



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:28 PM UTC

PDB ID : 7CIM / pdb_00007cim
Title : Crystal structure of L-methionine decarboxylase from Streptomyces sp.590 in complexed with 3-methlythiopropylamine (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 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

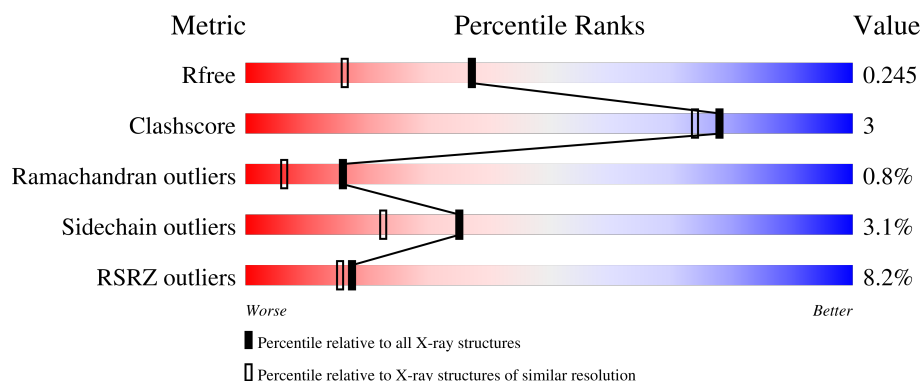
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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	
1	B	557	

2 Entry composition [i](#)

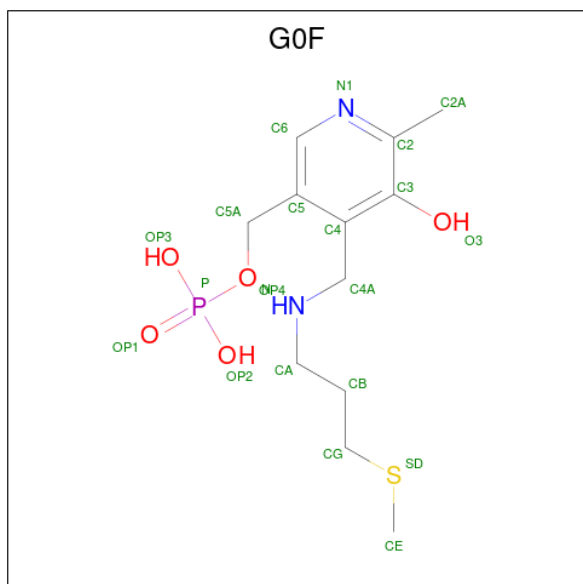
There are 3 unique types of molecules in this entry. The entry contains 8484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: G0F) (formula: C₁₂H₂₁N₂O₅PS) (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		

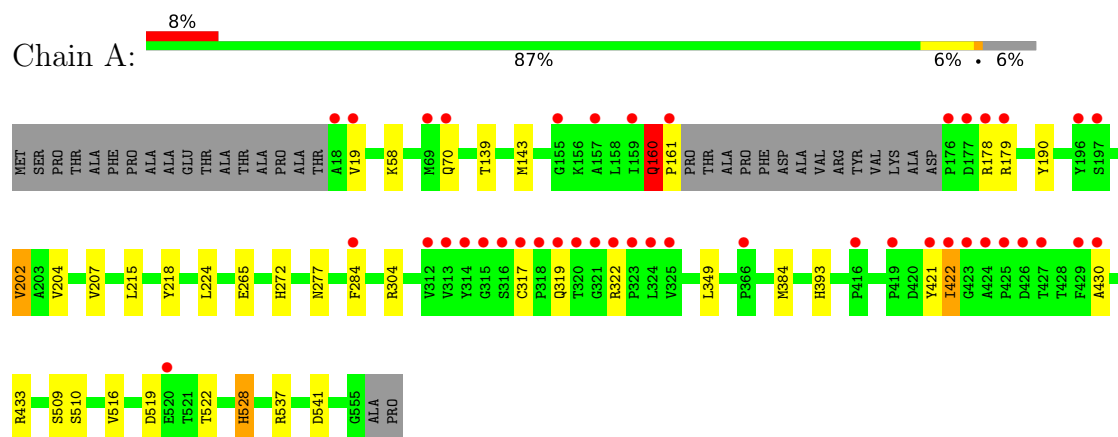
- Molecule 3 is water.

