



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:01 AM UTC

PDB ID : 9L63 / pdb_00009l63
Title : A novel allosteric covalent inhibitory site of fucosyltransferase 8 revealed by crystal structures
Authors : Jiang, J.; Fang, P.
Deposited on : 2024-12-24
Resolution : 2.66 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

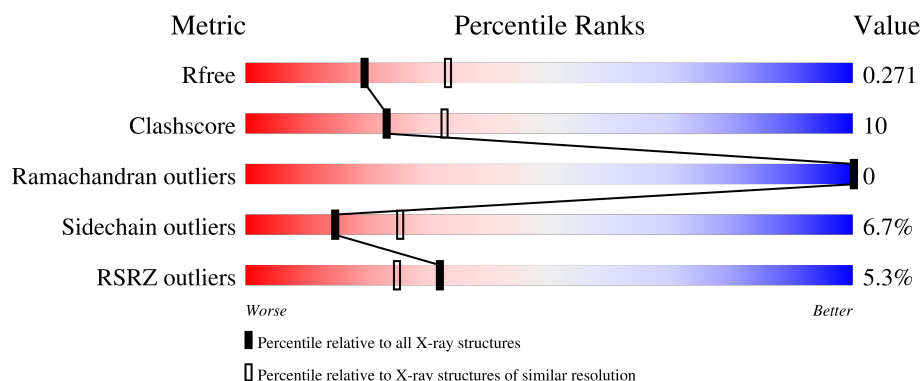
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	499	6% 57% 28% • 12%
1	B	499	4% 71% 16% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7214 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 Alpha-(1,6)-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3569	2276	626	653	14			
1	B	444	Total	C	N	O	S	0	0	0
			3613	2304	635	660	14			

There are 56 discrepancies between the modelled and reference sequences:

