



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 03:30 PM BST

PDB ID : 6K0W
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

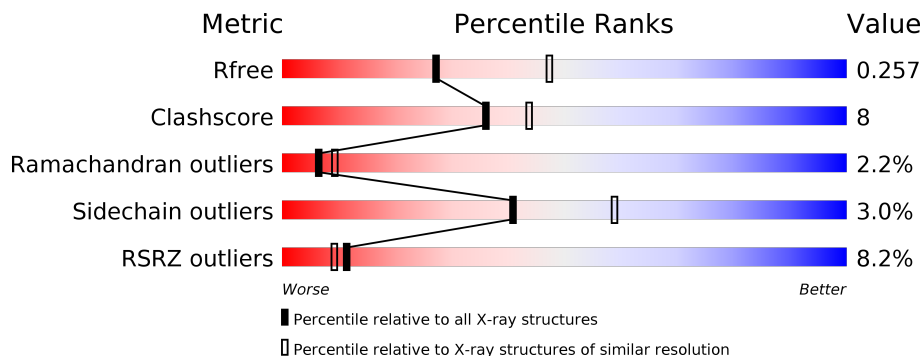
1 Overall quality at a glance

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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	<p>7% 70% 15% 15%</p>
1	B	618	<p>8% 64% 16% 19%</p>
1	C	618	<p>4% 56% 12% 30%</p>
1	D	618	<p>6% 58% 12% 30%</p>

2 Entry composition [i](#)

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

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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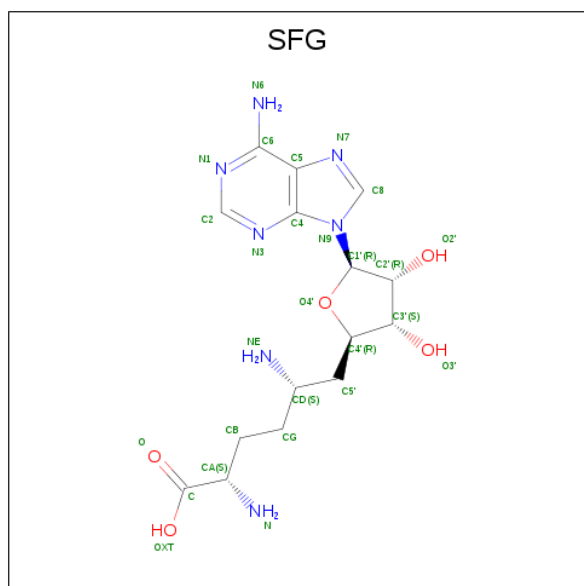
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O25315
A	-17	SER	-	expression tag	UNP O25315
A	-16	SER	-	expression tag	UNP O25315
A	-15	HIS	-	expression tag	UNP O25315
A	-14	HIS	-	expression tag	UNP O25315
A	-13	HIS	-	expression tag	UNP O25315
A	-12	HIS	-	expression tag	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 (three-letter code: SFG) (formula: C₁₅H₂₃N₇O₅) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
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		

LEU	HIS	V432	C545	LEU
GLU	ILE	Q433	E546	GLU
ASN	ASP	K439	D547	ASN
TYR	GLU	E440	A548	TYR
LYS	GLY	D441	TYR	LYS
ASN	ARG	Y445	F550	ASN
PRO	ILE	K449	C551	PRO
ASP	CYS	K453	I552	ASP
ASN	PHE	S454	V553	ASN
ASP	LYS	A556	C554	ASP
PRO	LYS	K456	D555	PRO
ALA	GLU	P457	E556	ALA
TRP	HIS	V458	E557	TRP
TRP	LYS	E465	A558	TRP
ILE	ASP	R466	Y561	ILE
ASN	GLU	R469	L562	ASN
ASP	ARG	D494	ALA	ASP
ASN	GLY	V496	K564	ASN
MET	PHE	G496	S565	MET
THR	ILE	GLN	K566	THR
THR	THR	ILE	K567	THR
LYS	THR	TYR	M568	LYS
GLY	THR	ILE	E569	GLY
VAL	Q346	ILE	I570	VAL
VAL	K347	ASN	F571	VAL
THR	T348	ASP	L572	THR
ASN	F349	LYS	D573	ASN
PRO	Q362	TYR	G574	PRO
TYR	A363	GLU	GLU	TYR
THR	K366	GLU	GLU	THR
ASN	E367	ILE	ILE	ASN
LYS	V383	ASP	ASP	LYS
VAL	K387	LEU	LEU	VAL
ASP	I390	LEU	ALA	ASP
TYR	A407	PHE	PHE	TYR
PRO	G408	ASN	LEU	PRO
PRO	S409	ARG	ASN	PRO
VAL	V416	ASN	LEU	VAL
GLY	L419	ASN	LEU	GLY
MET	M420	ASN	SER	MET
PHE	R427	THR	VAL	PHE
TRP		ILE	VAL	TRP
ARG		ILE	TYR	ARG
ARG		ILE		ARG
PHE		ILE		PHE
SER		ILE		SER
GLN		I538		GLN
ASN		K539		ASN
THR		L542		THR
ILE				ILE
GLN				GLN
LYS				LYS

