



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2026 – 08:22 AM JST

PDB ID : 9WAV / pdb_00009wav
Title : Crystal Structure of Munia coronavirus HKU13 Main Proteinase in Complex with a Broad-spectrum Inhibitor
Authors : Liu, L.; Chen, Z.F.; Yang, X.; Zhang, X.L.; Liu, H.; Bai, F.
Deposited on : 2025-08-12
Resolution : 2.25 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

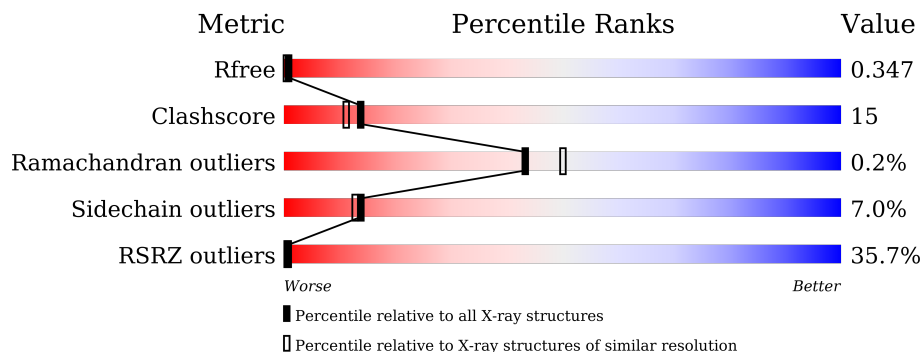
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	301	44% 69% 26% ..
1	B	301	26% 63% 29% ...

2 Entry composition [i](#)

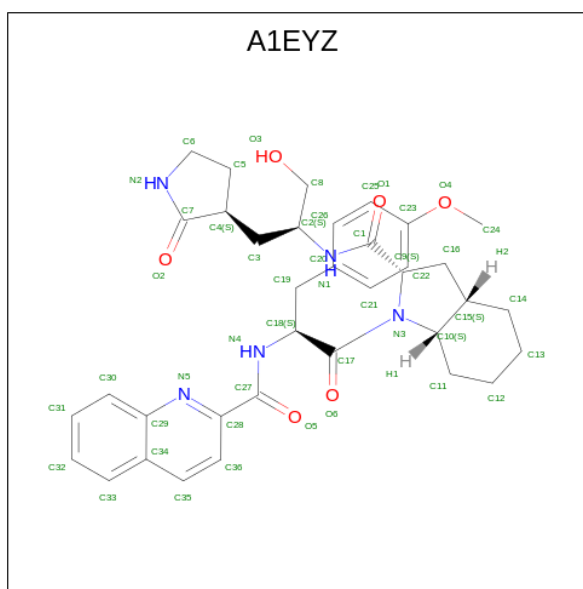
There are 3 unique types of molecules in this entry. The entry contains 4751 atoms, of which 83 are hydrogens and 0 are deuteriums.

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 Munia coronavirus HKU13 Main Proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2307	1476	387	425	19			
1	B	288	Total	C	N	O	S	0	0	0
			2258	1443	383	415	17			

- Molecule 2 is N-[(2S)-1-[(2S,3aS,7aS)-2-[(2S)-1-oxidanyl-3-[(3S)-2-oxidanylidene-pyrrolidin-3-yl]propan-2-yl]carbamoyl]-2,3,3a,4,5,6,7,7a-octahydroindol-1-yl]-3-(4-methoxyphenyl)-1-oxidanylidene-propan-2-yl]quinoline-2-carboxamide (CCD ID: A1EYZ) (formula: C₃₆H₄₃N₅O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			89	36	42	5	6		
2	B	1	Total	C	H	N	O	0	0
			88	36	41	5	6		

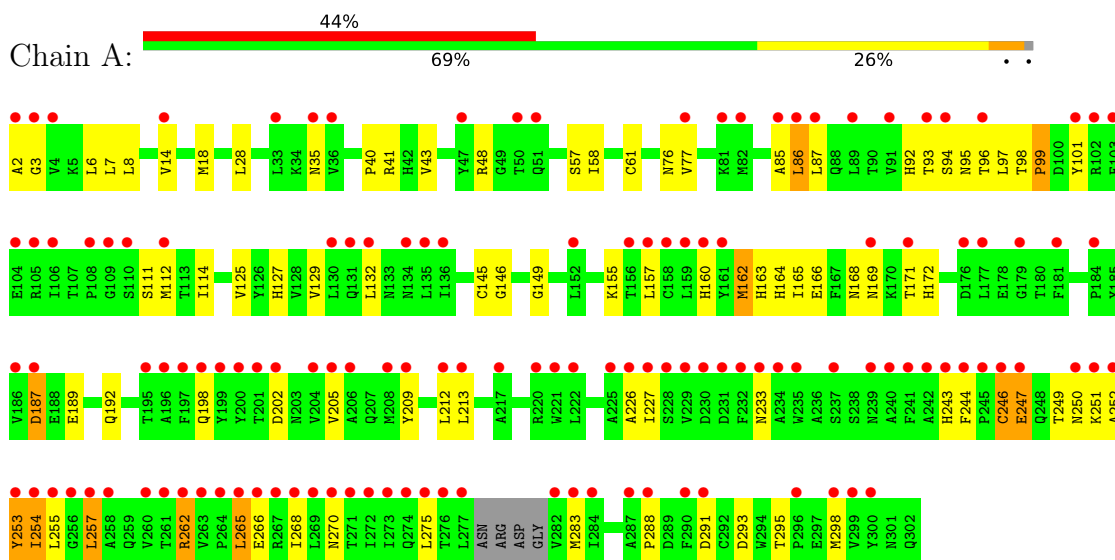
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	2	Total 2	O 2	0	0