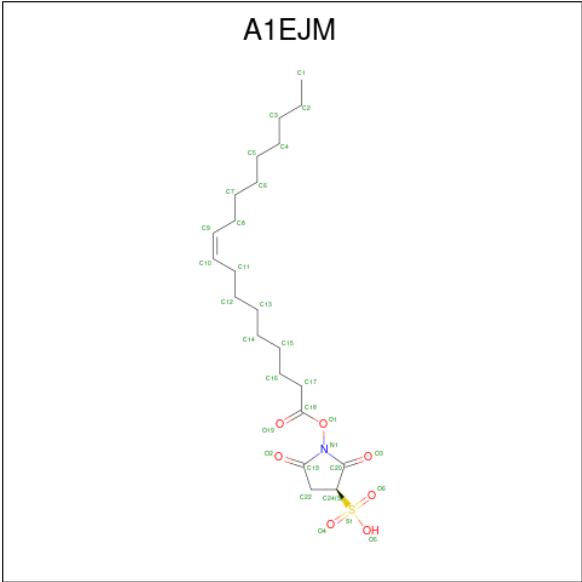
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ASP	-	expression tag	UNP Q9BYC5
A	78	ALA	-	expression tag	UNP Q9BYC5
A	79	ALA	-	expression tag	UNP Q9BYC5
A	80	GLN	-	expression tag	UNP Q9BYC5
A	81	PRO	-	expression tag	UNP Q9BYC5
A	82	ALA	-	expression tag	UNP Q9BYC5
A	83	ASP	-	expression tag	UNP Q9BYC5
A	84	TYR	-	expression tag	UNP Q9BYC5
A	85	LYS	-	expression tag	UNP Q9BYC5
A	86	ASP	-	expression tag	UNP Q9BYC5
A	87	HIS	-	expression tag	UNP Q9BYC5
A	88	ASP	-	expression tag	UNP Q9BYC5
A	89	GLY	-	expression tag	UNP Q9BYC5
A	90	ASP	-	expression tag	UNP Q9BYC5
A	91	TYR	-	expression tag	UNP Q9BYC5
A	92	LYS	-	expression tag	UNP Q9BYC5
A	93	ASP	-	expression tag	UNP Q9BYC5
A	94	HIS	-	expression tag	UNP Q9BYC5
A	95	ASP	-	expression tag	UNP Q9BYC5
A	96	ILE	-	expression tag	UNP Q9BYC5
A	97	ASP	-	expression tag	UNP Q9BYC5
A	98	TYR	-	expression tag	UNP Q9BYC5
A	99	LYS	-	expression tag	UNP Q9BYC5
A	100	ASP	-	expression tag	UNP Q9BYC5
A	101	ASP	-	expression tag	UNP Q9BYC5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ASP	-	expression tag	UNP Q9BYC5
A	103	ASP	-	expression tag	UNP Q9BYC5
A	104	LYS	-	expression tag	UNP Q9BYC5
B	77	ASP	-	expression tag	UNP Q9BYC5
B	78	ALA	-	expression tag	UNP Q9BYC5
B	79	ALA	-	expression tag	UNP Q9BYC5
B	80	GLN	-	expression tag	UNP Q9BYC5
B	81	PRO	-	expression tag	UNP Q9BYC5
B	82	ALA	-	expression tag	UNP Q9BYC5
B	83	ASP	-	expression tag	UNP Q9BYC5
B	84	TYR	-	expression tag	UNP Q9BYC5
B	85	LYS	-	expression tag	UNP Q9BYC5
B	86	ASP	-	expression tag	UNP Q9BYC5
B	87	HIS	-	expression tag	UNP Q9BYC5
B	88	ASP	-	expression tag	UNP Q9BYC5
B	89	GLY	-	expression tag	UNP Q9BYC5
B	90	ASP	-	expression tag	UNP Q9BYC5
B	91	TYR	-	expression tag	UNP Q9BYC5
B	92	LYS	-	expression tag	UNP Q9BYC5
B	93	ASP	-	expression tag	UNP Q9BYC5
B	94	HIS	-	expression tag	UNP Q9BYC5
B	95	ASP	-	expression tag	UNP Q9BYC5
B	96	ILE	-	expression tag	UNP Q9BYC5
B	97	ASP	-	expression tag	UNP Q9BYC5
B	98	TYR	-	expression tag	UNP Q9BYC5
B	99	LYS	-	expression tag	UNP Q9BYC5
B	100	ASP	-	expression tag	UNP Q9BYC5
B	101	ASP	-	expression tag	UNP Q9BYC5
B	102	ASP	-	expression tag	UNP Q9BYC5
B	103	ASP	-	expression tag	UNP Q9BYC5
B	104	LYS	-	expression tag	UNP Q9BYC5

- Molecule 2 is 1-[({Z})-octadec-9-enoyl]oxy-2,5-bis(oxidanylidene)pyrrolidine-3-sulfonic acid (CCD ID: A1EJM) (formula: C₂₂H₃₇NO₇S) (labeled as "Ligand of Interest" by depositor).

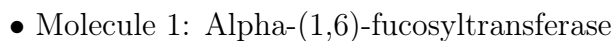


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			19	18	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	10	Total	O	0	0
			10	10		

- Molecule 1: Alpha-(1,6)-fucosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.43Å 69.74Å 141.69Å 90.00° 132.62° 90.00°	Depositor
Resolution (Å)	30.86 – 2.66 30.86 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.86-2.66) 99.3 (30.86-2.66)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.64Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.216 , 0.271 0.218 , 0.271	Depositor DCC
R_{free} test set	2086 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7214	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EJM

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	0.36	0/3659	0.56	0/4954
1	B	0.47	0/3705	0.68	3/5018 (0.1%)
All	All	0.42	0/7364	0.63	3/9972 (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	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	493	LEU	CA-C-N	-5.51	114.95	121.90
1	B	493	LEU	C-N-CA	-5.51	114.95	121.90
1	B	465	CYS	N-CA-C	5.24	114.76	107.73

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	ARG	Sidechain
1	A	403	ARG	Sidechain
1	B	260	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	337	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	3569	0	3499	98	0
1	B	3613	0	3534	60	0
2	B	19	0	0	0	0
3	A	3	0	0	0	0
3	B	10	0	0	0	0
All	All	7214	0	7033	147	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 10.

