



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2025 – 12:04 AM EDT

PDB ID : 9N50 / pdb_00009n50
Title : Crosslinked Crystal Structure of Human Mitochondrial Ketosynthase, OXSM, and Crosslinker-crypto Human Mitochondrial Acyl Carrier Protein, C8aBr-mACP
Authors : Suo, Y.; Jiang, Z.; Heberlig, G.W.; Wang, E.Y.; Chen, A.; Sankaran, B.; La Clair, J.J.; Burkart, M.D.
Deposited on : 2025-02-03
Resolution : 2.50 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

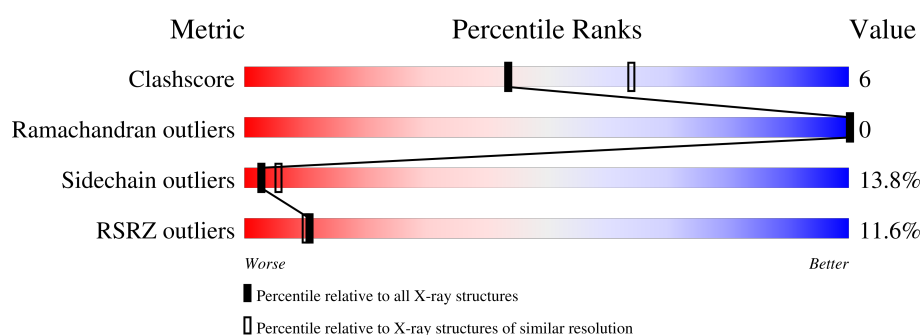
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	425	<div> <div>12%</div> <div>71%</div> <div>23%</div> <div>5%</div> </div>
1	B	425	<div> <div>8%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
2	C	88	<div> <div>24%</div> <div>61%</div> <div>27%</div> <div>• • 7%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6973 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 3-oxoacyl-[acyl-carrier-protein] synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	5	0
			3144	1985	544	596	19			
1	B	421	Total	C	N	O	S	0	1	0
			3132	1976	544	595	17			

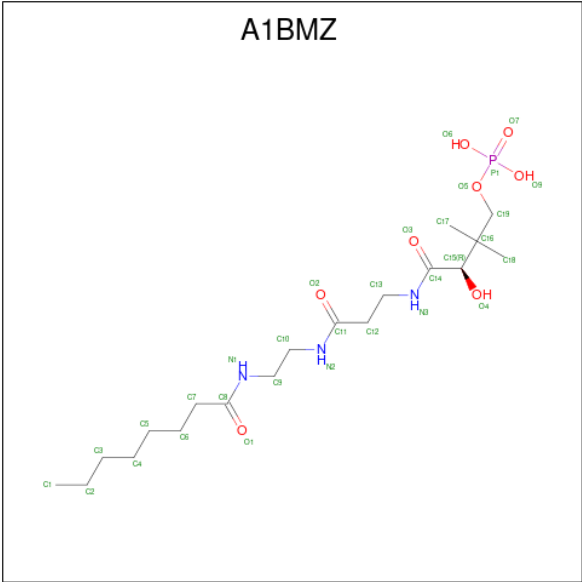
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLY	-	expression tag	UNP Q9NWU1
A	36	HIS	-	expression tag	UNP Q9NWU1
A	37	MET	-	expression tag	UNP Q9NWU1
B	35	GLY	-	expression tag	UNP Q9NWU1
B	36	HIS	-	expression tag	UNP Q9NWU1
B	37	MET	-	expression tag	UNP Q9NWU1

- Molecule 2 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	82	Total	C	N	O	S	0	0	0
			660	424	98	133	5			

- Molecule 3 is N 3 -[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-N-(2-octanami doethyl)-beta-alaninamide (CCD ID: A1BMZ) (formula: C₁₉H₃₈N₃O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			30	19	3	7	1		