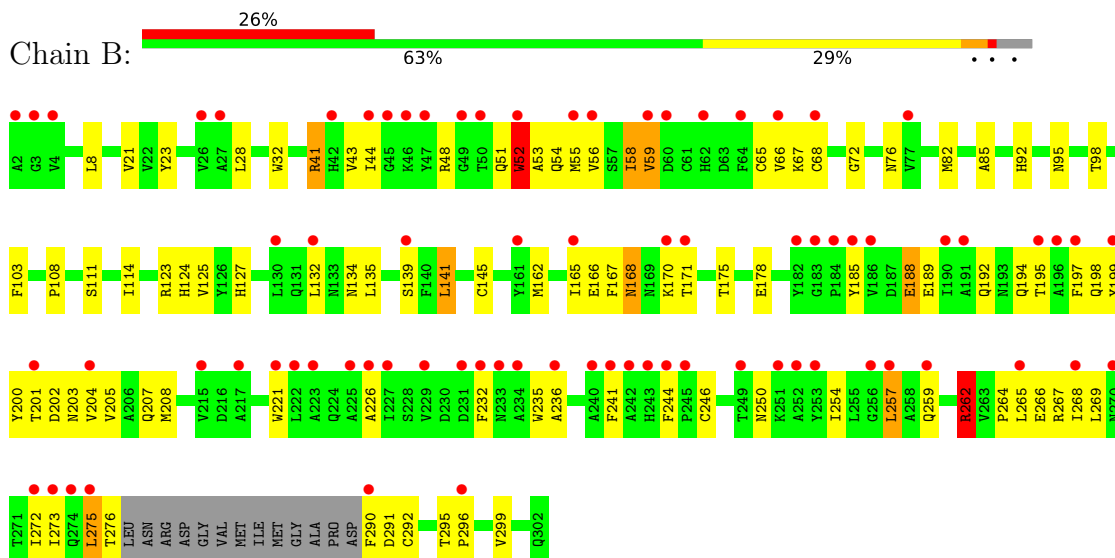
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Munia coronavirus HKU13 Main Proteinase



• Molecule 1: Munia coronavirus HKU13 Main Proteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.39Å 104.39Å 105.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 2.25 47.20 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.20-2.25) 92.0 (47.20-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.323 , 0.344 0.325 , 0.347	Depositor DCC
R_{free} test set	1999 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k 0.006 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4751	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: A1EYZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.73	0/2364	0.97	9/3230 (0.3%)
1	B	0.59	0/2314	0.83	4/3159 (0.1%)
All	All	0.66	0/4678	0.90	13/6389 (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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	TYR	N-CA-C	-7.12	103.71	113.18
1	B	41	ARG	CA-C-N	-6.63	112.05	122.73
1	B	41	ARG	C-N-CA	-6.63	112.05	122.73
1	A	164	HIS	CA-C-O	-6.57	111.12	120.51
1	A	146	GLY	N-CA-C	-6.27	107.23	114.69
1	B	145	CYS	CB-CA-C	5.69	119.80	109.62
1	A	99	PRO	N-CA-CB	-5.66	97.31	103.25
1	A	145	CYS	CB-CA-C	5.26	118.64	109.65
1	A	155	LYS	N-CA-C	-5.14	107.17	112.93
1	A	257	LEU	N-CA-C	-5.14	106.27	112.54
1	A	255	LEU	N-CA-C	-5.11	106.88	113.01
1	A	246	CYS	CB-CA-C	-5.09	102.93	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ARG	N-CA-C	-5.04	107.09	113.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	ARG	Sidechain
1	A	48	ARG	Sidechain
1	B	262	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	2307	0	2233	55	0
1	B	2258	0	2193	82	0
2	A	47	42	0	5	0
2	B	47	41	0	2	0
3	A	7	0	0	0	0
3	B	2	0	0	0	0
All	All	4668	83	4426	132	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 15.

