



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:23 AM UTC

PDB ID : 8X4P / pdb_00008x4p
Title : Crystal structure of the Y135A mutant of DIMT1 in complex with adenosylornithine (SFG) from *Pyrococcus horikoshii*
Authors : Saha, S.; Kanaujia, S.P.
Deposited on : 2023-11-15
Resolution : 2.60 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

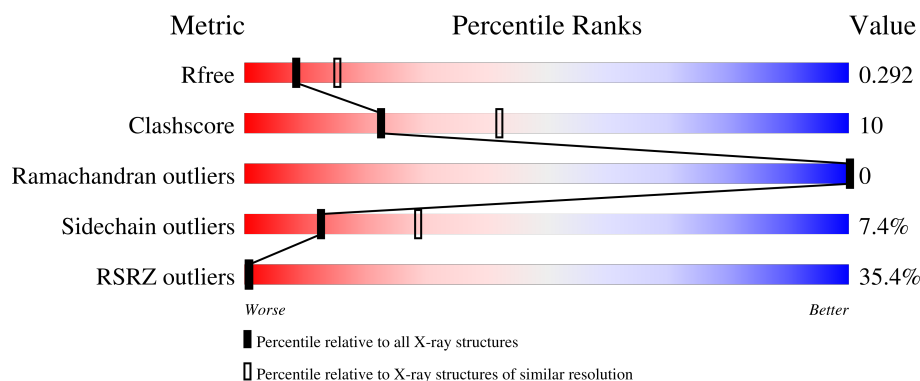
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	290	38% 66% 24% •• 7%
1	B	290	28% 66% 24% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4536 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 Probable ribosomal RNA small subunit methyltransferase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2188	1413	383	386	6			
1	B	270	Total	C	N	O	S	0	0	0
			2188	1413	383	386	6			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O59487
A	2	SER	-	expression tag	UNP O59487
A	3	SER	-	expression tag	UNP O59487
A	4	ARG	-	expression tag	UNP O59487
A	5	ILE	-	expression tag	UNP O59487
A	6	ARG	-	expression tag	UNP O59487
A	7	ILE	-	expression tag	UNP O59487
A	8	ASN	-	expression tag	UNP O59487
A	9	THR	-	expression tag	UNP O59487
A	10	LYS	-	expression tag	UNP O59487
A	11	SER	-	expression tag	UNP O59487
A	12	LEU	-	expression tag	UNP O59487
A	13	LEU	-	expression tag	UNP O59487
A	14	VAL	-	expression tag	UNP O59487
A	15	GLN	-	expression tag	UNP O59487
A	16	PRO	-	expression tag	UNP O59487
A	17	GLY	-	expression tag	UNP O59487
A	18	TYR	-	expression tag	UNP O59487
A	19	SER	-	expression tag	UNP O59487
A	20	GLY	-	expression tag	UNP O59487
A	21	SER	-	expression tag	UNP O59487
A	22	LYS	-	expression tag	UNP O59487
A	135	ALA	TYR	engineered mutation	UNP O59487
B	1	MET	-	initiating methionine	UNP O59487
B	2	SER	-	expression tag	UNP O59487

Continued on next page...

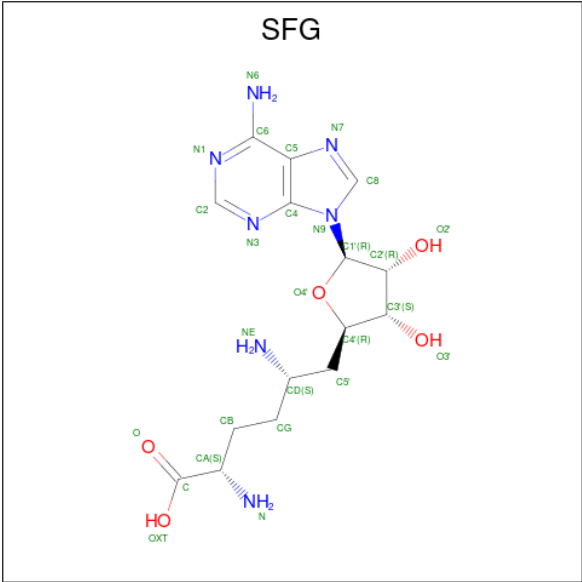
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	SER	-	expression tag	UNP O59487
B	4	ARG	-	expression tag	UNP O59487
B	5	ILE	-	expression tag	UNP O59487
B	6	ARG	-	expression tag	UNP O59487
B	7	ILE	-	expression tag	UNP O59487
B	8	ASN	-	expression tag	UNP O59487
B	9	THR	-	expression tag	UNP O59487
B	10	LYS	-	expression tag	UNP O59487
B	11	SER	-	expression tag	UNP O59487
B	12	LEU	-	expression tag	UNP O59487
B	13	LEU	-	expression tag	UNP O59487
B	14	VAL	-	expression tag	UNP O59487
B	15	GLN	-	expression tag	UNP O59487
B	16	PRO	-	expression tag	UNP O59487
B	17	GLY	-	expression tag	UNP O59487
B	18	TYR	-	expression tag	UNP O59487
B	19	SER	-	expression tag	UNP O59487
B	20	GLY	-	expression tag	UNP O59487
B	21	SER	-	expression tag	UNP O59487
B	22	LYS	-	expression tag	UNP O59487
B	135	ALA	TYR	engineered mutation	UNP O59487

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Zn 4 4	0	0

- Molecule 3 is SINEFUNGIN (CCD ID: SFG) (formula: C₁₅H₂₃N₇O₅) (labeled as "Ligand of Interest" by depositor).



