



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 18, 2021 – 10:11 AM JST

PDB ID : 7CIM
Title : Crystal structure of L-methionine decarboxylase from Streptomyces sp.590 in complexed with 3-methylthiopropylamine (geminal diamine form).
Authors : Okawa, A.; Shiba, T.; Hayashi, M.; Onoue, Y.; Murota, M.; Sato, D.; Inagaki, J.; Tamura, T.; Harada, S.; Inagaki, K.
Deposited on : 2020-07-07
Resolution : 1.80 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 : 2.16
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) : 2.16

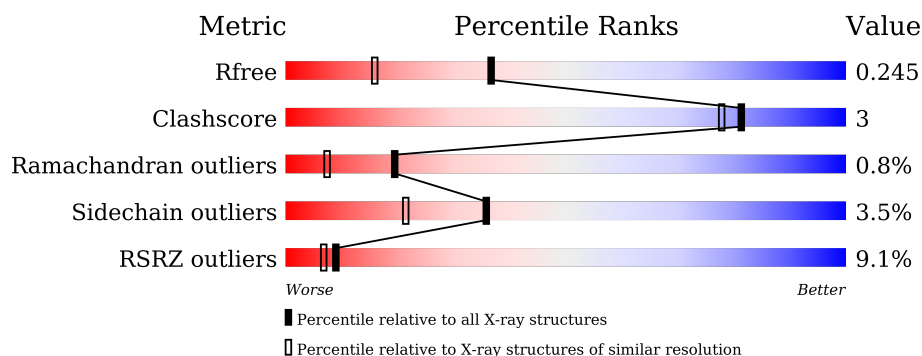
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	557	<div> <div>9%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	B	557	<div> <div>8%</div> <div>83%</div> <div>9%</div> <div>7%</div> </div>

2 Entry composition [i](#)

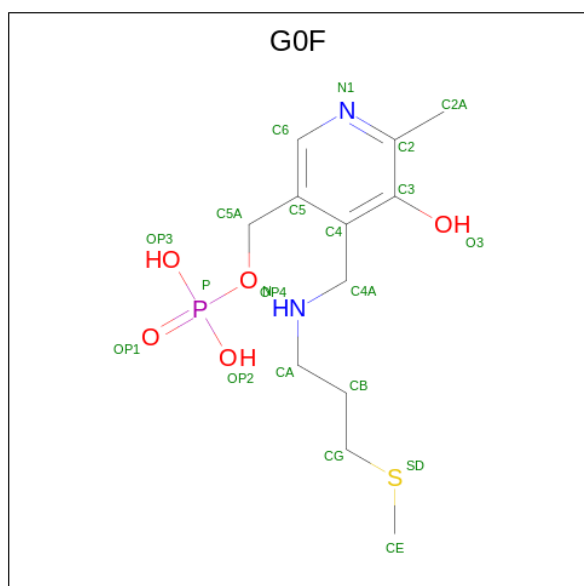
There are 3 unique types of molecules in this entry. The entry contains 8484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-methionine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	1	0
			4115	2618	718	764	15			
1	B	518	Total	C	N	O	S	0	0	0
			4056	2584	705	752	15			

- Molecule 2 is [6-methyl-4-[(3-methylsulfanylpropylamino)methyl]-5-oxidanyl-pyridin-3-yl]methyl dihydrogen phosphate (three-letter code: G0F) (formula: $C_{12}H_{21}N_2O_5PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			21	12	2	5	1 1		
2	B	1	Total	C	N	O	P S	0	0
			21	12	2	5	1 1		