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

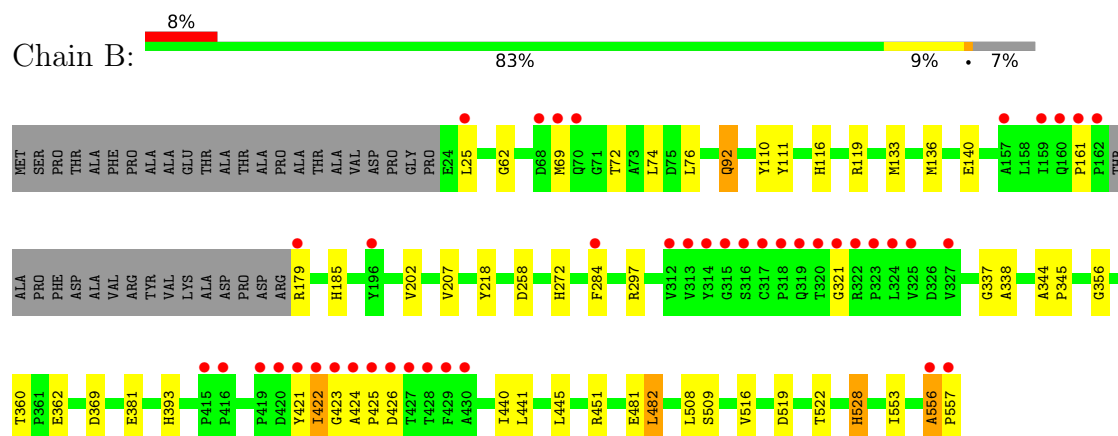
3 Residue-property plots

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) 99.6 (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 (5.00%)	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 , 33.1	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 [i](#)

5.1 Standard geometry [i](#)

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	0.73	0/4235	0.86	1/5772 (0.0%)
1	B	0.77	0/4175	0.88	2/5691 (0.0%)
All	All	0.75	0/8410	0.87	3/11463 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	426	ASP	N-CA-C	6.88	119.79	111.40
1	B	422	ILE	N-CA-C	6.42	117.36	108.89
1	A	384	MET	N-CA-C	5.06	117.91	111.69

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	20	0
1	B	4056	0	3911	27	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	45	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 (45) 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:337:GLY:O	1:B:338:ALA:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:MET:HE3	1:B:441:LEU:HD12	1.93	0.49
1:A:421:TYR:O	1:A:422:ILE:HG22	2.12	0.49
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:A:143:MET:HE1	1:A:204:VAL:HG11	1.97	0.46
1:B:393:HIS:CD2	1:B:393:HIS:H	2.32	0.46
1:B:62:GLY:HA3	1:B:508:LEU:HA	1.98	0.46
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.81	0.45
1:A:430:ALA:HB2	1:B:136:MET:SD	2.57	0.45
1:A:433[B]:ARG:HE	1:A:433[B]:ARG:HB3	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:B:136:MET:HE3	1:B:140:GLU:HB2	2.02	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%)	16 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	514/557 (92%)	489 (95%)	21 (4%)	4 (1%)	16	6
All	All	1035/1114 (93%)	988 (96%)	39 (4%)	8 (1%)	16	6

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 ⓘ

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%)	416 (97%)	12 (3%)	38	26
1	B	421/450 (94%)	407 (97%)	14 (3%)	33	21
All	All	849/900 (94%)	823 (97%)	26 (3%)	35	23

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	58	LYS
1	A	70	GLN
1	A	160	GLN
1	A	178	ARG
1	A	202	VAL
1	A	215	LEU
1	A	224	LEU