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

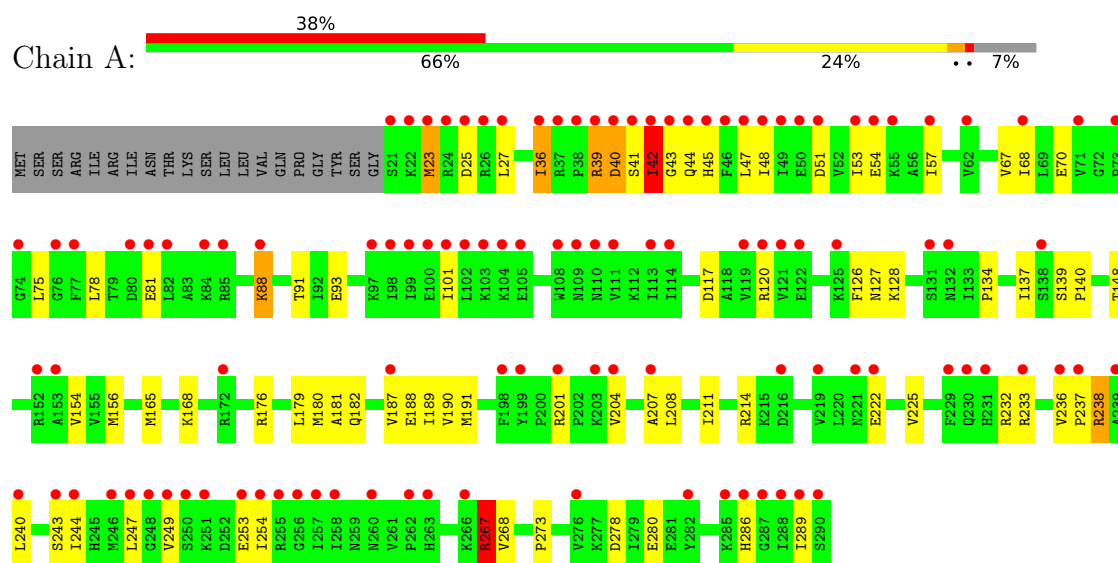
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	55	Total	O	0	0
			55	55		

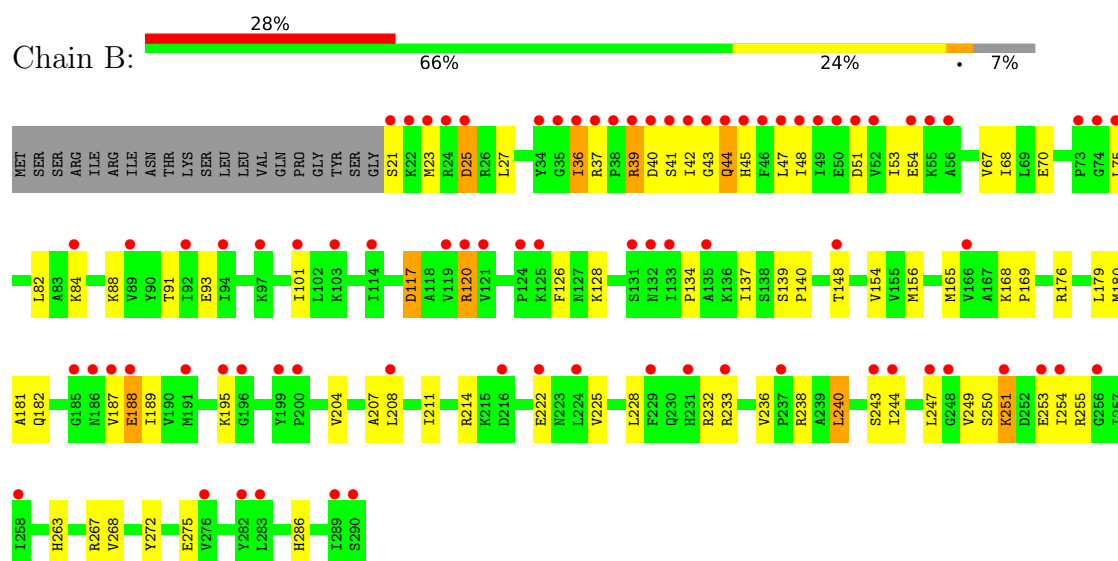
3 Residue-property plots [i](#)