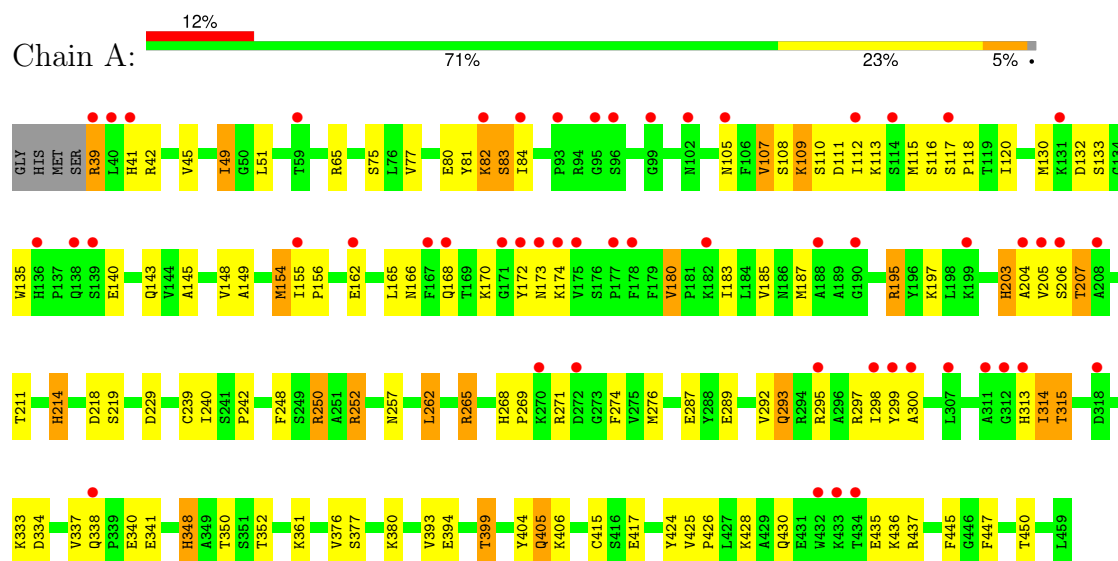
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	1	Total	O	0	0
			1	1		

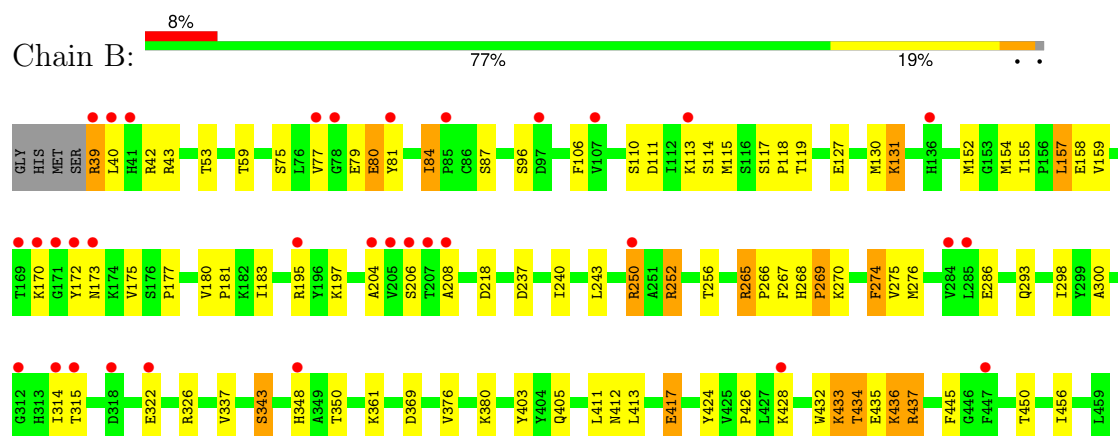
3 Residue-property plots [i](#)

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: 3-oxoacyl-[acyl-carrier-protein] synthase, mitochondrial

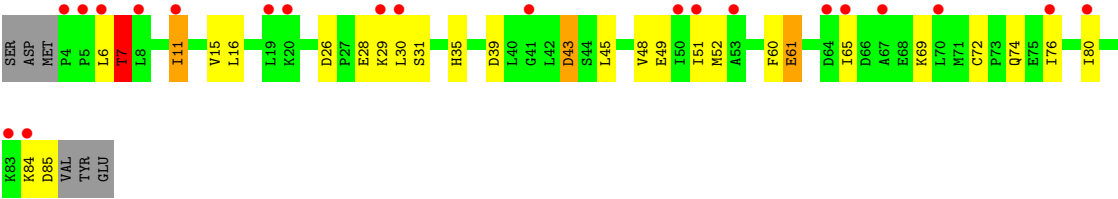


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase, mitochondrial



- Molecule 2: Acyl carrier protein, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.95Å 119.44Å 78.87Å 90.00° 103.29° 90.00°	Depositor
Resolution (Å)	62.98 – 2.50 62.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.98-2.50) 90.7 (62.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC v5.5	Depositor
R, R_{free}	0.220 , (Not available) 0.254 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6973	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: A1BMZ