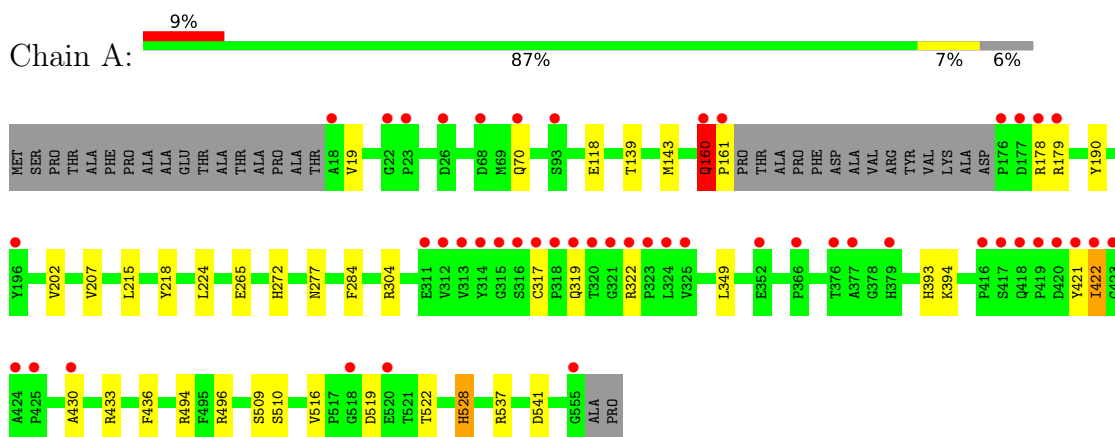
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total 132	O 132	0	0
3	B	139	Total 139	O 139	0	0

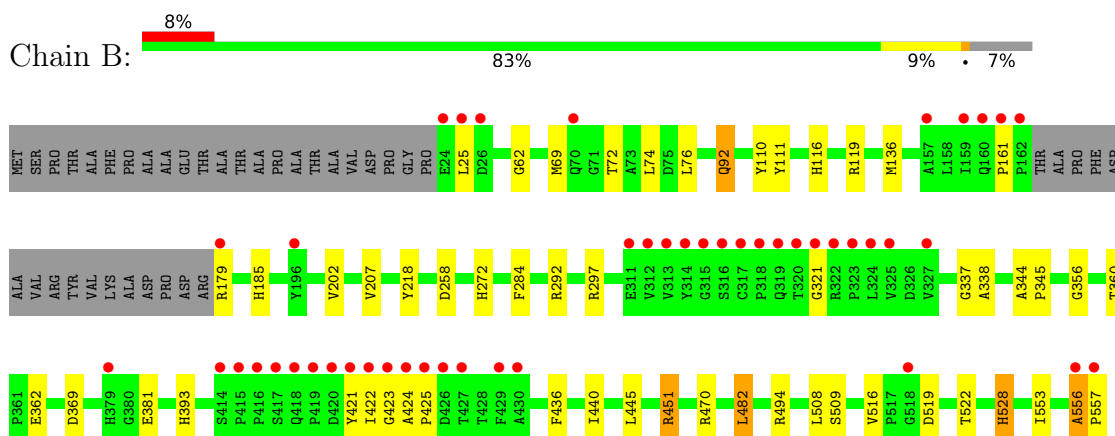
3 Residue-property plots

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

• Molecule 1: L-methionine decarboxylase



• Molecule 1: L-methionine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.64Å 147.81Å 54.19Å 90.00° 99.47° 90.00°	Depositor
Resolution (Å)	19.96 – 1.80 19.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.96-1.80) 99.7 (19.96-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.203 , 0.238 0.211 , 0.245	Depositor DCC
R_{free} test set	4496 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8484	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.73% 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: GOF

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	0.52	0/4235	0.73	3/5772 (0.1%)
1	B	0.56	0/4175	0.74	1/5691 (0.0%)
All	All	0.54	0/8410	0.74	4/11463 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	A	394	LYS	CD-CE-NZ	5.39	124.10	111.70
1	A	496	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	496	ARG	NE-CZ-NH2	-5.27	117.66	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	425	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4115	0	3968	19	0
1	B	4056	0	3911	25	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
3	A	132	0	0	0	0
3	B	139	0	0	0	0
All	All	8484	0	7879	42	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 3.