All (132) 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:48:ARG:HG2	1:B:188:GLU:HG2	1.55	0.88
1:B:185:TYR:CE2	1:B:194:GLN:HG3	2.09	0.88
1:B:201:THR:HG22	1:B:246:CYS:SG	2.13	0.87
1:B:21:VAL:HG12	1:B:43:VAL:HG21	1.57	0.84
1:A:3:GLY:H	1:B:139:SER:HA	1.43	0.81
1:A:205:VAL:HG23	1:A:268:ILE:HG21	1.64	0.79
1:B:236:ALA:HB1	1:B:241:PHE:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:CE1	1:B:290:PHE:HB2	2.19	0.78
1:A:295:THR:HG23	1:A:298:MET:H	1.50	0.75
1:B:201:THR:CG2	1:B:246:CYS:SG	2.74	0.74
1:A:227:ILE:HB	1:A:270:ASN:HD22	1.51	0.73
1:A:283:MET:HE2	1:A:288:PRO:HB3	1.71	0.72
1:B:44:ILE:HD11	1:B:52:TRP:HE3	1.55	0.71
1:B:264:PRO:HD2	1:B:267:ARG:HD3	1.73	0.71
1:A:8:LEU:HD22	1:B:8:LEU:HD22	1.74	0.70
1:A:7:LEU:H	1:A:298:MET:CE	2.06	0.69
1:A:165:ILE:HD12	2:A:401:A1EYZ:C30	2.23	0.69
1:A:251:LYS:HA	1:A:254:ILE:HG22	1.76	0.68
1:B:235:TRP:CE3	1:B:273:ILE:HG12	2.30	0.66
1:B:85:ALA:HB3	1:B:175:THR:HG21	1.77	0.66
1:B:21:VAL:HG22	1:B:66:VAL:HG22	1.79	0.65
1:B:166:GLU:HB2	2:B:401:A1EYZ:C7	2.27	0.65
1:A:61:CYS:HB3	1:A:77:VAL:HG12	1.79	0.64
1:A:7:LEU:H	1:A:298:MET:HE3	1.63	0.64
1:A:202:ASP:O	1:A:205:VAL:HG12	1.99	0.63
1:A:189:GLU:HA	2:A:401:A1EYZ:O5	1.98	0.62
1:A:28:LEU:HD13	1:A:40:PRO:HD2	1.80	0.62
1:A:209:TYR:O	1:A:213:LEU:HD12	2.00	0.61
1:B:185:TYR:CZ	1:B:194:GLN:HG3	2.34	0.61
1:A:2:ALA:HB2	1:B:141:LEU:HD22	1.82	0.61
1:A:247:GLU:HG2	1:A:250:ASN:HB2	1.83	0.60
1:A:112:MET:HE2	1:A:149:GLY:HA3	1.84	0.60
1:A:41:ARG:HD3	1:A:85:ALA:HA	1.83	0.60
1:B:55:MET:SD	1:B:55:MET:N	2.75	0.60
1:B:135:LEU:HD11	1:B:194:GLN:HB3	1.84	0.58
1:B:44:ILE:HD11	1:B:52:TRP:CE3	2.39	0.57
1:A:251:LYS:O	1:A:252:ALA:HB3	2.05	0.57
1:A:254:ILE:HD13	1:A:265:LEU:HD23	1.87	0.56
1:B:203:ASN:ND2	1:B:292:CYS:O	2.30	0.56
1:B:291:ASP:OD1	1:B:292:CYS:N	2.38	0.56
1:B:52:TRP:HB2	1:B:82:MET:SD	2.45	0.56
1:A:251:LYS:C	1:A:253:TYR:H	2.13	0.56
1:A:28:LEU:HD21	1:A:43:VAL:HB	1.88	0.55
1:B:201:THR:HA	1:B:204:VAL:HG22	1.89	0.54
1:A:111:SER:HB2	1:A:127:HIS:NE2	2.23	0.54
1:B:166:GLU:O	1:B:166:GLU:HG2	2.07	0.54
1:B:108:PRO:HB3	1:B:132:LEU:HA	1.90	0.53
1:B:48:ARG:HG2	1:B:188:GLU:CG	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PHE:HE2	1:B:199:TYR:CD1	2.26	0.53
1:A:166:GLU:HB2	2:A:401:A1EYZ:O2	2.09	0.53
1:B:208:MET:HE1	1:B:221:TRP:HZ3	1.73	0.53
1:B:52:TRP:H	1:B:52:TRP:CD1	2.26	0.52
1:B:244:PHE:CE2	1:B:265:LEU:HD21	2.45	0.52
1:B:103:PHE:HD2	1:B:178:GLU:HG2	1.74	0.51
1:A:76:ASN:H	1:A:92:HIS:CD2	2.29	0.51
1:A:209:TYR:HD1	1:A:212:LEU:HD12	1.76	0.51
1:A:233:ASN:OD1	1:A:244:PHE:HB3	2.11	0.51
1:B:56:VAL:HA	1:B:59:VAL:HG22	1.92	0.51
1:A:8:LEU:HD11	1:A:127:HIS:HB2	1.93	0.51
1:A:7:LEU:H	1:A:298:MET:HE1	1.76	0.50
1:A:41:ARG:HA	1:A:87:LEU:HD13	1.93	0.50
1:A:205:VAL:HG23	1:A:268:ILE:CG2	2.37	0.50
1:A:6:LEU:HA	1:A:298:MET:HE1	1.93	0.50
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.12	0.49
1:B:76:ASN:HB2	1:B:92:HIS:HB3	1.94	0.49
1:B:235:TRP:CH2	1:B:273:ILE:HA	2.48	0.49
1:B:114:ILE:O	1:B:125:VAL:HA	2.12	0.49
1:A:265:LEU:O	1:A:268:ILE:N	2.46	0.49
1:B:111:SER:HB2	1:B:127:HIS:CE1	2.48	0.49
1:B:32:TRP:CE2	1:B:95:ASN:HB2	2.47	0.48
1:A:114:ILE:O	1:A:125:VAL:HA	2.13	0.48
1:A:226:ALA:HB1	1:A:266:GLU:HB3	1.94	0.48
1:B:132:LEU:HD13	1:B:198:GLN:O	2.12	0.48
1:A:7:LEU:HD13	1:B:124:HIS:CD2	2.48	0.48
1:B:201:THR:O	1:B:205:VAL:HG23	2.13	0.48
1:A:3:GLY:N	1:B:139:SER:HA	2.22	0.47
1:A:129:VAL:HG11	1:A:293:ASP:HA	1.97	0.47
1:A:192:GLN:NE2	2:A:401:A1EYZ:C35	2.78	0.47
1:A:41:ARG:NE	1:A:187:ASP:OD2	2.48	0.46
1:B:132:LEU:H	1:B:132:LEU:HD12	1.79	0.46
1:B:232:PHE:CG	1:B:269:LEU:HD12	2.51	0.46
1:B:168:ASN:C	1:B:170:LYS:N	2.70	0.46
1:B:23:TYR:HB3	1:B:43:VAL:O	2.15	0.46
1:A:162:MET:HE3	1:A:162:MET:HB2	1.83	0.46
1:B:257:LEU:HD21	1:B:299:VAL:HG23	1.98	0.46
1:A:251:LYS:C	1:A:253:TYR:N	2.73	0.45
1:B:235:TRP:CD2	1:B:273:ILE:HG12	2.52	0.45
1:B:185:TYR:CD2	1:B:192:GLN:HG2	2.51	0.45
1:A:112:MET:CE	1:A:160:HIS:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD11	1:B:200:TYR:HD1	1.82	0.45
1:B:272:ILE:HG23	1:B:290:PHE:CZ	2.52	0.45
1:B:232:PHE:CD1	1:B:269:LEU:HD12	2.52	0.44
1:B:250:ASN:O	1:B:254:ILE:HG13	2.17	0.44
1:B:185:TYR:CE2	1:B:192:GLN:HG2	2.52	0.44
1:B:58:ILE:O	1:B:59:VAL:C	2.60	0.44
1:A:168:ASN:O	1:A:169:ASN:C	2.60	0.44
1:B:68:CYS:O	1:B:72:GLY:N	2.50	0.44
1:B:226:ALA:HB1	1:B:266:GLU:HB3	1.99	0.44
1:A:132:LEU:HD12	1:A:198:GLN:O	2.17	0.44
1:B:41:ARG:O	1:B:44:ILE:HG12	2.17	0.44
1:B:168:ASN:HD22	1:B:168:ASN:HA	1.55	0.44
1:B:207:GLN:HE22	1:B:291:ASP:HB3	1.82	0.44
1:B:23:TYR:CD2	1:B:44:ILE:HA	2.53	0.44
1:B:23:TYR:HB3	1:B:43:VAL:HG22	2.00	0.43
1:B:48:ARG:HA	1:B:188:GLU:OE2	2.18	0.43
1:B:162:MET:HE3	1:B:162:MET:HB2	1.85	0.43
1:B:103:PHE:CD2	1:B:178:GLU:HG2	2.52	0.43
1:B:167:PHE:CE1	2:B:401:A1EYZ:C35	3.02	0.43
1:B:232:PHE:CD2	1:B:269:LEU:HD12	2.54	0.43
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.18	0.43
1:B:202:ASP:OD1	1:B:246:CYS:HB2	2.19	0.43
1:B:123:ARG:O	1:B:124:HIS:ND1	2.51	0.43
1:B:262:ARG:HA	1:B:262:ARG:HD3	1.49	0.43
1:B:167:PHE:HZ	1:B:185:TYR:HB3	1.84	0.43
1:A:14:VAL:O	1:A:18:MET:HG2	2.19	0.42
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.54	0.42
1:B:23:TYR:CB	1:B:43:VAL:HG22	2.49	0.42
1:A:35:ASN:HB3	1:A:94:SER:HB2	2.02	0.42
1:B:132:LEU:C	1:B:134:ASN:H	2.28	0.42
1:A:166:GLU:HB2	2:A:401:A1EYZ:C7	2.49	0.41
1:B:295:THR:O	1:B:299:VAL:HG22	2.19	0.41
1:B:51:GLN:O	1:B:53:ALA:N	2.54	0.41
1:A:111:SER:HB2	1:A:127:HIS:CE1	2.56	0.41
1:B:202:ASP:HB3	1:B:296:PRO:HG2	2.03	0.41
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.79	0.41
1:B:21:VAL:HB	1:B:28:LEU:HD12	2.02	0.41
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.84	0.41
1:A:86:LEU:HD22	1:A:86:LEU:HA	1.95	0.41
1:B:208:MET:HB3	1:B:268:ILE:HD12	2.03	0.41
1:A:101:TYR:HA	1:A:157:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:CYS:SG	1:B:67:LYS:HE3	2.61	0.41
1:B:194:GLN:H	1:B:194:GLN:CD	2.28	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	293/301 (97%)	273 (93%)	20 (7%)	0	100	100
1	B	284/301 (94%)	269 (95%)	14 (5%)	1 (0%)	30	31
All	All	577/602 (96%)	542 (94%)	34 (6%)	1 (0%)	43	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	TRP