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	1.00	5/3217 (0.2%)	1.43	21/4365 (0.5%)
1	B	1.19	6/3202 (0.2%)	1.50	23/4343 (0.5%)
2	C	0.68	0/671	1.34	4/905 (0.4%)
All	All	1.07	11/7090 (0.2%)	1.46	48/9613 (0.5%)

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	10
1	B	0	4
All	All	0	14

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	SER	CA-CB	-7.00	1.42	1.53
1	A	203	HIS	CE1-NE2	-5.68	1.26	1.32
1	A	214	HIS	CG-CD2	-5.63	1.29	1.35
1	B	298	ILE	C-O	-5.45	1.17	1.24
1	B	43	ARG	CZ-NH2	-5.39	1.26	1.33
1	A	204	ALA	CA-CB	-5.33	1.45	1.53
1	B	403	TYR	C-O	-5.26	1.18	1.24
1	B	300	ALA	C-O	-5.12	1.18	1.23
1	B	275	VAL	C-O	-5.07	1.18	1.24
1	B	293	GLN	C-O	-5.03	1.18	1.24
1	A	334	ASP	C-O	-5.01	1.18	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	THR	CA-CB-OG1	-8.58	96.73	109.60
1	B	405	GLN	CG-CD-NE2	-8.48	103.68	116.40
1	B	437	ARG	NE-CZ-NH2	-7.33	112.60	119.20
1	A	257	ASN	CB-CA-C	7.09	121.40	109.84
1	B	39	ARG	CB-CA-C	7.06	123.51	110.10
2	C	60	PHE	CA-CB-CG	6.86	120.66	113.80
1	A	293	GLN	N-CA-CB	6.61	119.83	110.12
1	B	274	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	405	GLN	CB-CA-C	6.47	121.27	111.76
1	A	415	CYS	N-CA-CB	-6.37	99.46	111.00
1	B	106	PHE	CA-CB-CG	-6.37	107.43	113.80
1	A	399	THR	CA-CB-OG1	-6.18	100.33	109.60
1	A	274	PHE	CA-CB-CG	6.06	119.86	113.80
1	B	437	ARG	NH1-CZ-NH2	6.02	127.13	119.30
1	B	252	ARG	CD-NE-CZ	5.96	132.74	124.40
1	A	404	TYR	CA-C-N	-5.91	113.67	123.37
1	A	404	TYR	C-N-CA	-5.91	113.67	123.37
1	A	295	ARG	CD-NE-CZ	5.91	132.68	124.40
1	A	265	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	B	434	THR	OG1-CB-CG2	-5.84	97.61	109.30
1	A	218	ASP	CA-CB-CG	5.75	118.34	112.60
1	A	81	TYR	N-CA-CB	-5.72	101.07	110.40
2	C	26	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	265	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	B	59	THR	CA-CB-OG1	-5.68	101.08	109.60
1	B	269	PRO	N-CA-CB	-5.67	97.26	103.39
1	A	180	VAL	N-CA-CB	5.65	114.86	110.45
1	A	404	TYR	N-CA-C	-5.60	102.62	110.35
1	B	208	ALA	CB-CA-C	-5.55	109.68	117.23
1	B	131	LYS	CB-CA-C	5.53	119.97	110.79
1	B	426	PRO	N-CA-C	5.47	119.07	110.80
1	B	286	GLU	N-CA-CB	-5.45	101.38	111.52
1	A	348	HIS	N-CA-C	-5.44	106.84	112.93
1	B	433	LYS	CG-CD-CE	5.42	123.76	111.30
2	C	85	ASP	CB-CA-C	5.40	120.36	110.10
1	B	218	ASP	CA-CB-CG	5.30	117.90	112.60
2	C	7	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	132	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	394	GLU	CB-CA-C	5.29	120.82	110.67
1	B	270	LYS	CG-CD-CE	5.27	123.43	111.30
1	A	287	GLU	CB-CG-CD	5.23	121.50	112.60
1	A	115	MET	CG-SD-CE	5.21	112.36	100.90
1	B	326	ARG	CA-C-O	-5.20	115.04	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	TYR	N-CA-CB	-5.09	102.64	110.12
1	B	436	LYS	CA-C-N	5.09	128.07	120.90
1	B	436	LYS	C-N-CA	5.09	128.07	120.90
1	B	53	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	156	PRO	N-CA-CB	5.04	106.60	103.23

