



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2025 – 12:06 AM EDT

PDB ID : 9N51 / pdb_00009n51
Title : Crosslinked Crystal Structure of Human Mitochondrial Ketosynthase, OXSM, and Crosslinker-crypto Human Mitochondrial Acyl Carrier Protein, C8Cl-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 : 2.31 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

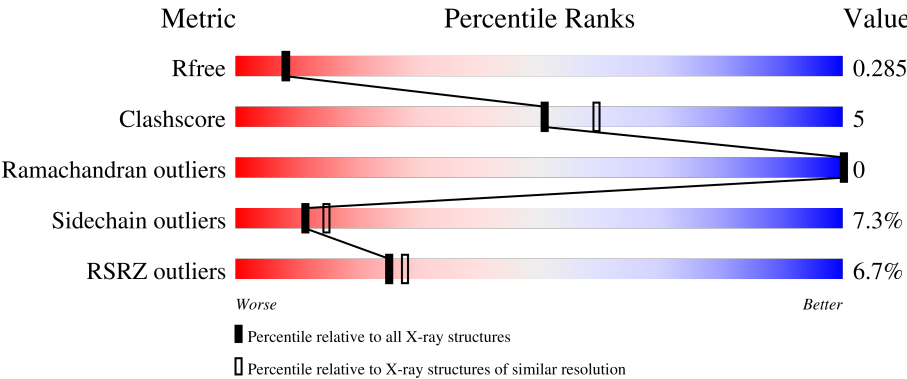
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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>5%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
1	B	425	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	D	425	<div> <div>6%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	E	425	<div> <div>6%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
2	C	88	<div> <div>14%</div> <div>81%</div> <div>13%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	88	<div><div></div><div>18%</div><div>81%</div><div>10%</div><div>• 7%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14066 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			
1	D	421	Total	C	N	O	S	0	5	0
			3144	1985	544	596	19			
1	E	421	Total	C	N	O	S	0	1	0
			3132	1976	544	595	17			

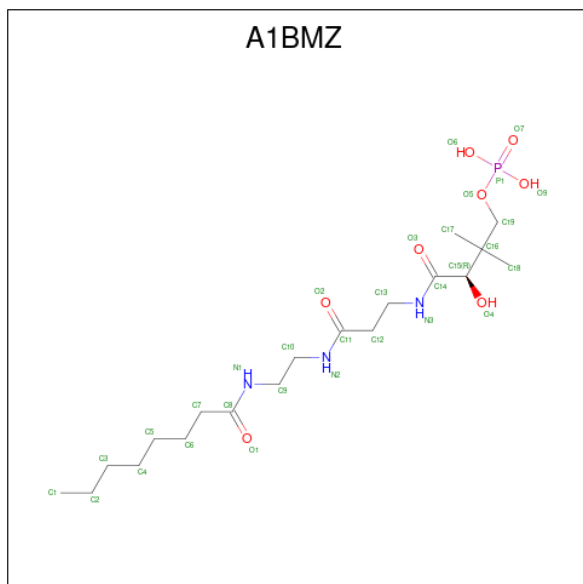
There are 12 discrepancies between the modelled and reference sequences:

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
D	35	GLY	-	expression tag	UNP Q9NWU1
D	36	HIS	-	expression tag	UNP Q9NWU1
D	37	MET	-	expression tag	UNP Q9NWU1
E	35	GLY	-	expression tag	UNP Q9NWU1
E	36	HIS	-	expression tag	UNP Q9NWU1
E	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			
2	F	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-(phosphonooxy)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		
3	F	1	Total	C	N	O	P	0	0
			30	19	3	7	1		

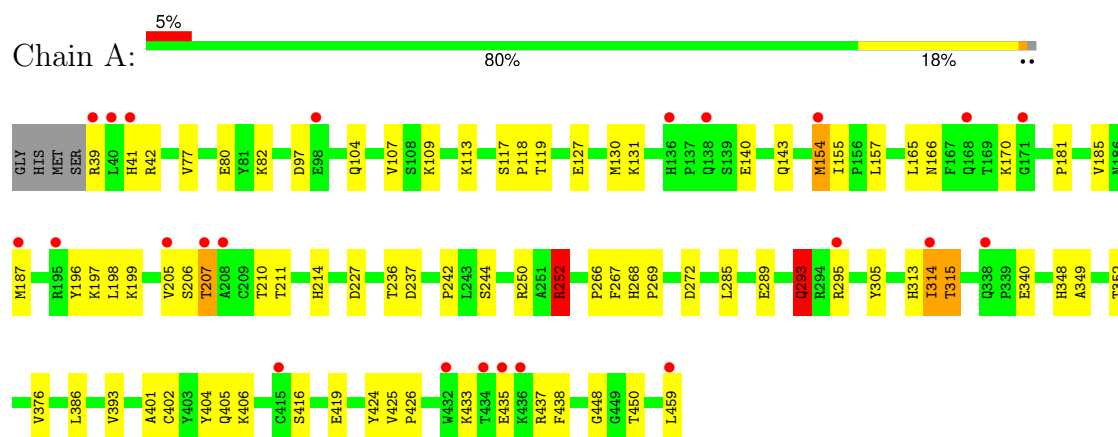
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	38	Total	O	0	0
			38	38		
4	C	2	Total	O	0	0
			2	2		
4	D	21	Total	O	0	0
			21	21		
4	E	46	Total	O	0	0
			46	46		
4	F	4	Total	O	0	0
			4	4		