All (42) 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:B:516:VAL:HG22	1:B:522:THR:HG21	1.63	0.78
1:A:516:VAL:HG22	1:A:522:THR:HG21	1.71	0.70
1:A:430:ALA:HB3	1:A:433[B]:ARG:NH1	2.08	0.66
1:B:284:PHE:O	1:B:528:HIS:HD2	1.78	0.66
1:B:556:ALA:HB1	1:B:557:PRO:CD	2.26	0.66
1:A:265:GLU:OE1	1:A:304:ARG:NH1	2.31	0.64
1:B:202:VAL:HG13	1:B:207:VAL:O	1.99	0.63
1:B:556:ALA:HB1	1:B:557:PRO:HD2	1.81	0.62
1:B:258:ASP:OD1	1:B:297:ARG:NH1	2.31	0.61
1:A:284:PHE:O	1:A:528:HIS:HD2	1.87	0.58
1:B:482:LEU:HD11	1:B:553:ILE:HG23	1.84	0.58
1:B:509:SER:HB3	1:B:528:HIS:CE1	2.42	0.55
1:B:218:TYR:OH	1:B:272:HIS:HE1	1.91	0.53
1:B:516:VAL:HG23	1:B:519:ASP:HB3	1.91	0.53
1:A:202:VAL:HG13	1:A:207:VAL:O	2.08	0.53
1:A:537:ARG:NH1	1:A:541:ASP:OD2	2.43	0.52
1:B:76:LEU:HD12	1:B:440:ILE:HD13	1.92	0.52
1:B:356:GLY:O	1:B:451:ARG:NH2	2.43	0.51
1:B:116:HIS:HD2	1:B:369:ASP:OD2	1.94	0.50
1:A:422:ILE:O	1:A:422:ILE:HG23	2.12	0.50
1:A:421:TYR:O	1:A:422:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:OH	1:A:272:HIS:HE1	1.96	0.48
1:B:92:GLN:HE21	1:B:424:ALA:HB1	1.80	0.47
1:B:337:GLY:O	1:B:338:ALA:C	2.54	0.46
1:B:393:HIS:H	1:B:393:HIS:CD2	2.32	0.46
1:B:62:GLY:HA3	1:B:508:LEU:HA	1.98	0.46
1:A:160:GLN:HA	1:A:160:GLN:HE21	1.81	0.45
1:A:430:ALA:HB2	1:B:136:MET:SD	2.57	0.45
1:A:433[B]:ARG:HB3	1:A:433[B]:ARG:HE	1.56	0.43
1:A:139:THR:O	1:A:143:MET:HG3	2.19	0.42
1:A:160:GLN:CB	1:A:161:PRO:CD	2.97	0.42
1:B:110:TYR:CE1	1:B:445:LEU:HD22	2.54	0.42
1:A:393:HIS:H	1:A:393:HIS:CD2	2.37	0.42
1:A:509:SER:HB3	1:A:528:HIS:CE1	2.55	0.42
1:A:510:SER:HB2	1:B:422:ILE:HD11	2.01	0.42
1:A:516:VAL:HG23	1:A:519:ASP:HB3	2.02	0.42
1:B:185:HIS:O	1:B:272:HIS:HD2	2.03	0.42
1:B:344:ALA:N	1:B:345:PRO:CD	2.83	0.41
1:B:516:VAL:CG2	1:B:519:ASP:HB3	2.51	0.41
1:A:190:TYR:HB3	1:A:277:ASN:HB3	2.03	0.41
1:B:111:TYR:CE2	1:B:445:LEU:HD11	2.56	0.40
1:B:516:VAL:HG22	1:B:522:THR:CG2	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	521/557 (94%)	499 (96%)	18 (4%)	4 (1%)	19	7
1	B	514/557 (92%)	489 (95%)	21 (4%)	4 (1%)	19	7
All	All	1035/1114 (93%)	988 (96%)	39 (4%)	8 (1%)	19	7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	422	ILE
1	B	556	ALA
1	B	161	PRO
1	B	321	GLY
1	B	423	GLY
1	A	179	ARG
1	A	319	GLN