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	251/259 (97%)	232 (92%)	19 (8%)	12	10
1	B	247/259 (95%)	231 (94%)	16 (6%)	15	14
All	All	498/518 (96%)	463 (93%)	35 (7%)	14	13

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	58	ILE
1	A	86	LEU
1	A	93	THR
1	A	96	THR
1	A	97	LEU
1	A	99	PRO
1	A	162	MET
1	A	171	THR
1	A	187	ASP
1	A	243	HIS
1	A	246	CYS
1	A	247	GLU
1	A	249	THR
1	A	254	ILE
1	A	257	LEU
1	A	262	ARG
1	A	265	LEU
1	A	291	ASP
1	B	52	TRP
1	B	54	GLN
1	B	58	ILE
1	B	59	VAL
1	B	141	LEU
1	B	165	ILE
1	B	168	ASN
1	B	171	THR
1	B	188	GLU
1	B	189	GLU
1	B	195	THR
1	B	257	LEU
1	B	259	GLN
1	B	262	ARG
1	B	275	LEU
1	B	276	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	54	GLN

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Mol	Chain	Res	Type
1	A	92	HIS
1	A	164	HIS
1	A	192	GLN
1	A	194	GLN
1	A	243	HIS
1	A	270	ASN
1	B	131	GLN
1	B	168	ASN
1	B	192	GLN
1	B	207	GLN
1	B	248	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1EYZ	A	401	-	52,52,52	4.81	26 (50%)	71,73,73	3.91	25 (35%)
2	A1EYZ	B	401	1	52,52,52	4.82	29 (55%)	71,73,73	4.28	37 (52%)

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	A1EYZ	A	401	-	-	4/36/69/69	0/6/6/6
2	A1EYZ	B	401	1	-	11/36/69/69	0/6/6/6