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Mol	Chain	Res	Type
1	A	317	CYS
1	A	322	ARG
1	A	349	LEU
1	A	528	HIS
1	B	25	LEU
1	B	69	MET
1	B	72	THR
1	B	74	LEU
1	B	92	GLN
1	B	119	ARG
1	B	179	ARG
1	B	360	THR
1	B	362	GLU
1	B	381	GLU
1	B	421	TYR
1	B	481	GLU
1	B	482	LEU
1	B	528	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	160	GLN
1	A	182	ASN
1	A	211	HIS
1	A	272	HIS
1	A	279	ASN
1	A	309	GLN
1	A	393	HIS
1	A	511	GLN
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	393	HIS
1	B	418	GLN
1	B	444	HIS
1	B	461	GLN
1	B	511	GLN

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Mol	Chain	Res	Type
1	B	528	HIS

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](#)

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	2.02	3 (14%)	26,28,28	2.39	9 (34%)
2	G0F	B	601	1	21,21,21	2.05	4 (19%)	26,28,28	2.34	10 (38%)

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	-	1/13/13/13	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	-7.63	1.40	1.52
2	B	601	G0F	C4A-C4	-7.29	1.41	1.52
2	B	601	G0F	C2-N1	2.88	1.39	1.33
2	B	601	G0F	P-OP2	-2.84	1.44	1.54
2	A	601	G0F	C2-N1	2.59	1.38	1.33
2	A	601	G0F	P-OP2	-2.35	1.46	1.54
2	B	601	G0F	C3-C2	-2.16	1.38	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	G0F	C4A-C4-C5	5.58	125.83	119.75
2	A	601	G0F	OP2-P-OP4	-5.37	92.68	106.67
2	B	601	G0F	C4A-N-CA	5.00	130.79	113.20
2	B	601	G0F	OP2-P-OP4	-4.55	94.81	106.67
2	A	601	G0F	C4-C4A-N	4.53	119.86	111.50
2	A	601	G0F	C4A-C4-C5	4.42	124.56	119.75
2	A	601	G0F	C4A-N-CA	3.51	125.56	113.20
2	B	601	G0F	C3-C2-N1	-3.40	116.67	120.96
2	A	601	G0F	C3-C2-N1	-3.22	116.90	120.96
2	A	601	G0F	OP4-P-OP1	-3.19	97.81	106.44
2	A	601	G0F	OP3-P-OP2	3.11	119.47	107.80
2	B	601	G0F	OP3-P-OP2	2.96	118.91	107.80
2	A	601	G0F	OP2-P-OP1	2.84	121.89	110.83
2	B	601	G0F	OP4-P-OP1	-2.27	100.29	106.44
2	B	601	G0F	C4-C3-C2	2.23	123.27	119.91
2	B	601	G0F	OP2-P-OP1	2.18	119.32	110.83
2	B	601	G0F	C4A-C4-C3	-2.06	117.24	119.98
2	B	601	G0F	OP4-C5A-C5	-2.03	105.56	109.36
2	A	601	G0F	OP3-P-OP4	-2.00	101.45	106.67

There are no chirality outliers.

