



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:40 PM EDT

PDB ID : 6MO0 / pdb_00006mo0
Title : Structure of dengue virus protease with an allosteric Inhibitor that blocks replication
Authors : Lin, Y.-L.; Nie, S.; Hua, Y.; Wu, J.; Wu, F.; Huo, T.; Yao, Y.; Song, Y.
Deposited on : 2018-10-03
Resolution : 2.70 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

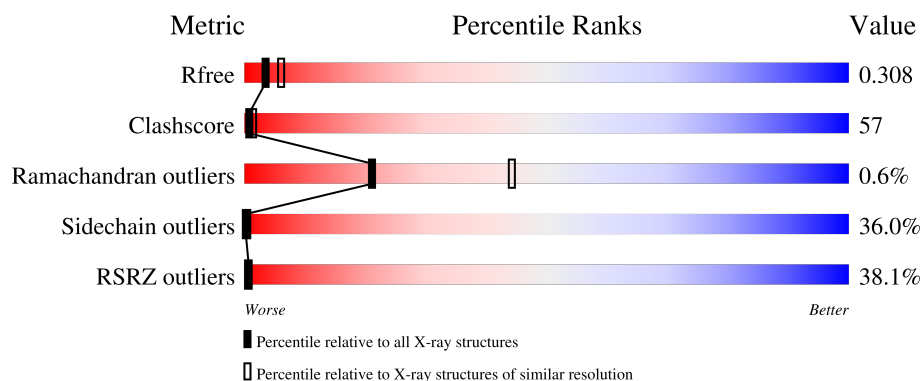
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	247	25% 22% 31% 13% 34%
1	B	247	26% 23% 29% 14% 34%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2578 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 FLAVIVIRUS_NS2B/Peptidase S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1256	796	217	240	3			
1	B	164	Total	C	N	O	S	0	0	0
			1256	796	217	240	3			

There are 32 discrepancies between the modelled and reference sequences:

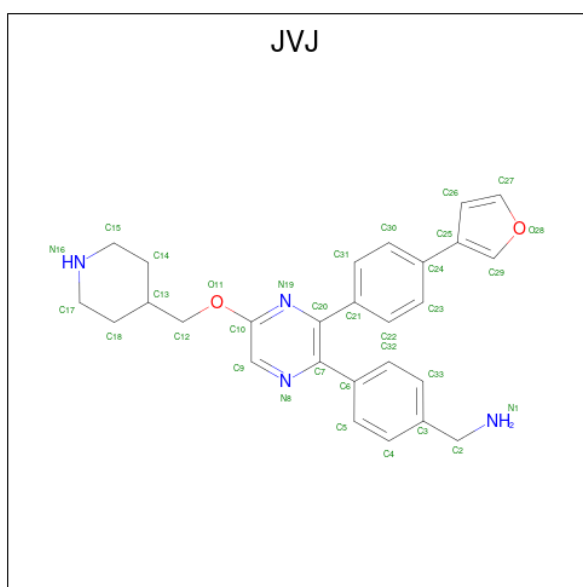
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	-	expression tag	UNP A0A0B4L2Y4
A	44	SER	-	expression tag	UNP A0A0B4L2Y4
A	45	HIS	-	expression tag	UNP A0A0B4L2Y4
A	46	MET	-	expression tag	UNP A0A0B4L2Y4
A	47	LEU	-	expression tag	UNP A0A0B4L2Y4
A	48	MET	-	expression tag	UNP A0A0B4L2Y4
A	992	GLY	-	linker	UNP A0A0B4L2Y4
A	993	GLY	-	linker	UNP A0A0B4L2Y4
A	994	GLY	-	linker	UNP A0A0B4L2Y4
A	995	GLY	-	linker	UNP A0A0B4L2Y4
A	996	SER	-	linker	UNP A0A0B4L2Y4
A	997	GLY	-	linker	UNP A0A0B4L2Y4
A	998	GLY	-	linker	UNP A0A0B4L2Y4
A	999	GLY	-	linker	UNP A0A0B4L2Y4
A	1000	GLY	-	linker	UNP A0A0B4L2Y4
A	1167	ASN	GLN	conflict	UNP Q91H74
B	43	GLY	-	expression tag	UNP A0A0B4L2Y4
B	44	SER	-	expression tag	UNP A0A0B4L2Y4
B	45	HIS	-	expression tag	UNP A0A0B4L2Y4
B	46	MET	-	expression tag	UNP A0A0B4L2Y4
B	47	LEU	-	expression tag	UNP A0A0B4L2Y4
B	48	MET	-	expression tag	UNP A0A0B4L2Y4
B	992	GLY	-	linker	UNP A0A0B4L2Y4
B	993	GLY	-	linker	UNP A0A0B4L2Y4
B	994	GLY	-	linker	UNP A0A0B4L2Y4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	995	GLY	-	linker	UNP A0A0B4L2Y4
B	996	SER	-	linker	UNP A0A0B4L2Y4
B	997	GLY	-	linker	UNP A0A0B4L2Y4
B	998	GLY	-	linker	UNP A0A0B4L2Y4
B	999	GLY	-	linker	UNP A0A0B4L2Y4
B	1000	GLY	-	linker	UNP A0A0B4L2Y4
B	1167	ASN	GLN	conflict	UNP Q91H74