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1EYZ	C7-N2	15.47	1.50	1.33
2	B	401	A1EYZ	C7-N2	15.04	1.49	1.33
2	A	401	A1EYZ	C34-C29	14.74	1.65	1.42
2	B	401	A1EYZ	C34-C29	14.14	1.64	1.42
2	B	401	A1EYZ	C36-C28	-9.52	1.21	1.39
2	B	401	A1EYZ	C26-C25	8.77	1.54	1.38
2	A	401	A1EYZ	C36-C28	-8.69	1.22	1.39
2	A	401	A1EYZ	C26-C25	8.60	1.54	1.38
2	A	401	A1EYZ	C29-N5	-7.59	1.25	1.37
2	B	401	A1EYZ	C27-N4	7.56	1.50	1.34
2	B	401	A1EYZ	C29-N5	-7.53	1.25	1.37
2	B	401	A1EYZ	C22-C23	7.50	1.53	1.38
2	A	401	A1EYZ	C22-C23	7.47	1.53	1.38
2	B	401	A1EYZ	C17-N3	7.05	1.50	1.35
2	A	401	A1EYZ	C27-N4	6.95	1.49	1.34
2	A	401	A1EYZ	C17-N3	6.77	1.50	1.35
2	A	401	A1EYZ	C1-N1	6.70	1.48	1.34
2	B	401	A1EYZ	C30-C29	6.69	1.53	1.41
2	B	401	A1EYZ	C1-N1	6.68	1.48	1.34
2	A	401	A1EYZ	C21-C20	6.63	1.53	1.38
2	A	401	A1EYZ	C30-C29	6.61	1.53	1.41
2	B	401	A1EYZ	C28-N5	-6.16	1.15	1.33
2	B	401	A1EYZ	C21-C20	6.15	1.52	1.38
2	A	401	A1EYZ	C35-C34	6.13	1.56	1.41
2	A	401	A1EYZ	C28-N5	-6.09	1.15	1.33
2	B	401	A1EYZ	C35-C34	5.85	1.56	1.41
2	A	401	A1EYZ	C4-C7	-5.72	1.45	1.52
2	B	401	A1EYZ	C4-C7	-5.64	1.45	1.52
2	B	401	A1EYZ	C32-C33	-5.10	1.25	1.36
2	A	401	A1EYZ	C32-C33	-5.05	1.25	1.36
2	B	401	A1EYZ	C31-C32	-4.48	1.26	1.38
2	A	401	A1EYZ	C31-C32	-4.32	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1EYZ	C6-N2	3.41	1.53	1.46
2	A	401	A1EYZ	C6-N2	3.39	1.53	1.46
2	B	401	A1EYZ	O6-C17	-3.39	1.16	1.22
2	B	401	A1EYZ	C9-N3	3.17	1.51	1.46
2	A	401	A1EYZ	C33-C34	-2.86	1.35	1.41
2	B	401	A1EYZ	C33-C34	-2.85	1.35	1.41
2	A	401	A1EYZ	C22-C21	-2.79	1.33	1.38
2	A	401	A1EYZ	O2-C7	-2.78	1.17	1.23
2	B	401	A1EYZ	O2-C7	-2.78	1.17	1.23
2	B	401	A1EYZ	C22-C21	-2.72	1.33	1.38
2	B	401	A1EYZ	C25-C23	-2.64	1.33	1.38
2	A	401	A1EYZ	C26-C20	-2.63	1.33	1.38
2	B	401	A1EYZ	C15-C10	-2.56	1.49	1.53
2	A	401	A1EYZ	C35-C36	2.52	1.41	1.36
2	A	401	A1EYZ	C28-C27	2.48	1.56	1.50
2	A	401	A1EYZ	O6-C17	-2.48	1.18	1.22
2	B	401	A1EYZ	O5-C27	-2.40	1.18	1.23
2	A	401	A1EYZ	C25-C23	-2.32	1.34	1.38
2	B	401	A1EYZ	C26-C20	-2.16	1.34	1.38
2	B	401	A1EYZ	C35-C36	2.14	1.41	1.36
2	B	401	A1EYZ	O1-C1	-2.04	1.19	1.23
2	A	401	A1EYZ	O5-C27	-2.02	1.19	1.23
2	B	401	A1EYZ	C19-C20	2.01	1.56	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	A1EYZ	C30-C29-N5	19.57	148.53	118.69
2	A	401	A1EYZ	C30-C29-N5	19.00	147.66	118.69
2	B	401	A1EYZ	C30-C29-C34	-17.04	101.11	119.04
2	A	401	A1EYZ	C30-C29-C34	-16.34	101.84	119.04
2	A	401	A1EYZ	C28-N5-C29	10.23	132.55	117.51
2	B	401	A1EYZ	C28-N5-C29	10.07	132.32	117.51
2	B	401	A1EYZ	C36-C28-N5	8.28	133.65	123.42
2	B	401	A1EYZ	C34-C29-N5	-8.00	110.36	122.26
2	A	401	A1EYZ	C34-C29-N5	-7.90	110.50	122.26
2	B	401	A1EYZ	C18-C17-N3	7.35	132.01	118.61
2	A	401	A1EYZ	C36-C28-N5	7.33	132.48	123.42
2	B	401	A1EYZ	C35-C34-C29	-6.06	109.90	118.45
2	A	401	A1EYZ	C35-C34-C29	-5.46	110.75	118.45
2	B	401	A1EYZ	O6-C17-N3	-5.13	113.89	121.68
2	B	401	A1EYZ	C28-C27-N4	4.67	123.88	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1EYZ	C16-C9-N3	4.43	109.09	103.47
2	B	401	A1EYZ	C35-C36-C28	-4.07	114.26	118.81
2	A	401	A1EYZ	C3-C2-C8	-4.05	106.02	111.65
2	B	401	A1EYZ	C33-C34-C29	3.76	123.76	118.45
2	B	401	A1EYZ	C5-C4-C7	3.73	107.73	102.88
2	A	401	A1EYZ	C9-N3-C10	-3.67	106.27	112.22
2	B	401	A1EYZ	C9-N3-C17	3.57	133.28	121.07
2	A	401	A1EYZ	C6-N2-C7	-3.41	107.14	113.84
2	B	401	A1EYZ	C16-C9-C1	-3.39	104.55	111.32
2	B	401	A1EYZ	C15-C10-N3	3.36	107.21	102.24
2	B	401	A1EYZ	C31-C30-C29	3.31	124.84	120.08
2	B	401	A1EYZ	O5-C27-C28	-3.19	114.14	121.08
2	A	401	A1EYZ	C5-C4-C7	3.10	106.90	102.88
2	A	401	A1EYZ	C33-C34-C29	3.09	122.81	118.45
2	B	401	A1EYZ	O6-C17-C18	-3.09	114.08	119.66
2	A	401	A1EYZ	C31-C30-C29	3.06	124.48	120.08
2	A	401	A1EYZ	C27-C28-N5	-3.06	108.98	116.94
2	B	401	A1EYZ	C9-N3-C10	-3.05	107.28	112.22
2	B	401	A1EYZ	C6-N2-C7	-2.94	108.06	113.84
2	A	401	A1EYZ	C3-C4-C7	-2.81	106.72	112.89
2	B	401	A1EYZ	C19-C18-N4	2.74	116.56	110.79
2	A	401	A1EYZ	C12-C11-C10	2.66	116.88	109.91
2	B	401	A1EYZ	C16-C15-C10	2.63	108.12	103.17
2	B	401	A1EYZ	C27-C28-N5	-2.63	110.09	116.94
2	B	401	A1EYZ	C24-O4-C23	-2.62	111.83	117.51
2	A	401	A1EYZ	C35-C36-C28	-2.56	115.94	118.81
2	B	401	A1EYZ	C3-C4-C5	-2.56	107.89	117.31
2	B	401	A1EYZ	C10-N3-C17	-2.54	119.35	126.84
2	B	401	A1EYZ	C17-C18-N4	2.46	114.56	108.81
2	A	401	A1EYZ	C32-C33-C34	2.40	124.20	120.44
2	B	401	A1EYZ	C19-C18-C17	2.38	114.95	109.93
2	B	401	A1EYZ	C3-C4-C7	-2.26	107.92	112.89
2	A	401	A1EYZ	C12-C13-C14	-2.24	106.85	111.42
2	A	401	A1EYZ	C8-C2-N1	-2.24	104.59	109.60
2	B	401	A1EYZ	C32-C33-C34	2.21	123.89	120.44
2	B	401	A1EYZ	C16-C9-N3	2.19	106.25	103.47
2	B	401	A1EYZ	C18-N4-C27	-2.17	116.29	121.60
2	A	401	A1EYZ	C32-C31-C30	2.16	123.47	120.44
2	A	401	A1EYZ	O3-C8-C2	-2.13	106.45	111.95
2	A	401	A1EYZ	C24-O4-C23	-2.12	112.90	117.51
2	A	401	A1EYZ	C15-C10-N3	2.11	105.35	102.24
2	A	401	A1EYZ	C16-C15-C14	-2.11	110.71	116.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	A1EYZ	C36-C28-C27	-2.08	116.18	119.57
2	B	401	A1EYZ	C32-C31-C30	2.05	123.32	120.44
2	B	401	A1EYZ	O1-C1-N1	-2.05	119.14	122.93
2	B	401	A1EYZ	C20-C19-C18	-2.03	107.78	113.39
2	B	401	A1EYZ	C19-C20-C21	-2.02	116.90	120.91

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1EYZ	C3-C2-C8-O3
2	B	401	A1EYZ	O5-C27-C28-N5
2	B	401	A1EYZ	O5-C27-C28-C36
2	B	401	A1EYZ	N4-C27-C28-N5
2	B	401	A1EYZ	N4-C27-C28-C36
2	B	401	A1EYZ	C3-C2-C8-O3
2	A	401	A1EYZ	C25-C23-O4-C24
2	A	401	A1EYZ	C22-C23-O4-C24
2	B	401	A1EYZ	C25-C23-O4-C24
2	B	401	A1EYZ	C22-C23-O4-C24
2	A	401	A1EYZ	N1-C2-C8-O3
2	B	401	A1EYZ	O6-C17-C18-C19
2	B	401	A1EYZ	N3-C17-C18-C19
2	B	401	A1EYZ	N1-C2-C8-O3
2	B	401	A1EYZ	N4-C18-C19-C20