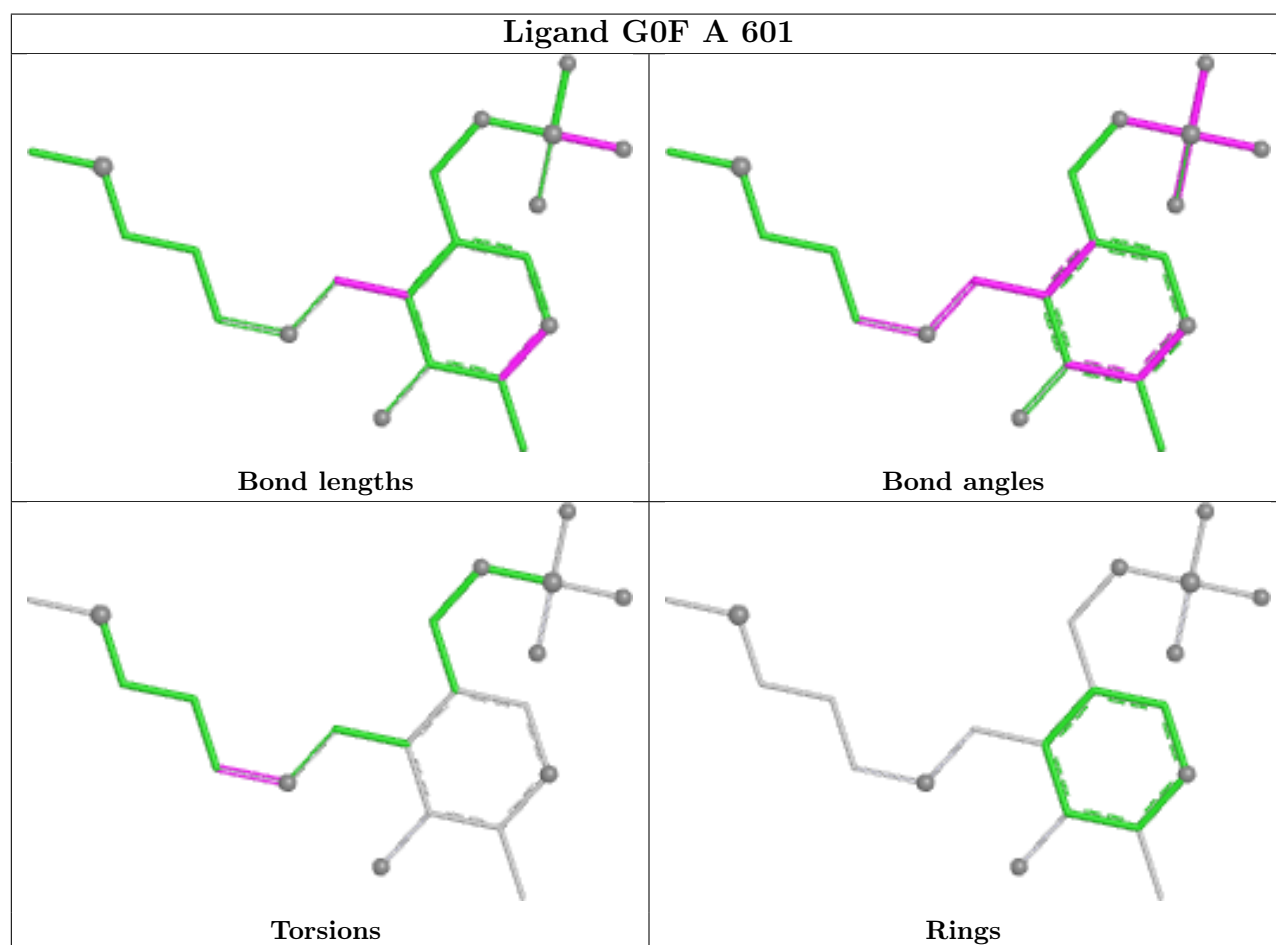
All (2) torsion outliers are listed below:

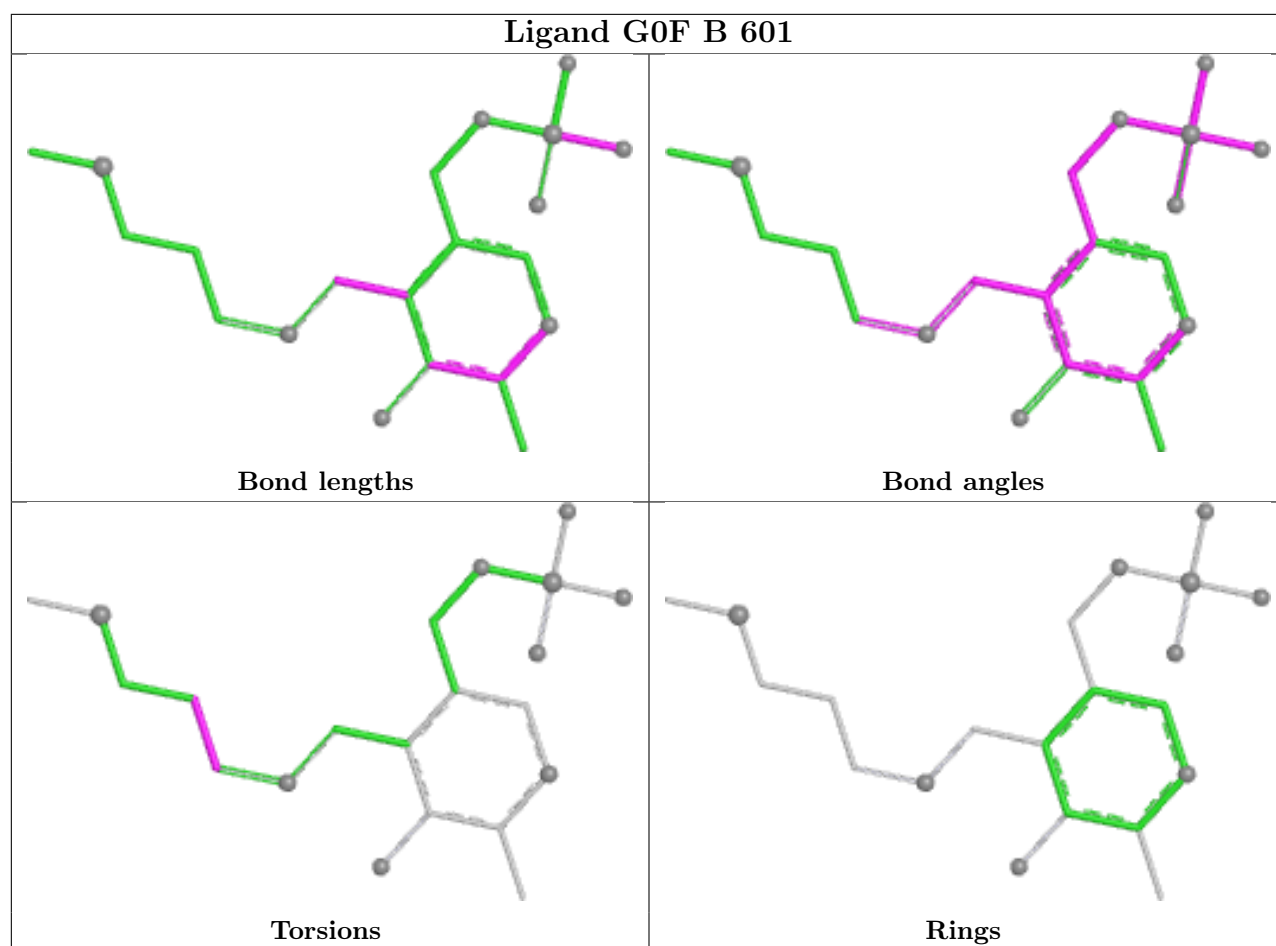
Mol	Chain	Res	Type	Atoms
2	B	601	G0F	N-CA-CB-CG
2	A	601	G0F	CB-CA-N-C4A

