



Full wwPDB EM Validation Report ⓘ

Oct 19, 2025 – 12:15 AM JST

PDB ID : 9LA9 / pdb_00009la9
EMDB ID : EMD-62922
Title : Munc13-4-Rab27a complex with GppNHp
Authors : Zheng, X.; Liu, C.Q.; Wang, S.; Guan, J.L.; He, J.; Ma, C.
Deposited on : 2025-01-02
Resolution : 4.38 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

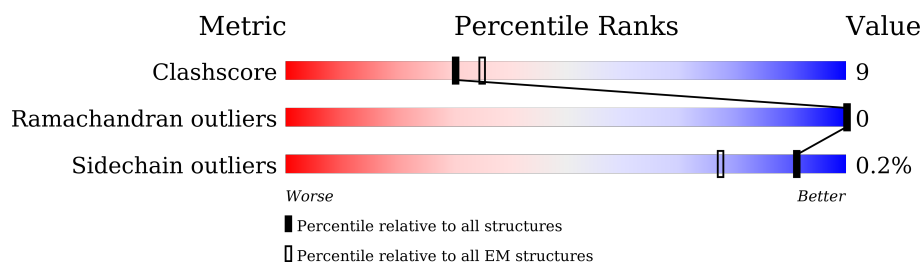
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.38 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1118	
2	B	263	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GNP	B	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9283 atoms, of which 16 are hydrogens and 0 are deuteriums.

In the tables below, 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 Protein unc-13 homolog D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	974	7761	4911	1369	1448	33	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q70J99
A	-26	SER	-	expression tag	UNP Q70J99
A	-25	TYR	-	expression tag	UNP Q70J99
A	-24	TYR	-	expression tag	UNP Q70J99
A	-23	HIS	-	expression tag	UNP Q70J99
A	-22	HIS	-	expression tag	UNP Q70J99
A	-21	HIS	-	expression tag	UNP Q70J99
A	-20	HIS	-	expression tag	UNP Q70J99
A	-19	HIS	-	expression tag	UNP Q70J99
A	-18	HIS	-	expression tag	UNP Q70J99
A	-17	ASP	-	expression tag	UNP Q70J99
A	-16	TYR	-	expression tag	UNP Q70J99
A	-15	ASP	-	expression tag	UNP Q70J99
A	-14	ILE	-	expression tag	UNP Q70J99
A	-13	PRO	-	expression tag	UNP Q70J99
A	-12	THR	-	expression tag	UNP Q70J99
A	-11	THR	-	expression tag	UNP Q70J99
A	-10	GLU	-	expression tag	UNP Q70J99
A	-9	ASN	-	expression tag	UNP Q70J99
A	-8	LEU	-	expression tag	UNP Q70J99
A	-7	TYR	-	expression tag	UNP Q70J99
A	-6	PHE	-	expression tag	UNP Q70J99
A	-5	GLN	-	expression tag	UNP Q70J99
A	-4	GLY	-	expression tag	UNP Q70J99
A	-3	ALA	-	expression tag	UNP Q70J99
A	-2	MET	-	expression tag	UNP Q70J99
A	-1	GLY	-	expression tag	UNP Q70J99
A	0	SER	-	expression tag	UNP Q70J99

- Molecule 2 is a protein called Ras-related protein Rab-27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	184	Total	C	N	O	S	0	0
			1474	936	252	278	8		

There are 42 discrepancies between the modelled and reference sequences:

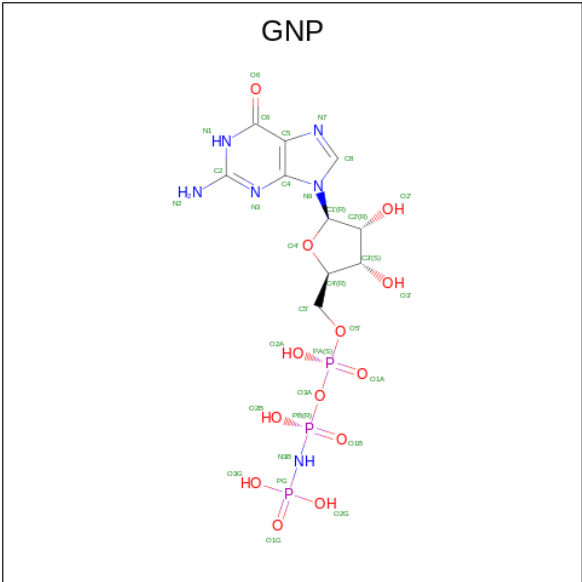
Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	MET	-	initiating methionine	UNP P51159
B	-32	GLY	-	expression tag	UNP P51159
B	-31	SER	-	expression tag	UNP P51159
B	-30	SER	-	expression tag	UNP P51159
B	-29	HIS	-	expression tag	UNP P51159
B	-28	HIS	-	expression tag	UNP P51159
B	-27	HIS	-	expression tag	UNP P51159
B	-26	HIS	-	expression tag	UNP P51159
B	-25	HIS	-	expression tag	UNP P51159
B	-24	HIS	-	expression tag	UNP P51159
B	-23	SER	-	expression tag	UNP P51159
B	-22	SER	-	expression tag	UNP P51159
B	-21	GLY	-	expression tag	UNP P51159
B	-20	LEU	-	expression tag	UNP P51159
B	-19	VAL	-	expression tag	UNP P51159
B	-18	PRO	-	expression tag	UNP P51159
B	-17	ARG	-	expression tag	UNP P51159
B	-16	GLY	-	expression tag	UNP P51159
B	-15	SER	-	expression tag	UNP P51159
B	-14	HIS	-	expression tag	UNP P51159
B	-13	MET	-	expression tag	UNP P51159
B	-12	ALA	-	expression tag	UNP P51159
B	-11	SER	-	expression tag	UNP P51159
B	-10	MET	-	expression tag	UNP P51159
B	-9	THR	-	expression tag	UNP P51159
B	-8	GLY	-	expression tag	UNP P51159
B	-7	GLY	-	expression tag	UNP P51159
B	-6	GLN	-	expression tag	UNP P51159
B	-5	GLN	-	expression tag	UNP P51159
B	-4	MET	-	expression tag	UNP P51159
B	-3	GLY	-	expression tag	UNP P51159
B	-2	ARG	-	expression tag	UNP P51159
B	-1	GLY	-	expression tag	UNP P51159
B	0	SER	-	expression tag	UNP P51159
B	222	LEU	-	expression tag	UNP P51159
B	223	GLU	-	expression tag	UNP P51159

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Chain	Residue	Modelled	Actual	Comment	Reference
B	224	HIS	-	expression tag	UNP P51159
B	225	HIS	-	expression tag	UNP P51159
B	226	HIS	-	expression tag	UNP P51159
B	227	HIS	-	expression tag	UNP P51159
B	228	HIS	-	expression tag	UNP P51159
B	229	HIS	-	expression tag	UNP P51159