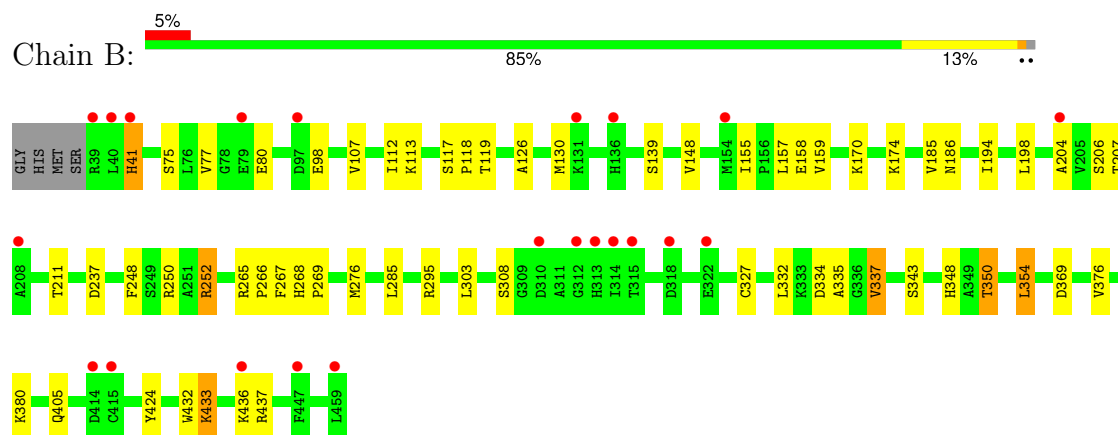
3 Residue-property plots

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.

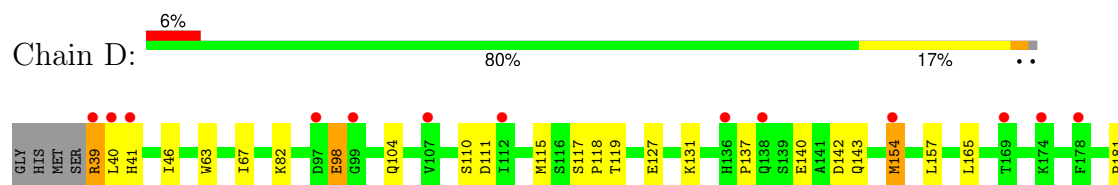
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase, mitochondrial

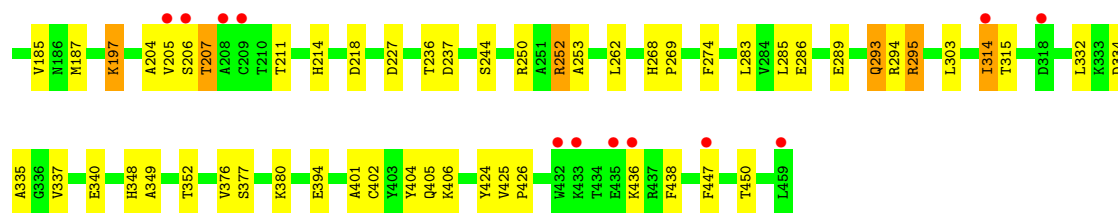


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase, mitochondrial

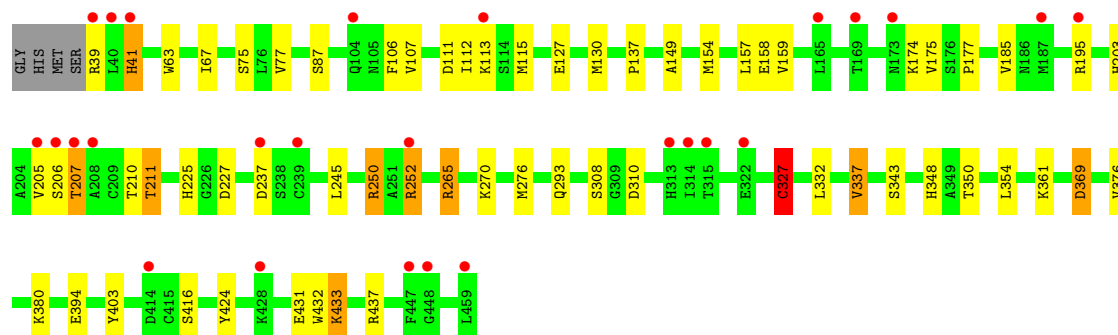
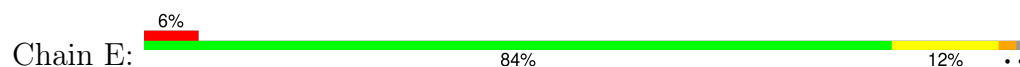


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase, mitochondrial

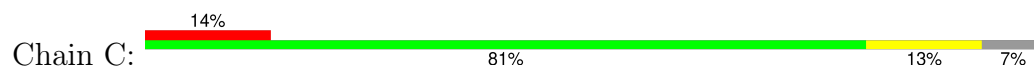




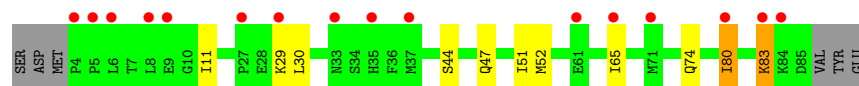
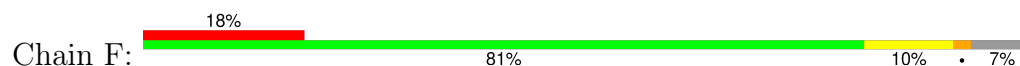
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase, mitochondrial