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%)	0.44	42 (8%) 18 16	11, 30, 79, 147	1 (0%)
1	B	518/557 (92%)	0.41	43 (8%) 17 15	19, 29, 84, 157	0
All	All	1042/1114 (93%)	0.43	85 (8%) 17 15	11, 30, 81, 157	1 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	GLY	10.9
1	B	422	ILE	9.9
1	A	424	ALA	7.3
1	A	422	ILE	7.1
1	B	421	TYR	7.1
1	B	419	PRO	6.4
1	B	324	LEU	6.1
1	A	425	PRO	6.0
1	B	424	ALA	6.0
1	B	425	PRO	5.7
1	A	320	THR	5.4
1	A	324	LEU	5.1
1	A	176	PRO	4.9
1	A	161	PRO	4.8
1	B	318	PRO	4.8
1	A	315	GLY	4.7
1	B	430	ALA	4.7
1	A	430	ALA	4.4
1	A	419	PRO	4.4
1	A	177	ASP	4.4
1	B	313	VAL	4.3
1	A	421	TYR	4.3
1	A	313	VAL	4.2
1	B	429	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	323	PRO	4.0
1	B	325	VAL	4.0
1	B	556	ALA	3.9
1	B	162	PRO	3.7
1	A	18	ALA	3.6
1	B	557	PRO	3.6
1	B	323	PRO	3.6
1	B	312	VAL	3.5
1	B	157	ALA	3.4
1	B	427	THR	3.3
1	B	315	GLY	3.3
1	A	312	VAL	3.2
1	A	70	GLN	3.2
1	B	314	TYR	3.2
1	B	321	GLY	3.2
1	A	416	PRO	3.2
1	A	325	VAL	3.1
1	A	429	PHE	3.1
1	B	70	GLN	3.0
1	B	161	PRO	3.0
1	B	196	TYR	2.9
1	B	284	PHE	2.9
1	A	314	TYR	2.9
1	A	318	PRO	2.9
1	B	415	PRO	2.8
1	B	322	ARG	2.8
1	A	317	CYS	2.7
1	B	426	ASP	2.7
1	A	179	ARG	2.7
1	A	284	PHE	2.7
1	B	69	MET	2.7
1	B	416	PRO	2.7
1	A	321	GLY	2.6
1	A	423	GLY	2.6
1	B	327	VAL	2.6
1	B	320	THR	2.6
1	B	160	GLN	2.5
1	A	196	TYR	2.5
1	A	426	ASP	2.5
1	B	179	ARG	2.4
1	A	366	PRO	2.4
1	A	316	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	317	CYS	2.4
1	B	420	ASP	2.4
1	B	159	ILE	2.4
1	A	178	ARG	2.3
1	A	19	VAL	2.3
1	B	25	LEU	2.3
1	A	159	ILE	2.2
1	A	322	ARG	2.2
1	A	427	THR	2.2
1	A	197	SER	2.2
1	B	316	SER	2.2
1	A	69	MET	2.1
1	A	520	GLU	2.1
1	A	157	ALA	2.1
1	A	319	GLN	2.1
1	B	428	THR	2.0
1	A	155	GLY	2.0
1	B	319	GLN	2.0
1	B	68	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

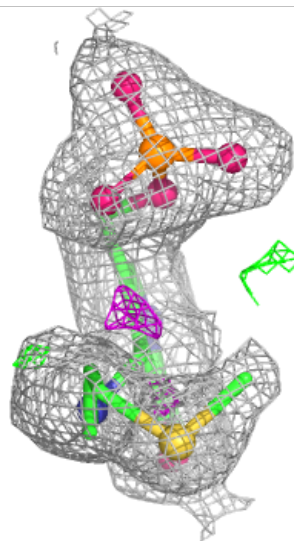
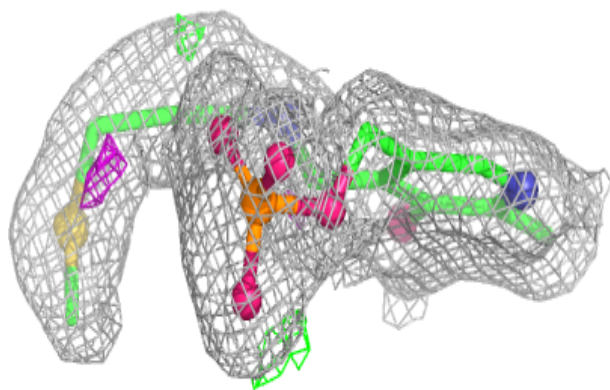
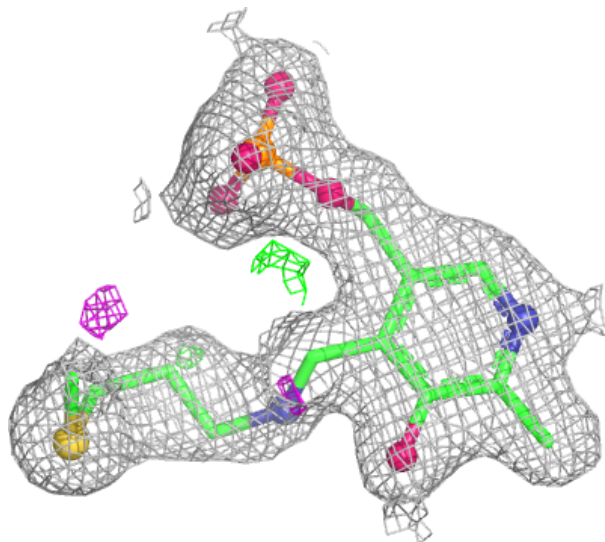
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G0F	A	601	21/21	0.95	0.08	25,28,40,43	0
2	G0F	B	601	21/21	0.95	0.09	24,26,48,50	0