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) 100.0 (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)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.206 , 0.258 0.208 , 0.257	Depositor DCC
R_{free} test set	5095 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtrriage
Anisotropy	0.585	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14455	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage'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 i

5.1 Standard geometry i

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	0.42	0/4062	0.60	3/5497 (0.1%)
1	B	0.42	0/3844	0.62	6/5192 (0.1%)
1	C	0.43	0/3304	0.59	0/4464
1	D	0.41	0/3288	0.56	1/4438 (0.0%)
All	All	0.42	0/14498	0.59	10/19591 (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	C	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	66	PRO	N-CA-CB	7.41	112.19	103.30
1	B	483	LEU	CA-CB-CG	6.58	130.44	115.30
1	B	264	PRO	N-CA-CB	6.29	110.84	103.30
1	A	260	PRO	N-CA-CB	6.13	110.66	103.30
1	B	298	PRO	N-CA-CB	5.90	110.38	103.30
1	A	264	PRO	N-CA-CB	5.66	110.09	103.30
1	D	66	PRO	N-CA-CB	5.54	109.95	103.30
1	A	290	PRO	N-CA-CB	5.50	109.89	103.30
1	B	17	LEU	CA-CB-CG	5.40	127.71	115.30
1	B	58	LEU	CA-CB-CG	5.16	127.18	115.30

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	46	0
1	B	3779	0	3513	60	0
1	C	3251	0	3014	67	0
1	D	3239	0	2976	55	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	222	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 8.