- Molecule 2: Acyl carrier protein, mitochondrial



- Molecule 2: Acyl carrier protein, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.00Å 118.63Å 132.51Å 90.00° 103.57° 90.00°	Depositor
Resolution (Å)	53.64 – 2.31 53.64 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.64-2.31) 99.9 (53.64-2.31)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.245 , 0.273 0.259 , 0.285	Depositor DCC
R_{free} test set	5385 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14066	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4865e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.60	0/3217	1.05	6/4365 (0.1%)
1	B	0.61	0/3202	1.06	5/4343 (0.1%)
1	D	0.61	0/3217	1.05	11/4365 (0.3%)
1	E	0.64	0/3202	1.05	6/4343 (0.1%)
2	C	0.52	0/671	1.16	0/905
2	F	0.50	0/671	1.15	1/905 (0.1%)
All	All	0.61	0/14180	1.06	29/19226 (0.2%)

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	3
1	B	0	2
1	E	0	3
All	All	0	8

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	HIS	CB-CA-C	7.77	121.58	110.24
1	A	405	GLN	CB-CA-C	7.15	122.66	111.72
1	D	405	GLN	CB-CA-C	7.02	122.47	111.72
1	E	227	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	227	ASP	CA-CB-CG	6.31	118.91	112.60
1	D	227	ASP	CA-CB-CG	6.24	118.84	112.60
2	F	83	LYS	N-CA-C	-6.11	103.53	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	295	ARG	CG-CD-NE	6.04	125.28	112.00
1	D	218	ASP	CA-CB-CG	6.03	118.63	112.60
1	D	236	THR	CA-CB-OG1	-6.02	100.57	109.60
1	D	98	GLU	CB-CG-CD	6.00	122.79	112.60
1	E	327	CYS	CB-CA-C	5.84	120.78	110.85
1	D	41	HIS	CA-CB-CG	5.83	119.63	113.80
1	E	369	ASP	CA-CB-CG	5.75	118.35	112.60
1	D	119	THR	CA-CB-OG1	-5.68	101.08	109.60
1	B	211	THR	CA-CB-OG1	-5.63	101.16	109.60
1	E	211	THR	CA-CB-OG1	-5.58	101.23	109.60
1	E	310	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	42	ARG	N-CA-CB	-5.46	102.85	110.38
1	B	119	THR	CA-CB-OG1	-5.32	101.62	109.60
1	D	293	GLN	CB-CA-C	-5.32	100.79	110.63
1	D	334	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	119	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	293	GLN	N-CA-CB	5.20	118.23	110.22
1	D	98	GLU	N-CA-CB	5.11	117.48	109.97
1	E	130	MET	CG-SD-CE	-5.10	89.67	100.90
1	A	236	THR	CA-CB-OG1	-5.09	101.97	109.60
1	B	350	THR	CA-CB-OG1	-5.07	102.00	109.60
1	B	334	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	ARG	Sidechain
1	A	252	ARG	Sidechain
1	A	437	ARG	Sidechain
1	B	250	ARG	Sidechain
1	B	437	ARG	Sidechain
1	E	250	ARG	Sidechain
1	E	265	ARG	Sidechain
1	E	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	35	0
1	B	3132	0	3105	32	0
1	D	3144	0	3109	40	0
1	E	3132	0	3105	34	0
2	C	660	0	655	3	0
2	F	660	0	655	6	0
3	C	30	0	0	0	0
3	F	30	0	0	5	0
4	A	23	0	0	2	0
4	B	38	0	0	1	0
4	C	2	0	0	0	0
4	D	21	0	0	1	0
4	E	46	0	0	4	0
4	F	4	0	0	2	0
All	All	14066	0	13738	140	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 5.