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.

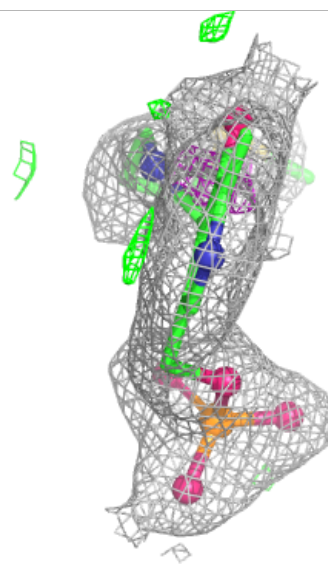
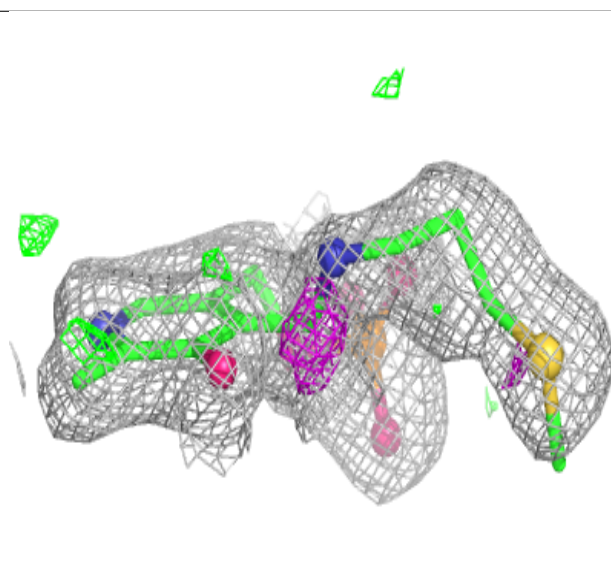
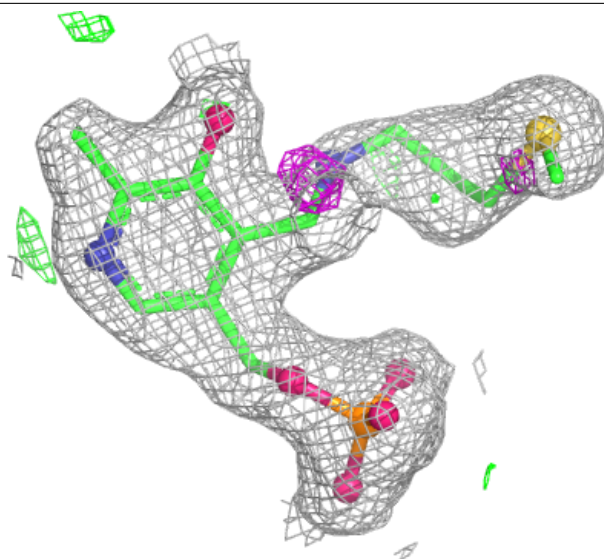
Electron density around G0F A 601:

$2mF_o-DF_c$ (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.