All (147) 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:202:LYS:H	1:B:202:LYS:HD2	1.27	0.97
1:A:554:PRO:HG2	1:A:557:LYS:HE3	1.58	0.86
1:B:511:TYR:HB2	1:B:557:LYS:HG2	1.66	0.77
1:B:553:TYR:HE2	1:B:558:VAL:HG21	1.50	0.74
1:A:334:TYR:O	1:A:337:ARG:NH1	2.21	0.73
1:A:294:VAL:HG21	1:A:501:GLY:HA3	1.71	0.70
1:B:113:GLU:OE1	1:B:116:ARG:NH2	2.22	0.70
1:A:363:HIS:HB2	1:A:457:LEU:HD11	1.73	0.70
1:A:365:ARG:HD3	1:A:469:SER:HB3	1.72	0.69
1:A:315:ARG:O	1:A:319:VAL:HG12	1.94	0.67
1:A:333:LYS:HB2	1:A:481:THR:HG21	1.76	0.67
1:A:360:ILE:HG12	1:A:462:PHE:HB3	1.77	0.67
1:A:317:VAL:O	1:B:117:ARG:NH2	2.27	0.67
1:A:467:PHE:CD2	1:A:492:SER:HB2	2.30	0.66
1:A:196:THR:HG22	1:A:334:TYR:HE2	1.61	0.66
1:A:273:SER:HB2	1:A:287:GLN:H	1.62	0.65
1:A:113:GLU:OE2	1:A:116:ARG:NH2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:VAL:HG12	1:A:451:ILE:HD12	1.79	0.64
1:B:325:VAL:HG13	1:B:497:TYR:CZ	2.32	0.63
1:B:202:LYS:H	1:B:202:LYS:CD	2.09	0.63
1:A:310:GLU:HB3	1:A:564:THR:HB	1.80	0.63
1:A:555:SER:HB2	1:B:125:GLU:HG2	1.81	0.62
1:B:507:GLN:HB3	1:B:558:VAL:HG11	1.83	0.60
1:A:145:LEU:HD21	1:B:138:LYS:HA	1.83	0.59
1:B:345:GLU:OE2	1:B:448:ARG:NH1	2.35	0.59
1:B:507:GLN:HB3	1:B:558:VAL:CG1	2.33	0.59
1:A:161:ARG:HB3	1:A:395:ARG:HD2	1.85	0.59
1:B:130:LEU:HD11	1:B:156:LEU:HD11	1.85	0.59
1:A:508:ILE:HD11	1:A:561:LYS:HD2	1.86	0.58
1:A:313:ALA:O	1:A:317:VAL:HG22	2.05	0.56
1:A:350:THR:HG22	1:A:456:PHE:HE1	1.70	0.56
1:A:467:PHE:HD2	1:A:492:SER:HB2	1.69	0.56
1:A:321:GLY:O	1:A:323:PRO:HD3	2.07	0.55
1:A:403:ARG:NH1	1:A:403:ARG:HG2	2.21	0.55
1:B:232:MET:HG3	1:B:331:PHE:CE2	2.42	0.55
1:B:365:ARG:NH2	1:B:469:SER:HA	2.23	0.54
1:B:188:THR:HG22	1:B:326:TRP:HZ2	1.73	0.54
1:B:228:VAL:HG21	1:B:332:VAL:HG22	1.90	0.54
1:B:345:GLU:OE2	1:B:448:ARG:HD3	2.08	0.53
1:A:403:ARG:HH12	1:A:425:GLU:CD	2.15	0.53
1:A:360:ILE:HD12	1:A:390:PHE:CE2	2.44	0.53
1:A:383:MET:HE2	1:A:421:TYR:CD2	2.45	0.52
1:A:220:TYR:CE1	1:A:447:LEU:HD23	2.44	0.52
1:A:220:TYR:CZ	1:A:447:LEU:HD23	2.44	0.52
1:A:516:ARG:NH2	1:B:151:GLU:HB3	2.25	0.52
1:A:494:ASP:OD1	1:A:495:ASP:N	2.43	0.52
1:A:305:PRO:HG2	1:A:499:PHE:CD2	2.45	0.52
1:B:281:VAL:HG23	1:B:282:LYS:H	1.75	0.52
1:A:231:PHE:O	1:A:234:ALA:HB3	2.10	0.52
1:A:403:ARG:HG2	1:A:403:ARG:HH11	1.74	0.51
1:B:184:ALA:O	1:B:188:THR:HG23	2.10	0.51
1:A:239:ARG:NH2	1:A:289:VAL:HG23	2.26	0.50