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

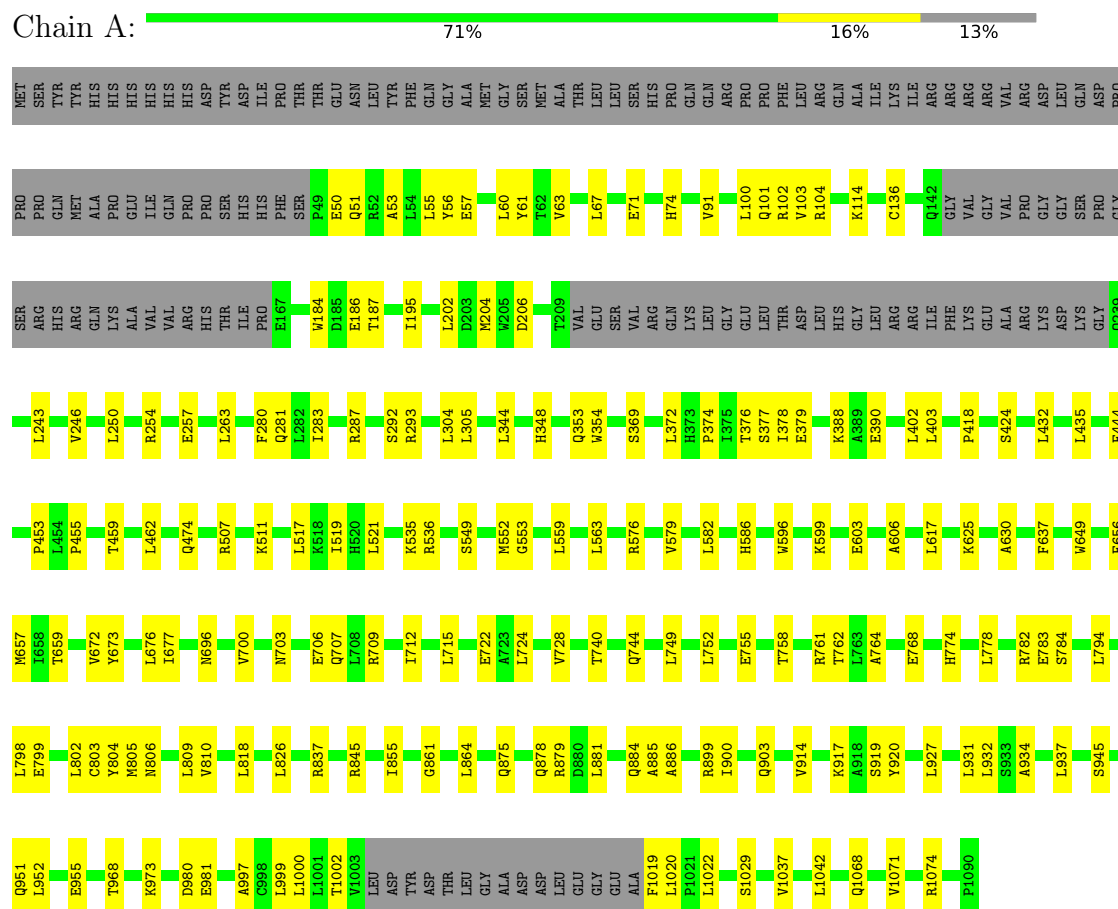


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
3	B	1	48	10	16	6	13	3	0

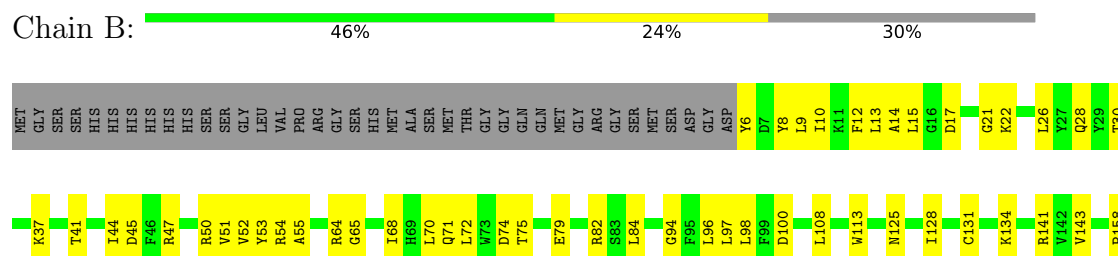
3 Residue-property plots

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. 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. 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: Protein unc-13 homolog D



• Molecule 2: Ras-related protein Rab-27A



S163	A164	A165	S171	Q172	A173	I174	E175	M176	D179	L180	I181	M182	K183	R184	V189	ASP	LYS	SER	TRP	ILE	PRO	GLU	GLY	VAL	ARG	SER	ASN	GLY	HIS	ALA	SER	THR	ASP	GLN	LEU	SER	GLU	GLU	LYS	GLU	LYS	GLY	ALA	CYS	GLY	CYS	LEU	GLU	HIS	HIS	HIS	HIS	HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102381	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP

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	0.23	1/7926 (0.0%)	0.64	9/10756 (0.1%)
2	B	0.21	0/1501	0.62	2/2023 (0.1%)
All	All	0.22	1/9427 (0.0%)	0.64	11/12779 (0.1%)