- Molecule 2 is 1-(4-{3-[4-(furan-3-yl)phenyl]-5-[(piperidin-4-yl)methoxy]pyrazin-2-yl}phenyl) methanamine (CCD ID: JVJ) (formula: C₂₇H₂₈N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	27	4	2		
2	B	1	Total	C	N	O	0	0
			33	27	4	2		

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.11Å 109.11Å 75.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.13 – 2.70 40.13 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.13-2.70) 99.8 (40.13-2.70)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.256 , 0.311 0.279 , 0.308	Depositor DCC
R_{free} test set	709 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2578	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: JVJ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.08	0/1280	1.37	7/1721 (0.4%)
1	B	1.10	0/1280	1.33	8/1721 (0.5%)
All	All	1.09	0/2560	1.35	15/3442 (0.4%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1066	GLU	CB-CA-C	10.23	121.55	109.47
1	A	1112	LYS	CB-CA-C	8.71	120.16	110.15
1	A	65	ALA	CA-C-O	-6.53	114.14	121.00
1	B	1139	ILE	CA-C-O	-5.99	114.12	120.53
1	B	1066	GLU	CA-C-N	5.97	125.91	119.76
1	B	1066	GLU	C-N-CA	5.97	125.91	119.76
1	A	65	ALA	N-CA-C	5.56	117.03	110.97
1	A	65	ALA	O-C-N	5.43	127.68	122.03
1	B	1117	LYS	N-CA-C	-5.34	103.43	110.43
1	A	1053	THR	CA-CB-OG1	-5.33	101.61	109.60
1	B	1067	PRO	CA-C-O	-5.19	115.42	121.34
1	A	1139	ILE	CA-C-O	-5.16	115.01	120.53
1	B	1139	ILE	O-C-N	5.12	129.09	123.10
1	B	1081	GLY	CA-C-O	-5.11	116.62	121.83
1	A	1081	GLY	CA-C-O	-5.02	116.19	121.56

There are no chirality outliers.

There are no planarity outliers.

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	1256	0	1252	141	3
1	B	1256	0	1252	153	3
2	A	33	0	0	3	0
2	B	33	0	0	5	0
All	All	2578	0	2504	288	6

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 57.

