N9	-2.16	1.33	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	SFG	N3-C2-N1	-5.67	120.00	128.58
4	D	301	SFG	N3-C2-N1	-5.64	120.05	128.58
4	D	301	SFG	C5-C4-N3	-4.88	120.00	126.72
4	B	301	SFG	C5-C4-N3	-4.87	120.01	126.72
4	B	301	SFG	N6-C6-N1	-4.61	108.10	118.38
4	D	301	SFG	N6-C6-N1	-4.59	108.15	118.38
4	B	301	SFG	N9-C8-N7	-4.18	108.01	113.94
4	D	301	SFG	N9-C8-N7	-4.09	108.13	113.94
4	D	301	SFG	C5-C6-N6	3.47	131.89	123.29
4	B	301	SFG	C5-C6-N6	3.47	131.87	123.29
4	B	301	SFG	C2-N3-C4	3.38	120.10	111.83
4	D	301	SFG	C2-N3-C4	3.37	120.05	111.83
4	D	301	SFG	N3-C4-N9	2.92	132.13	127.17
4	B	301	SFG	C5-N7-C8	2.90	108.01	103.45
4	D	301	SFG	C5-N7-C8	2.88	107.97	103.45
4	B	301	SFG	N3-C4-N9	2.84	132.00	127.17
4	D	301	SFG	C3'-C2'-C1'	2.38	105.97	101.46
4	B	301	SFG	C4-C5-N7	-2.29	107.96	110.58
4	D	301	SFG	C4-C5-N7	-2.26	108.00	110.58
4	B	301	SFG	C4-N9-C8	2.18	108.03	105.74
4	D	301	SFG	C4-N9-C8	2.18	108.03	105.74
4	B	301	SFG	C5-C4-N9	2.00	107.99	105.81

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	SFG	N-CA-CB-CG
4	D	301	SFG	C5'-CD-CG-CB
4	D	301	SFG	C4'-C5'-CD-CG
4	D	301	SFG	C4'-C5'-CD-NE
4	D	301	SFG	C3'-C4'-C5'-CD
4	D	301	SFG	OXT-C-CA-N
4	C	301	SFG	C2'-C1'-N9-C8
4	D	301	SFG	C2'-C1'-N9-C8
4	B	301	SFG	C-CA-CB-CG
4	D	301	SFG	C-CA-CB-CG