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

- Molecule 1: Probable ribosomal RNA small subunit methyltransferase A



- Molecule 1: Probable ribosomal RNA small subunit methyltransferase A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.06Å 79.96Å 85.41Å 90.00° 116.28° 90.00°	Depositor
Resolution (Å)	76.58 – 2.60 76.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.8 (76.58-2.60) 93.8 (76.58-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.262 , 0.289 0.268 , 0.292	Depositor DCC
R_{free} test set	1065 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.938	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4536	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 18.21% 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: ZN, 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	0.62	0/2228	1.29	11/2998 (0.4%)
1	B	0.63	0/2228	1.33	12/2998 (0.4%)
All	All	0.62	0/4456	1.31	23/5996 (0.4%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ILE	N-CA-C	-17.25	95.28	111.67
1	A	42	ILE	N-CA-C	-16.45	75.11	109.34
1	A	41	SER	N-CA-C	14.51	141.70	110.80
1	B	43	GLY	N-CA-C	-13.80	90.35	110.91
1	B	41	SER	N-CA-C	10.62	133.42	110.80
1	B	44	GLN	N-CA-C	-10.18	89.89	107.61
1	B	44	GLN	N-CA-CB	9.25	124.86	110.71
1	B	40	ASP	CB-CA-C	9.23	125.48	110.90
1	B	25	ASP	CA-CB-CG	9.00	121.60	112.60
1	A	42	ILE	CB-CA-C	8.92	125.91	111.29
1	A	41	SER	CB-CA-C	-8.73	93.04	110.42
1	A	40	ASP	CB-CA-C	8.23	123.91	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ASP	N-CA-C	-7.60	102.93	111.14
1	B	41	SER	N-CA-CB	-6.59	99.35	110.49
1	A	40	ASP	N-CA-C	-6.52	104.09	111.14
1	B	188	GLU	CB-CA-C	6.42	120.82	110.16
1	A	41	SER	N-CA-CB	-6.12	100.14	110.49
1	A	51	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	39	ARG	N-CA-CB	5.49	119.71	110.77
1	A	39	ARG	N-CA-CB	5.42	119.28	110.77
1	A	253	GLU	CB-CG-CD	5.33	121.66	112.60
1	A	25	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	25	ASP	N-CA-C	-5.21	106.88	113.18

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	ARG	Sidechain
1	A	267	ARG	Sidechain
1	B	238	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	2188	0	2301	47	2
1	B	2188	0	2301	50	2
2	A	4	0	0	0	0
3	A	27	0	22	1	0
3	B	27	0	22	4	0
4	A	47	0	0	5	0
4	B	55	0	0	5	0
All	All	4536	0	4646	95	2