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	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	453	PRO	CG-CD	-5.13	1.33	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	886	ALA	N-CA-CB	-22.63	76.45	110.40
1	A	885	ALA	CB-CA-C	-18.08	73.89	109.68
1	A	885	ALA	N-CA-C	15.64	135.50	108.75
1	A	453	PRO	CA-N-CD	-12.41	94.63	112.00
1	A	886	ALA	N-CA-C	10.10	139.28	111.00
1	A	453	PRO	N-CD-CG	-7.02	92.67	103.20
2	B	53	TYR	CA-C-N	6.84	134.61	121.54
2	B	53	TYR	C-N-CA	6.84	134.61	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	VAL	CA-C-N	6.76	130.09	120.49
1	A	91	VAL	C-N-CA	6.76	130.09	120.49
1	A	453	PRO	N-CA-C	5.90	119.92	111.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	755	GLU	Peptide
2	B	54	ARG	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	7761	0	7740	108	0
2	B	1474	0	1452	55	0
3	B	32	16	13	17	0
All	All	9267	16	9205	162	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 9.

All (162) 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)
2:B:100:ASP:OD2	2:B:134:LYS:CE	1.93	1.16
2:B:100:ASP:OD2	2:B:134:LYS:NZ	1.88	1.04
2:B:21:GLY:HA2	3:B:301:GNP:PA	2.04	0.98
2:B:100:ASP:OD2	2:B:134:LYS:HE3	1.66	0.95
2:B:100:ASP:CG	2:B:134:LYS:HE3	1.91	0.94
2:B:41:THR:OG1	3:B:301:GNP:O2G	1.88	0.91
2:B:134:LYS:HG2	3:B:301:GNP:C6	2.02	0.88
2:B:21:GLY:HA2	3:B:301:GNP:O3A	1.73	0.87
2:B:100:ASP:CG	2:B:134:LYS:CE	2.49	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LYS:HG2	3:B:301:GNP:C5	2.14	0.78
2:B:21:GLY:HA2	3:B:301:GNP:O1A	1.86	0.75
2:B:100:ASP:OD1	2:B:134:LYS:HE3	1.87	0.73
1:A:53:ALA:O	1:A:56:TYR:HB3	1.90	0.70
2:B:47:ARG:HB2	2:B:72:LEU:HB2	1.79	0.64
1:A:630:ALA:HB1	1:A:707:GLN:HG2	1.80	0.64
1:A:740:THR:O	1:A:744:GLN:NE2	2.31	0.64
1:A:61:TYR:HE2	1:A:287:ARG:HB3	1.63	0.64
2:B:158:PRO:HG2	2:B:180:LEU:HD11	1.79	0.64
2:B:41:THR:OG1	3:B:301:GNP:PG	2.57	0.63
1:A:951:GLN:HB2	1:A:1002:THR:HB	1.79	0.63
1:A:917:LYS:HD3	1:A:932:LEU:HD11	1.81	0.63
2:B:97:LEU:HD23	2:B:128:ILE:HG23	1.81	0.62
1:A:657:MET:HG3	2:B:84:LEU:HD22	1.80	0.62
1:A:703:ASN:HD22	1:A:810:VAL:HG23	1.66	0.61
1:A:474:GLN:HE22	1:A:536:ARG:HE	1.47	0.60
1:A:388:LYS:HG3	1:A:390:GLU:H	1.67	0.60
2:B:14:ALA:HA	2:B:96:LEU:HB2	1.83	0.60
2:B:21:GLY:CA	3:B:301:GNP:O3A	2.48	0.60
1:A:999:LEU:HD12	1:A:1020:LEU:HD11	1.83	0.59
2:B:12:PHE:HE2	2:B:174:ILE:HG23	1.67	0.59
2:B:45:ASP:HB2	2:B:74:ASP:HB3	1.83	0.59
1:A:136:CYS:HB3	1:A:202:LEU:HD11	1.86	0.58
2:B:13:LEU:HB3	2:B:15:LEU:HD23	1.86	0.58
1:A:67:LEU:O	1:A:254:ARG:NH1	2.38	0.57
1:A:712:ILE:HD12	1:A:752:LEU:HD11	1.87	0.57
2:B:64:ARG:NH1	2:B:65:GLY:O	2.38	0.57
1:A:57:GLU:OE2	1:A:102:ARG:NH1	2.39	0.56
1:A:758:THR:HA	1:A:761:ARG:HB2	1.87	0.56
1:A:703:ASN:HD21	1:A:809:LEU:HA	1.71	0.56