1:B:202:LYS:HD2	1:B:202:LYS:N	2.11	0.50
1:A:384:VAL:O	1:A:388:GLU:HG3	2.12	0.50
1:B:485:ASP:OD1	1:B:487:SER:OG	2.28	0.50
1:A:387:GLU:OE2	1:A:424:TYR:OH	2.29	0.50
1:A:179:TRP:HH2	1:A:318:ARG:HG2	1.77	0.50
1:A:405:TYR:HE1	1:A:407:ALA:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TYR:O	1:A:173:THR:HG23	2.13	0.49
1:A:258:VAL:HG22	1:A:342:LEU:HD22	1.95	0.49
1:A:167:LEU:HD13	1:B:120:GLU:HA	1.95	0.49
1:B:315:ARG:O	1:B:319:VAL:HG23	2.13	0.49
1:A:420:LYS:HB3	1:A:421:TYR:HD1	1.78	0.48
1:A:516:ARG:CZ	1:B:151:GLU:HB3	2.43	0.48
1:A:164:MET:HE3	1:A:164:MET:HA	1.95	0.48
1:A:227:VAL:O	1:A:231:PHE:N	2.40	0.48
1:A:458:SER:HB2	1:A:478:ILE:HB	1.96	0.48
1:A:515:PRO:HG3	1:A:522:PRO:HD3	1.96	0.48
1:B:258:VAL:HG23	1:B:259:PHE:N	2.29	0.47
1:A:188:THR:HG23	1:A:330:GLN:OE1	2.14	0.47
1:A:207:ALA:O	1:A:209:LYS:HG3	2.13	0.47
1:A:421:TYR:HB3	1:A:424:TYR:HD2	1.78	0.47
1:B:147:ARG:NE	1:B:151:GLU:OE2	2.48	0.47
1:A:132:SER:HB2	1:B:537:ASP:HB2	1.96	0.47
1:B:131:GLN:O	1:B:132:SER:C	2.58	0.47
1:B:232:MET:SD	1:B:305:PRO:HD3	2.55	0.46
1:B:295:ASP:OD1	1:B:295:ASP:N	2.48	0.46
1:A:348:GLU:O	1:A:352:LYS:HB2	2.16	0.46
1:A:522:PRO:HG2	1:A:547:LEU:HD21	1.97	0.46
1:A:132:SER:CB	1:B:537:ASP:HB2	2.46	0.46
1:A:383:MET:HE3	1:A:383:MET:HB3	1.78	0.46
1:B:229:TYR:CE2	1:B:294:VAL:HB	2.51	0.46
1:A:210:LEU:HD11	1:A:291:LEU:HD13	1.97	0.45
1:A:415:LYS:O	1:A:419:THR:HG23	2.17	0.45
1:A:470:GLN:O	1:A:474:VAL:HG23	2.16	0.45
1:A:541:LYS:HE2	1:A:550:THR:HG23	1.99	0.45
1:B:118:ARG:HD2	1:B:166:ASP:OD2	2.17	0.45
1:B:325:VAL:HG13	1:B:497:TYR:CE2	2.51	0.45
1:A:228:VAL:HG21	1:A:332:VAL:HG22	1.97	0.45
1:A:541:LYS:HE2	1:A:550:THR:CG2	2.46	0.45
1:B:447:LEU:HA	1:B:450:VAL:HG12	1.99	0.45
1:B:519:ASP:N	1:B:519:ASP:OD1	2.49	0.45
1:A:409:ASP:O	1:A:411:PRO:HD3	2.17	0.45
1:A:380:GLU:O	1:A:383:MET:N	2.50	0.45
1:A:172:GLN:OE1	1:A:177:GLY:HA3	2.18	0.44
1:A:466:THR:HG23	1:A:469:SER:OG	2.16	0.44
1:A:490:PHE:CD1	1:A:490:PHE:C	2.94	0.44
1:B:220:TYR:CE1	1:B:447:LEU:HD13	2.52	0.44
1:A:403:ARG:NH1	1:A:425:GLU:OE2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:VAL:HG22	1:B:454:ILE:HD12	2.00	0.44
1:A:543:VAL:HG22	1:A:550:THR:OG1	2.18	0.44
1:B:316:LEU:HD23	1:B:316:LEU:HA	1.81	0.44
1:A:541:LYS:HD3	1:A:541:LYS:C	2.42	0.44
1:A:332:VAL:O	1:A:336:ILE:HG12	2.17	0.44