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 10.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD12	1:A:75:LEU:HD12	1.24	1.17
1:B:27:LEU:HD12	1:B:75:LEU:HD12	1.23	1.16
1:B:93:GLU:OE1	3:B:301:SFG:O2'	1.62	1.13
1:B:25:ASP:OD1	4:B:401:HOH:O	1.77	1.03
1:B:188:GLU:OE1	4:B:402:HOH:O	1.80	0.97
1:B:36:ILE:HD11	1:B:101:ILE:CD1	2.09	0.82
1:A:267:ARG:HH11	1:A:267:ARG:HG2	1.45	0.82
1:B:51:ASP:OD1	4:B:403:HOH:O	1.98	0.82
1:A:36:ILE:HD11	1:A:101:ILE:CD1	2.12	0.80
1:A:23:MET:HE1	1:A:53:ILE:HD12	1.65	0.79
1:A:237:PRO:HG2	4:A:444:HOH:O	1.82	0.78
1:B:27:LEU:CD1	1:B:75:LEU:HD12	2.11	0.76
1:A:93:GLU:OE1	3:A:305:SFG:O2'	2.01	0.75
1:B:23:MET:HE1	1:B:53:ILE:HD12	1.68	0.74
1:A:27:LEU:CD1	1:A:75:LEU:HD12	2.12	0.74
1:A:267:ARG:HH11	1:A:267:ARG:CG	2.09	0.66
1:A:267:ARG:HG2	1:A:267:ARG:NH1	2.11	0.65
1:A:27:LEU:HD12	1:A:75:LEU:CD1	2.15	0.62
1:A:45:HIS:NE2	1:B:253:GLU:OE1	2.29	0.62
1:B:44:GLN:HG3	3:B:301:SFG:H5'2	1.81	0.61
1:B:126:PHE:CZ	1:B:148:THR:HG21	2.35	0.60
1:B:139:SER:HB3	1:B:140:PRO:HD3	1.83	0.60
1:A:139:SER:HB3	1:A:140:PRO:HD3	1.84	0.59
1:B:27:LEU:HD12	1:B:75:LEU:CD1	2.15	0.59
1:B:93:GLU:CD	3:B:301:SFG:HO2'	2.04	0.59
1:B:39:ARG:HH21	1:B:45:HIS:CE1	2.21	0.59
1:A:249:VAL:HG11	1:A:254:ILE:HD13	1.84	0.58
1:B:249:VAL:HG11	1:B:254:ILE:HD13	1.85	0.58
1:B:255:ARG:HG3	1:B:255:ARG:HH11	1.67	0.58
1:A:42:ILE:HG13	1:A:43:GLY:H	1.71	0.56
1:A:67:VAL:HG13	1:A:88:LYS:HB3	1.88	0.55
1:A:126:PHE:CZ	1:A:148:THR:HG21	2.41	0.55
1:B:68:ILE:HD13	1:B:128:LYS:HB2	1.88	0.55
1:B:67:VAL:HG13	1:B:88:LYS:HB3	1.89	0.54
1:B:176:ARG:HG3	1:B:225:VAL:HG12	1.88	0.54
1:B:182:GLN:O	1:B:214:ARG:NH1	2.37	0.53
1:B:244:ILE:HA	1:B:247:LEU:HD12	1.92	0.52
1:A:78:LEU:HB3	4:A:416:HOH:O	2.09	0.52
1:B:47:LEU:CD2	1:B:156:MET:HE1	2.40	0.52
1:A:47:LEU:CD2	1:A:156:MET:HE1	2.40	0.52
1:A:39:ARG:HH21	1:A:45:HIS:CE1	2.27	0.52
1:B:25:ASP:CG	4:B:401:HOH:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD13	1:A:128:LYS:HB2	1.91	0.51
1:A:182:GLN:O	1:A:214:ARG:NH1	2.42	0.50
1:B:39:ARG:HH21	1:B:45:HIS:HE1	1.58	0.50
1:A:36:ILE:HD11	1:A:101:ILE:HD13	1.90	0.50
1:A:39:ARG:HH21	1:A:45:HIS:HE1	1.60	0.50
1:B:36:ILE:HD11	1:B:101:ILE:HD13	1.91	0.50
1:A:48:ILE:HD12	1:A:48:ILE:O	2.13	0.49
1:A:70:GLU:O	1:A:91:THR:HA	2.12	0.49
1:A:120:ARG:HH21	1:A:120:ARG:HG3	1.77	0.49
1:B:36:ILE:HD11	1:B:101:ILE:HD11	1.92	0.49
1:A:189:ILE:HG23	1:A:207:ALA:HB1	1.94	0.49
1:A:45:HIS:HE2	1:B:253:GLU:CD	2.17	0.48
1:B:48:ILE:HD12	1:B:48:ILE:O	2.13	0.48
1:B:70:GLU:O	1:B:91:THR:HA	2.13	0.48
1:A:244:ILE:HA	1:A:247:LEU:HD12	1.95	0.48
1:A:181:ALA:HB1	1:A:187:VAL:HG21	1.95	0.48
1:A:57:ILE:CD1	1:A:81:GLU:HB3	2.44	0.47
1:A:244:ILE:O	1:A:247:LEU:HB2	2.14	0.47
1:B:176:ARG:O	1:B:180:MET:HG2	2.14	0.47
1:B:244:ILE:O	1:B:247:LEU:HB2	2.14	0.47
1:A:36:ILE:HD11	1:A:101:ILE:HD11	1.93	0.47
1:A:134:PRO:HB2	1:A:137:ILE:HG12	1.96	0.47
1:B:195:LYS:HG2	4:B:409:HOH:O	2.13	0.47
1:A:154:VAL:CG1	1:A:208:LEU:HD11	2.46	0.46
1:B:117:ASP:OD2	1:B:120:ARG:HB2	2.16	0.46
1:A:176:ARG:O	1:A:180:MET:HG2	2.17	0.45
1:B:134:PRO:HB2	1:B:137:ILE:HG12	1.97	0.45
1:B:189:ILE:HG23	1:B:207:ALA:HB1	2.00	0.44
1:A:39:ARG:HD3	1:A:42:ILE:O	2.18	0.44
1:A:232:ARG:HA	1:A:268:VAL:HB	2.00	0.44
1:B:181:ALA:HB1	1:B:187:VAL:HG21	1.98	0.44
1:A:280:GLU:HG3	1:A:289:ILE:HD11	2.00	0.43
1:A:201:ARG:HG3	4:A:414:HOH:O	2.18	0.43
1:A:176:ARG:HG3	1:A:225:VAL:HG12	2.00	0.43
1:B:232:ARG:HA	1:B:268:VAL:HB	2.00	0.43
1:B:251:LYS:NZ	1:B:255:ARG:HH22	2.16	0.43
1:B:154:VAL:CG1	1:B:208:LEU:HD11	2.49	0.43
1:B:169:PRO:HB2	1:B:272:TYR:CE1	2.54	0.42
1:A:182:GLN:HG2	1:A:273:PRO:HG2	2.01	0.42
1:A:165:MET:HE1	1:A:211:ILE:HD11	2.01	0.42
1:A:278:ASP:HA	4:A:408:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:HG12	1:B:250:SER:O	2.19	0.42
1:B:27:LEU:HD22	1:B:48:ILE:HG21	2.02	0.42
1:B:255:ARG:HG3	1:B:255:ARG:NH1	2.34	0.42
1:B:68:ILE:HG21	1:B:82:LEU:HD13	2.01	0.41
1:A:190:VAL:HG12	1:A:191:MET:HG2	2.02	0.41
1:B:45:HIS:HB2	3:B:301:SFG:HA	2.03	0.41
1:A:39:ARG:NH2	1:A:45:HIS:CE1	2.89	0.41
1:B:47:LEU:HD21	1:B:156:MET:HE1	2.02	0.40
1:B:165:MET:HE1	1:B:211:ILE:HD11	2.03	0.40
1:B:263:HIS:CE1	1:B:275:GLU:HG2	2.55	0.40
1:A:48:ILE:HD11	4:A:406:HOH:O	2.21	0.40
1:B:228:LEU:HD21	1:B:240:LEU:CD2	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:HIS:NE2	1:B:188:GLU:OE1[4_555]	1.71	0.49
1:A:188:GLU:OE1	1:B:286:HIS:NE2[4_556]	2.10	0.10