5.3.2 Protein sidechains [i](#)

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	428/450 (95%)	415 (97%)	13 (3%)	41	27
1	B	421/450 (94%)	404 (96%)	17 (4%)	31	16
All	All	849/900 (94%)	819 (96%)	30 (4%)	36	21

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	70	GLN
1	A	118	GLU
1	A	160	GLN
1	A	178	ARG
1	A	215	LEU
1	A	224	LEU
1	A	317	CYS
1	A	322	ARG
1	A	349	LEU
1	A	436	PHE
1	A	494	ARG
1	A	528	HIS
1	B	25	LEU
1	B	69	MET

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Mol	Chain	Res	Type
1	B	72	THR
1	B	74	LEU
1	B	92	GLN
1	B	119	ARG
1	B	179	ARG
1	B	292	ARG
1	B	360	THR
1	B	362	GLU
1	B	381	GLU
1	B	421	TYR
1	B	436	PHE
1	B	451	ARG
1	B	482	LEU
1	B	494	ARG
1	B	528	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	92	GLN
1	A	160	GLN
1	A	182	ASN
1	A	272	HIS
1	A	279	ASN
1	A	393	HIS
1	A	528	HIS
1	B	59	HIS
1	B	92	GLN
1	B	116	HIS
1	B	272	HIS
1	B	279	ASN
1	B	309	GLN
1	B	393	HIS
1	B	444	HIS
1	B	461	GLN
1	B	528	HIS

5.3.3 RNA ⓘ

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](#)

2 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	G0F	A	601	1	21,21,21	2.20	3 (14%)	26,28,28	2.37	9 (34%)
2	G0F	B	601	1	21,21,21	2.21	4 (19%)	26,28,28	2.36	9 (34%)

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	G0F	A	601	1	-	2/13/13/13	0/1/1/1
2	G0F	B	601	1	-	1/13/13/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	G0F	C4A-C4	-8.73	1.40	1.51
2	B	601	G0F	C4A-C4	-8.34	1.41	1.51
2	B	601	G0F	P-OP2	-2.75	1.44	1.54
2	B	601	G0F	C2-N1	2.72	1.39	1.33
2	A	601	G0F	C2-N1	2.45	1.38	1.33
2	A	601	G0F	P-OP2	-2.27	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	G0F	C3-C2	-2.18	1.38	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	G0F	C4A-C4-C5	5.50	125.83	119.71
2	A	601	G0F	OP2-P-OP4	-5.28	92.68	106.73
2	B	601	G0F	C4A-N-CA	5.07	130.79	113.41
2	B	601	G0F	OP2-P-OP4	-4.48	94.81	106.73
2	A	601	G0F	C4-C4A-N	4.43	119.86	111.58
2	A	601	G0F	C4A-C4-C5	4.36	124.56	119.71
2	A	601	G0F	C4A-N-CA	3.55	125.56	113.41
2	B	601	G0F	C3-C2-N1	-3.17	116.67	120.77
2	A	601	G0F	OP3-P-OP2	3.10	119.47	107.64
2	A	601	G0F	OP4-P-OP1	-3.09	97.81	106.47
2	A	601	G0F	C3-C2-N1	-3.00	116.90	120.77
2	B	601	G0F	OP3-P-OP2	2.95	118.91	107.64
2	A	601	G0F	OP2-P-OP1	2.86	121.89	110.68
2	B	601	G0F	C4A-C4-C3	-2.62	117.24	120.04
2	A	601	G0F	C4A-C4-C3	-2.35	117.53	120.04
2	B	601	G0F	OP2-P-OP1	2.21	119.32	110.68
2	B	601	G0F	OP4-P-OP1	-2.20	100.29	106.47
2	B	601	G0F	C4-C3-C2	2.10	123.27	120.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