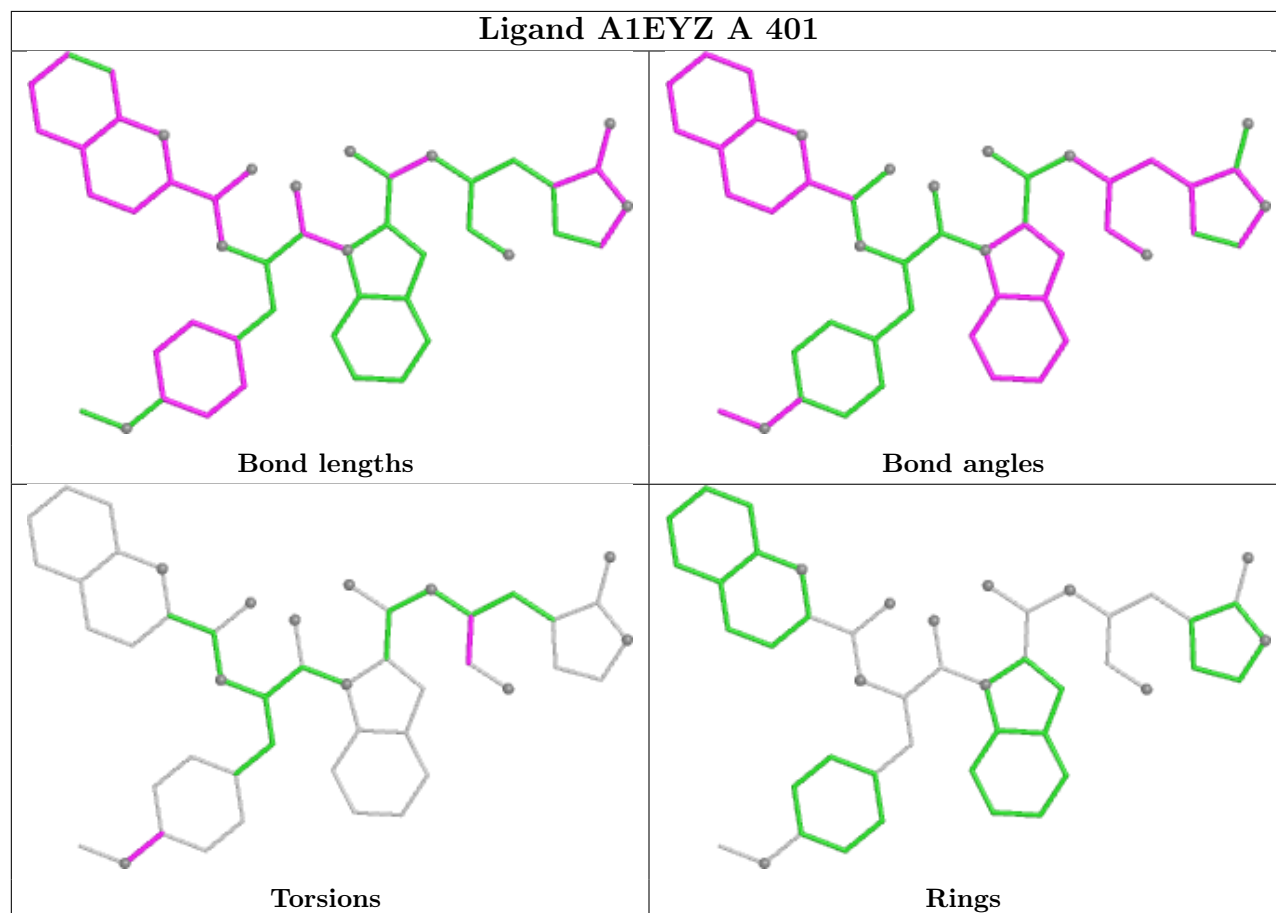
There are no ring outliers.