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	268/290 (92%)	255 (95%)	13 (5%)	0	100	100
1	B	268/290 (92%)	259 (97%)	9 (3%)	0	100	100
All	All	536/580 (92%)	514 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	242/260 (93%)	223 (92%)	19 (8%)	11	26
1	B	242/260 (93%)	225 (93%)	17 (7%)	14	31
All	All	484/520 (93%)	448 (93%)	36 (7%)	13	29

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	36	ILE
1	A	40	ASP
1	A	42	ILE
1	A	44	GLN
1	A	54	GLU
1	A	88	LYS
1	A	117	ASP
1	A	127	ASN
1	A	168	LYS
1	A	179	LEU
1	A	204	VAL
1	A	222	GLU
1	A	233	ARG
1	A	236	VAL
1	A	238	ARG
1	A	240	LEU
1	A	243	SER
1	A	267	ARG
1	B	21	SER
1	B	36	ILE
1	B	37	ARG
1	B	54	GLU
1	B	84	LYS
1	B	117	ASP
1	B	120	ARG
1	B	168	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	179	LEU
1	B	204	VAL
1	B	222	GLU
1	B	233	ARG
1	B	236	VAL
1	B	240	LEU
1	B	243	SER
1	B	251	LYS
1	B	267	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SFG	A	305	-	28,29,29	0.65	1 (3%)	34,42,42	0.92	2 (5%)
3	SFG	B	301	-	28,29,29	0.59	0	34,42,42	0.93	2 (5%)

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
3	SFG	A	305	-	-	5/17/33/33	0/3/3/3
3	SFG	B	301	-	-	5/17/33/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	305	SFG	OXT-C	-2.01	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	SFG	O3'-C3'-C2'	-3.28	101.31	111.82
3	A	305	SFG	O4'-C4'-C5'	-2.33	105.39	109.41
3	A	305	SFG	C4'-O4'-C1'	-2.31	104.36	109.47
3	B	301	SFG	O4'-C4'-C5'	-2.13	105.73	109.41

There are no chirality outliers.

All (10) torsion outliers are listed below:

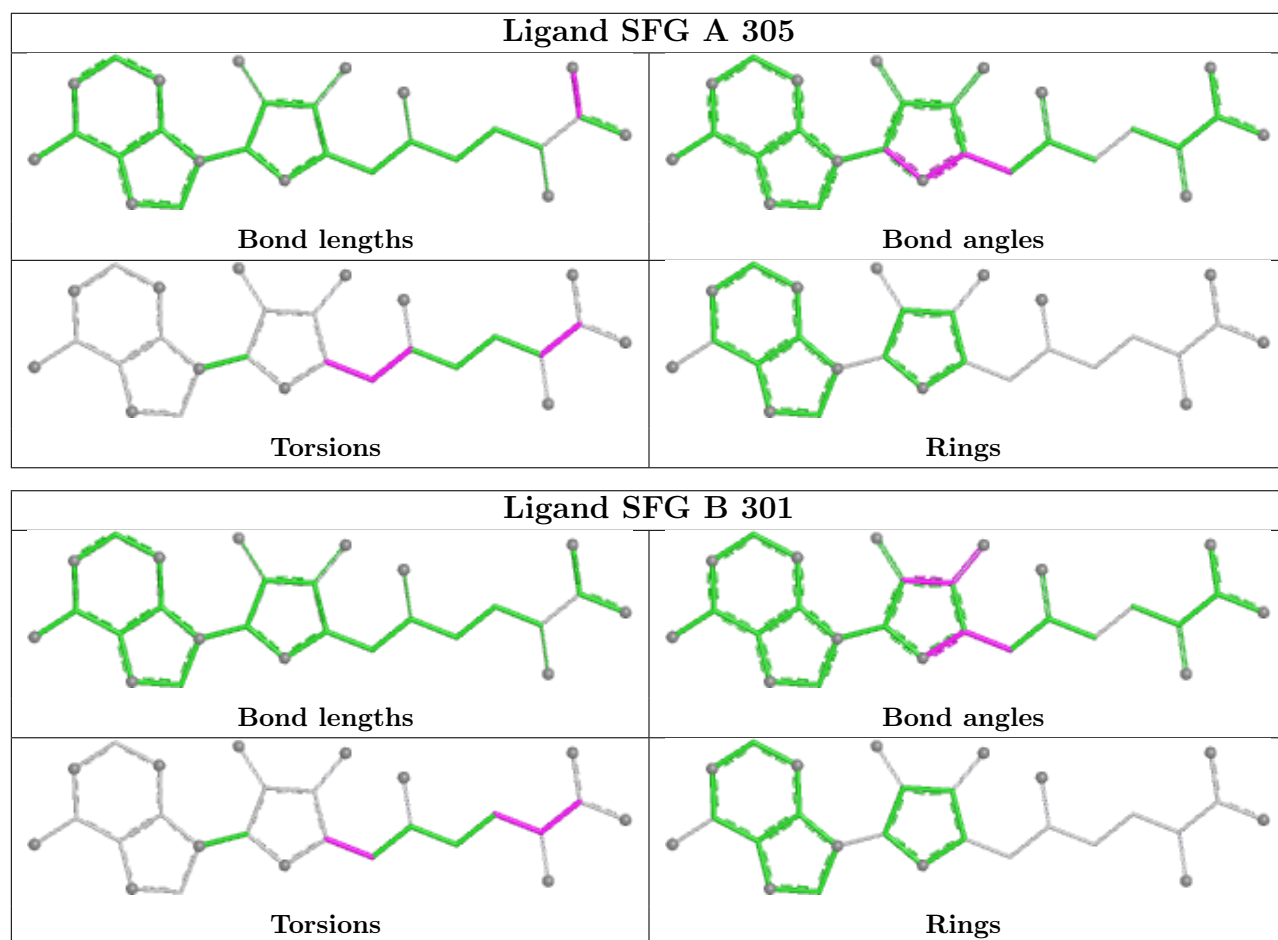
Mol	Chain	Res	Type	Atoms
3	A	305	SFG	C4'-C5'-CD-NE
3	A	305	SFG	O4'-C4'-C5'-CD
3	A	305	SFG	C3'-C4'-C5'-CD
3	B	301	SFG	O4'-C4'-C5'-CD
3	B	301	SFG	OXT-C-CA-CB
3	B	301	SFG	N-CA-CB-CG
3	B	301	SFG	O-C-CA-CB
3	A	305	SFG	O-C-CA-N
3	A	305	SFG	C4'-C5'-CD-CG
3	B	301	SFG	C3'-C4'-C5'-CD