1:A:246:VAL:HG23	1:A:263:LEU:HD23	1.87	0.56
1:A:305:LEU:HD21	1:A:353:GLN:HA	1.88	0.55
1:A:517:LEU:HG	1:A:519:ILE:HG12	1.88	0.55
1:A:806:ASN:ND2	1:A:861:GLY:O	2.39	0.55
1:A:603:GLU:O	1:A:606:ALA:HB3	2.07	0.54
1:A:900:ILE:HD13	1:A:1019:PHE:HB2	1.89	0.54
1:A:783:GLU:HG2	1:A:837:ARG:HH22	1.70	0.54
2:B:22:LYS:NZ	3:B:301:GNP:N3B	2.54	0.54
1:A:955:GLU:HG3	1:A:1000:LEU:HD13	1.89	0.54
1:A:257:GLU:HB2	1:A:280:PHE:HB2	1.89	0.54
1:A:919:SER:HB2	1:A:1037:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LYS:O	1:A:603:GLU:N	2.40	0.53
1:A:403:LEU:HD22	1:A:444:PHE:HZ	1.73	0.53
1:A:354:TRP:HH2	1:A:402:LEU:HD22	1.74	0.53
1:A:945:SER:HA	1:A:973:LYS:HD3	1.91	0.53
1:A:617:LEU:HD11	1:A:677:ILE:HG22	1.90	0.53
2:B:98:LEU:HD13	2:B:131:CYS:HB2	1.91	0.53
1:A:374:PRO:O	1:A:377:SER:HB3	2.09	0.52
1:A:774:HIS:HB3	1:A:794:LEU:HB2	1.90	0.52
1:A:722:GLU:OE2	1:A:722:GLU:N	2.43	0.52
2:B:30:THR:HG21	2:B:47:ARG:HE	1.75	0.51
1:A:114:LYS:HB3	1:A:281:GLN:HB2	1.93	0.51
2:B:9:LEU:HD21	2:B:71:GLN:HE21	1.75	0.50
1:A:206:ASP:HB2	1:A:243:LEU:HD11	1.94	0.50
2:B:134:LYS:CG	3:B:301:GNP:C5	2.86	0.50
2:B:51:VAL:HG23	2:B:68:ILE:HB	1.93	0.50
1:A:875:GLN:HA	1:A:878:GLN:HG2	1.93	0.50
1:A:1029:SER:O	1:A:1029:SER:OG	2.30	0.50
1:A:292:SER:OG	1:A:293:ARG:NH1	2.45	0.49
1:A:459:THR:HA	1:A:462:LEU:HD12	1.93	0.49
1:A:55:LEU:HD21	1:A:304:LEU:HA	1.94	0.49
1:A:749:LEU:HA	1:A:752:LEU:HD12	1.95	0.49
2:B:134:LYS:HG2	3:B:301:GNP:N1	2.27	0.49
1:A:114:LYS:HB2	1:A:283:ILE:HG23	1.95	0.49
1:A:637:PHE:HD2	1:A:715:LEU:HD21	1.78	0.49
2:B:28:GLN:NE2	2:B:164:ALA:O	2.40	0.49
2:B:163:SER:OG	3:B:301:GNP:O6	2.22	0.49
1:A:903:GLN:HG2	1:A:1042:LEU:HD23	1.95	0.48
1:A:673:TYR:O	1:A:677:ILE:HG12	2.13	0.48
2:B:26:LEU:HD12	2:B:74:ASP:HB2	1.95	0.48
2:B:165:ALA:HB2	3:B:301:GNP:C2	2.43	0.48
1:A:799:GLU:O	1:A:803:CYS:CB	2.62	0.48
1:A:920:TYR:HD1	1:A:927:LEU:HD13	1.79	0.48
1:A:549:SER:HB3	1:A:552:MET:HB2	1.94	0.48
1:A:673:TYR:HA	1:A:676:LEU:HD12	1.96	0.48
1:A:507:ARG:O	1:A:511:LYS:NZ	2.40	0.47
2:B:179:ASP:O	2:B:183:LYS:HG3	2.13	0.47
1:A:71:GLU:HB2	1:A:74:HIS:HB2	1.96	0.47
1:A:344:LEU:HD11	1:A:348:HIS:HB2	1.95	0.47
1:A:369:SER:HA	1:A:372:LEU:HD12	1.96	0.47
2:B:55:ALA:HB1	2:B:179:ASP:HA	1.96	0.47
2:B:171:SER:OG	2:B:175:GLU:OE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LYS:HB3	2:B:37:LYS:HE3	1.71	0.46
1:A:418:PRO:O	1:A:424:SER:OG	2.25	0.46
1:A:462:LEU:HD22	1:A:521:LEU:HD13	1.97	0.46
2:B:21:GLY:H	3:B:301:GNP:PB	2.39	0.46
1:A:799:GLU:O	1:A:803:CYS:HB2	2.16	0.46
1:A:204:MET:HB3	1:A:243:LEU:HD12	1.98	0.46
2:B:79:GLU:HA	2:B:82:ARG:HG3	1.97	0.46
2:B:17:ASP:OD1	2:B:113:TRP:NE1	2.43	0.46
1:A:931:LEU:O	1:A:980:ASP:N	2.49	0.45
1:A:659:THR:HG21	1:A:724:LEU:HD22	1.99	0.45
1:A:672:VAL:O	1:A:676:LEU:HG	2.16	0.45