All (140) 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:405:GLN:NE2	1:E:293:GLN:HG2	1.73	1.04
1:E:41:HIS:O	4:E:501:HOH:O	1.87	0.92
1:D:289:GLU:O	1:D:293:GLN:HG2	1.85	0.76
1:A:313:HIS:HB2	4:A:522:HOH:O	1.85	0.75
1:D:252:ARG:NH2	2:F:47:GLN:OE1	2.20	0.73
1:B:405:GLN:NE2	1:E:293:GLN:CG	2.53	0.71
1:D:314:ILE:HD12	1:D:315:THR:HG23	1.72	0.70
1:A:185:VAL:HG11	1:A:206:SER:HB2	1.75	0.69
1:E:376:VAL:O	1:E:424:TYR:HA	1.96	0.66
1:B:376:VAL:O	1:B:424:TYR:HA	1.96	0.65
1:E:308:SER:HB3	1:E:327:CYS:HB3	1.79	0.65
1:D:376:VAL:O	1:D:424:TYR:HA	1.98	0.64
1:E:350:THR:HG22	1:E:380:LYS:HD2	1.80	0.64
1:A:376:VAL:O	1:A:424:TYR:HA	1.97	0.64
1:B:350:THR:HG22	1:B:380:LYS:HD2	1.80	0.63
1:B:185:VAL:HG11	1:B:206:SER:HB2	1.80	0.63
1:D:181:PRO:O	1:D:187:MET:HG3	1.99	0.62
1:A:181:PRO:O	1:A:187:MET:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:PRO:HD3	2:F:52:MET:HE1	1.81	0.61
1:A:289:GLU:O	1:A:293:GLN:HG2	1.99	0.61
1:B:248:PHE:CE1	1:B:276:MET:HE1	2.36	0.60
1:E:185:VAL:HG11	1:E:206:SER:HB2	1.84	0.59
1:E:111:ASP:HB3	1:E:115:MET:HE2	1.84	0.58
1:D:185:VAL:HG11	1:D:206:SER:HB2	1.86	0.57
1:A:252:ARG:HH21	1:A:252:ARG:HG2	1.69	0.56
2:F:11:ILE:HD12	2:F:80:ILE:HG23	1.86	0.56
3:F:101:A1BMZ:C9	4:F:201:HOH:O	2.53	0.56
1:A:207:THR:HG21	1:A:214:HIS:CE1	2.41	0.56
1:B:248:PHE:CD1	1:B:276:MET:HE1	2.41	0.56
1:D:111:ASP:HB3	1:D:115:MET:HE3	1.87	0.56
1:E:107:VAL:HG23	1:E:112:ILE:HG13	1.88	0.54
1:D:207:THR:HG21	1:D:214:HIS:CE1	2.42	0.54
1:B:354:LEU:H	1:B:354:LEU:HD12	1.72	0.54
1:E:332:LEU:HD22	1:E:337:VAL:HG12	1.90	0.53
1:D:46:ILE:HD13	1:D:283:LEU:HD23	1.91	0.53
1:B:343:SER:OG	1:B:432:TRP:NE1	2.41	0.53
1:A:402:CYS:HA	1:A:438:PHE:CD1	2.44	0.52
1:B:308:SER:HB3	1:B:327:CYS:HB3	1.90	0.52
1:D:154:MET:HA	1:D:154:MET:HE2	1.91	0.52
1:A:210:THR:HG22	1:A:214:HIS:CE1	2.45	0.52
1:A:140:GLU:HA	1:A:143:GLN:HE21	1.74	0.52
1:A:214:HIS:HD2	1:A:305:TYR:OH	1.93	0.51
1:A:295:ARG:HG2	4:A:521:HOH:O	2.10	0.51
1:E:270:LYS:NZ	4:E:505:HOH:O	2.40	0.51
1:D:143:GLN:OE1	1:D:197:LYS:HB3	2.10	0.51
1:E:63:TRP:CZ2	1:E:67:ILE:HD11	2.46	0.51
1:D:40:LEU:HA	4:D:507:HOH:O	2.11	0.50
1:B:295:ARG:HG2	1:E:403:TYR:CE1	2.45	0.50
1:D:447:PHE:CD2	3:F:101:A1BMZ:C2	2.94	0.50
1:E:149:ALA:HA	1:E:203:HIS:O	2.12	0.49
1:A:314:ILE:HG22	1:A:448:GLY:HA2	1.93	0.49
1:D:137:PRO:HB3	1:D:142:ASP:HB3	1.93	0.49
1:E:354:LEU:H	1:E:354:LEU:HD12	1.77	0.49
1:A:401:ALA:O	1:A:404:TYR:O	2.31	0.49
1:A:127:GLU:HB2	1:A:196:TYR:OH	2.13	0.49
1:D:402:CYS:HA	1:D:438:PHE:CD1	2.47	0.49
1:D:157:LEU:HD12	1:D:244:SER:HB3	1.95	0.49
1:D:401:ALA:O	1:D:404:TYR:O	2.31	0.49
1:B:433:LYS:HA	1:B:433:LYS:HD3	1.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:PRO:HD2	4:E:513:HOH:O	2.12	0.49
1:D:250:ARG:NH1	2:F:52:MET:HE2	2.28	0.48
1:A:386:LEU:HD13	1:A:393:VAL:HG11	1.95	0.48
1:B:252:ARG:NH2	4:B:503:HOH:O	2.38	0.48
1:D:117:SER:N	1:D:118:PRO:HD2	2.28	0.48
1:A:205:VAL:O	1:A:211:THR:HG23	2.13	0.48
1:E:250:ARG:NH2	4:E:506:HOH:O	2.46	0.48
1:E:380:LYS:HE3	1:E:394:GLU:OE2	2.12	0.48
1:A:117:SER:N	1:A:118:PRO:HD2	2.29	0.47
1:E:127:GLU:OE1	1:E:195[A]:ARG:NH2	2.48	0.47
1:D:253:ALA:HB1	1:D:274:PHE:CE1	2.50	0.47
1:A:154:MET:HE3	1:A:154:MET:HB2	1.68	0.47
1:D:286:GLU:OE1	1:D:294:ARG:NH2	2.43	0.47
1:A:80:GLU:HG2	1:A:242:PRO:HG3	1.97	0.46
1:E:252:ARG:O	1:E:252:ARG:CG	2.62	0.46
1:B:252:ARG:CG	1:B:252:ARG:O	2.62	0.46
1:D:250:ARG:HD2	1:E:175:VAL:O	2.14	0.46
1:E:154:MET:HE3	1:E:154:MET:HB2	1.79	0.46