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	305	SFG	1	0
3	B	301	SFG	4	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	270/290 (93%)	1.90	111 (41%) 0 0	34, 51, 78, 131	0
1	B	270/290 (93%)	1.73	80 (29%) 1 1	33, 49, 76, 147	0
All	All	540/580 (93%)	1.81	191 (35%) 1 1	33, 50, 77, 147	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	7.5
1	A	38	PRO	6.6
1	B	41	SER	6.6
1	B	42	ILE	6.6
1	B	21	SER	6.5
1	B	40	ASP	5.8
1	B	38	PRO	5.7
1	B	43	GLY	5.6
1	A	45	HIS	5.5
1	A	43	GLY	5.4
1	B	39	ARG	5.3
1	A	40	ASP	5.2
1	A	41	SER	5.1
1	A	44	GLN	5.0
1	A	77	PHE	4.9
1	A	254	ILE	4.8
1	A	250	SER	4.8
1	A	258	ILE	4.6
1	A	248	GLY	4.6
1	B	199	TYR	4.5
1	A	39	ARG	4.5
1	B	74	GLY	4.3
1	B	25	ASP	4.1
1	A	236	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	36	ILE	4.0
1	A	25	ASP	4.0
1	A	21	SER	3.9
1	B	254	ILE	3.9
1	A	37	ARG	3.7
1	A	251	LYS	3.7
1	A	257	ILE	3.7
1	A	199	TYR	3.5
1	B	253	GLU	3.5
1	B	36	ILE	3.4
1	A	74	GLY	3.4
1	B	46	PHE	3.4
1	B	50	GLU	3.4
1	A	47	LEU	3.4
1	A	216	ASP	3.4
1	B	131	SER	3.3
1	A	46	PHE	3.3
1	B	35	GLY	3.3
1	B	119	VAL	3.2
1	B	132	ASN	3.2
1	A	81	GLU	3.2
1	A	253	GLU	3.2
1	A	121	VAL	3.2
1	B	47	LEU	3.2
1	B	289	ILE	3.2
1	A	51	ASP	3.2
1	A	222	GLU	3.2
1	A	204	VAL	3.2
1	B	121	VAL	3.1
1	A	104	LYS	3.1
1	B	22	LYS	3.1
1	B	37	ARG	3.1
1	B	23	MET	3.1
1	B	45	HIS	3.1
1	B	243	SER	3.1
1	A	249	VAL	3.1
1	B	188	GLU	3.0
1	A	153	ALA	3.0
1	B	54	GLU	3.0
1	B	51	ASP	3.0
1	B	251	LYS	3.0
1	B	55	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	247	LEU	2.9
1	B	49	ILE	2.9
1	A	244	ILE	2.9
1	A	289	ILE	2.9
1	B	120	ARG	2.9
1	A	290	SER	2.9
1	A	256	GLY	2.9
1	A	287	GLY	2.9
1	B	148	THR	2.9
1	A	240	LEU	2.9
1	A	233	ARG	2.8
1	A	243	SER	2.8
1	A	84	LYS	2.8
1	B	125	LYS	2.8
1	A	108	TRP	2.8
1	B	290	SER	2.8
1	A	24	ARG	2.8
1	A	97	LYS	2.8
1	A	101	ILE	2.7
1	A	138	SER	2.7
1	A	85	ARG	2.7
1	A	120	ARG	2.7
1	A	73	PRO	2.7
1	A	172	ARG	2.7
1	A	239	ALA	2.7
1	B	56	ALA	2.7
1	B	196	GLY	2.7
1	B	248	GLY	2.7
1	A	201	ARG	2.7
1	A	49	ILE	2.6
1	A	98	ILE	2.6
1	A	26	ARG	2.6
1	B	34	TYR	2.6
1	B	187	VAL	2.6
1	A	230	GLN	2.6
1	B	44	GLN	2.6
1	A	23	MET	2.5
1	A	48	ILE	2.5
1	B	97	LYS	2.5
1	A	71	VAL	2.5
1	A	111	VAL	2.5
1	A	262	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	207	ALA	2.5
1	A	88	LYS	2.5
1	A	102	LEU	2.5
1	A	103	LYS	2.5
1	B	24	ARG	2.5
1	A	55	LYS	2.5
1	A	152	ARG	2.5
1	A	62	VAL	2.5
1	A	53	ILE	2.5
1	A	114	ILE	2.5
1	A	286	HIS	2.5
1	B	89	VAL	2.5
1	A	203	LYS	2.4
1	B	186	ASN	2.4
1	A	80	ASP	2.4
1	B	216	ASP	2.4
1	B	48	ILE	2.4
1	B	258	ILE	2.4
1	B	256	GLY	2.4
1	A	247	LEU	2.3
1	A	131	SER	2.3
1	B	195	LYS	2.3
1	B	73	PRO	2.3
1	B	283	LEU	2.3
1	B	124	PRO	2.3
1	A	276	VAL	2.3
1	A	99	ILE	2.3
1	A	231	HIS	2.3
1	A	246	MET	2.3
1	A	113	ILE	2.2
1	B	244	ILE	2.2
1	B	231	HIS	2.2
1	A	125	LYS	2.2
1	A	282	TYR	2.2
1	A	76	GLY	2.2
1	A	219	VAL	2.2
1	B	229	PHE	2.2
1	B	237	PRO	2.2
1	A	229	PHE	2.2
1	A	132	ASN	2.2
1	B	282	TYR	2.2
1	B	185	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	52	VAL	2.2
1	A	68	ILE	2.2
1	A	288	ILE	2.2
1	B	114	ILE	2.2
1	A	22	LYS	2.2
1	A	119	VAL	2.2
1	A	100	GLU	2.1
1	B	233	ARG	2.1
1	B	200	PRO	2.1
1	A	221	ASN	2.1
1	A	260	ASN	2.1
1	A	57	ILE	2.1
1	A	187	VAL	2.1
1	A	263	HIS	2.1
1	A	255	ARG	2.1
1	B	103	LYS	2.1
1	B	133	ILE	2.1
1	A	105	GLU	2.1
1	B	84	LYS	2.1
1	B	92	ILE	2.1
1	A	198	PHE	2.1
1	B	222	GLU	2.1
1	A	237	PRO	2.1
1	B	191	MET	2.1
1	A	82	LEU	2.1
1	B	75	LEU	2.1
1	B	208	LEU	2.1
1	B	276	VAL	2.1
1	A	50	GLU	2.0
1	B	135	ALA	2.0
1	A	266	LYS	2.0
1	A	285	LYS	2.0
1	A	109	ASN	2.0
1	A	54	GLU	2.0
1	A	122	GLU	2.0
1	A	27	LEU	2.0
1	B	224	LEU	2.0
1	A	110	ASN	2.0
1	B	94	ILE	2.0
1	B	101	ILE	2.0
1	B	166	VAL	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](#)