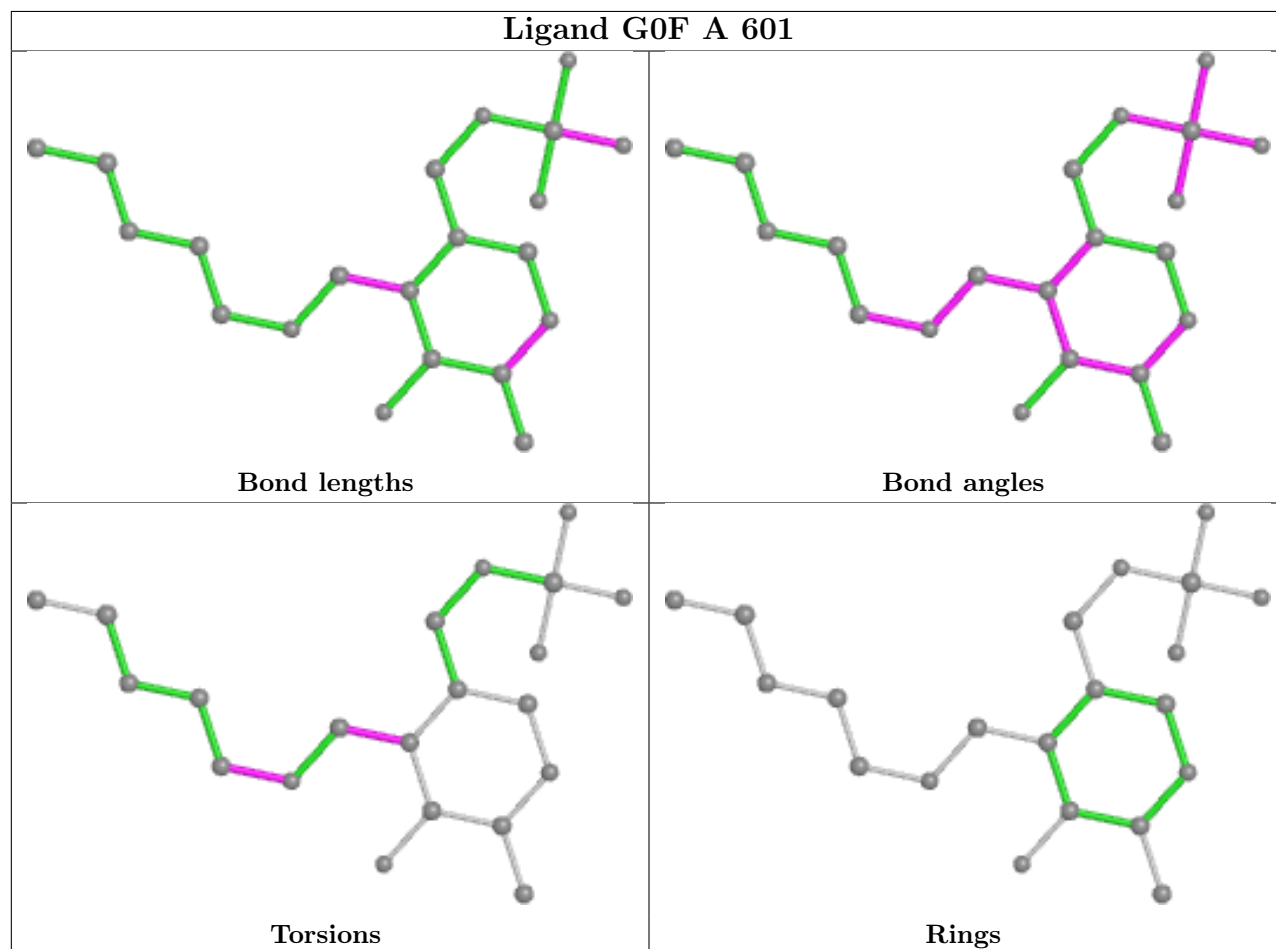
Mol	Chain	Res	Type	Atoms
2	B	601	G0F	N-CA-CB-CG
2	A	601	G0F	CB-CA-N-C4A
2	A	601	G0F	C5-C4-C4A-N