1:B:268:HIS:CG	1:B:269:PRO:HD2	2.50	0.46
1:E:348:HIS:O	1:E:350:THR:HG23	2.15	0.46
1:B:126:ALA:O	1:B:130:MET:HG3	2.16	0.45
1:E:205:VAL:HG23	1:E:211:THR:HG23	1.99	0.45
1:B:252:ARG:O	1:B:252:ARG:HG2	2.17	0.45
1:D:39:ARG:NH1	1:D:40:LEU:HG	2.32	0.45
1:B:405:GLN:HE21	1:E:293:GLN:HG2	1.72	0.45
1:A:315:THR:HG21	2:C:43:ASP:HB2	1.98	0.44
1:D:425:VAL:N	1:D:426:PRO:HD3	2.33	0.44
1:A:425:VAL:N	1:A:426:PRO:HD3	2.32	0.44
1:E:245:LEU:HD23	1:E:276:MET:HE3	1.99	0.44
1:E:343:SER:OG	1:E:432:TRP:NE1	2.49	0.44
1:A:155:ILE:HD11	1:B:155:ILE:HD11	2.00	0.44
1:A:157:LEU:HD12	1:A:244:SER:HB3	2.00	0.44
1:D:315:THR:HG22	1:D:447:PHE:HZ	1.82	0.44
1:B:348:HIS:O	1:B:350:THR:HG23	2.18	0.44
1:D:332:LEU:HD22	1:D:337[A]:VAL:HG23	2.00	0.44
1:B:332:LEU:HD22	1:B:337:VAL:HG12	2.00	0.44
1:D:315:THR:HG22	1:D:447:PHE:CZ	2.53	0.44
1:B:148:VAL:HG22	1:B:198:LEU:HD12	2.00	0.43
1:D:63:TRP:CZ2	1:D:67:ILE:HD11	2.54	0.43
1:E:39:ARG:HH12	1:E:225:HIS:CD2	2.36	0.43
1:A:210:THR:CG2	1:A:214:HIS:CE1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:HA	1:A:109:LYS:HD2	1.90	0.43
1:B:107:VAL:HG23	1:B:112:ILE:HG13	2.00	0.43
1:A:314:ILE:H	1:A:314:ILE:HG13	1.44	0.42
2:C:11:ILE:HD12	2:C:80:ILE:HG22	2.00	0.42
1:D:380:LYS:HZ1	1:D:394:GLU:CD	2.26	0.42
1:B:308:SER:CB	1:B:327:CYS:HB3	2.49	0.42
1:D:303:LEU:HB3	1:D:335:ALA:HB1	2.01	0.42
1:B:117:SER:HB3	1:B:118:PRO:HD3	2.02	0.42
1:D:314:ILE:H	1:D:314:ILE:HG13	1.49	0.42
1:E:106:PHE:O	1:E:195[A]:ARG:NH1	2.34	0.42
1:A:285:LEU:HD12	1:A:285:LEU:N	2.34	0.42
1:A:348:HIS:O	1:A:349:ALA:C	2.63	0.42
2:C:51:ILE:C	2:C:51:ILE:HD12	2.45	0.42
1:E:433:LYS:HA	1:E:433:LYS:HD3	1.45	0.42
1:A:268:HIS:CG	1:A:269:PRO:HD2	2.55	0.41
1:D:286:GLU:CD	1:D:294:ARG:HH21	2.28	0.41
1:E:207:THR:HB	1:E:210:THR:OG1	2.19	0.41
3:F:101:A1BMZ:C9	3:F:101:A1BMZ:C13	2.98	0.41
2:F:51:ILE:C	2:F:51:ILE:HD12	2.45	0.41
1:A:130:MET:HE1	1:A:198:LEU:HD21	2.00	0.41
1:B:266:PRO:O	1:B:267:PHE:HB2	2.20	0.41
1:B:285:LEU:HD12	1:B:285:LEU:N	2.35	0.41
1:D:205:VAL:HG23	1:D:211:THR:HG23	2.02	0.41
1:D:335:ALA:HB3	1:D:337[A]:VAL:HG22	2.02	0.41
2:F:80:ILE:O	2:F:83:LYS:HG2	2.20	0.41
1:D:140:GLU:HA	1:D:143:GLN:HE21	1.86	0.41
1:A:314:ILE:HG23	1:B:194:ILE:CD1	2.50	0.41
1:D:285:LEU:N	1:D:285:LEU:HD12	2.36	0.41
1:D:447:PHE:HB2	3:F:101:A1BMZ:C4	2.50	0.41
1:A:143:GLN:OE1	1:A:197:LYS:HB3	2.20	0.40
1:B:186:ASN:HB3	1:B:204:ALA:CB	2.51	0.40
1:D:268:HIS:CG	1:D:269:PRO:HD2	2.56	0.40
1:E:207:THR:HB	1:E:210:THR:HG1	1.86	0.40
1:A:266:PRO:O	1:A:267:PHE:HB2	2.22	0.40
1:D:348:HIS:O	1:D:349:ALA:C	2.64	0.40
1:B:186:ASN:HB3	1:B:204:ALA:HB3	2.03	0.40
3:F:101:A1BMZ:C11	4:F:201:HOH:O	2.69	0.40
1:A:314:ILE:HG23	1:B:194:ILE:HD11	2.04	0.40
1:B:303:LEU:HB3	1:B:335:ALA:HB1	2.04	0.40
1:D:204:ALA:HB3	1:E:207:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	410 (97%)	13 (3%)	0	100	100
1	B	420/425 (99%)	406 (97%)	14 (3%)	0	100	100
1	D	423/425 (100%)	408 (96%)	15 (4%)	0	100	100
1	E	420/425 (99%)	408 (97%)	12 (3%)	0	100	100
2	C	80/88 (91%)	78 (98%)	2 (2%)	0	100	100
2	F	80/88 (91%)	78 (98%)	2 (2%)	0	100	100
All	All	1846/1876 (98%)	1788 (97%)	58 (3%)	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	327/327 (100%)	297 (91%)	30 (9%)	7	9
1	B	325/327 (99%)	304 (94%)	21 (6%)	14	19
1	D	327/327 (100%)	305 (93%)	22 (7%)	13	18
1	E	325/327 (99%)	305 (94%)	20 (6%)	15	21
2	C	76/82 (93%)	69 (91%)	7 (9%)	7	9
2	F	76/82 (93%)	70 (92%)	6 (8%)	10	13
All	All	1456/1472 (99%)	1350 (93%)	106 (7%)	11	15