All (222) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:179:LYS:NZ	1:D:181:ASP:CG	2.43	0.72
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: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: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:B:452:LEU:C	1:B:453:LYS:HD2	2.17	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:197:LYS:NZ	1:C:201:ASP:OD1	2.30	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: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:D:179:LYS:HZ2	1:D:181:ASP:CG	2.01	0.61
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: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:C:352:LEU:O	1:C:355:SER:OG	2.20	0.58
1:D:179:LYS:HE2	1:D:181:ASP:OD1	2.03	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:B:395:THR:HG22	1:B:400:ASP:OD2	2.04	0.58
1:C:85:ASP:CG	1:C:121:ARG:HH22	2.07	0.58
1:D:83:ASN:OD1	1:D:170:ARG:HD3	2.04	0.57
1:A:55:GLN:OE1	1:A:55:GLN:N	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:N	1:C:494:ASP:OD1	2.35	0.56
1:C:533:ALA:C	1:C:535:GLU:H	2.09	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: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: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:C:583:PHE:C	1:C:585:ASN:H	2.11	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:D:179:LYS:HZ3	1:D:181:ASP:CG	2.12	0.53
1:A:514:THR:HG23	1:A:517:ASP:H	1.74	0.53
1:B:578:ILE:HD12	1:B:579:ASP:H	1.74	0.52
1:B:73:HIS:CD2	1:B:534:LEU:H	2.27	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
1:B:73:HIS:CD2	1:B:533:ALA:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:346:GLN:N	1:D:347:LYS:HZ3	2.08	0.51
1:D:456:LYS:HD3	1:D:456:LYS:O	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:C:102:TYR:CG	1:C:386:MET:HE1	2.46	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: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: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:B:17:LEU:CD2	1:B:19:ALA:HB3	2.44	0.48
1:D:445:TYR:CD2	1:D:457:PRO:HG2	2.49	0.48
1:C:409:SER:HG	1:C:466:ARG:NH2	2.11	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: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:B:481:SER:C	1:B:483:LEU:H	2.17	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
1:A:436:GLU:HB3	1:A:459:ILE:HD12	1.97	0.47
1:B:107:TYR:CD1	1:B:107:TYR:N	2.83	0.47
1:C:516:PHE:HE1	1:C:535:GLU:CB	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:407:ALA:HB3	1:A:433:GLN:HB2	1.97	0.46
1:B:60:LEU:HD23	1:B:61:GLN:N	2.30	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:D:545:CYS:HB3	1:D:550:PHE:HE2	1.81	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:514:THR:HG22	1:A:517:ASP:CG	2.37	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:C:121:ARG:HB3	1:C:123:ASP:OD1	2.17	0.45
1:D:239:ALA:HB1	1:D:245:THR:HG21	1.99	0.44
1:D:441:ASP:N	1:D:441:ASP:OD1	2.44	0.44
1:A:407:ALA:CB	1:A:431:LEU:HD22	2.47	0.44
1:B:409:SER:O	1:B:466:ARG:HD2	2.17	0.44
1:A:386:MET:HB3	1:A:386:MET:HE2	1.90	0.44
1:C:456:LYS:HA	1:C:456:LYS:HD2	1.73	0.44
1:D:79:ILE:O	1:D:432:VAL:HA	2.17	0.44
1:A:102:TYR:OH	1:A:104:ASP:HB2	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:B:360:MET:HB3	1:B:362:GLN:OE1	2.18	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:A:215:ARG:HA	1:A:354:PHE:O	2.18	0.43
1:A:537:ILE:C	1:A:538:ILE:HD13	2.38	0.43
1:B:578:ILE:HD12	1:B:579:ASP:N	2.32	0.43
1:A:458:VAL:O	1:A:461:ASP:HB2	2.19	0.43
1:B:586:LEU:HD12	1:B:586:LEU:HA	1.88	0.43
1:A:107:TYR:CD1	1:A:107:TYR:N	2.86	0.43
1:A:198:ILE:HD12	1:C:198:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:OE1	1:A:253:ASN:N	2.52	0.43
1:B:27:ASN:OD1	1:D:27:ASN:ND2	2.52	0.43
1:A:439:LYS:HG2	1:A:441:ASP:H	1.84	0.43
1:A:369:LEU:HD23	1:A:374:GLY:HA3	2.01	0.43
1:B:448:CYS:HA	1:B:452:LEU:HB2	2.01	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:35:GLY:HA2	1:D:41:THR:CG2	2.49	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:A:536:ILE:CB	1:A:544:LYS:HB3	2.48	0.42
1:B:405:PHE:HA	1:B:432:VAL:HB	2.01	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:116:TYR:CZ	1:B:118:ASP:HB2	2.55	0.42
1:C:127:ILE:C	1:C:129:ARG:H	2.24	0.42
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:D:366:LYS:HA	1:D:366:LYS:HD2	1.90	0.41
1:A:125:GLN:C	1:A:127:ILE:H	2.23	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:B:100:MET:HE3	1:B:102:TYR:HB2	2.02	0.41
1:C:408:GLY:N	1:C:433:GLN:OE1	2.52	0.41
1:A:118:ASP:HA	1:A:121:ARG:HG3	2.02	0.41
1:A:91:LYS:HE3	1:A:176:ASP:OD2	2.21	0.41
1:B:445:TYR:CD2	1:B:457:PRO:HG2	2.56	0.41
1:A:99:LYS:O	1:A:182:GLY:HA2	2.21	0.41
1:B:208:ASN:HB3	1:B:239:ALA:O	2.20	0.41
1:C:433:GLN:HE22	2:C:801:SFG:H1'	1.86	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:C:539:LYS:C	1:C:541:LYS:H	2.24	0.41
1:C:76:ASN:HB3	1:C:429:PHE:CE1	2.56	0.41
1:A:357:ASN:O	1:A:360:MET:HG3	2.21	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:A:56:LYS:HE2	1:A:494:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:HA	1:B:354:PHE:O	2.21	0.40
1:A:480:ASP:C	1:A:482:GLY:H	2.25	0.40
1:D:46:ALA:O	1:D:169:PRO:HG3	2.22	0.40
1:A:404:ASP:HB3	1:A:431:LEU:HD23	2.02	0.40
1:B:465:GLU:O	1:B:469:ARG:HG3	2.20	0.40
1:C:533:ALA:C	1:C:535:GLU:N	2.73	0.40
1:D:546:GLU:CD	1:D:547:ASP:H	2.24	0.40
1:A:353:ILE:HA	1:A:353:ILE:HD12	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	520/618 (84%)	463 (89%)	44 (8%)	13 (2%)	5	7
1	B	485/618 (78%)	433 (89%)	40 (8%)	12 (2%)	5	7
1	C	421/618 (68%)	383 (91%)	28 (7%)	10 (2%)	6	7
1	D	421/618 (68%)	377 (90%)	38 (9%)	6 (1%)	11	16
All	All	1847/2472 (75%)	1656 (90%)	150 (8%)	41 (2%)	6	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

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Mol	Chain	Res	Type
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
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%)	384 (98%)	8 (2%)	55	73
1	B	376/549 (68%)	364 (97%)	12 (3%)	39	56
1	C	320/549 (58%)	307 (96%)	13 (4%)	30	46
1	D	319/549 (58%)	310 (97%)	9 (3%)	43	61
All	All	1407/2196 (64%)	1365 (97%)	42 (3%)	41	59

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	16	SER
1	B	29	SER
1	B	34	SER
1	B	218	LYS
1	B	349	PHE
1	B	453	LYS
1	B	456	LYS
1	B	466	ARG
1	B	479	LYS
1	B	512	ASP
1	B	539	LYS
1	B	593	ARG
1	A	265	ASN
1	A	293	ASN
1	A	349	PHE
1	A	362	GLN
1	A	466	ARG
1	A	513	LEU
1	A	520	LEU
1	A	555	ASP
1	C	37	GLU
1	C	90	LEU
1	C	91	LYS
1	C	173	LEU
1	C	252	LYS
1	C	349	PHE
1	C	409	SER
1	C	466	ARG
1	C	483	LEU
1	C	494	ASP
1	C	525	GLN