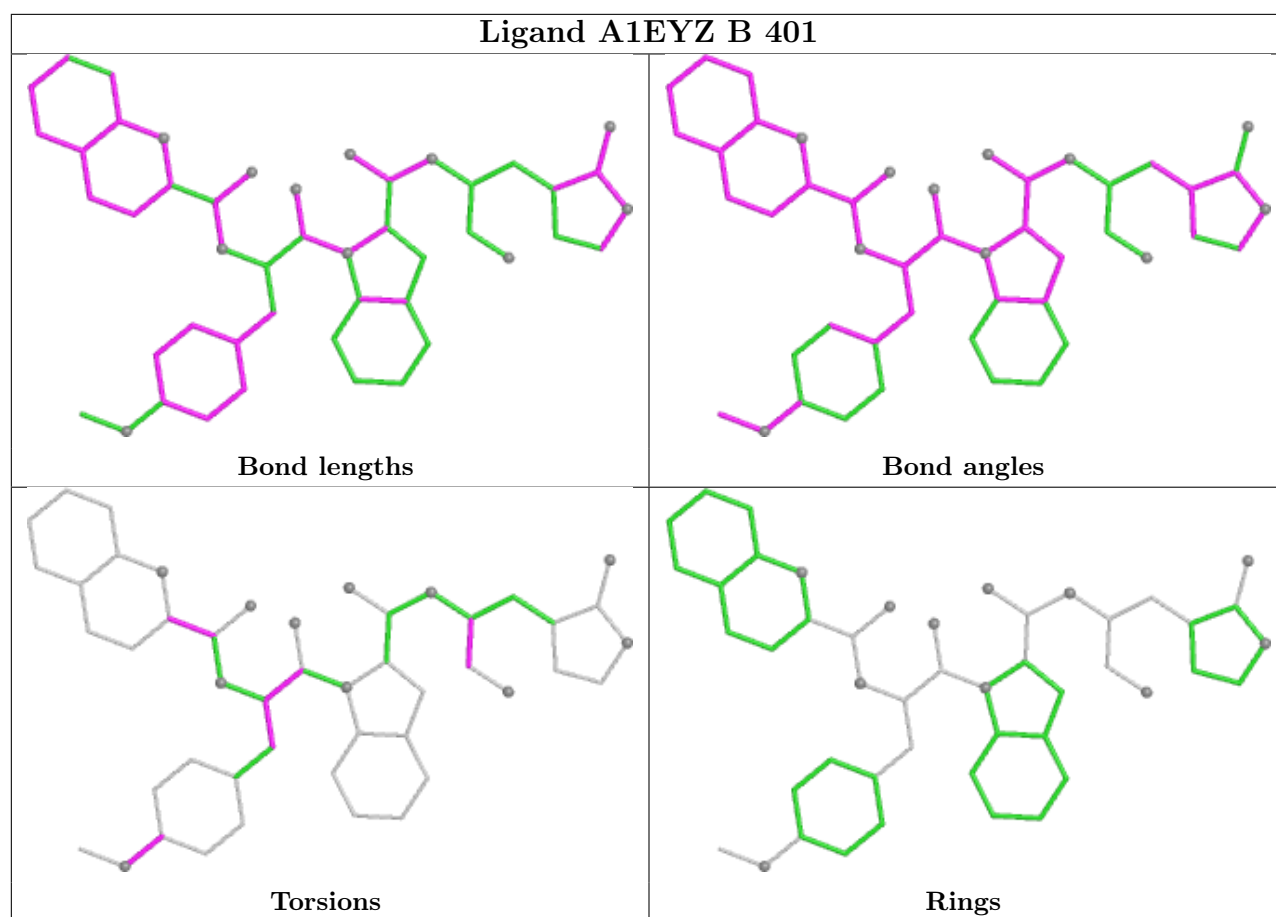
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	A1EYZ	5	0
2	B	401	A1EYZ	2	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	297/301 (98%)	1.89	131 (44%) 0 0	29, 68, 141, 168	0
1	B	288/301 (95%)	1.53	78 (27%) 1 1	38, 76, 133, 149	0
All	All	585/602 (97%)	1.71	209 (35%) 1 0	29, 72, 137, 168	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	PHE	9.2
1	B	268	ILE	6.0
1	A	232	PHE	5.8
1	B	197	PHE	5.2
1	A	265	LEU	5.2
1	B	272	ILE	5.0
1	A	282	VAL	4.8
1	A	229	VAL	4.8
1	A	268	ILE	4.7
1	A	205	VAL	4.7
1	A	269	LEU	4.7
1	A	241	PHE	4.6
1	A	226	ALA	4.5
1	A	240	ALA	4.5
1	A	255	LEU	4.4
1	A	252	ALA	4.3
1	B	244	PHE	4.3
1	A	257	LEU	4.1
1	A	227	ILE	4.1
1	A	242	ALA	4.1
1	A	263	VAL	4.1
1	B	290	PHE	4.0
1	A	260	VAL	4.0
1	A	200	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	201	THR	4.0
1	A	272	ILE	3.9
1	A	201	THR	3.9
1	A	251	LYS	3.8
1	B	190	ILE	3.8
1	B	217	ALA	3.8
1	A	221	TRP	3.8
1	A	253	TYR	3.7
1	B	165	ILE	3.7
1	A	3	GLY	3.7
1	A	157	LEU	3.7
1	A	106	ILE	3.7
1	A	273	ILE	3.7
1	B	56	VAL	3.7
1	B	185	TYR	3.7
1	B	275	LEU	3.6
1	A	264	PRO	3.6
1	A	250	ASN	3.6
1	A	101	TYR	3.6
1	B	196	ALA	3.6
1	A	89	LEU	3.5
1	A	277	LEU	3.5
1	A	228	SER	3.5
1	A	33	LEU	3.5
1	A	275	LEU	3.5
1	A	254	ILE	3.5
1	A	212	LEU	3.5
1	B	204	VAL	3.4
1	A	256	GLY	3.4
1	A	204	VAL	3.4
1	A	233	ASN	3.4
1	B	52	TRP	3.4
1	A	91	VAL	3.4
1	B	229	VAL	3.4
1	A	208	MET	3.3
1	A	199	TYR	3.3
1	A	36	VAL	3.3
1	B	49	GLY	3.3
1	A	245	PRO	3.3
1	A	103	PHE	3.3
1	A	235	TRP	3.3
1	A	276	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	87	LEU	3.2
1	A	152	LEU	3.2
1	A	290	PHE	3.1
1	A	2	ALA	3.1
1	A	284	ILE	3.0
1	A	202	ASP	3.0
1	A	246	CYS	3.0
1	B	191	ALA	3.0
1	B	226	ALA	3.0
1	B	50	THR	3.0
1	B	256	GLY	3.0
1	A	222	LEU	2.9
1	B	170	LYS	2.9
1	A	231	ASP	2.9
1	A	135	LEU	2.9
1	A	225	ALA	2.9
1	A	4	VAL	2.9
1	A	156	THR	2.9
1	A	209	TYR	2.8
1	B	265	LEU	2.8
1	B	241	PHE	2.8
1	A	299	VAL	2.8
1	B	59	VAL	2.8
1	B	227	ILE	2.8
1	A	270	ASN	2.8
1	B	62	HIS	2.8
1	A	102	ARG	2.8
1	B	60	ASP	2.8
1	A	296	PRO	2.8
1	A	86	LEU	2.8
1	B	130	LEU	2.8
1	B	47	TYR	2.8
1	A	243	HIS	2.7
1	B	252	ALA	2.7
1	A	298	MET	2.7
1	A	287	ALA	2.7
1	A	300	TYR	2.7
1	A	50	THR	2.7
1	A	169	ASN	2.7
1	A	213	LEU	2.7
1	B	234	ALA	2.7
1	B	195	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	139	SER	2.7
1	A	47	TYR	2.6
1	B	215	VAL	2.6
1	A	104	GLU	2.6
1	B	66	VAL	2.6
1	A	198	GLN	2.6
1	B	222	LEU	2.6
1	A	262	ARG	2.6
1	B	55	MET	2.6
1	B	68	CYS	2.6
1	A	217	ALA	2.6
1	A	230	ASP	2.6
1	A	108	PRO	2.6
1	A	179	GLY	2.6
1	B	296	PRO	2.6
1	A	160	HIS	2.6
1	B	251	LYS	2.6
1	B	257	LEU	2.5
1	A	181	PHE	2.5
1	B	184	PRO	2.5
1	A	261	THR	2.5
1	B	77	VAL	2.5
1	A	161	TYR	2.5
1	A	93	THR	2.4
1	A	197	PHE	2.4
1	B	232	PHE	2.4
1	B	44	ILE	2.4
1	B	221	TRP	2.4
1	A	81	LYS	2.4
1	B	46	LYS	2.4
1	A	291	ASP	2.4
1	B	4	VAL	2.4
1	B	186	VAL	2.4
1	A	132	LEU	2.4
1	B	270	ASN	2.4
1	B	27	ALA	2.4
1	B	225	ALA	2.4
1	A	96	THR	2.4
1	B	245	PRO	2.3
1	B	242	ALA	2.3
1	B	243	HIS	2.3
1	B	132	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	247	GLU	2.3
1	B	199	TYR	2.3
1	A	94	SER	2.3
1	A	14	VAL	2.3
1	A	288	PRO	2.3
1	A	112	MET	2.3
1	A	234	ALA	2.3
1	A	283	MET	2.3
1	A	271	THR	2.3
1	A	220	ARG	2.3
1	A	237	SER	2.3
1	A	77	VAL	2.3
1	A	130	LEU	2.3
1	A	158	CYS	2.3
1	B	233	ASN	2.3
1	B	45	GLY	2.3
1	B	183	GLY	2.3
1	A	184	PRO	2.2
1	A	85	ALA	2.2
1	A	131	GLN	2.2
1	B	171	THR	2.2
1	B	274	GLN	2.2
1	B	273	ILE	2.2
1	A	35	ASN	2.2
1	A	239	ASN	2.2
1	B	240	ALA	2.2
1	B	161	TYR	2.2
1	B	26	VAL	2.2
1	B	64	PHE	2.2
1	A	109	GLY	2.2
1	A	171	THR	2.2
1	B	249	THR	2.2
1	A	105	ARG	2.1
1	A	136	ILE	2.1
1	A	187	ASP	2.1
1	A	176	ASP	2.1
1	A	186	VAL	2.1
1	A	206	ALA	2.1
1	B	2	ALA	2.1
1	A	134	ASN	2.1
1	B	231	ASP	2.1
1	B	253	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	110	SER	2.1
1	B	223	ALA	2.1
1	A	266	GLU	2.1
1	A	51	GLN	2.1
1	B	182	TYR	2.1
1	A	195	THR	2.0
1	A	82	MET	2.0
1	A	196	ALA	2.0
1	A	258	ALA	2.0
1	B	236	ALA	2.0
1	A	274	GLN	2.0
1	A	177	LEU	2.0
1	A	267	ARG	2.0
1	B	3	GLY	2.0
1	B	42	HIS	2.0
1	B	259	GLN	2.0
1	A	159	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](#)