1:A:141:GLU:OE2	1:A:141:GLU:HA	2.18	0.43
1:A:463:LEU:HD12	1:A:463:LEU:HA	1.88	0.43
1:A:465:CYS:SG	1:A:466:THR:N	2.92	0.43
1:B:112:HIS:CD2	1:B:170:LEU:HD11	2.53	0.43
1:B:147:ARG:CZ	1:B:151:GLU:OE2	2.66	0.43
1:B:333:LYS:HB2	1:B:481:THR:HG21	2.00	0.43
1:B:508:ILE:HG13	1:B:561:LYS:HB2	2.00	0.43
1:A:385:HIS:CD2	1:A:491:HIS:CD2	3.06	0.43
1:A:181:GLU:HG3	1:A:484:PRO:HG3	2.00	0.43
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.73	0.43
1:A:467:PHE:HD1	1:A:473:ARG:HG2	1.84	0.43
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.82	0.42
1:A:214:ILE:HD11	1:A:243:LEU:HD23	2.01	0.42
1:B:188:THR:HG22	1:B:326:TRP:CZ2	2.52	0.42
1:B:205:SER:O	1:B:287:GLN:NE2	2.42	0.42
1:A:467:PHE:HB2	1:A:495:ASP:O	2.20	0.42
1:B:319:VAL:O	1:B:319:VAL:HG12	2.19	0.42
1:A:185:LYS:HA	1:A:185:LYS:HD3	1.79	0.42
1:A:457:LEU:HD23	1:A:457:LEU:HA	1.90	0.42
1:A:537:ASP:HB2	1:B:132:SER:HB2	2.01	0.42
1:A:216:LYS:HA	1:A:223:GLN:NE2	2.34	0.42
1:B:151:GLU:HA	1:B:154:LEU:HB2	2.02	0.42
1:B:188:THR:O	1:B:192:GLN:HG2	2.20	0.41
1:A:245:SER:O	1:A:246:GLN:HB2	2.21	0.41
1:A:318:ARG:HD2	1:B:108:LEU:O	2.20	0.41
1:A:547:LEU:HD23	1:A:549:ARG:HG3	2.02	0.41
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.90	0.41
1:B:556:TYR:CD1	1:B:556:TYR:C	2.98	0.41
1:A:305:PRO:HA	1:A:306:LEU:HA	1.75	0.41
1:A:108:LEU:HB3	1:A:109:GLY:H	1.57	0.41
1:A:154:LEU:HD22	1:B:516:ARG:HH12	1.85	0.41
1:B:234:ALA:HB1	1:B:239:ARG:O	2.21	0.41
1:A:316:LEU:HG	1:A:323:PRO:HB3	2.03	0.41
1:A:127:TRP:CE2	1:A:131:GLN:NE2	2.89	0.41
1:A:420:LYS:HB3	1:A:421:TYR:CD1	2.55	0.40
1:B:316:LEU:HD11	1:B:326:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:HIS:HB3	1:B:523:MET:HB2	2.03	0.40
1:B:522:PRO:HD3	1:B:549:ARG:NH1	2.36	0.40
1:B:547:LEU:HD13	1:B:547:LEU:HA	1.90	0.40
1:A:139:ASN:O	1:A:140:LEU:HD23	2.20	0.40
1:B:336:ILE:O	1:B:337:ARG:C	2.63	0.40
1:A:211:VAL:HG22	1:A:242:ILE:HB	2.03	0.40
1:A:377:HIS:ND1	1:A:381:GLU:OE1	2.53	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	430/499 (86%)	413 (96%)	17 (4%)	0	100	100
1	B	436/499 (87%)	416 (95%)	20 (5%)	0	100	100
All	All	866/998 (87%)	829 (96%)	37 (4%)	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	387/437 (89%)	360 (93%)	27 (7%)	14	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	391/437 (90%)	366 (94%)	25 (6%)	16	28
All	All	778/874 (89%)	726 (93%)	52 (7%)	15	25