All (288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:LEU:HD23	1:A:1060:HIS:CD2	1.58	1.39
1:A:1112:LYS:HE2	1:A:1113:PRO:O	1.35	1.26
1:B:1053:THR:HG21	1:B:1079:TYR:OH	1.37	1.22
1:A:1018:LEU:O	1:A:1023:TYR:OH	1.64	1.15
1:A:1101:GLU:OE2	1:A:1101:GLU:N	1.82	1.12
1:B:1026:LYS:HZ2	1:B:1035:GLN:HB3	0.94	1.09
1:A:1091:GLU:HB2	1:A:1168:THR:CG2	1.85	1.06
1:A:1091:GLU:HB2	1:A:1168:THR:HG23	1.34	1.05
1:B:1026:LYS:NZ	1:B:1035:GLN:HB3	1.72	1.04
1:B:1070:ALA:HB2	1:B:1077:ILE:HD12	1.41	1.03
1:A:1018:LEU:HD23	1:A:1060:HIS:NE2	1.73	1.02
1:B:1065:ILE:CG2	1:B:1079:TYR:HB3	1.89	1.02
1:A:51:LEU:HD21	1:A:1025:ILE:CG2	1.90	1.01
1:A:1105:ASN:OD1	1:A:1106:PRO:HD2	1.60	1.01
1:A:1030:ILE:HG23	1:A:1031:LEU:HD13	1.40	0.99
1:B:56:ALA:HB3	1:B:1100:LEU:HD21	1.38	0.98
1:B:1053:THR:CG2	1:B:1079:TYR:OH	2.13	0.96
1:B:1105:ASN:OD1	1:B:1106:PRO:HD2	1.66	0.96
1:A:1151:GLY:C	1:A:1165:ILE:HD12	1.91	0.94
1:A:1026:LYS:HE3	1:A:1035:GLN:HB2	1.50	0.94
1:A:1116:PHE:HE2	1:A:1125:ALA:HB2	1.31	0.93
1:B:1124:GLY:O	1:B:1166:ALA:HB3	1.67	0.93
1:B:1090:LYS:NZ	1:B:1093:GLU:OE1	2.01	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:ALA:O	1:A:1079:TYR:OH	1.88	0.91
1:B:1057:VAL:HG21	1:B:1064:ARG:NE	1.84	0.91
1:A:55:ARG:NH1	1:A:1020:ASP:O	2.03	0.90
1:B:56:ALA:CB	1:B:1100:LEU:HD21	2.01	0.90
1:B:1019:GLU:O	1:B:1023:TYR:OH	1.89	0.90
1:B:1118:THR:HG21	1:B:1123:ILE:HG12	1.52	0.89
1:B:1091:GLU:HB2	1:B:1168:THR:CG2	2.02	0.89
1:A:1018:LEU:CD2	1:A:1060:HIS:CD2	2.53	0.89
1:A:55:ARG:HB3	1:B:64:GLN:NE2	1.88	0.88
1:A:1116:PHE:CE2	1:A:1125:ALA:HB2	2.08	0.88
1:A:1101:GLU:HG2	1:A:1104:LYS:HB2	1.57	0.87
1:A:1027:GLN:O	1:A:1027:GLN:NE2	2.08	0.86
1:A:65:ALA:O	1:A:66:GLU:HB2	1.72	0.86
1:B:1101:GLU:N	1:B:1101:GLU:OE1	2.07	0.86
1:A:50:ASP:OD2	1:A:1028:LYS:HE3	1.76	0.84
1:A:51:LEU:CD2	1:A:1025:ILE:HG23	2.08	0.84
1:A:1037:GLY:HA3	1:A:1052:VAL:HG11	1.60	0.83
1:A:1101:GLU:H	1:A:1101:GLU:CD	1.86	0.83
1:A:51:LEU:CD2	1:A:1025:ILE:CG2	2.56	0.83
1:A:51:LEU:HD22	1:A:1058:LEU:HD11	1.59	0.83
1:B:1026:LYS:HZ2	1:B:1035:GLN:CB	1.85	0.82
1:B:1091:GLU:HB2	1:B:1168:THR:HG23	1.61	0.80
1:A:1097:VAL:CG1	1:A:1109:VAL:HG13	2.12	0.80
1:B:1057:VAL:HG21	1:B:1064:ARG:HE	1.45	0.80
1:A:1101:GLU:HG2	1:A:1104:LYS:CB	2.13	0.79
1:B:1049:MET:HE1	1:B:1150:TYR:O	1.83	0.79
1:A:1070:ALA:HB2	1:A:1077:ILE:HD12	1.64	0.79
1:A:1061:LYS:HG3	1:A:1062:GLY:H	1.48	0.78
1:B:1048:THR:HG23	1:B:1077:ILE:CG2	2.12	0.78
1:B:1070:ALA:HB2	1:B:1077:ILE:CD1	2.13	0.78
1:A:1097:VAL:HG12	1:A:1109:VAL:HG13	1.64	0.78
1:A:1101:GLU:HG3	1:A:1104:LYS:HE2	1.66	0.78
1:B:1070:ALA:CB	1:B:1077:ILE:HD12	2.14	0.78
1:B:1036:ILE:HD12	1:B:1036:ILE:H	1.49	0.77
1:B:1101:GLU:CD	1:B:1101:GLU:H	1.90	0.77
1:B:1090:LYS:O	1:B:1091:GLU:HB3	1.83	0.76
1:A:1053:THR:CG2	1:A:1079:TYR:OH	2.34	0.76
1:A:55:ARG:HD3	1:B:64:GLN:HE22	1.49	0.76
1:A:1090:LYS:HD3	1:A:1093:GLU:HB2	1.68	0.76
1:A:1088:GLU:O	1:A:1088:GLU:HG2	1.84	0.76
1:A:1099:ALA:C	1:A:1100:LEU:HD12	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:LEU:HD13	1:A:1031:LEU:N	2.02	0.75
1:A:1053:THR:HG21	1:A:1079:TYR:OH	1.86	0.75
1:A:1030:ILE:HG23	1:A:1031:LEU:CD1	2.17	0.75
1:A:1116:PHE:HE2	1:A:1125:ALA:CB	1.99	0.75
1:A:1037:GLY:HA3	1:A:1052:VAL:CG1	2.16	0.75
1:B:56:ALA:CB	1:B:1100:LEU:CD2	2.64	0.75
1:A:55:ARG:HB3	1:B:64:GLN:HE21	1.51	0.74
1:B:1151:GLY:O	1:B:1165:ILE:HG13	1.87	0.74