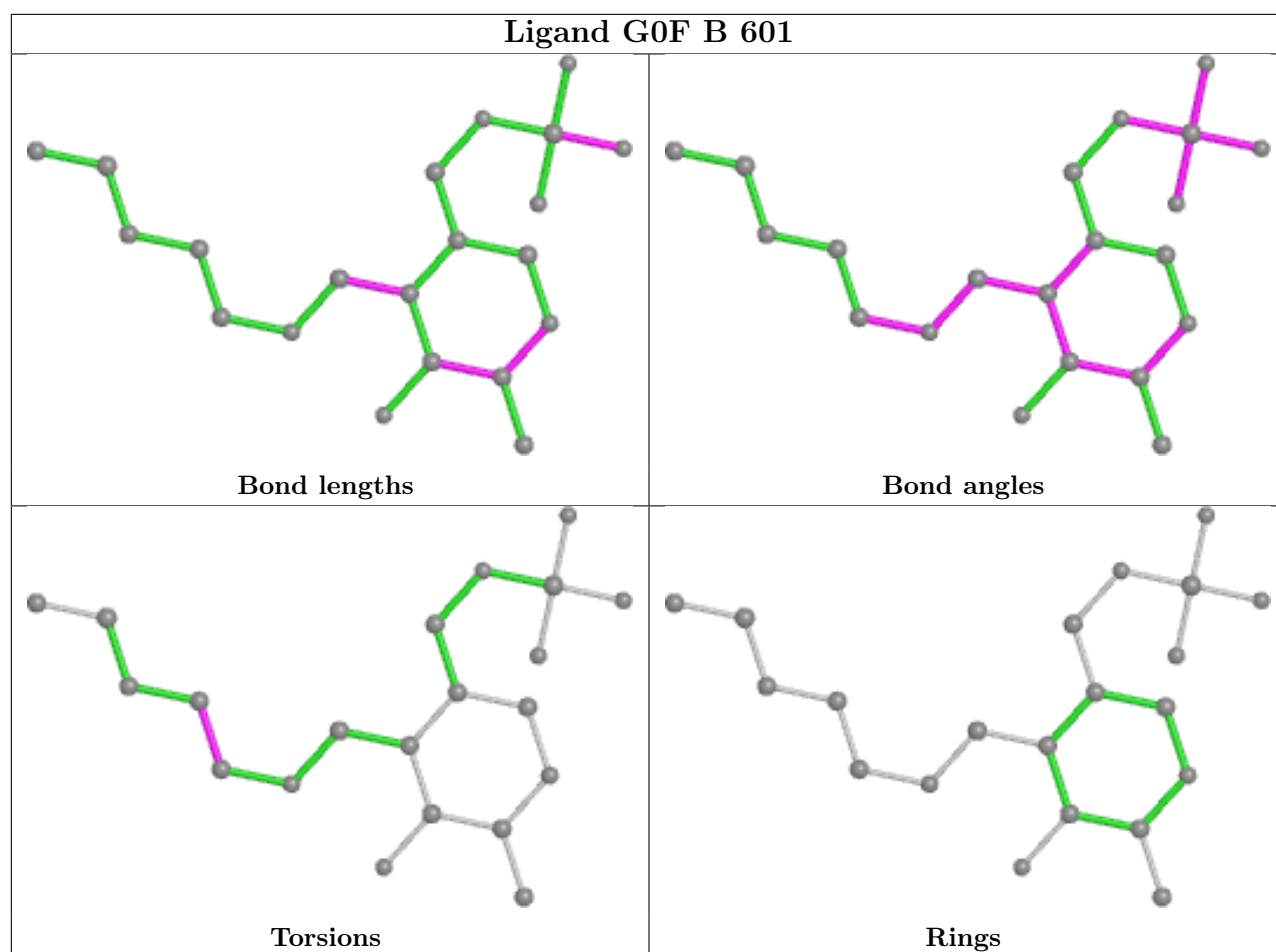
There are no ring outliers.