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ARG	Sidechain
1	A	250	ARG	Sidechain
1	A	252	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	271	ARG	Sidechain
1	A	297	ARG	Sidechain
1	A	39	ARG	Sidechain
1	A	42	ARG	Sidechain
1	A	437	ARG	Sidechain
1	A	65	ARG	Sidechain
1	B	252	ARG	Sidechain
1	B	265	ARG	Sidechain
1	B	42	ARG	Sidechain
1	B	437	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	3144	0	3109	51	0
1	B	3132	0	3105	33	0
2	C	660	0	655	9	0
3	C	30	0	0	1	0
4	A	6	0	0	2	0
4	B	1	0	0	0	0
All	All	6973	0	6869	83	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 6.

All (83) 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:170:LYS:HB2	1:A:174:LYS:HG3	1.41	0.99
1:B:343:SER:HB2	1:B:432:TRP:HE1	1.42	0.84
1:A:185:VAL:HG11	1:A:206:SER:HB2	1.69	0.75
1:A:170:LYS:CB	1:A:174:LYS:HG3	2.21	0.70
1:B:177:PRO:HB2	2:C:45:LEU:HG	1.77	0.66
1:B:376:VAL:O	1:B:424:TYR:HA	1.96	0.66
1:B:111:ASP:O	1:B:115:MET:HG2	1.97	0.65
1:A:207:THR:HG21	1:A:214:HIS:CE1	2.33	0.63
1:A:80:GLU:HG3	1:A:242:PRO:HG3	1.80	0.62
1:A:107:VAL:HG13	1:A:111:ASP:HB2	1.80	0.62
1:A:376:VAL:O	1:A:424:TYR:HA	1.99	0.62
1:A:117:SER:N	1:A:118:PRO:HD2	2.15	0.61
1:A:39:ARG:NH1	4:A:501:HOH:O	2.32	0.61
1:A:155:ILE:HG12	1:B:155:ILE:HG12	1.82	0.61
1:A:315:THR:HG21	2:C:43:ASP:HB2	1.83	0.60
1:A:149:ALA:HA	1:A:203:HIS:O	2.01	0.60
1:B:250:ARG:HG3	1:B:250:ARG:HH11	1.66	0.59
1:A:425:VAL:HG13	1:A:430:GLN:HG3	1.85	0.58
1:A:172:TYR:CE1	1:B:250:ARG:HD3	2.40	0.57
1:B:111:ASP:HB3	1:B:115:MET:HE2	1.85	0.56
1:A:248:PHE:CD2	1:A:276[A]:MET:HE1	2.40	0.56
1:B:127:GLU:HB2	1:B:195[A]:ARG:HH21	1.71	0.55
1:A:140:GLU:HA	1:A:143:GLN:HE21	1.72	0.55
1:B:350:THR:HG22	1:B:380:LYS:HD2	1.89	0.55
1:A:166:ASN:HD21	1:A:174:LYS:HB3	1.72	0.54
1:A:45:VAL:HB	1:A:298:ILE:CG2	2.37	0.54
1:B:269:PRO:HG3	1:B:417:GLU:HG2	1.92	0.52
1:B:343:SER:CB	1:B:432:TRP:HE1	2.18	0.52
1:A:80:GLU:HG3	1:A:242:PRO:CG	2.40	0.51
1:A:289:GLU:O	1:A:293:GLN:HG2	2.11	0.51
1:B:266:PRO:O	1:B:267:PHE:HB2	2.11	0.50
2:C:76:ILE:O	2:C:80:ILE:HG12	2.12	0.50
1:A:173:ASN:O	1:B:250:ARG:NH2	2.44	0.50
1:A:130:MET:HE2	1:A:135:TRP:O	2.13	0.49
1:A:250:ARG:NH1	2:C:52:MET:SD	2.85	0.49
2:C:7:THR:O	2:C:11:ILE:HG23	2.13	0.49
1:A:250:ARG:HG2	1:B:172:TYR:CE2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:TYR:O	1:B:84:ILE:HB	2.13	0.48
1:A:268:HIS:CG	1:A:269:PRO:HD2	2.49	0.48
1:A:425:VAL:N	1:A:426:PRO:HD3	2.29	0.48