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	41	HIS
1	A	77	VAL
1	A	82	LYS
1	A	97	ASP
1	A	104	GLN
1	A	107	VAL
1	A	113	LYS
1	A	131	LYS
1	A	154	MET
1	A	165	LEU
1	A	166	ASN
1	A	170	LYS
1	A	199	LYS
1	A	207	THR
1	A	237	ASP
1	A	252	ARG
1	A	272	ASP
1	A	293	GLN
1	A	314	ILE
1	A	315	THR
1	A	340	GLU
1	A	352	THR
1	A	406	LYS
1	A	416	SER
1	A	419	GLU
1	A	433	LYS
1	A	435	GLU
1	A	450	THR
1	A	459	LEU
1	B	41	HIS
1	B	75	SER
1	B	77	VAL
1	B	80	GLU
1	B	98	GLU
1	B	113	LYS
1	B	139	SER
1	B	157	LEU
1	B	158	GLU
1	B	159	VAL
1	B	170	LYS
1	B	174	LYS

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Mol	Chain	Res	Type
1	B	207	THR
1	B	237	ASP
1	B	252	ARG
1	B	265	ARG
1	B	337	VAL
1	B	354	LEU
1	B	369	ASP
1	B	433	LYS
1	B	436	LYS
2	C	16	LEU
2	C	28	GLU
2	C	29	LYS
2	C	30	LEU
2	C	61	GLU
2	C	65	ILE
2	C	74	GLN
1	D	39	ARG
1	D	82	LYS
1	D	98	GLU
1	D	104	GLN
1	D	110	SER
1	D	127	GLU
1	D	131	LYS
1	D	154	MET
1	D	165	LEU
1	D	197	LYS
1	D	207	THR
1	D	237	ASP
1	D	252	ARG
1	D	262	LEU
1	D	295	ARG
1	D	314	ILE
1	D	340	GLU
1	D	352	THR
1	D	377	SER
1	D	406	LYS
1	D	436	LYS
1	D	450	THR
1	E	41	HIS
1	E	75	SER
1	E	77	VAL
1	E	87	SER

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Mol	Chain	Res	Type
1	E	113	LYS
1	E	157	LEU
1	E	158	GLU
1	E	159	VAL
1	E	174	LYS
1	E	207	THR
1	E	237	ASP
1	E	252	ARG
1	E	265	ARG
1	E	327	CYS
1	E	337	VAL
1	E	361	LYS
1	E	369	ASP
1	E	416	SER
1	E	431	GLU
1	E	433	LYS
2	F	29	LYS
2	F	30	LEU
2	F	44	SER
2	F	65	ILE
2	F	74	GLN
2	F	80	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	214	HIS
1	A	346	ASN
1	A	405	GLN
1	B	41	HIS
1	B	60	HIS
1	B	143	GLN
1	B	173	ASN
1	B	293	GLN
1	B	346	ASN
1	B	405	GLN
1	B	451	ASN
2	C	74	GLN
1	D	451	ASN
1	E	136	HIS
1	E	143	GLN

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Mol	Chain	Res	Type
1	E	214	HIS
1	E	225	HIS
1	E	293	GLN
1	E	451	ASN
2	F	33	ASN
2	F	74	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](#)

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	$\# Z > 2$
3	A1BMZ	F	101	2,1	24,29,30	1.20	2 (8%)	29,36,39	2.69	8 (27%)
3	A1BMZ	C	101	2,1	24,29,30	1.09	1 (4%)	29,36,39	1.66	7 (24%)

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	F	101	2,1	-	19/34/36/37	-
3	A1BMZ	C	101	2,1	-	19/34/36/37	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	101	A1BMZ	C6-C7	-4.86	1.34	1.52
3	C	101	A1BMZ	C6-C7	-4.40	1.36	1.52
3	F	101	A1BMZ	C19-C16	2.22	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	A1BMZ	C6-C7-C8	10.76	143.04	113.19
3	F	101	A1BMZ	C7-C8-N1	-5.20	106.88	116.34
3	F	101	A1BMZ	C13-C12-C11	4.34	119.62	112.39
3	C	101	A1BMZ	C6-C7-C8	3.62	123.24	113.19
3	C	101	A1BMZ	C12-C11-N2	-3.42	110.11	116.34
3	C	101	A1BMZ	C7-C8-N1	-3.37	110.21	116.34
3	F	101	A1BMZ	O1-C8-C7	3.21	127.84	122.02
3	F	101	A1BMZ	C5-C6-C7	3.02	124.21	113.13
3	C	101	A1BMZ	C10-C9-N1	2.75	120.11	111.54
3	C	101	A1BMZ	C5-C6-C7	2.74	123.18	113.13
3	C	101	A1BMZ	C9-C10-N2	-2.61	103.42	111.54
3	F	101	A1BMZ	C9-C10-N2	-2.39	104.11	111.54
3	F	101	A1BMZ	C18-C16-C19	-2.20	104.60	108.22
3	F	101	A1BMZ	C18-C16-C17	-2.03	105.16	109.20
3	C	101	A1BMZ	C12-C13-N3	-2.01	107.71	112.00

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	101	A1BMZ	C7-C8-N1-C9
3	C	101	A1BMZ	C12-C11-N2-C10
3	C	101	A1BMZ	C15-C14-N3-C13
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