No monomer is involved in short contacts.

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	524/557 (94%)	0.61	48 (9%) 9 6	21, 30, 79, 147	0
1	B	518/557 (92%)	0.56	47 (9%) 9 7	19, 29, 84, 157	0
All	All	1042/1114 (93%)	0.59	95 (9%) 9 7	19, 30, 81, 157	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	GLY	20.7
1	B	422	ILE	17.4
1	A	422	ILE	16.3
1	A	320	THR	15.2
1	B	421	TYR	14.5
1	A	321	GLY	14.4
1	B	424	ALA	12.4
1	A	317	CYS	12.4
1	B	318	PRO	12.3
1	A	315	GLY	12.2
1	A	176	PRO	11.3
1	B	324	LEU	11.3
1	B	322	ARG	10.8
1	B	315	GLY	10.8
1	A	424	ALA	10.6
1	B	320	THR	10.6
1	B	419	PRO	10.2
1	B	161	PRO	10.0
1	A	421	TYR	9.7
1	B	325	VAL	9.5
1	A	319	GLN	9.1
1	B	317	CYS	8.9
1	B	162	PRO	8.8
1	A	318	PRO	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	321	GLY	8.6
1	A	177	ASP	8.1
1	A	322	ARG	7.9
1	A	425	PRO	7.7
1	A	178	ARG	7.5
1	B	557	PRO	7.3
1	A	324	LEU	7.2
1	B	319	GLN	7.2
1	B	417	SER	6.9
1	A	417	SER	6.9
1	A	179	ARG	6.8
1	A	423	GLY	6.8
1	B	425	PRO	6.7
1	B	420	ASP	6.5
1	A	316	SER	6.4
1	A	314	TYR	6.3
1	B	323	PRO	6.0
1	A	420	ASP	5.9
1	B	179	ARG	5.8
1	A	18	ALA	5.8
1	B	314	TYR	5.7
1	B	316	SER	5.7
1	A	161	PRO	5.7
1	A	419	PRO	5.6
1	A	323	PRO	5.3
1	A	377	ALA	5.3
1	A	160	GLN	5.3
1	B	418	GLN	5.1
1	B	313	VAL	4.9
1	A	418	GLN	4.7
1	B	160	GLN	4.7
1	A	325	VAL	4.6
1	A	313	VAL	4.5
1	A	70	GLN	4.4
1	B	556	ALA	4.3
1	B	70	GLN	4.1
1	A	416	PRO	4.1
1	A	379	HIS	3.8
1	B	416	PRO	3.8
1	B	312	VAL	3.7
1	A	196	TYR	3.4
1	A	555	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	520	GLU	3.3
1	B	26	ASP	3.2
1	B	415	PRO	3.2
1	B	25	LEU	3.1
1	B	426	ASP	3.1
1	A	312	VAL	3.1
1	B	518	GLY	3.1
1	A	518	GLY	3.1
1	B	429	PHE	3.0
1	A	68	ASP	2.9
1	B	379	HIS	2.9
1	B	157	ALA	2.9
1	B	196	TYR	2.9
1	B	327	VAL	2.9
1	A	430	ALA	2.8
1	B	430	ALA	2.7
1	A	376	THR	2.7
1	A	311	GLU	2.5
1	A	22	GLY	2.4
1	A	366	PRO	2.4
1	B	311	GLU	2.3
1	B	159	ILE	2.3
1	B	24	GLU	2.2
1	A	23	PRO	2.2
1	A	93	SER	2.1
1	B	414	SER	2.1
1	B	427	THR	2.1
1	A	26	ASP	2.1
1	A	352	GLU	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 ⓘ