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Mol	Chain	Res	Type
1	C	551	CYS
1	C	581	GLU
1	D	34	SER
1	D	347	LYS
1	D	349	PHE
1	D	362	GLN
1	D	439	LYS
1	D	456	LYS
1	D	466	ARG
1	D	551	CYS
1	D	565	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
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 monosaccharides 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	B	601	-	22,29,29	4.82	11 (50%)	18,42,42	2.18	3 (16%)
2	SFG	C	801	-	22,29,29	4.87	10 (45%)	18,42,42	2.32	4 (22%)
2	SFG	A	701	-	22,29,29	5.02	11 (50%)	18,42,42	2.84	4 (22%)
2	SFG	D	901	-	22,29,29	4.88	11 (50%)	18,42,42	2.72	3 (16%)

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	B	601	-	-	1/9/33/33	0/3/3/3
2	SFG	C	801	-	-	0/9/33/33	0/3/3/3
2	SFG	A	701	-	-	0/9/33/33	0/3/3/3
2	SFG	D	901	-	-	0/9/33/33	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	SFG	C2'-C1'	-14.74	1.31	1.53
2	D	901	SFG	C2'-C1'	-14.55	1.31	1.53
2	A	701	SFG	O4'-C1'	14.33	1.61	1.41
2	B	601	SFG	C2'-C1'	-14.06	1.32	1.53
2	C	801	SFG	C2'-C1'	-14.02	1.32	1.53
2	C	801	SFG	O4'-C1'	13.92	1.60	1.41
2	D	901	SFG	O4'-C1'	13.53	1.60	1.41
2	B	601	SFG	O4'-C1'	13.38	1.59	1.41
2	B	601	SFG	O4'-C4'	-6.39	1.30	1.45
2	A	701	SFG	O4'-C4'	-6.12	1.31	1.45
2	C	801	SFG	O4'-C4'	-6.10	1.31	1.45
2	D	901	SFG	O4'-C4'	-6.07	1.31	1.45
2	B	601	SFG	O2'-C2'	4.70	1.54	1.43
2	C	801	SFG	O2'-C2'	4.57	1.53	1.43
2	D	901	SFG	O2'-C2'	4.30	1.53	1.43
2	A	701	SFG	C5'-CD	4.21	1.60	1.53
2	A	701	SFG	O2'-C2'	4.18	1.52	1.43
2	D	901	SFG	C5'-CD	3.98	1.59	1.53
2	C	801	SFG	C5'-CD	3.91	1.59	1.53
2	B	601	SFG	C5'-CD	3.79	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	SFG	C6-N6	3.57	1.47	1.34
2	B	601	SFG	C6-N6	3.54	1.47	1.34
2	A	701	SFG	C6-N6	3.47	1.46	1.34
2	C	801	SFG	C6-N6	3.41	1.46	1.34
2	C	801	SFG	C2-N3	3.04	1.37	1.32
2	D	901	SFG	O3'-C3'	-3.00	1.35	1.43
2	B	601	SFG	O3'-C3'	-2.86	1.36	1.43
2	A	701	SFG	O3'-C3'	-2.84	1.36	1.43
2	C	801	SFG	O3'-C3'	-2.81	1.36	1.43
2	D	901	SFG	C5'-C4'	2.80	1.57	1.52
2	A	701	SFG	CG-CD	-2.79	1.49	1.53
2	A	701	SFG	C2-N3	2.64	1.36	1.32
2	B	601	SFG	C2-N3	2.63	1.36	1.32
2	A	701	SFG	C5'-C4'	2.58	1.57	1.52
2	D	901	SFG	C5-C4	-2.55	1.34	1.40
2	D	901	SFG	C2-N3	2.50	1.36	1.32
2	B	601	SFG	C5-C4	-2.47	1.34	1.40
2	C	801	SFG	C5'-C4'	2.36	1.56	1.52
2	A	701	SFG	C5-C4	-2.11	1.35	1.40
2	C	801	SFG	C5-C4	-2.10	1.35	1.40
2	B	601	SFG	C5'-C4'	2.08	1.56	1.52
2	B	601	SFG	CD-NE	-2.02	1.40	1.46
2	D	901	SFG	CG-CD	-2.02	1.50	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	SFG	C5-C6-N6	8.07	132.62	120.35
2	D	901	SFG	C5-C6-N6	7.29	131.43	120.35
2	D	901	SFG	N3-C2-N1	-6.08	119.18	128.68
2	C	801	SFG	C5-C6-N6	5.88	129.28	120.35
2	A	701	SFG	N6-C6-N1	-5.74	106.66	118.57
2	B	601	SFG	N3-C2-N1	-5.69	119.79	128.68
2	A	701	SFG	N3-C2-N1	-5.62	119.89	128.68
2	B	601	SFG	C5-C6-N6	5.54	128.77	120.35
2	C	801	SFG	N3-C2-N1	-5.47	120.13	128.68
2	D	901	SFG	N6-C6-N1	-5.33	107.51	118.57
2	C	801	SFG	N6-C6-N1	-4.29	109.67	118.57
2	B	601	SFG	N6-C6-N1	-3.89	110.51	118.57
2	C	801	SFG	O4'-C1'-C2'	-2.26	103.62	106.93
2	A	701	SFG	C4-C5-N7	-2.01	107.30	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