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

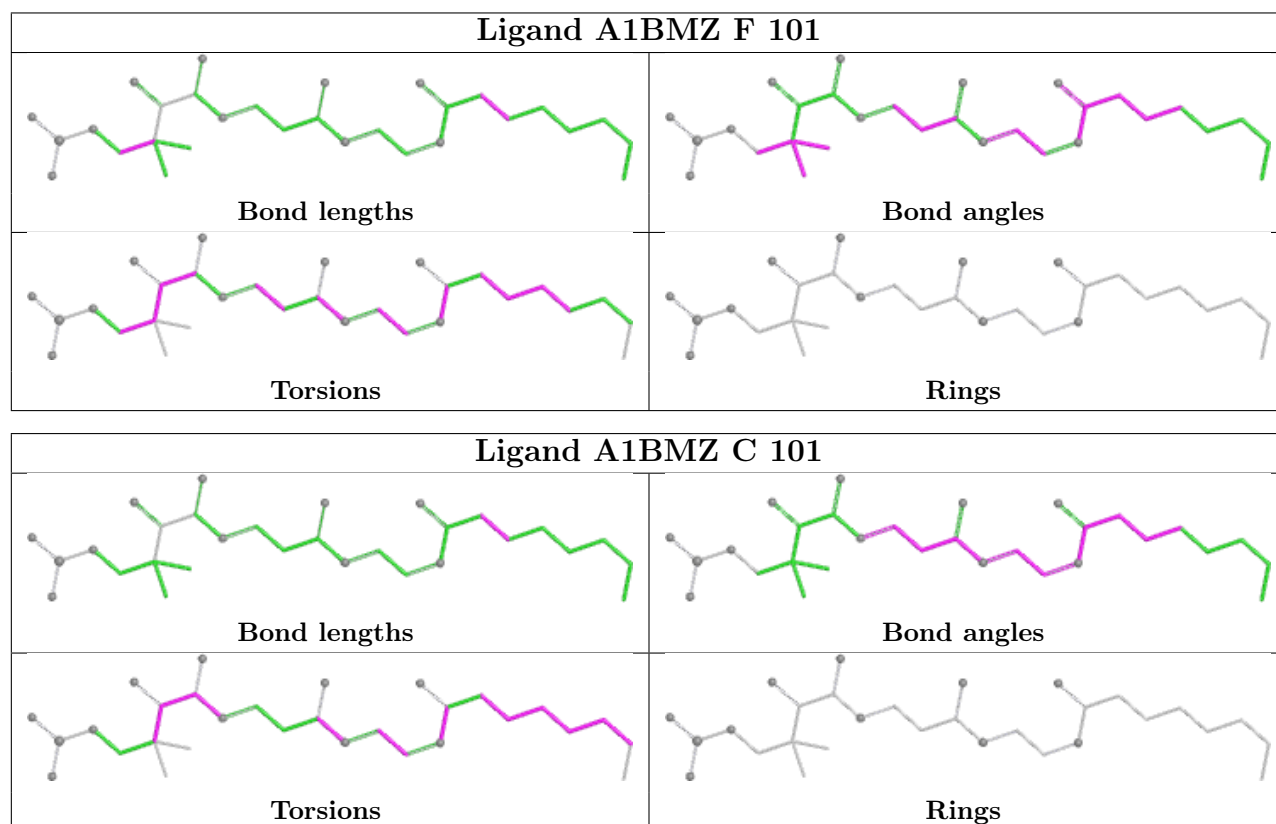
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	101	A1BMZ	5	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%)	0.41	23 (5%)	32	34	11, 21, 46, 113	4 (0%)
1	B	421/425 (99%)	0.33	22 (5%)	34	36	10, 19, 41, 103	1 (0%)
1	D	421/425 (99%)	0.36	25 (5%)	29	32	10, 19, 46, 98	4 (0%)
1	E	421/425 (99%)	0.34	26 (6%)	28	31	10, 19, 44, 107	1 (0%)
2	C	82/88 (93%)	0.83	12 (14%)	7	8	16, 32, 51, 72	0
2	F	82/88 (93%)	1.03	16 (19%)	4	5	15, 31, 57, 64	0
All	All	1848/1876 (98%)	0.41	124 (6%)	25	28	10, 21, 47, 113	10 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	LEU	8.7
1	A	41	HIS	7.0
1	E	40	LEU	6.9
1	D	40	LEU	6.5
2	C	5	PRO	6.4
1	B	40	LEU	6.2
1	B	41	HIS	5.9
1	D	154	MET	5.5
1	A	171	GLY	5.3
1	E	39	ARG	5.3
1	B	447	PHE	5.1
1	E	41	HIS	5.1
1	A	39	ARG	4.9
1	E	322	GLU	4.8
2	F	5	PRO	4.7
1	D	41	HIS	4.5
1	D	432	TRP	4.4
1	B	39	ARG	4.2
1	B	313	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	4	PRO	4.1
1	E	206	SER	3.9
1	A	208	ALA	3.9
2	C	4	PRO	3.6
1	D	39	ARG	3.6
1	B	414	ASP	3.6
2	F	6	LEU	3.6
1	D	447	PHE	3.6
1	E	195[A]	ARG	3.5
1	D	97	ASP	3.5
1	D	136	HIS	3.5
1	D	208	ALA	3.4
1	A	338[A]	GLN	3.3
1	B	310	ASP	3.3
1	A	435	GLU	3.2
1	E	207	THR	3.1
1	D	178	PHE	3.1
1	B	315	THR	3.1
1	E	208	ALA	3.1
1	E	239	CYS	3.0
1	D	169	THR	3.0
1	A	295	ARG	3.0
1	A	432	TRP	3.0
2	F	83	LYS	2.9
2	F	65	ILE	2.9
1	B	208	ALA	2.9
1	D	318	ASP	2.8
2	C	35	HIS	2.8
1	E	428	LYS	2.8
2	C	84	LYS	2.7
1	A	434	THR	2.7
1	B	459	LEU	2.7
1	B	436	LYS	2.7
1	D	435	GLU	2.7
1	E	113	LYS	2.7
2	F	84	LYS	2.7
1	A	459	LEU	2.7
1	A	154	MET	2.7
1	B	314	ILE	2.7
1	A	136	HIS	2.7
1	D	209	CYS	2.6
1	A	314	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	138	GLN	2.6
1	A	168	GLN	2.6
1	E	447	PHE	2.6
2	C	85	ASP	2.6
2	F	8	LEU	2.6
2	F	33	ASN	2.6
1	A	415	CYS	2.6
1	E	314	ILE	2.6
1	E	414	ASP	2.6
1	E	252	ARG	2.6
1	B	79	GLU	2.6
1	E	448	GLY	2.6
1	E	173	ASN	2.6
2	F	29	LYS	2.6
2	F	37	MET	2.5
1	D	138	GLN	2.5
1	B	154	MET	2.5
1	B	322	GLU	2.4
2	C	71	MET	2.4
2	F	9	GLU	2.4
2	C	64	ASP	2.4
2	C	83	LYS	2.4
2	C	6	LEU	2.4
1	E	459	LEU	2.4
1	A	207	THR	2.3
2	C	27	PRO	2.3
1	D	174	LYS	2.3
1	D	433	LYS	2.3
1	E	104	GLN	2.3
1	A	98	GLU	2.3
1	D	436	LYS	2.3
2	C	29	LYS	2.3
1	D	112	ILE	2.3
1	A	187	MET	2.3
1	B	415	CYS	2.3
2	F	80	ILE	2.3
1	E	315	THR	2.3
1	D	206	SER	2.3
1	A	436	LYS	2.2
1	B	312	GLY	2.2
1	E	165	LEU	2.2
1	A	205	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	314	ILE	2.2
2	C	65	ILE	2.2
1	D	99	GLY	2.2
1	B	136	HIS	2.2
1	E	205	VAL	2.2
1	B	131	LYS	2.2
1	B	97	ASP	2.2
2	F	71	MET	2.2
2	F	27	PRO	2.1
1	B	204	ALA	2.1
1	D	107	VAL	2.1
1	D	205	VAL	2.1
1	E	313	HIS	2.1
2	F	35	HIS	2.1
1	A	195	ARG	2.1
1	E	237	ASP	2.1
1	D	459	LEU	2.1
1	B	318	ASP	2.1
1	E	169	THR	2.1
1	E	187	MET	2.0
2	F	61	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