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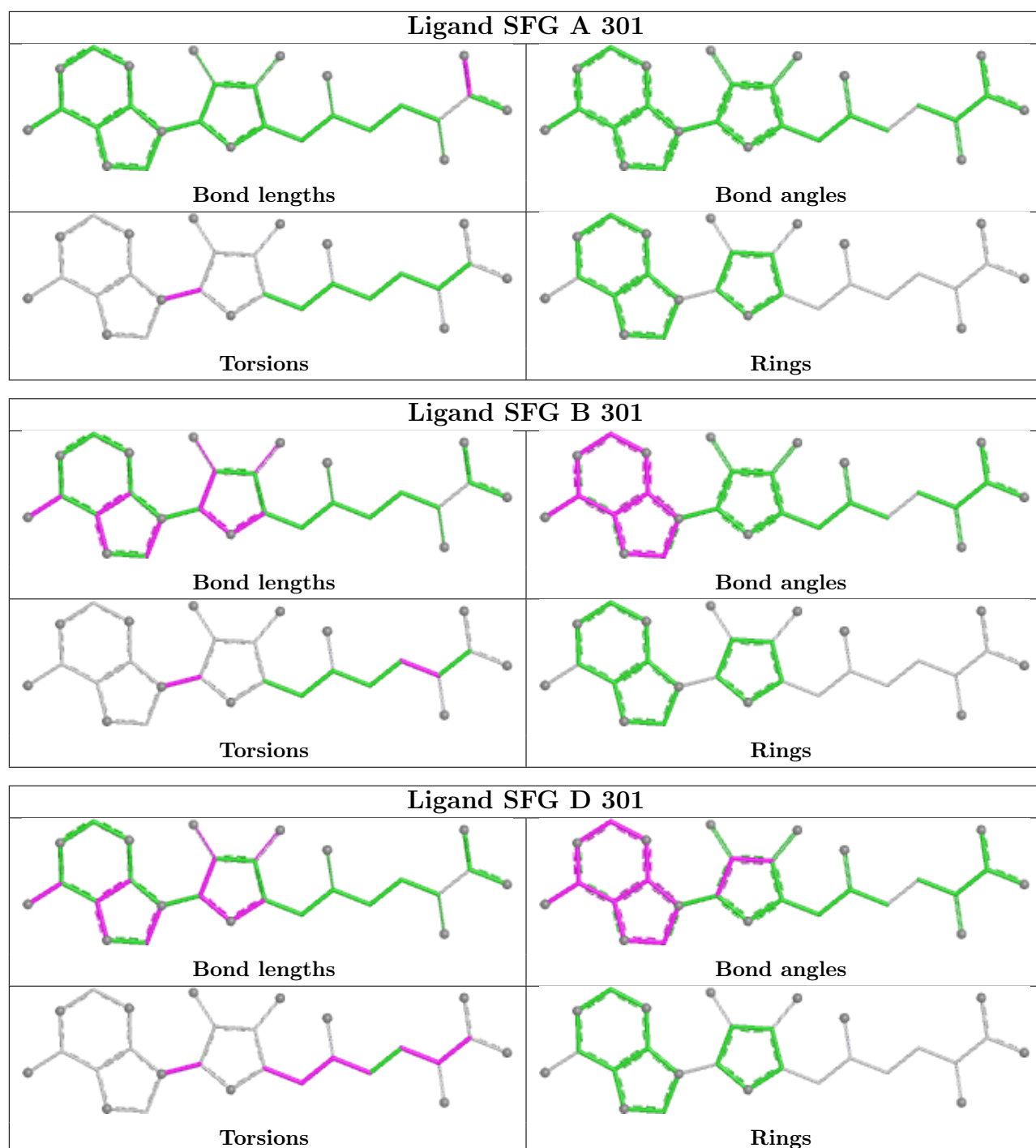
Mol	Chain	Res	Type	Atoms
4	A	301	SFG	C2'-C1'-N9-C8
4	B	301	SFG	C2'-C1'-N9-C8
4	D	301	SFG	NE-CD-CG-CB
4	C	301	SFG	C2'-C1'-N9-C4
4	D	301	SFG	C2'-C1'-N9-C4
4	C	301	SFG	O4'-C4'-C5'-CD
4	C	301	SFG	O-C-CA-N
4	D	301	SFG	O-C-CA-CB
4	B	301	SFG	O4'-C1'-N9-C8
4	D	301	SFG	OXT-C-CA-CB
4	C	301	SFG	O4'-C1'-N9-C8
4	D	301	SFG	O4'-C1'-N9-C8
4	C	301	SFG	C4'-C5'-CD-CG
4	C	301	SFG	C3'-C4'-C5'-CD