1:A:625:LYS:HB2	1:A:625:LYS:HE2	1.79	0.44
1:A:968:THR:OG1	1:A:981:GLU:OE1	2.34	0.44
1:A:881:LEU:HA	1:A:884:GLN:HB2	1.98	0.44
1:A:60:LEU:HA	1:A:63:VAL:HG12	1.99	0.44
1:A:818:LEU:HD22	1:A:864:LEU:HB2	2.00	0.44
1:A:586:HIS:HB2	1:A:649:TRP:CZ3	2.53	0.44
1:A:764:ALA:O	1:A:768:GLU:HB3	2.16	0.44
1:A:782:ARG:NH1	1:A:784:SER:OG	2.50	0.44
1:A:997:ALA:HB1	1:A:1022:LEU:HD23	2.00	0.44
1:A:879:ARG:HA	1:A:879:ARG:HD2	1.81	0.44
1:A:354:TRP:HB2	1:A:378:ILE:HD11	2.00	0.44
1:A:914:VAL:HA	1:A:934:ALA:HA	1.98	0.44
1:A:934:ALA:HB1	1:A:937:LEU:HD21	1.99	0.44
1:A:376:THR:O	1:A:379:GLU:HB3	2.18	0.44
1:A:778:LEU:O	1:A:845:ARG:NH2	2.50	0.44
2:B:9:LEU:HD21	2:B:71:GLN:NE2	2.32	0.43
1:A:100:LEU:HA	1:A:103:VAL:HG12	2.00	0.43
1:A:798:LEU:HG	1:A:802:LEU:HD13	1.99	0.43
2:B:21:GLY:HA3	3:B:301:GNP:H5'1	2.00	0.43
1:A:293:ARG:HD3	1:A:293:ARG:HA	1.83	0.43
2:B:52:VAL:HG22	2:B:65:GLY:H	1.84	0.43
2:B:94:GLY:HA3	2:B:181:ILE:HD11	2.00	0.43
1:A:899:ARG:HH21	1:A:1074:ARG:HH22	1.67	0.42
2:B:141:ARG:NH1	2:B:143:VAL:O	2.52	0.42
1:A:369:SER:O	1:A:372:LEU:HB2	2.20	0.42
2:B:10:ILE:HB	2:B:70:LEU:HD23	2.01	0.42
2:B:125:ASN:O	2:B:184:ARG:NH1	2.51	0.42
2:B:158:PRO:HB3	2:B:176:MET:HE1	2.01	0.42
1:A:101:GLN:N	1:A:104:ARG:HH21	2.17	0.42
1:A:455:PRO:HB3	1:A:519:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LYS:HA	1:A:535:LYS:HD3	1.77	0.42
1:A:696:ASN:O	1:A:700:VAL:HG12	2.20	0.42
1:A:931:LEU:HD22	1:A:952:LEU:HD11	2.02	0.42
1:A:559:LEU:HD12	1:A:559:LEU:HA	1.94	0.42
1:A:563:LEU:HD22	1:A:582:LEU:HD11	2.02	0.42
2:B:44:ILE:HG22	2:B:75:THR:HA	2.02	0.41
2:B:6:TYR:HB3	2:B:50:ARG:HH21	1.85	0.41
1:A:553:GLY:O	1:A:596:TRP:NE1	2.50	0.41
1:A:706:GLU:OE2	1:A:709:ARG:NH2	2.53	0.41
1:A:576:ARG:HH21	1:A:579:VAL:HG21	1.85	0.41
1:A:703:ASN:ND2	1:A:810:VAL:HG23	2.35	0.41
1:A:114:LYS:HD3	1:A:283:ILE:HD13	2.01	0.41
2:B:172:GLN:H	2:B:172:GLN:HG2	1.71	0.41
1:A:67:LEU:HD12	1:A:195:ILE:HB	2.03	0.41
1:A:114:LYS:HG3	1:A:187:THR:HG21	2.02	0.41
1:A:195:ILE:HG13	1:A:250:LEU:HB3	2.03	0.41
1:A:656:PHE:HB2	1:A:728:VAL:HG11	2.02	0.41
2:B:8:TYR:HB2	2:B:68:ILE:HD13	2.02	0.41
2:B:21:GLY:CA	3:B:301:GNP:H5'1	2.50	0.41
1:A:50:GLU:OE2	1:A:51:GLN:NE2	2.51	0.41
1:A:184:TRP:CD1	1:A:186:GLU:HB2	2.55	0.41
1:A:826:LEU:HD23	1:A:826:LEU:HA	1.94	0.40
1:A:855:ILE:HD12	1:A:855:ILE:HA	1.93	0.40
1:A:204:MET:HB2	1:A:243:LEU:HB2	2.04	0.40
1:A:432:LEU:HA	1:A:435:LEU:HB2	2.03	0.40
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.94	0.40
1:A:805:MET:HE3	1:A:805:MET:HB2	1.89	0.40
2:B:165:ALA:HB2	3:B:301:GNP:N1	2.36	0.40
1:A:1068:GLN:HA	1:A:1071:VAL:HG22	2.04	0.40
1:A:758:THR:O	1:A:762:THR:OG1	2.39	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 PDB entries followed by that with respect to all EM entries.