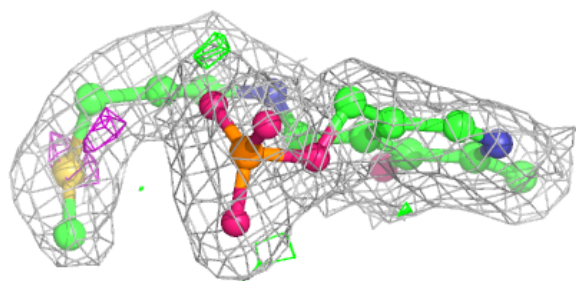
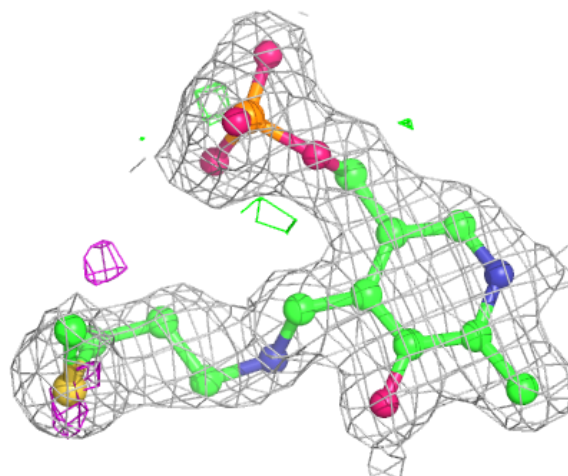
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G0F	A	601	21/21	0.96	0.09	25,28,40,43	0
2	G0F	B	601	21/21	0.96	0.10	24,26,48,50	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.

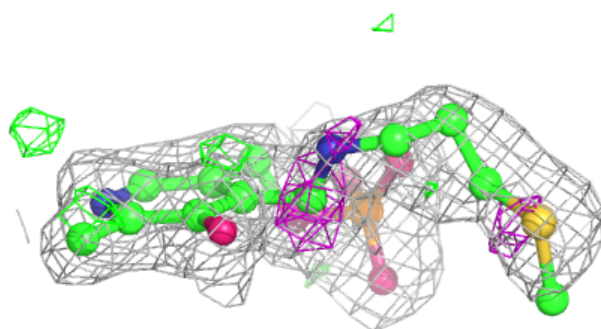
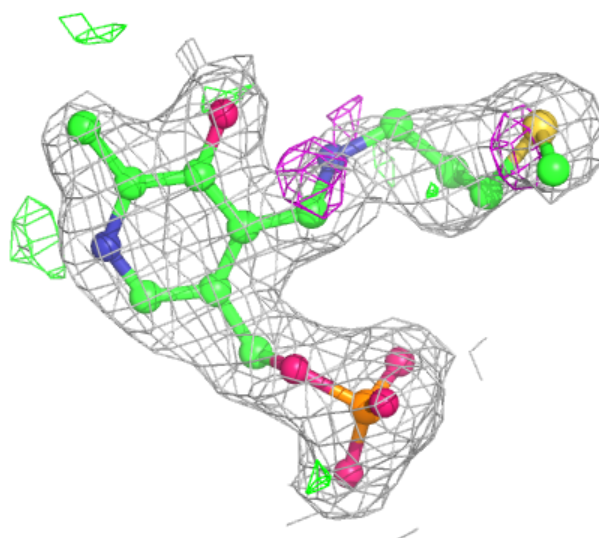
Electron density around G0F A 601:

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 G0F 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.