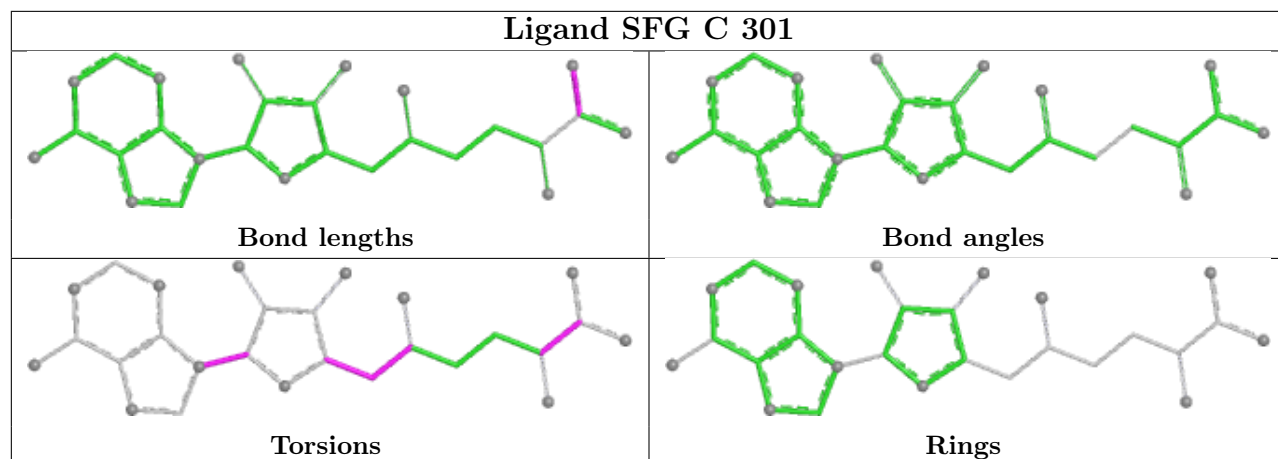
There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	SFG	2	0
4	B	301	SFG	4	0
4	D	301	SFG	7	0
4	C	301	SFG	3	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	249/283 (87%)	0.04	3 (1%) 76 76	14, 39, 66, 87	0
1	B	249/283 (87%)	-0.10	0 100 100	14, 35, 57, 73	0
1	C	250/283 (88%)	0.65	10 (4%) 42 42	39, 68, 90, 113	0
1	D	244/283 (86%)	0.66	14 (5%) 29 28	38, 63, 89, 106	0
2	E	14/14 (100%)	-0.68	0 100 100	30, 43, 71, 75	0
2	G	14/14 (100%)	-0.54	0 100 100	27, 42, 66, 67	0
2	I	14/14 (100%)	-0.37	0 100 100	49, 56, 66, 67	0
2	K	14/14 (100%)	-0.02	0 100 100	60, 71, 92, 99	0
3	F	14/14 (100%)	-0.21	0 100 100	30, 43, 77, 80	0
3	H	14/14 (100%)	-0.41	0 100 100	30, 42, 75, 77	0
3	J	14/14 (100%)	-0.48	0 100 100	40, 53, 67, 73	0
3	L	14/14 (100%)	-0.08	0 100 100	54, 69, 86, 88	0
All	All	1104/1244 (88%)	0.24	27 (2%) 59 59	14, 51, 85, 113	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	68	TYR	6.6
1	D	105	CYS	3.0
1	D	258	PHE	2.9
1	D	97	PRO	2.9
1	C	185	GLY	2.8
1	C	97	PRO	2.7
1	D	71	ASP	2.7
1	A	32	SER	2.7
1	D	91	ALA	2.6
1	D	266	SER	2.6
1	D	65	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	41	PHE	2.4
1	D	237	VAL	2.3
1	D	262	GLU	2.3
1	A	70	ASN	2.3
1	C	69	GLY	2.2
1	C	243	GLY	2.1
1	C	158	ALA	2.1
1	D	36	LEU	2.1
1	D	56	ILE	2.1
1	D	37	HIS	2.1
1	D	114	PHE	2.1
1	C	186	SER	2.1
1	C	45	ALA	2.1
1	C	34	ILE	2.1
1	A	278	LEU	2.0
1	C	77	GLY	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.

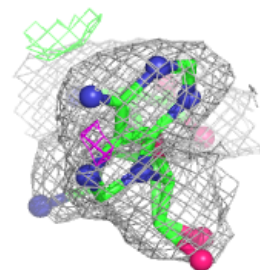
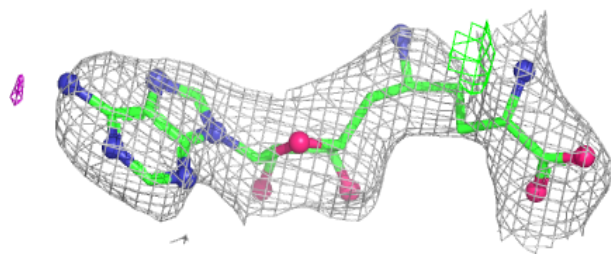
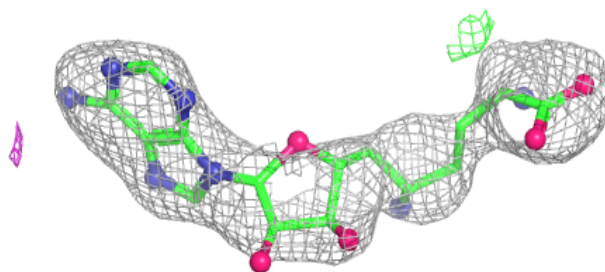
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SFG	D	301	27/27	0.87	0.11	55,76,87,100	0
4	SFG	C	301	27/27	0.90	0.10	58,70,80,86	0
4	SFG	A	301	27/27	0.92	0.08	23,39,45,46	0
4	SFG	B	301	27/27	0.97	0.05	26,29,41,45	0

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.