1:A:1091:GLU:HB2	1:A:1168:THR:HG21	1.70	0.73
1:B:1067:PRO:HG3	1:B:1079:TYR:CE2	2.23	0.73
1:A:1018:LEU:CD2	1:A:1060:HIS:NE2	2.51	0.73
1:B:1040:VAL:CG2	1:B:1138:PRO:HG3	2.19	0.73
1:B:51:LEU:HB3	1:B:1058:LEU:HD12	1.71	0.72
1:B:1053:THR:HG22	1:B:1055:GLY:H	1.54	0.72
1:A:1047:HIS:HE1	1:A:1084:LYS:H	1.37	0.72
1:B:63:GLU:OE2	1:B:63:GLU:N	2.21	0.72
1:B:66:GLU:HG2	1:B:70:SER:OG	1.88	0.72
1:A:1031:LEU:HD13	1:A:1031:LEU:H	1.54	0.71
1:A:1025:ILE:HG22	1:A:1036:ILE:HD11	1.70	0.71
1:A:1090:LYS:HD3	1:A:1093:GLU:CB	2.20	0.71
1:B:1026:LYS:HD2	1:B:1035:GLN:HB2	1.72	0.71
1:B:1065:ILE:HG22	1:B:1079:TYR:HB3	1.71	0.71
1:B:1050:TRP:CE3	1:B:1077:ILE:HD13	2.26	0.71
1:A:1071:ASP:OD2	1:A:1074:LYS:HE3	1.91	0.71
1:A:51:LEU:HD22	1:A:1058:LEU:CD1	2.21	0.70
1:A:1112:LYS:CE	1:A:1113:PRO:O	2.28	0.70
1:B:1151:GLY:O	1:B:1165:ILE:CD1	2.41	0.69
1:B:1101:GLU:OE2	1:B:1107:ARG:CZ	2.41	0.69
1:A:1040:VAL:HG21	1:A:1138:PRO:HB3	1.76	0.68
1:A:1067:PRO:HG3	1:A:1079:TYR:CE2	2.29	0.68
1:B:1049:MET:CE	1:B:1151:GLY:HA3	2.23	0.68
1:B:1165:ILE:HD11	2:B:1201:JVJ:C33	2.24	0.67
1:B:1065:ILE:CG2	1:B:1079:TYR:CB	2.71	0.67
1:A:1053:THR:HG21	1:A:1079:TYR:CE1	2.30	0.66
1:B:1091:GLU:HB2	1:B:1168:THR:HG21	1.76	0.66
1:A:1078:SER:OG	1:A:1081:GLY:O	2.14	0.66
1:A:68:SER:OG	1:A:69:GLY:N	2.13	0.65
1:A:1057:VAL:CG2	1:A:1064:ARG:HG3	2.27	0.65
1:B:1091:GLU:O	1:B:1091:GLU:HG2	1.96	0.64
1:B:1057:VAL:CG2	1:B:1064:ARG:NE	2.60	0.64
1:A:1090:LYS:O	1:A:1091:GLU:HB3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD21	1:A:1025:ILE:HG22	1.78	0.64
1:B:1089:TRP:HH2	1:B:1115:LEU:HD11	1.62	0.64
1:B:1041:TYR:CD2	1:B:1046:PHE:HD1	2.16	0.63
1:A:1040:VAL:CG2	1:A:1138:PRO:HB3	2.29	0.63
1:B:1026:LYS:HZ1	1:B:1035:GLN:N	1.97	0.63
1:A:1061:LYS:HG3	1:A:1062:GLY:N	2.14	0.63
1:A:1057:VAL:HG21	1:A:1064:ARG:HG3	1.81	0.62
1:A:1031:LEU:H	1:A:1031:LEU:HD22	1.62	0.62
1:B:1030:ILE:N	1:B:1030:ILE:HD12	2.14	0.62
1:A:55:ARG:HD3	1:B:64:GLN:NE2	2.14	0.62
1:A:1065:ILE:HG22	1:A:1079:TYR:CD2	2.35	0.61
1:A:1053:THR:HG22	1:A:1055:GLY:H	1.65	0.61
1:B:1054:ARG:HH11	1:B:1054:ARG:CG	2.14	0.61
1:A:1151:GLY:C	1:A:1165:ILE:CD1	2.71	0.61
1:B:1026:LYS:HE3	1:B:1034:SER:C	2.26	0.60
1:B:1040:VAL:HG23	1:B:1138:PRO:HG3	1.84	0.60
1:B:1030:ILE:HD12	1:B:1030:ILE:H	1.67	0.60
1:B:1048:THR:HG23	1:B:1077:ILE:HG21	1.83	0.60
1:B:1151:GLY:O	1:B:1165:ILE:CG1	2.50	0.59
1:A:1025:ILE:HD13	1:A:1037:GLY:C	2.28	0.59
1:A:1025:ILE:N	1:A:1025:ILE:HD12	2.18	0.59
1:A:55:ARG:CD	1:B:64:GLN:HE22	2.15	0.59
1:B:1105:ASN:OD1	1:B:1106:PRO:CD	2.45	0.59
1:A:1053:THR:HG21	1:A:1079:TYR:CZ	2.38	0.59
1:A:1047:HIS:CE1	1:A:1084:LYS:H	2.19	0.58
1:B:1050:TRP:HE3	1:B:1077:ILE:HD13	1.68	0.58
1:B:1089:TRP:CH2	1:B:1115:LEU:HD11	2.38	0.58
1:A:1127:SER:O	1:A:1128:LEU:HD23	2.03	0.58
1:A:1067:PRO:HG3	1:A:1079:TYR:CZ	2.39	0.58
1:B:56:ALA:HB3	1:B:1100:LEU:CD2	2.22	0.57
1:A:1033:TYR:N	1:A:1033:TYR:CD1	2.72	0.57
1:A:1098:LEU:HB3	1:A:1138:PRO:HG2	1.87	0.57
1:A:1033:TYR:N	1:A:1033:TYR:HD1	2.02	0.56
1:B:1048:THR:CG2	1:B:1077:ILE:CG2	2.83	0.56
1:B:1090:LYS:O	1:B:1091:GLU:CB	2.53	0.56
1:B:1026:LYS:NZ	1:B:1035:GLN:CB	2.56	0.56
1:A:1036:ILE:HG12	1:A:1052:VAL:HG13	1.87	0.56
1:A:1042:LYS:HE2	1:A:1085:LEU:CD2	2.35	0.56
1:A:1093:GLU:HG3	1:A:1094:GLU:N	2.21	0.56
1:B:1054:ARG:NH1	1:B:1054:ARG:HG2	2.21	0.56
1:B:1037:GLY:HA3	1:B:1052:VAL:CG1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1058:LEU:HD22	1:A:1079:TYR:CZ	2.41	0.55