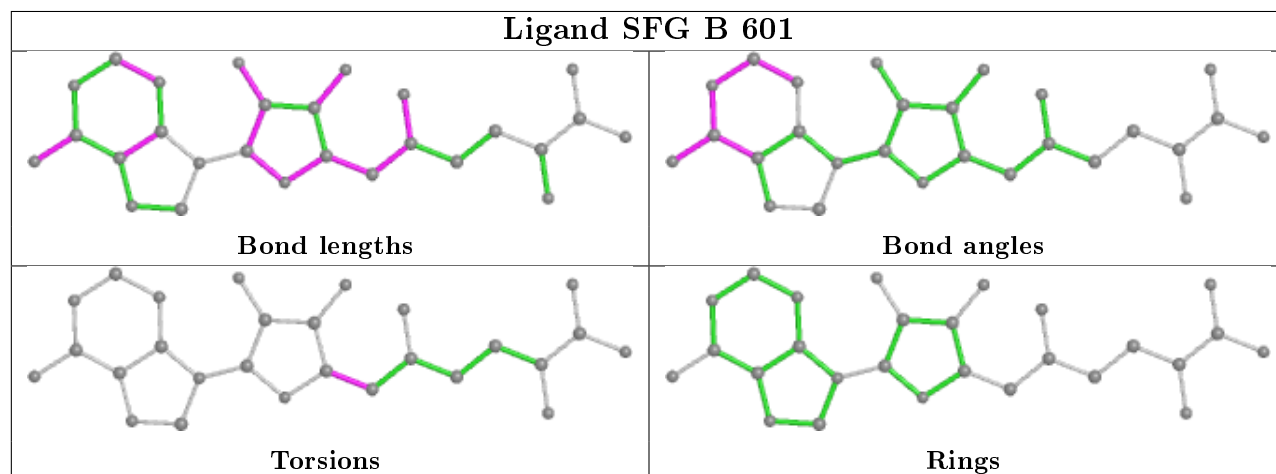
Mol	Chain	Res	Type	Atoms
2	B	601	SFG	O4'-C4'-C5'-CD

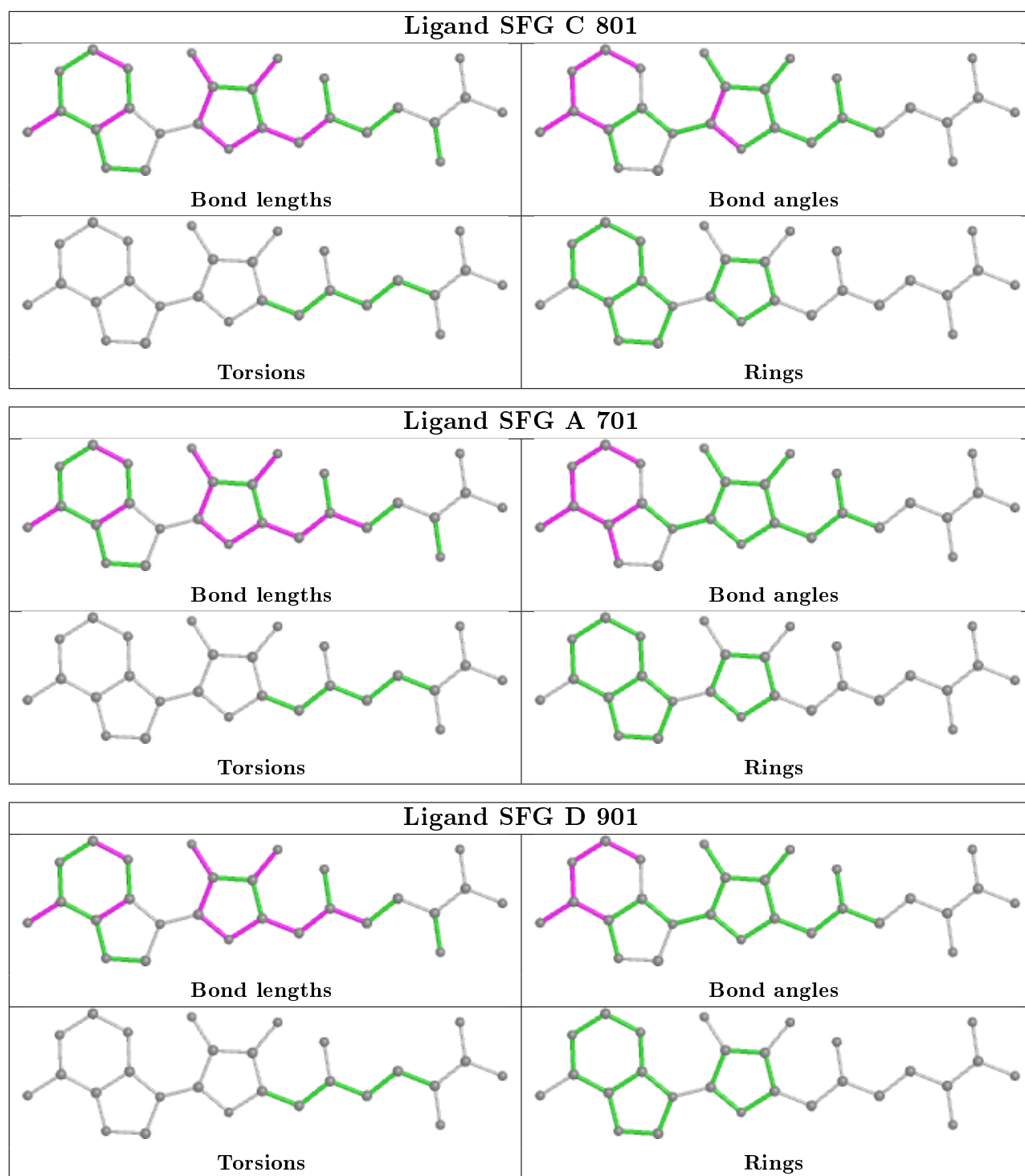
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	SFG	2	0
2	C	801	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