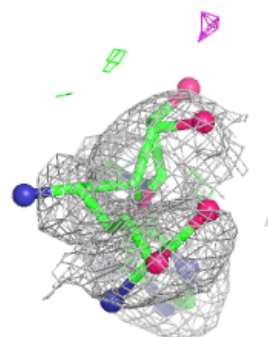
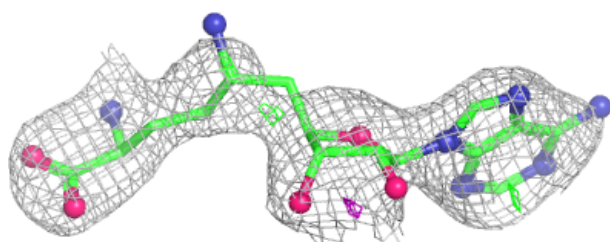
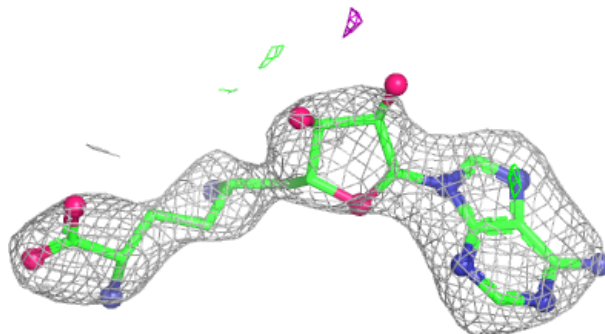
Electron density around SFG D 301:

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

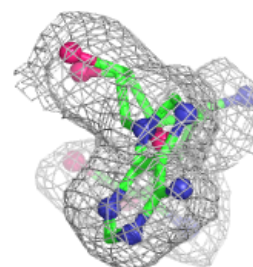
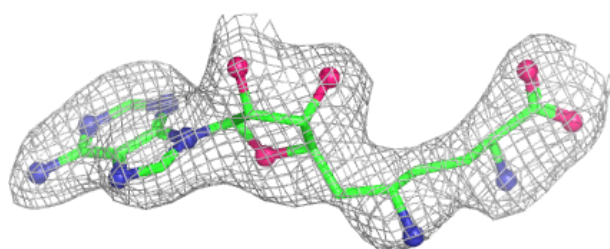
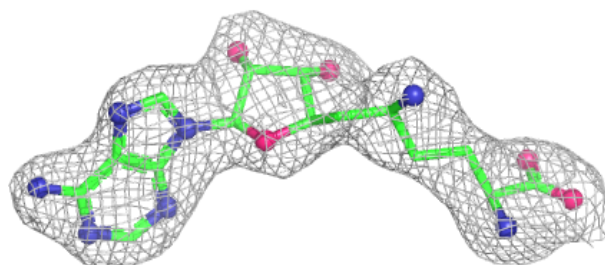


Electron density around SFG C 301:

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

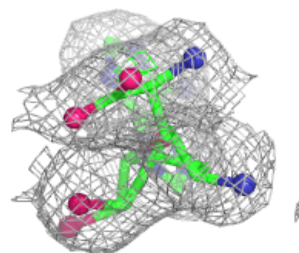
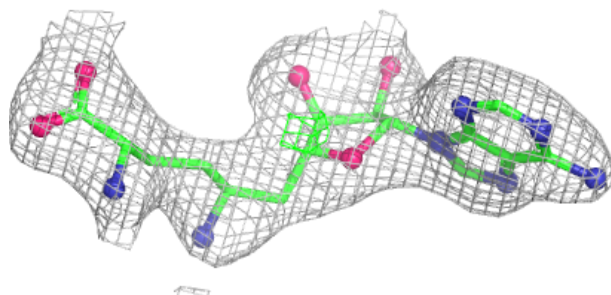
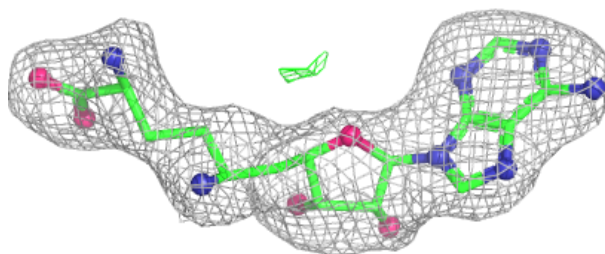
**Electron density around SFG A 301:**

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



Electron density around SFG B 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.