1:B:1028:LYS:HG3	1:B:1033:TYR:HB3	1.88	0.55
1:B:1065:ILE:HG22	1:B:1079:TYR:CD2	2.41	0.55
1:A:1036:ILE:HD13	1:A:1036:ILE:H	1.72	0.55
1:B:1049:MET:HE1	1:B:1151:GLY:HA3	1.88	0.55
1:A:1042:LYS:HE2	1:A:1085:LEU:HD23	1.87	0.55
1:A:1099:ALA:O	1:A:1100:LEU:HD12	2.07	0.55
1:B:1098:LEU:C	1:B:1098:LEU:HD12	2.31	0.55
1:A:1129:ASP:OD1	1:A:1129:ASP:C	2.50	0.55
1:B:1118:THR:CG2	1:B:1123:ILE:HG12	2.32	0.55
1:A:1065:ILE:HG22	1:A:1079:TYR:HD2	1.71	0.54
1:A:1067:PRO:HA	1:A:1079:TYR:HA	1.89	0.54
1:A:55:ARG:CB	1:B:64:GLN:NE2	2.67	0.54
1:A:1057:VAL:HG23	1:A:1065:ILE:O	2.08	0.54
1:B:1018:LEU:CD2	1:B:1044:GLY:HA2	2.38	0.54
1:A:1025:ILE:CG2	1:A:1036:ILE:HD11	2.38	0.53
2:A:1201:JVJ:C31	2:A:1201:JVJ:C6	2.85	0.53
1:B:1025:ILE:HD12	1:B:1025:ILE:N	2.24	0.53
1:B:1041:TYR:CD2	1:B:1046:PHE:CD1	2.96	0.53
1:B:1115:LEU:CD1	1:B:1115:LEU:N	2.71	0.53
1:A:51:LEU:HB3	1:A:1058:LEU:HD12	1.91	0.53
1:B:1026:LYS:HD2	1:B:1035:GLN:CB	2.39	0.53
1:B:1065:ILE:HG21	1:B:1079:TYR:CB	2.39	0.52
1:B:1090:LYS:NZ	1:B:1093:GLU:CD	2.67	0.52
1:A:1091:GLU:O	1:A:1091:GLU:HG2	2.09	0.52
1:B:1141:ASP:OD2	1:B:1145:LYS:HE3	2.10	0.52
1:B:1053:THR:HG22	1:B:1055:GLY:N	2.21	0.52
1:B:1067:PRO:HG3	1:B:1079:TYR:HE2	1.74	0.52
1:A:1061:LYS:CG	1:A:1062:GLY:H	2.17	0.52
1:B:1058:LEU:HB3	1:B:1065:ILE:HD12	1.91	0.52
1:B:1065:ILE:HG21	1:B:1079:TYR:HB3	1.85	0.52
1:A:1030:ILE:CG2	1:A:1031:LEU:HD13	2.28	0.52
1:B:1037:GLY:HA3	1:B:1052:VAL:HG11	1.92	0.51
1:A:1090:LYS:HG3	1:A:1092:GLY:H	1.75	0.51
1:B:1042:LYS:HD3	1:B:1085:LEU:CD2	2.40	0.51
1:A:1053:THR:HG21	1:A:1079:TYR:HE1	1.76	0.51
1:B:1025:ILE:HD11	1:B:1046:PHE:HZ	1.75	0.51
1:B:1026:LYS:CD	1:B:1035:GLN:HB2	2.40	0.51
1:B:1028:LYS:HA	1:B:1033:TYR:HB3	1.92	0.51
1:A:1050:TRP:O	1:A:1054:ARG:N	2.41	0.51
1:B:1070:ALA:CB	1:B:1077:ILE:CD1	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1054:ARG:HH11	1:B:1054:ARG:HG2	1.74	0.51
1:B:1065:ILE:HG23	1:B:1079:TYR:HB3	1.88	0.51
1:B:1141:ASP:OD2	1:B:1145:LYS:HB2	2.11	0.51
1:B:52:GLU:HA	1:B:1059:MET:O	2.11	0.50
1:B:1026:LYS:NZ	1:B:1035:GLN:N	2.58	0.50
1:A:1033:TYR:HD1	1:A:1033:TYR:H	1.60	0.50
1:A:1048:THR:HG23	1:A:1077:ILE:CG2	2.42	0.50
1:B:1058:LEU:HD22	1:B:1079:TYR:CZ	2.46	0.50
1:B:1127:SER:C	1:B:1128:LEU:HD13	2.36	0.50
1:B:1018:LEU:HD21	1:B:1044:GLY:HA2	1.93	0.50
1:B:52:GLU:HB2	1:B:1059:MET:HE2	1.92	0.50
1:B:1018:LEU:CD2	1:B:1041:TYR:CE1	2.95	0.50
1:B:66:GLU:CG	1:B:70:SER:OG	2.59	0.50
1:B:1018:LEU:HD23	1:B:1041:TYR:CE1	2.47	0.50
1:A:1025:ILE:HD13	1:A:1038:ALA:N	2.27	0.49
1:B:1169:GLU:O	1:B:1170:LYS:HB3	2.13	0.49
1:B:1051:HIS:ND1	1:B:1075:ASP:OD2	2.40	0.49
1:A:1053:THR:HG23	1:A:1079:TYR:OH	2.13	0.49
1:B:56:ALA:HB1	1:B:1106:PRO:HG3	1.94	0.49
1:B:61:TRP:CE3	1:B:1142:LYS:HA	2.47	0.49
1:A:70:SER:O	1:A:70:SER:OG	2.14	0.49
1:B:1069:TRP:HE3	1:B:1078:SER:HB3	1.78	0.48
1:B:1057:VAL:HG21	1:B:1064:ARG:CZ	2.40	0.48
1:B:51:LEU:HD23	1:B:1058:LEU:HD11	1.95	0.48
1:A:1097:VAL:CG1	1:A:1109:VAL:CG1	2.90	0.48
1:B:1018:LEU:HD23	1:B:1018:LEU:O	2.13	0.48
1:B:1114:GLY:C	1:B:1115:LEU:HD12	2.39	0.48
1:A:63:GLU:H	1:A:63:GLU:HG2	1.34	0.47
1:A:1101:GLU:HG2	1:A:1104:LYS:HB3	1.92	0.47
1:A:67:ILE:HG13	1:A:1110:GLN:HB3	1.96	0.47
1:A:1058:LEU:HD22	1:A:1079:TYR:CE1	2.50	0.47
1:A:51:LEU:HD23	1:A:1025:ILE:HG23	1.94	0.47
1:A:1018:LEU:HA	1:A:1060:HIS:CE1	2.49	0.47
1:A:1025:ILE:HG22	1:A:1036:ILE:CD1	2.41	0.47