1:A:107:VAL:HG12	1:A:112:ILE:HG13	1.96	0.47
1:A:154:MET:HB2	1:A:154:MET:HE3	1.68	0.47
1:A:248:PHE:CD2	1:A:276[B]:MET:HE1	2.49	0.47
1:A:337[B]:VAL:HG13	1:A:341:GLU:HB2	1.96	0.47
1:A:116:SER:O	1:A:120:ILE:HG13	2.15	0.46
1:A:361:LYS:NZ	4:A:502:HOH:O	2.48	0.46
1:A:350:THR:HG22	1:A:380:LYS:HD2	1.97	0.46
1:A:45:VAL:HB	1:A:298:ILE:HG21	1.98	0.46
1:A:205:VAL:O	1:A:211:THR:HG23	2.16	0.46
1:A:348:HIS:CD2	1:A:445:PHE:H	2.34	0.46
1:B:173:ASN:OD1	2:C:61:GLU:HG3	2.16	0.46
2:C:48:VAL:O	2:C:51:ILE:HG13	2.15	0.46
1:A:145:ALA:HB1	1:A:229:ASP:HB2	1.98	0.45
1:B:348:HIS:CD2	1:B:445:PHE:H	2.34	0.45
1:A:276[B]:MET:HB2	1:A:276[B]:MET:HE3	1.44	0.45
1:A:300:ALA:HB3	1:A:399:THR:HG23	1.98	0.45
1:A:51:LEU:HD22	1:A:393:VAL:HG23	1.98	0.44
1:A:447:PHE:N	3:C:101:A1BMZ:O1	2.50	0.44
1:A:109:LYS:HA	1:A:109:LYS:HD2	1.75	0.44
1:B:411:LEU:O	1:B:412:ASN:HB2	2.18	0.44
1:A:49:ILE:HG13	1:A:299:TYR:CE1	2.53	0.43
1:B:250:ARG:HG3	1:B:250:ARG:NH1	2.30	0.43
1:A:314:ILE:H	1:A:314:ILE:HG13	1.50	0.43
2:C:49:GLU:HA	2:C:52:MET:HE2	2.01	0.43
1:A:276[A]:MET:HB2	1:A:276[A]:MET:HE3	1.63	0.43
1:B:157:LEU:HB3	1:B:243:LEU:HD23	2.01	0.43
1:B:180:VAL:O	1:B:183:ILE:HG12	2.18	0.43
1:B:80:GLU:H	1:B:80:GLU:HG3	1.27	0.42
1:B:180:VAL:HB	1:B:181:PRO:HD3	2.01	0.42
1:B:39:ARG:HE	1:B:39:ARG:HB3	1.63	0.42
1:A:82:LYS:HE2	1:A:83:SER:H	1.85	0.42
1:B:276:MET:HB2	1:B:276:MET:HE3	1.65	0.42
2:C:6:LEU:HD22	2:C:11:ILE:HG22	2.01	0.42
1:B:117:SER:N	1:B:118:PRO:CD	2.83	0.41
1:A:207:THR:HG23	1:B:204:ALA:O	2.20	0.41
1:B:152:MET:O	1:B:206:SER:HB2	2.20	0.41
1:A:269:PRO:HG3	1:A:417:GLU:HG3	2.03	0.41
1:A:117:SER:N	1:A:118:PRO:CD	2.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:HD2	1:B:175:VAL:O	2.21	0.41
1:A:262:LEU:HD13	1:A:262:LEU:HA	1.93	0.41
1:B:268:HIS:CG	1:B:269:PRO:HD2	2.57	0.40
1:B:154:MET:HB2	1:B:154:MET:HE3	1.76	0.40
1:B:413:LEU:HD12	1:B:413:LEU:HA	1.90	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	423/425 (100%)	412 (97%)	11 (3%)	0	100	100
1	B	420/425 (99%)	410 (98%)	10 (2%)	0	100	100
2	C	80/88 (91%)	80 (100%)	0	0	100	100
All	All	923/938 (98%)	902 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	327/327 (100%)	282 (86%)	45 (14%)	3	5
1	B	325/327 (99%)	286 (88%)	39 (12%)	4	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	76/82 (93%)	59 (78%)	17 (22%)	1	1
All	All	728/736 (99%)	627 (86%)	101 (14%)	3	5