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%)	0.33	45 (8%) 10 8	35, 81, 158, 191	0
1	B	499/618 (80%)	0.38	49 (9%) 7 5	42, 81, 152, 221	0
1	C	433/618 (70%)	0.10	25 (5%) 23 19	39, 73, 143, 195	0
1	D	435/618 (70%)	0.34	37 (8%) 10 8	40, 81, 160, 210	0
All	All	1895/2472 (76%)	0.29	156 (8%) 11 9	35, 79, 156, 221	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	554	CYS	9.8
1	D	558	ALA	6.5
1	B	306	PHE	6.4
1	B	588	ALA	6.1
1	A	330	GLU	5.9
1	D	547	ASP	5.9
1	B	534	LEU	5.4
1	D	553	VAL	5.3
1	D	565	SER	5.2
1	B	552	ILE	5.1
1	C	481	SER	5.0
1	B	537	ILE	4.7
1	D	545	CYS	4.7
1	B	299	PRO	4.7
1	C	552	ILE	4.7
1	B	300	VAL	4.5
1	A	72	LYS	4.5
1	D	552	ILE	4.5
1	D	550	PHE	4.5
1	C	551	CYS	4.4
1	C	589	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	564	LYS	4.2
1	B	554	CYS	4.2
1	A	318	GLY	4.1
1	A	301	GLY	4.0
1	A	332	GLY	4.0
1	A	329	ASN	4.0
1	A	328	ASP	4.0
1	D	71	SER	4.0
1	B	284	TYR	3.9
1	A	534	LEU	3.9
1	C	150	PHE	3.9
1	A	326	HIS	3.9
1	D	551	CYS	3.9
1	B	271	ASP	3.9
1	B	293	ASN	3.9
1	A	331	ARG	3.8
1	A	327	LYS	3.8
1	B	269	ILE	3.7
1	B	542	LEU	3.7
1	B	481	SER	3.6
1	B	551	CYS	3.5
1	C	148	LEU	3.5
1	D	533	ALA	3.4
1	A	294	LYS	3.4
1	B	567	ASN	3.4
1	B	536	ILE	3.4
1	D	568	GLU	3.3
1	D	570	ILE	3.3
1	A	582	ALA	3.3
1	C	534	LEU	3.3
1	D	561	TYR	3.2
1	D	68	THR	3.2
1	D	556	GLU	3.2
1	C	570	ILE	3.2
1	A	572	LEU	3.2
1	A	302	MET	3.2
1	D	511	SER	3.2
1	B	131	VAL	3.1
1	A	266	GLY	3.1
1	A	319	ARG	3.1
1	A	291	TYR	3.1
1	C	107	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	553	VAL	3.1
1	C	548	ALA	3.1
1	B	590	PHE	3.1
1	B	578	ILE	3.0
1	B	270	ASN	3.0
1	A	571	PHE	3.0
1	A	323	LYS	3.0
1	A	342	LEU	3.0
1	B	301	GLY	3.0
1	B	264	PRO	3.0
1	B	570	ILE	3.0
1	D	496	VAL	3.0
1	C	554	CYS	3.0
1	B	583	PHE	2.9
1	D	562	LEU	2.9
1	A	554	CYS	2.9
1	B	343	LYS	2.9
1	C	553	VAL	2.9
1	C	550	PHE	2.9
1	D	569	MET	2.9
1	C	561	TYR	2.9
1	C	571	PHE	2.9
1	C	151	PHE	2.8
1	A	324	LYS	2.8
1	A	325	GLU	2.8
1	B	304	TRP	2.7
1	B	547	ASP	2.7
1	A	551	CYS	2.7
1	D	566	LYS	2.7
1	A	290	PRO	2.7
1	A	555	ASP	2.7
1	B	265	ASN	2.7
1	D	516	PHE	2.7
1	B	539	LYS	2.7
1	C	586	LEU	2.6
1	A	312	GLN	2.6
1	C	253	ASN	2.6
1	C	574	GLY	2.6
1	B	559	GLN	2.6
1	D	73	HIS	2.6
1	A	315	ILE	2.6
1	A	261	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	273	PRO	2.5
1	A	268	TRP	2.5
1	A	299	PRO	2.5
1	A	570	ILE	2.5
1	A	145	SER	2.5
1	C	149	LYS	2.5
1	B	296	ASP	2.5
1	D	548	ALA	2.5
1	A	287	VAL	2.5
1	C	558	ALA	2.5
1	B	297	TYR	2.5
1	D	546	GLU	2.4
1	D	19	ALA	2.4
1	D	515	PRO	2.4
1	B	533	ALA	2.4
1	D	557	GLU	2.4
1	B	543	TYR	2.3
1	B	535	GLU	2.3
1	A	321	CYS	2.3
1	A	322	PHE	2.3
1	A	590	PHE	2.3
1	A	333	PHE	2.3
1	B	33	ILE	2.3
1	B	268	TRP	2.3
1	D	144	GLU	2.3
1	B	302	MET	2.3
1	A	289	ASN	2.3
1	B	568	GLU	2.3
1	B	397	ASN	2.2
1	C	536	ILE	2.2
1	D	72	LYS	2.2
1	A	293	ASN	2.2
1	D	572	LEU	2.2
1	B	562	LEU	2.2
1	B	569	MET	2.2
1	B	565	SER	2.2
1	A	587	ASN	2.2
1	D	495	LYS	2.2
1	D	45	PHE	2.2
1	B	16	SER	2.1
1	D	223	ASP	2.1
1	C	569	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	152	LYS	2.1
1	D	526	CYS	2.1
1	A	297	TYR	2.1
1	A	559	GLN	2.1
1	D	571	PHE	2.1
1	B	223	ASP	2.1
1	C	158	GLY	2.0
1	A	550	PHE	2.0
1	B	23	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