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	966/1118 (86%)	925 (96%)	41 (4%)	0	100	100
2	B	182/263 (69%)	166 (91%)	16 (9%)	0	100	100
All	All	1148/1381 (83%)	1091 (95%)	57 (5%)	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 PDB entries followed by that with respect to all EM entries.

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	855/979 (87%)	854 (100%)	1 (0%)	92	95
2	B	157/221 (71%)	156 (99%)	1 (1%)	84	88
All	All	1012/1200 (84%)	1010 (100%)	2 (0%)	91	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	804	TYR
2	B	108	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	703	ASN
1	A	746	GLN
1	A	971	HIS
2	B	69	HIS
2	B	105	GLN
2	B	125	ASN
2	B	140	GLN

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Mol	Chain	Res	Type
2	B	166	ASN

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](#)

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	GNP	B	301	-	29,34,34	1.62	7 (24%)	33,54,54	2.23	6 (18%)

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	GNP	B	301	-	-	3/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	GNP	PB-O3A	4.47	1.64	1.59
3	B	301	GNP	C6-N1	3.11	1.38	1.33
3	B	301	GNP	PB-O1B	3.10	1.51	1.46
3	B	301	GNP	PG-N3B	2.95	1.71	1.63
3	B	301	GNP	PG-O1G	2.76	1.50	1.46
3	B	301	GNP	PB-O2B	-2.14	1.51	1.56
3	B	301	GNP	C5-C6	2.05	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	GNP	C5-C6-N1	-8.43	111.90	123.43
3	B	301	GNP	C2-N1-C6	5.86	125.24	115.93
3	B	301	GNP	N3-C2-N1	-2.79	123.50	127.22
3	B	301	GNP	C4-C5-C6	-2.56	118.36	120.80
3	B	301	GNP	PB-O3A-PA	-2.33	124.39	132.62
3	B	301	GNP	C2-N3-C4	-2.14	112.91	115.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	GNP	PB-N3B-PG-O1G
3	B	301	GNP	C5'-O5'-PA-O1A
3	B	301	GNP	O4'-C4'-C5'-O5'