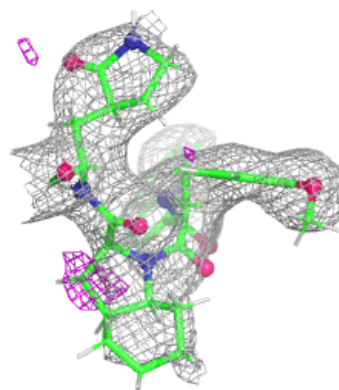
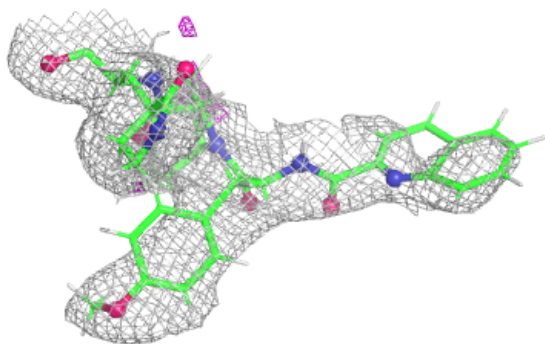
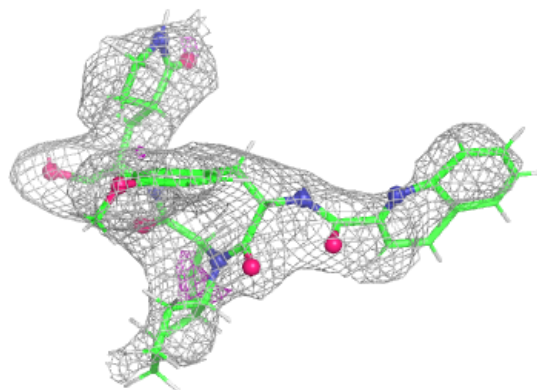
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1EYZ	B	401	47/47	0.72	0.15	51,88,123,139	0
2	A1EYZ	A	401	47/47	0.76	0.12	30,43,55,61	0

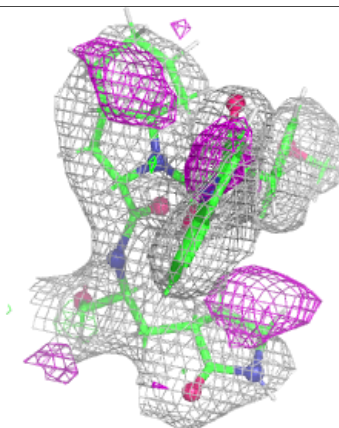
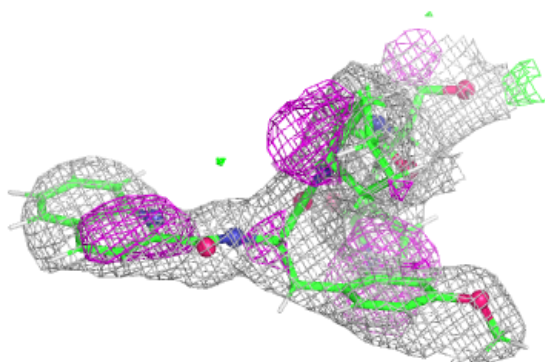
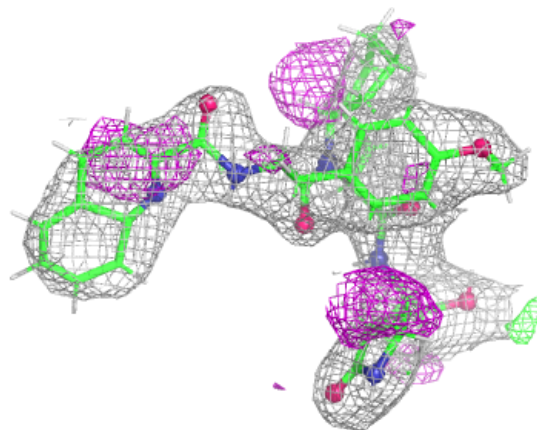
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1EYZ B 401:

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

**Electron density around A1EYZ A 401:**

$2mF_o-DF_c$ (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.