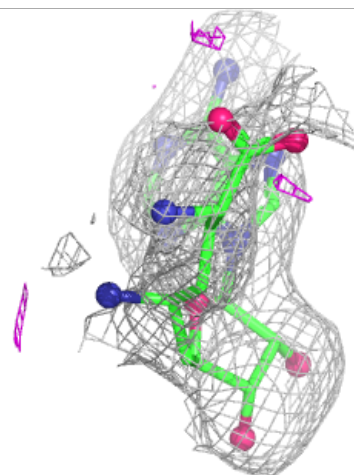
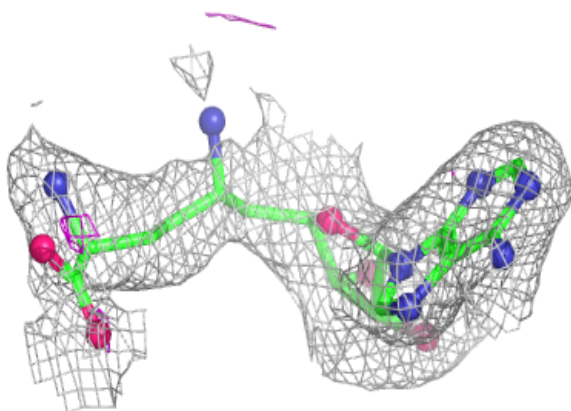
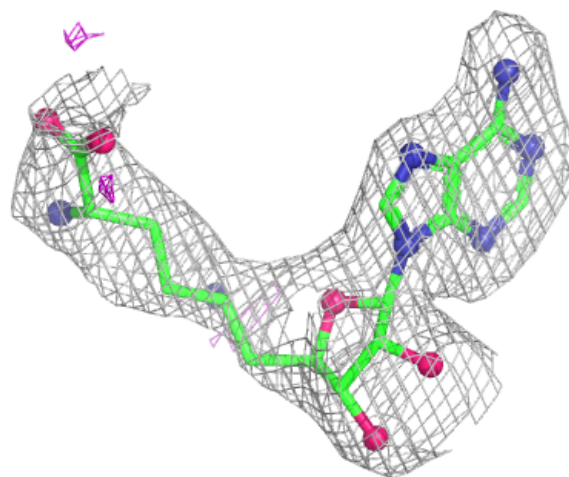
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SFG	A	305	27/27	0.81	0.16	39,48,63,82	0
3	SFG	B	301	27/27	0.86	0.16	32,45,62,78	0
2	ZN	A	304	1/1	0.92	0.06	71,71,71,71	0
2	ZN	A	303	1/1	0.94	0.07	59,59,59,59	0
2	ZN	A	301	1/1	0.95	0.07	63,63,63,63	0
2	ZN	A	302	1/1	0.97	0.04	61,61,61,61	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.

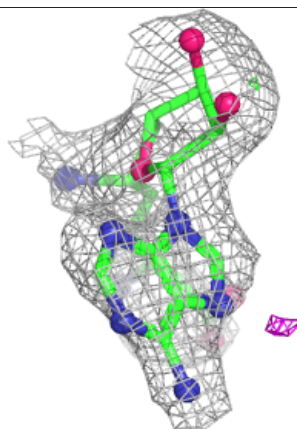
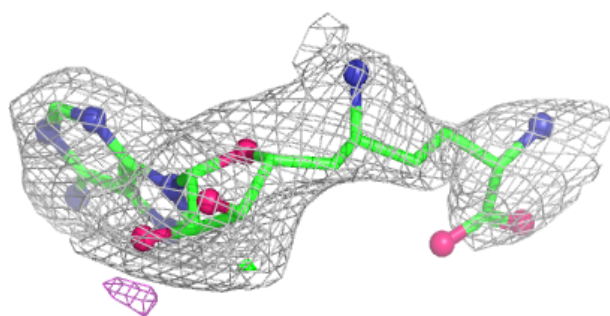
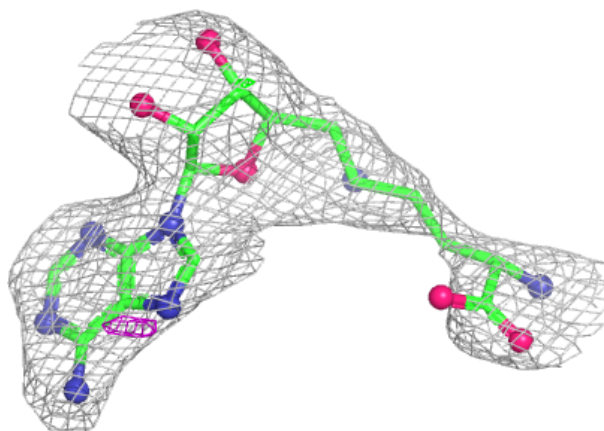
Electron density around SFG A 305:

$2mF_o-DF_c$ (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.