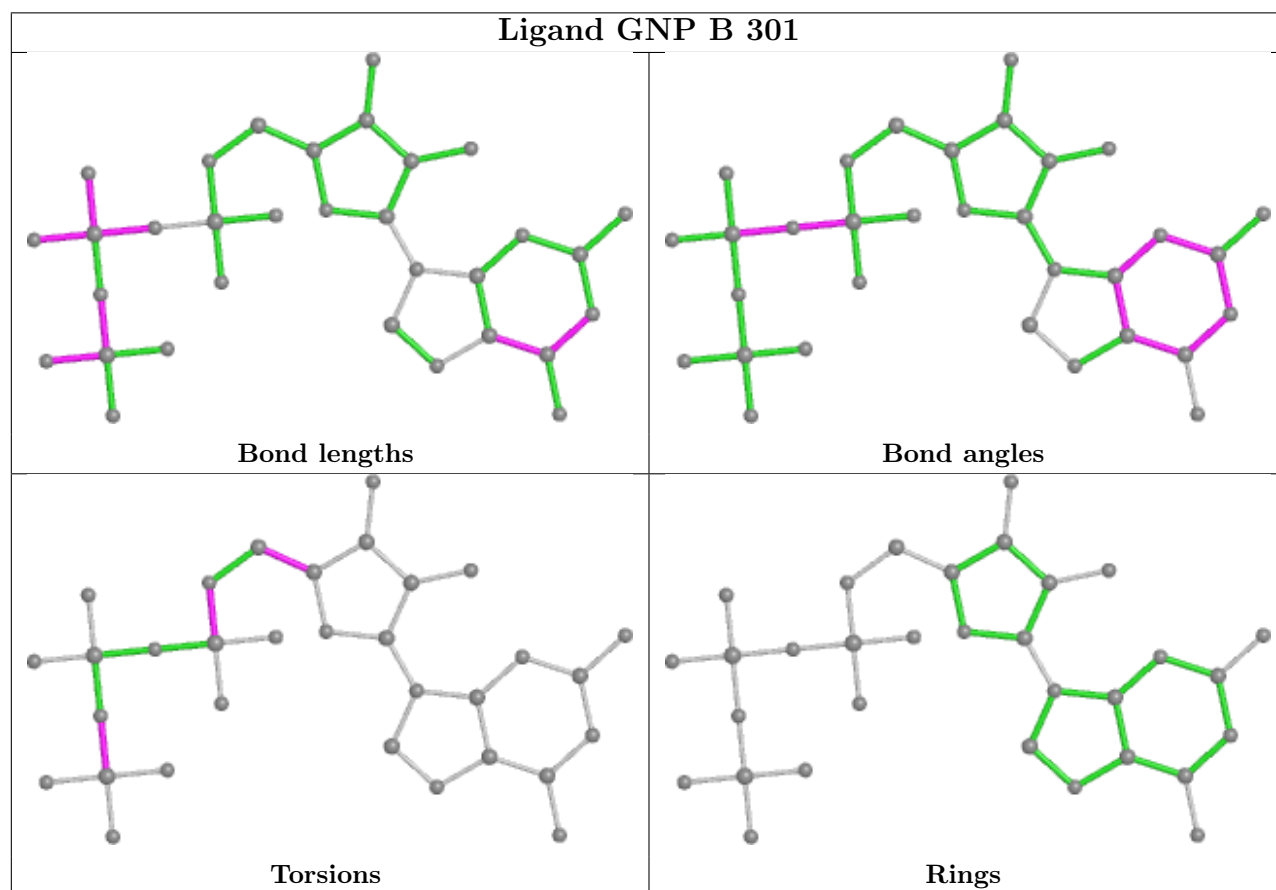
There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	GNP	17	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.