1:A:1074:LYS:HB3	1:A:1076:LEU:HD12	1.97	0.47
1:B:1042:LYS:HD3	1:B:1085:LEU:HD23	1.96	0.46
1:A:1086:GLU:H	1:A:1086:GLU:HG3	1.58	0.46
1:B:1149:LEU:HB2	2:B:1201:JVJ:C27	2.45	0.46
1:A:1116:PHE:CD2	1:A:1116:PHE:N	2.84	0.46
1:A:51:LEU:HD21	1:A:1025:ILE:HG21	1.90	0.46
1:B:1057:VAL:CG2	1:B:1064:ARG:CZ	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:GLY:HA3	1:B:1046:PHE:CZ	2.51	0.46
1:A:1036:ILE:H	1:A:1036:ILE:CD1	2.29	0.46
1:A:1054:ARG:HE	1:A:1054:ARG:HB2	1.50	0.46
1:A:1140:VAL:HA	1:A:1145:LYS:O	2.15	0.46
1:B:56:ALA:CB	1:B:1100:LEU:HD23	2.46	0.46
1:A:50:ASP:HB3	1:A:1028:LYS:HB2	1.98	0.45
1:B:1025:ILE:N	1:B:1025:ILE:CD1	2.79	0.45
1:A:1031:LEU:N	1:A:1031:LEU:HD22	2.31	0.45
1:B:1049:MET:HE3	1:B:1151:GLY:HA3	1.96	0.45
1:B:1078:SER:OG	1:B:1081:GLY:O	2.35	0.45
1:A:1039:GLY:HA3	1:A:1046:PHE:CZ	2.52	0.45
1:A:1058:LEU:HD12	1:A:1058:LEU:HA	1.78	0.45
1:B:1026:LYS:CD	1:B:1035:GLN:CB	2.93	0.45
1:B:1107:ARG:HH21	1:B:1107:ARG:CG	2.29	0.45
1:B:1050:TRP:CZ3	1:B:1077:ILE:HD13	2.51	0.45
1:B:1114:GLY:C	1:B:1115:LEU:CD1	2.89	0.45
1:A:1027:GLN:NE2	1:A:1027:GLN:C	2.73	0.45
1:B:51:LEU:HD22	1:B:1056:ALA:HB3	1.99	0.45
1:A:1026:LYS:HE3	1:A:1035:GLN:CB	2.35	0.45
1:A:55:ARG:HB3	1:B:64:GLN:HE22	1.79	0.45
1:A:1149:LEU:H	2:A:1201:JVJ:C27	2.30	0.44
1:B:60:ARG:HD2	1:B:60:ARG:HA	1.85	0.44
1:B:1104:LYS:HD2	1:B:1104:LYS:HA	1.49	0.44
1:A:1067:PRO:HB3	1:A:1077:ILE:HD11	1.98	0.44
1:B:61:TRP:CE2	1:B:1096:GLN:NE2	2.86	0.44
1:B:1030:ILE:H	1:B:1030:ILE:CD1	2.23	0.44
1:A:1100:LEU:HD12	1:A:1100:LEU:N	2.33	0.43
1:B:1051:HIS:HD1	1:B:1075:ASP:CG	2.26	0.43
1:B:1107:ARG:HG2	1:B:1107:ARG:NH2	2.33	0.43
1:A:64:GLN:O	1:A:64:GLN:HG3	2.18	0.43
1:B:51:LEU:HD12	1:B:1027:GLN:HB2	1.98	0.43
1:B:1069:TRP:CZ2	1:B:1071:ASP:HB2	2.53	0.43
1:B:51:LEU:CD1	1:B:1027:GLN:HB2	2.47	0.43
1:B:1066:GLU:HA	1:B:1067:PRO:HD3	1.73	0.43
1:B:1074:LYS:O	2:B:1201:JVJ:C31	2.67	0.43
1:A:1018:LEU:CA	1:A:1060:HIS:NE2	2.82	0.43
1:B:1091:GLU:CB	1:B:1168:THR:HG23	2.41	0.43
1:A:1047:HIS:HB3	1:A:1083:TRP:CH2	2.53	0.42
1:B:1145:LYS:HE3	1:B:1145:LYS:HB2	1.80	0.42
1:B:1115:LEU:N	1:B:1115:LEU:HD13	2.34	0.42
1:B:1140:VAL:HG12	1:B:1144:GLY:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1201:JVJ:C31	2:A:1201:JVJ:C32	2.98	0.42
1:B:1165:ILE:CD1	2:B:1201:JVJ:C33	2.97	0.42
1:A:54:GLU:O	1:A:1023:TYR:HA	2.20	0.41
1:A:1018:LEU:N	1:A:1060:HIS:CE1	2.88	0.41
1:B:51:LEU:HB3	1:B:1058:LEU:CD1	2.44	0.41
1:A:1100:LEU:N	1:A:1100:LEU:CD1	2.82	0.41
1:B:53:LEU:HA	1:B:53:LEU:HD12	1.84	0.41
1:A:1053:THR:HG22	1:A:1055:GLY:N	2.30	0.41
1:A:1131:SER:OG	1:A:1132:PRO:HD2	2.20	0.41
1:B:60:ARG:NH2	1:B:1144:GLY:HA3	2.36	0.41
1:A:1129:ASP:O	1:A:1129:ASP:CG	2.62	0.41
1:B:61:TRP:CD1	1:B:61:TRP:C	2.98	0.41
1:A:1122:THR:O	1:A:1168:THR:HB	2.20	0.41
1:B:1137:SER:HA	1:B:1138:PRO:HD3	1.89	0.40
1:B:1165:ILE:HD13	2:B:1201:JVJ:C30	2.51	0.40
1:A:53:LEU:HD13	1:A:1058:LEU:HG	2.04	0.40
1:A:55:ARG:CG	1:B:64:GLN:NE2	2.85	0.40
1:B:1064:ARG:NH1	1:B:1066:GLU:HB3	2.36	0.40
1:B:1091:GLU:CB	1:B:1168:THR:HG21	2.48	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:MET:N	1:A:71:SER:O[2_445]	0.67	1.53
1:B:48:MET:N	1:B:71:SER:O[3_655]	1.12	1.08
1:B:1143:LYS:CG	1:B:1143:LYS:CG[6_556]	1.75	0.45
1:A:48:MET:N	1:A:71:SER:C[2_445]	1.91	0.29
1:A:48:MET:CA	1:A:71:SER:O[2_445]	2.11	0.09
1:B:48:MET:CA	1:B:71:SER:O[3_655]	2.18	0.02