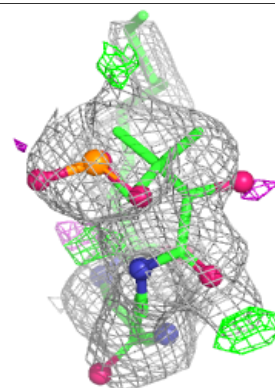
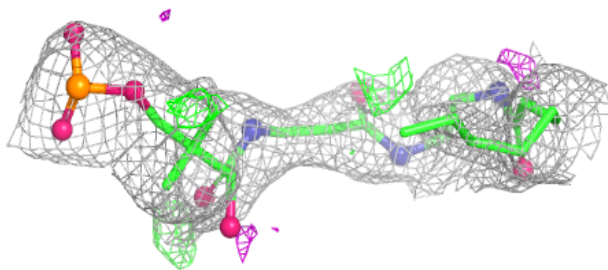
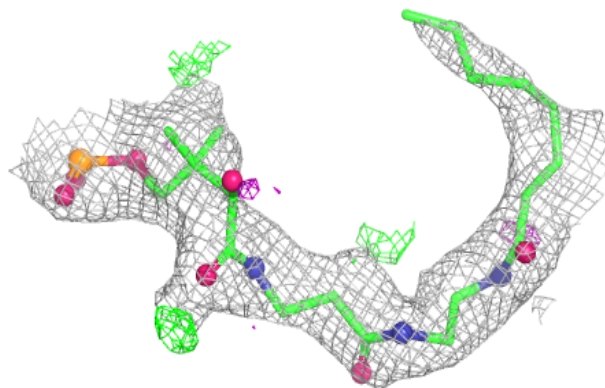
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1BMZ	C	101	30/31	0.75	0.19	41,58,68,74	0
3	A1BMZ	F	101	30/31	0.84	0.20	48,66,80,87	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.

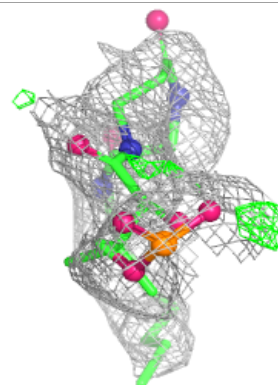
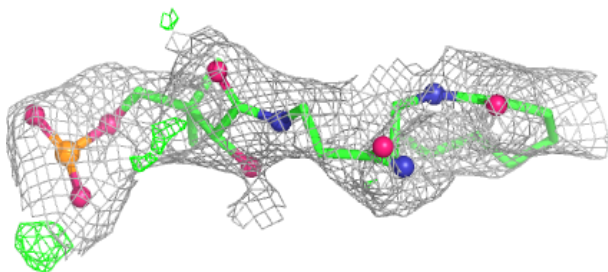
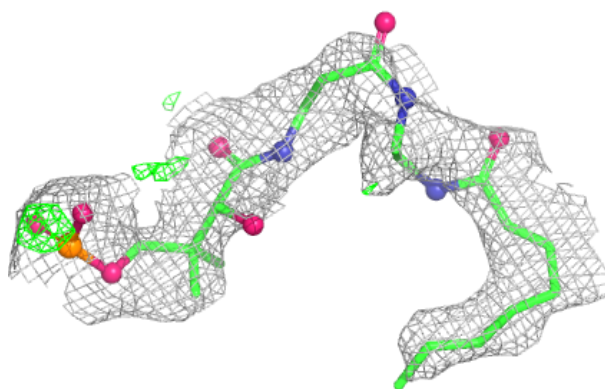
Electron density around A1BMZ C 101:

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



Electron density around A1BMZ F 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.