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	146	GLN
1	A	186	ASP
1	A	191	VAL
1	A	205	SER
1	A	206	LYS
1	A	227	VAL
1	A	258	VAL
1	A	273	SER
1	A	281	VAL
1	A	287	GLN
1	A	346	ILE
1	A	351	LYS
1	A	376	PHE
1	A	399	VAL
1	A	400	ASP
1	A	406	LEU
1	A	414	LEU
1	A	423	ASN
1	A	429	ASP
1	A	446	SER
1	A	450	VAL
1	A	469	SER
1	A	470	GLN
1	A	471	VAL
1	A	478	ILE
1	A	517	THR
1	B	108	LEU
1	B	130	LEU
1	B	131	GLN
1	B	132	SER
1	B	171	SER
1	B	173	THR
1	B	222	CYS
1	B	229	TYR
1	B	270	SER

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Mol	Chain	Res	Type
1	B	276	HIS
1	B	295	ASP
1	B	296	SER
1	B	325	VAL
1	B	342	LEU
1	B	384	VAL
1	B	429	ASP
1	B	446	SER
1	B	454	ILE
1	B	466	THR
1	B	471	VAL
1	B	519	ASP
1	B	531	VAL
1	B	545	ARG
1	B	555	SER
1	B	558	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	146	GLN
1	A	148	HIS
1	A	223	GLN
1	A	287	GLN
1	A	298	HIS
1	A	491	HIS
1	B	148	HIS
1	B	276	HIS
1	B	389	HIS
1	B	514	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
2	A1EJM	B	601	1	17,18,31	0.17	0	16,17,39	0.38	0