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	158/247 (64%)	152 (96%)	5 (3%)	1 (1%)	21	44
1	B	158/247 (64%)	153 (97%)	4 (2%)	1 (1%)	21	44
All	All	316/494 (64%)	305 (96%)	9 (3%)	2 (1%)	21	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	B	1091	GLU

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	129/194 (66%)	84 (65%)	45 (35%)	0	0
1	B	129/194 (66%)	81 (63%)	48 (37%)	0	0
All	All	258/388 (66%)	165 (64%)	93 (36%)	0	0

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	52	GLU
1	A	53	LEU
1	A	60	ARG
1	A	62	GLU
1	A	63	GLU
1	A	64	GLN
1	A	66	GLU
1	A	67	ILE
1	A	68	SER
1	A	71	SER
1	A	1018	LEU

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Mol	Chain	Res	Type
1	A	1019	GLU
1	A	1026	LYS
1	A	1028	LYS
1	A	1030	ILE
1	A	1031	LEU
1	A	1033	TYR
1	A	1036	ILE
1	A	1040	VAL
1	A	1041	TYR
1	A	1042	LYS
1	A	1054	ARG
1	A	1058	LEU
1	A	1063	LYS
1	A	1064	ARG
1	A	1066	GLU
1	A	1074	LYS
1	A	1077	ILE
1	A	1078	SER
1	A	1086	GLU
1	A	1098	LEU
1	A	1101	GLU
1	A	1109	VAL
1	A	1112	LYS
1	A	1117	LYS
1	A	1123	ILE
1	A	1129	ASP
1	A	1135	SER
1	A	1140	VAL
1	A	1142	LYS
1	A	1147	VAL
1	A	1167	ASN
1	A	1169	GLU
1	A	1170	LYS
1	B	48	MET
1	B	51	LEU
1	B	52	GLU
1	B	53	LEU
1	B	54	GLU
1	B	66	GLU
1	B	67	ILE
1	B	71	SER
1	B	1024	ARG

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Mol	Chain	Res	Type
1	B	1025	ILE
1	B	1027	GLN
1	B	1028	LYS
1	B	1030	ILE
1	B	1031	LEU
1	B	1033	TYR
1	B	1035	GLN
1	B	1036	ILE
1	B	1041	TYR
1	B	1049	MET
1	B	1053	THR
1	B	1054	ARG
1	B	1058	LEU
1	B	1061	LYS
1	B	1063	LYS
1	B	1066	GLU
1	B	1073	LYS
1	B	1074	LYS
1	B	1078	SER
1	B	1088	GLU
1	B	1090	LYS
1	B	1091	GLU
1	B	1098	LEU
1	B	1101	GLU
1	B	1104	LYS
1	B	1107	ARG
1	B	1115	LEU
1	B	1117	LYS
1	B	1118	THR
1	B	1119	ASN
1	B	1120	THR
1	B	1122	THR
1	B	1128	LEU
1	B	1131	SER
1	B	1134	THR
1	B	1135	SER
1	B	1140	VAL
1	B	1169	GLU
1	B	1170	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	1047	HIS
1	B	64	GLN
1	B	1119	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](#)