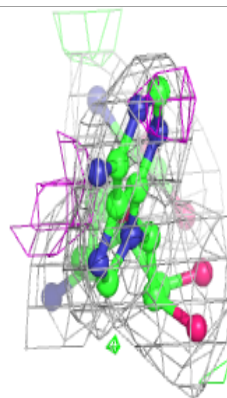
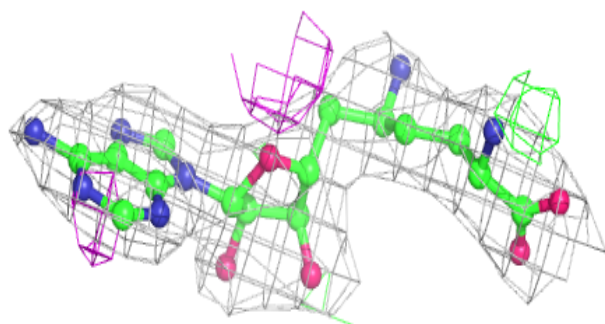
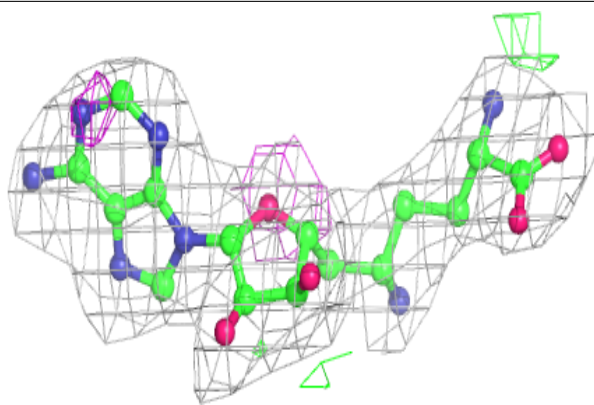
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SFG	B	601	27/27	0.95	0.18	40,47,61,64	0
2	SFG	A	701	27/27	0.95	0.19	34,46,57,62	0
2	SFG	C	801	27/27	0.96	0.17	43,51,62,68	0
2	SFG	D	901	27/27	0.96	0.18	46,58,67,71	0