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	A1EJM	B	601	1	-	7/16/16/43	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

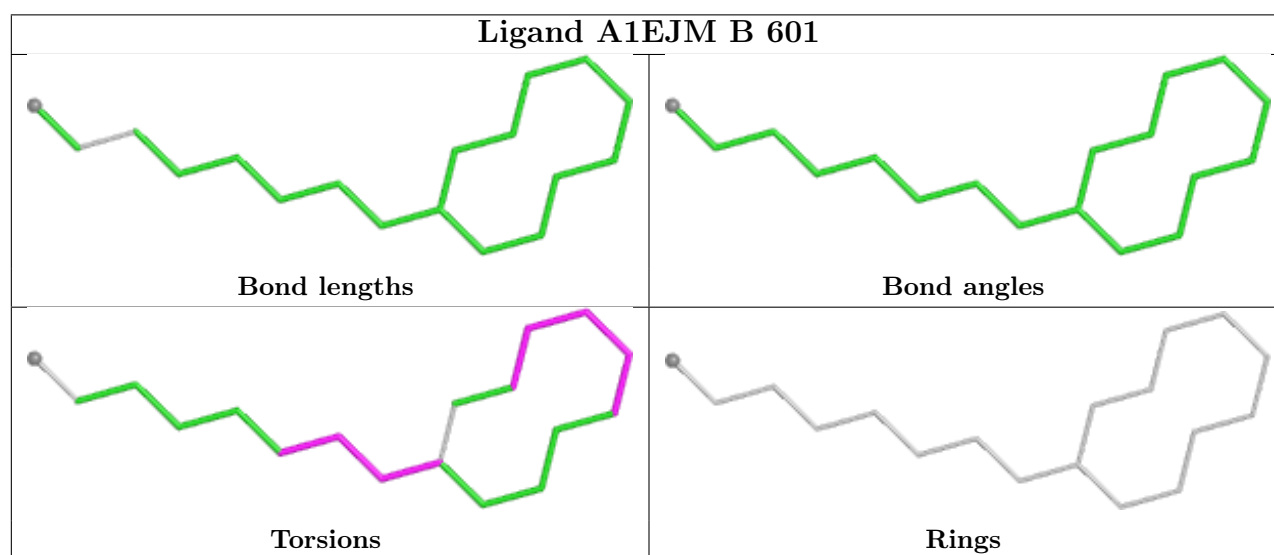
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	A1EJM	C4-C5-C6-C7
2	B	601	A1EJM	C3-C4-C5-C6
2	B	601	A1EJM	C5-C6-C7-C8
2	B	601	A1EJM	C10-C11-C12-C13
2	B	601	A1EJM	C11-C12-C13-C14
2	B	601	A1EJM	C12-C13-C14-C15
2	B	601	A1EJM	C2-C3-C4-C5

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	438/499 (87%)	0.87	29 (6%) 24 18	55, 86, 118, 134	0
1	B	444/499 (88%)	0.45	18 (4%) 41 33	49, 69, 101, 132	0
All	All	882/998 (88%)	0.66	47 (5%) 32 25	49, 77, 114, 134	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	LEU	6.4
1	A	108	LEU	4.3
1	B	336	ILE	3.9
1	A	274	THR	3.8
1	B	253	GLY	3.3
1	B	375	ALA	3.3
1	A	221	GLY	3.3
1	A	222	CYS	3.0
1	B	432	ILE	2.9
1	A	342	LEU	2.6
1	A	375	ALA	2.6
1	B	127	TRP	2.6
1	B	266	CYS	2.6
1	A	464	VAL	2.5
1	A	212	CYS	2.5
1	A	214	ILE	2.5
1	A	271	GLY	2.5
1	A	272	ILE	2.4
1	A	145	LEU	2.4
1	B	204	CYS	2.4
1	A	388	GLU	2.3
1	A	414	LEU	2.3
1	A	532	ALA	2.3
1	B	149	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	337	ARG	2.3
1	A	518	ALA	2.3
1	A	365	ARG	2.3
1	A	289	VAL	2.3
1	A	254	GLY	2.3
1	B	130	LEU	2.3
1	B	281	VAL	2.3
1	A	421	TYR	2.2
1	B	145	LEU	2.2
1	A	311	ASP	2.2
1	B	295	ASP	2.2
1	A	213	ASN	2.1
1	B	298	HIS	2.1
1	A	142	GLY	2.1
1	A	454	ILE	2.1
1	B	409	ASP	2.1
1	A	134	LEU	2.1
1	B	148	HIS	2.1
1	A	427	ILE	2.0
1	A	376	PHE	2.0
1	A	390	PHE	2.0
1	B	431	SER	2.0
1	A	210	LEU	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.