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	49	ILE
1	A	75	SER
1	A	77	VAL
1	A	82	LYS
1	A	83	SER
1	A	84	ILE
1	A	105	ASN
1	A	107	VAL
1	A	108	SER
1	A	109	LYS
1	A	110	SER
1	A	113	LYS
1	A	133	SER
1	A	148	VAL
1	A	154	MET
1	A	162	GLU
1	A	165	LEU
1	A	168	GLN
1	A	180	VAL
1	A	183	ILE
1	A	187	MET
1	A	195	ARG
1	A	197	LYS
1	A	207	THR
1	A	239	CYS
1	A	240	ILE
1	A	252	ARG
1	A	262	LEU
1	A	292	VAL
1	A	313	HIS
1	A	314	ILE
1	A	315	THR
1	A	333	LYS
1	A	338[A]	GLN
1	A	338[B]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	GLU
1	A	352	THR
1	A	377	SER
1	A	405	GLN
1	A	406	LYS
1	A	428	LYS
1	A	435	GLU
1	A	436	LYS
1	A	450	THR
1	B	40	LEU
1	B	75	SER
1	B	77	VAL
1	B	79	GLU
1	B	80	GLU
1	B	84	ILE
1	B	87	SER
1	B	96	SER
1	B	110	SER
1	B	113	LYS
1	B	114	SER
1	B	130	MET
1	B	131	LYS
1	B	157	LEU
1	B	158	GLU
1	B	159	VAL
1	B	170	LYS
1	B	197	LYS
1	B	237	ASP
1	B	240	ILE
1	B	250	ARG
1	B	256	THR
1	B	265	ARG
1	B	274	PHE
1	B	314	ILE
1	B	315	THR
1	B	322	GLU
1	B	337	VAL
1	B	343	SER
1	B	361	LYS
1	B	369	ASP
1	B	417	GLU
1	B	428	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	433	LYS
1	B	434	THR
1	B	435	GLU
1	B	436	LYS
1	B	450	THR
1	B	456	ILE
2	C	7	THR
2	C	11	ILE
2	C	15	VAL
2	C	16	LEU
2	C	28	GLU
2	C	29	LYS
2	C	30	LEU
2	C	31	SER
2	C	35	HIS
2	C	39	ASP
2	C	43	ASP
2	C	61	GLU
2	C	65	ILE
2	C	69	LYS
2	C	72	CYS
2	C	74	GLN
2	C	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	102	ASN
1	A	105	ASN
1	A	136	HIS
1	A	214	HIS
1	A	405	GLN
1	B	136	HIS
1	B	143	GLN
1	B	214	HIS
1	B	346	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	A1BMZ	C	101	1,2	24,29,30	1.00	2 (8%)	29,36,39	1.23	4 (13%)

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	A1BMZ	C	101	1,2	-	22/34/36/37	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	101	A1BMZ	C19-C16	3.12	1.57	1.52
3	C	101	A1BMZ	O3-C14	2.03	1.27	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	101	A1BMZ	C12-C11-N2	-3.09	110.72	116.34
3	C	101	A1BMZ	C9-C10-N2	-3.07	101.97	111.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	101	A1BMZ	C13-C12-C11	2.36	116.32	112.39
3	C	101	A1BMZ	O2-C11-N2	2.31	127.56	123.03