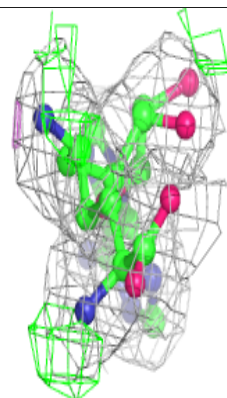
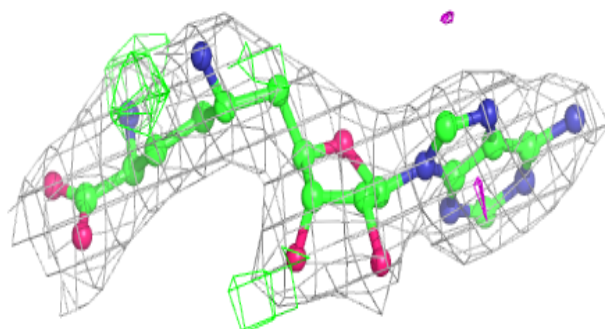
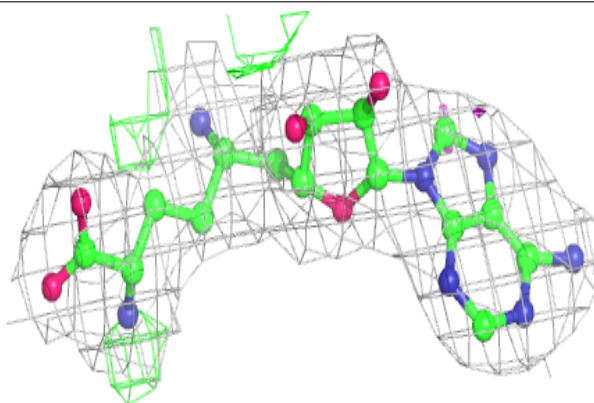
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

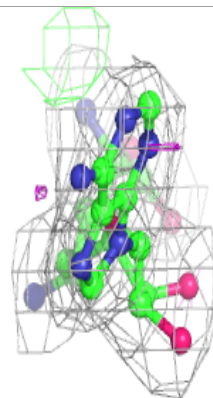
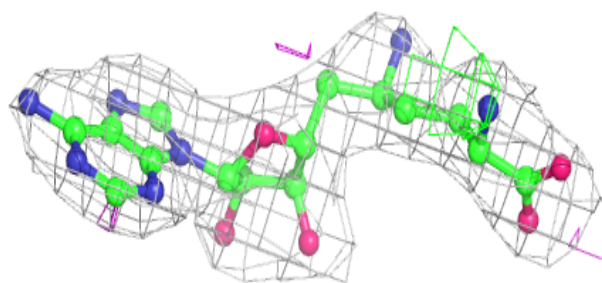
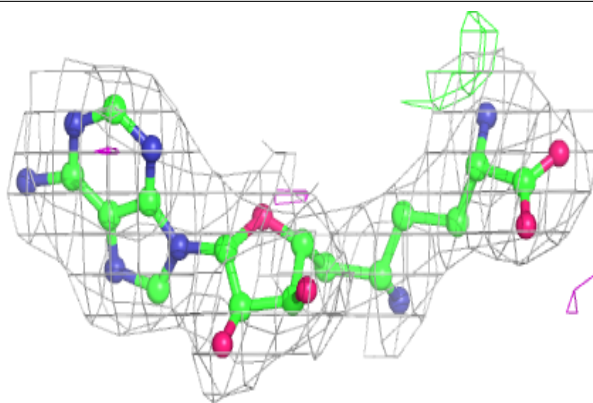
**Electron density around SFG A 701:**

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

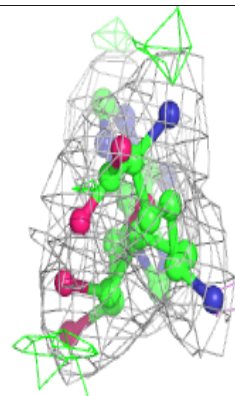
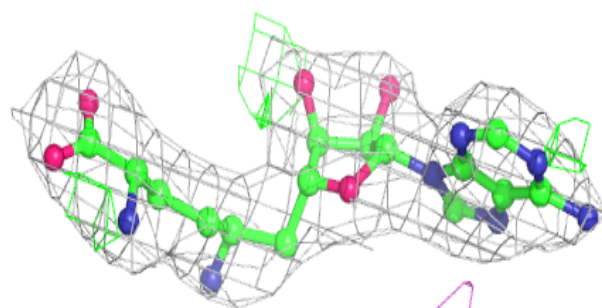
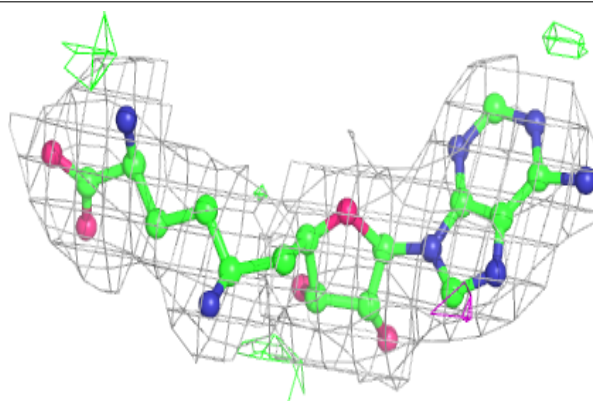


Electron density around SFG C 801:

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

**Electron density around SFG 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)



6.5 Other polymers

There are no such residues in this entry.