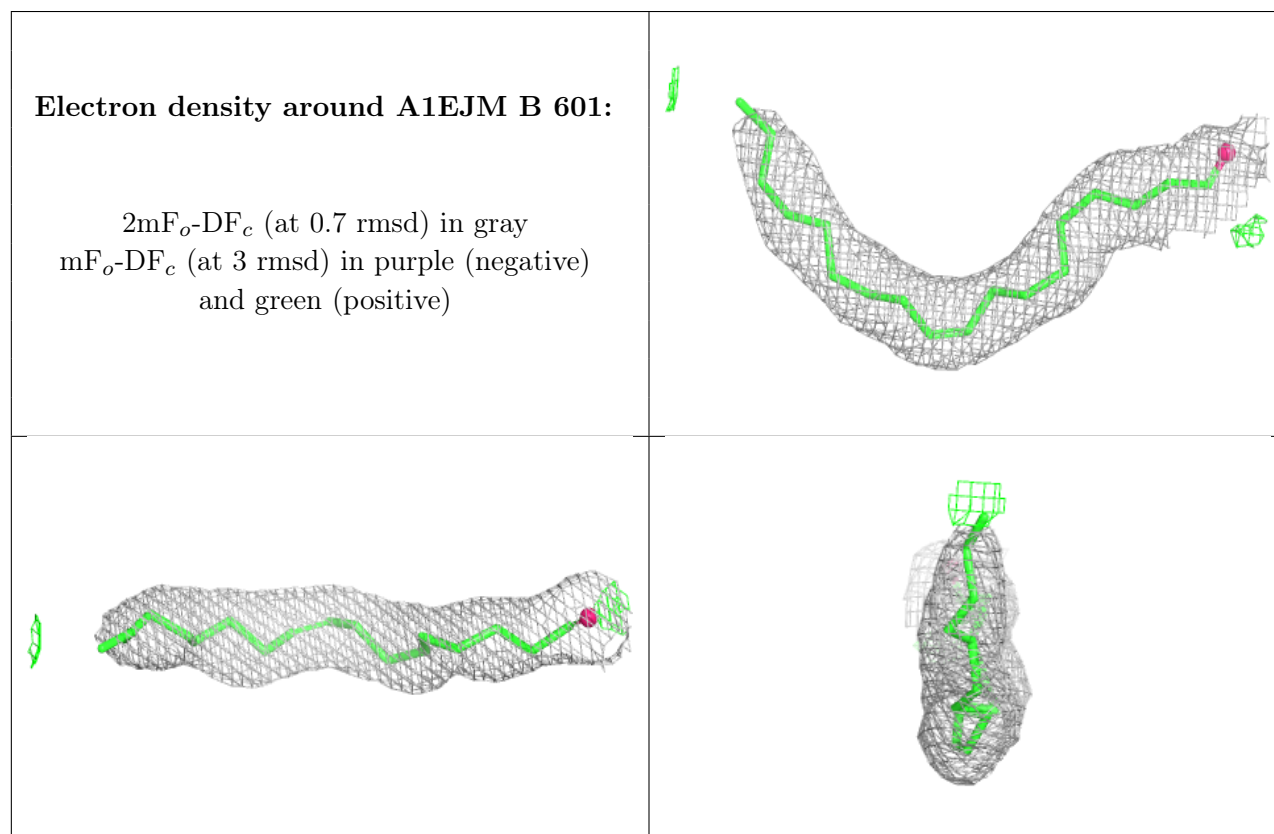
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1EJM	B	601	19/31	0.95	0.13	53,63,76,78	0

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.



6.5 Other polymers ⓘ

There are no such residues in this entry.