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	101	A1BMZ	C12-C11-N2-C10
3	C	101	A1BMZ	C14-C15-C16-C17
3	C	101	A1BMZ	C14-C15-C16-C18
3	C	101	A1BMZ	C14-C15-C16-C19
3	C	101	A1BMZ	O4-C15-C16-C17
3	C	101	A1BMZ	O4-C15-C16-C18
3	C	101	A1BMZ	O4-C15-C16-C19
3	C	101	A1BMZ	C15-C16-C19-O5
3	C	101	A1BMZ	C17-C16-C19-O5
3	C	101	A1BMZ	C18-C16-C19-O5
3	C	101	A1BMZ	O2-C11-N2-C10
3	C	101	A1BMZ	N2-C10-C9-N1
3	C	101	A1BMZ	C1-C2-C3-C4
3	C	101	A1BMZ	C4-C5-C6-C7
3	C	101	A1BMZ	C6-C7-C8-N1
3	C	101	A1BMZ	C12-C13-N3-C14
3	C	101	A1BMZ	C15-C14-N3-C13
3	C	101	A1BMZ	C6-C7-C8-O1
3	C	101	A1BMZ	C2-C3-C4-C5
3	C	101	A1BMZ	C11-C12-C13-N3
3	C	101	A1BMZ	O3-C14-N3-C13
3	C	101	A1BMZ	O2-C11-C12-C13

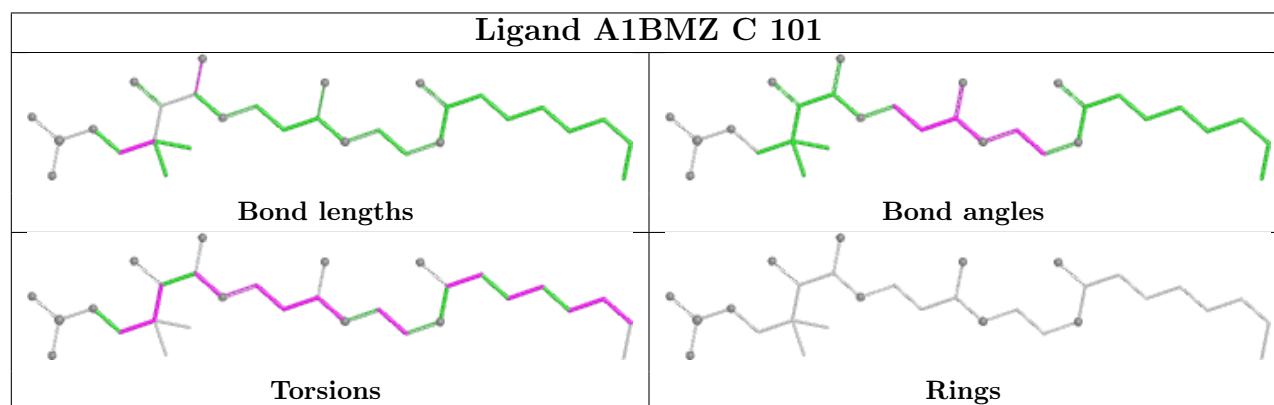
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	101	A1BMZ	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 [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	421/425 (99%)	0.89	53 (12%) 9 9	19, 40, 70, 113	4 (0%)
1	B	421/425 (99%)	0.65	33 (7%) 20 19	19, 35, 65, 102	1 (0%)
2	C	82/88 (93%)	1.37	21 (25%) 2 2	31, 54, 74, 86	0
All	All	924/938 (98%)	0.82	107 (11%) 11 10	19, 39, 70, 113	5 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	LEU	7.2
1	A	41	HIS	4.7
2	C	6	LEU	4.7
1	B	447	PHE	4.5
1	B	40	LEU	4.3
1	A	174	LYS	4.2
1	A	312	GLY	4.2
1	B	136	HIS	3.8
2	C	65	ILE	3.8
2	C	53	ALA	3.7
1	A	131	LYS	3.6
1	A	167	PHE	3.6
1	B	195[A]	ARG	3.6
1	A	162	GLU	3.5
1	B	206	SER	3.4
1	B	208	ALA	3.4
1	A	84	ILE	3.4
2	C	80	ILE	3.4
2	C	4	PRO	3.3
1	A	177	PRO	3.2
1	A	138	GLN	3.2
1	A	93	PRO	3.1
1	A	39	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	76	ILE	3.0
1	B	107	VAL	3.0
2	C	84	LYS	3.0
2	C	20	LYS	3.0
1	B	250	ARG	2.9
2	C	83	LYS	2.9
1	A	96	SER	2.9
2	C	64	ASP	2.9
1	A	59	THR	2.9
1	B	314	ILE	2.9
1	B	78	GLY	2.8
1	A	313	HIS	2.8
1	A	99	GLY	2.8
1	B	41	HIS	2.8
1	A	208	ALA	2.8
1	B	169	THR	2.8
1	A	136	HIS	2.8
1	A	272	ASP	2.8
1	B	81	TYR	2.8
2	C	11	ILE	2.7
1	B	315	THR	2.7
1	B	171	GLY	2.7
1	A	182	LYS	2.7
2	C	30	LEU	2.6
1	B	113	LYS	2.6
1	A	173	ASN	2.6
1	B	428	LYS	2.6
2	C	51	ILE	2.6
1	B	207	THR	2.6
1	A	270	LYS	2.5
1	A	300	ALA	2.5
2	C	41	GLY	2.5
2	C	29	LYS	2.5
1	B	348	HIS	2.5
1	A	175	VAL	2.5
1	A	188	ALA	2.5
1	A	298	ILE	2.5
1	A	95	GLY	2.5
1	A	199	LYS	2.5
1	A	178	PHE	2.5
2	C	19	LEU	2.4
1	A	205	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	2.4
1	A	112	ILE	2.4
1	A	190	GLY	2.4
1	B	77	VAL	2.4
1	B	284	VAL	2.4
1	B	85	PRO	2.4
1	A	338[A]	GLN	2.4
1	A	171	GLY	2.4
1	B	172	TYR	2.3
1	B	170	LYS	2.3
1	A	295	ARG	2.3
1	B	318	ASP	2.3
1	A	206	SER	2.3
1	B	285	LEU	2.3
1	B	322	GLU	2.3
1	A	172	TYR	2.3
1	B	205	VAL	2.3
1	A	433	LYS	2.2
1	A	102	ASN	2.2
2	C	50	ILE	2.2
2	C	67	ALA	2.2
2	C	70	LEU	2.2
1	B	97	ASP	2.2
1	B	204	ALA	2.2
1	A	307	LEU	2.2
1	B	312	GLY	2.2
1	A	434	THR	2.2
2	C	5	PRO	2.2
1	A	105	ASN	2.2
2	C	8	LEU	2.2
1	A	114	SER	2.2
1	A	168	GLN	2.2
1	A	311	ALA	2.1
1	B	39	ARG	2.1
1	A	139	SER	2.1
1	A	155	ILE	2.1
1	B	173	ASN	2.1
1	A	82	LYS	2.0
1	A	117	SER	2.0
1	A	318	ASP	2.0
1	A	432	TRP	2.0
1	A	299	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

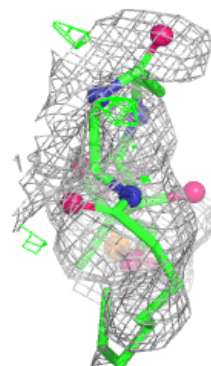
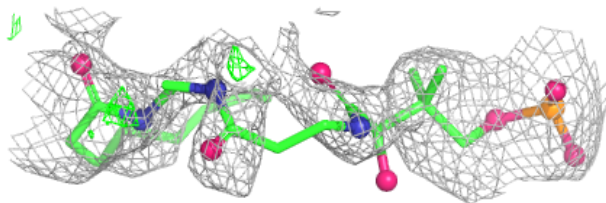
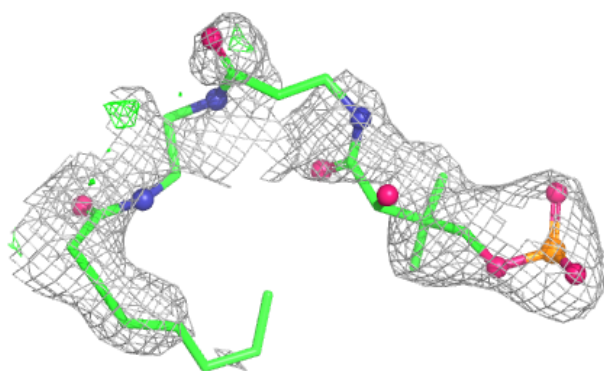
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1BMZ	C	101	30/31	0.80	0.26	84,110,124,129	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 A1BMZ C 101:

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.