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	JVJ	B	1201	-	36,37,37	2.49	15 (41%)	49,50,50	1.94	11 (22%)
2	JVJ	A	1201	-	36,37,37	2.49	15 (41%)	49,50,50	2.43	16 (32%)

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	JVJ	B	1201	-	-	0/19/27/27	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JVJ	A	1201	-	-	5/19/27/27	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	JVJ	C30-C24	6.71	1.49	1.39
2	B	1201	JVJ	C21-C20	6.45	1.56	1.49
2	A	1201	JVJ	C20-N19	5.42	1.43	1.34
2	A	1201	JVJ	C30-C31	4.35	1.45	1.38
2	B	1201	JVJ	C30-C24	4.12	1.45	1.39
2	B	1201	JVJ	C30-C31	3.97	1.45	1.38
2	A	1201	JVJ	O11-C10	3.81	1.43	1.36
2	B	1201	JVJ	C26-C27	3.63	1.43	1.34
2	A	1201	JVJ	C22-C21	3.63	1.46	1.39
2	B	1201	JVJ	C20-N19	3.61	1.40	1.34
2	B	1201	JVJ	C32-C33	3.53	1.44	1.38
2	B	1201	JVJ	O28-C29	3.46	1.43	1.36
2	A	1201	JVJ	C21-C20	3.40	1.52	1.49
2	B	1201	JVJ	C23-C24	3.35	1.44	1.39
2	A	1201	JVJ	C6-C7	-3.34	1.45	1.49
2	A	1201	JVJ	C4-C5	3.30	1.44	1.38
2	B	1201	JVJ	C24-C25	3.26	1.54	1.48
2	B	1201	JVJ	C22-C23	3.22	1.44	1.38
2	B	1201	JVJ	C6-C7	-3.20	1.45	1.49
2	B	1201	JVJ	C10-N19	3.08	1.38	1.33
2	B	1201	JVJ	C22-C21	2.92	1.45	1.39
2	A	1201	JVJ	O28-C29	2.83	1.42	1.36
2	B	1201	JVJ	C33-C3	2.61	1.44	1.38
2	A	1201	JVJ	C26-C27	2.56	1.40	1.34
2	A	1201	JVJ	C10-N19	2.55	1.37	1.33
2	A	1201	JVJ	C32-C6	2.45	1.44	1.39
2	A	1201	JVJ	C4-C3	2.43	1.43	1.38
2	A	1201	JVJ	C31-C21	2.41	1.44	1.39
2	A	1201	JVJ	C9-C10	2.37	1.43	1.39
2	B	1201	JVJ	C4-C5	2.16	1.42	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	JVJ	C9-C10-N19	-9.00	116.72	122.99
2	B	1201	JVJ	C33-C32-C6	-6.70	112.52	121.12
2	B	1201	JVJ	C12-O11-C10	-5.15	110.96	117.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	JVJ	C4-C5-C6	-4.76	115.02	121.12
2	A	1201	JVJ	C22-C23-C24	-4.64	115.84	120.80
2	A	1201	JVJ	C5-C6-C32	4.56	125.83	117.68
2	B	1201	JVJ	C5-C6-C32	4.33	125.42	117.68
2	A	1201	JVJ	C23-C24-C30	3.83	123.44	118.57
2	B	1201	JVJ	C17-C18-C13	-3.75	106.33	112.14
2	A	1201	JVJ	C30-C24-C25	-3.35	116.47	121.16
2	A	1201	JVJ	C30-C31-C21	-3.09	117.16	121.12
2	A	1201	JVJ	C21-C20-N19	2.93	119.09	115.10
2	A	1201	JVJ	C15-N16-C17	2.91	118.61	110.40
2	A	1201	JVJ	C32-C6-C7	-2.84	116.01	120.62
2	A	1201	JVJ	C4-C3-C33	2.84	122.45	118.23
2	A	1201	JVJ	C26-C25-C29	2.82	110.97	105.76
2	B	1201	JVJ	C5-C4-C3	-2.81	117.31	121.00
2	B	1201	JVJ	C6-C7-C20	-2.78	120.02	124.08
2	A	1201	JVJ	O28-C29-C25	-2.51	106.77	110.20
2	A	1201	JVJ	C33-C32-C6	-2.47	117.95	121.12
2	A	1201	JVJ	C12-O11-C10	2.44	120.88	117.69
2	B	1201	JVJ	C32-C6-C7	-2.40	116.72	120.62
2	B	1201	JVJ	C14-C13-C12	-2.33	105.22	111.42
2	B	1201	JVJ	C23-C24-C25	2.15	124.18	121.16
2	A	1201	JVJ	C32-C33-C3	-2.08	118.26	121.00
2	B	1201	JVJ	C30-C24-C25	-2.06	118.27	121.16
2	B	1201	JVJ	C32-C33-C3	2.04	123.68	121.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

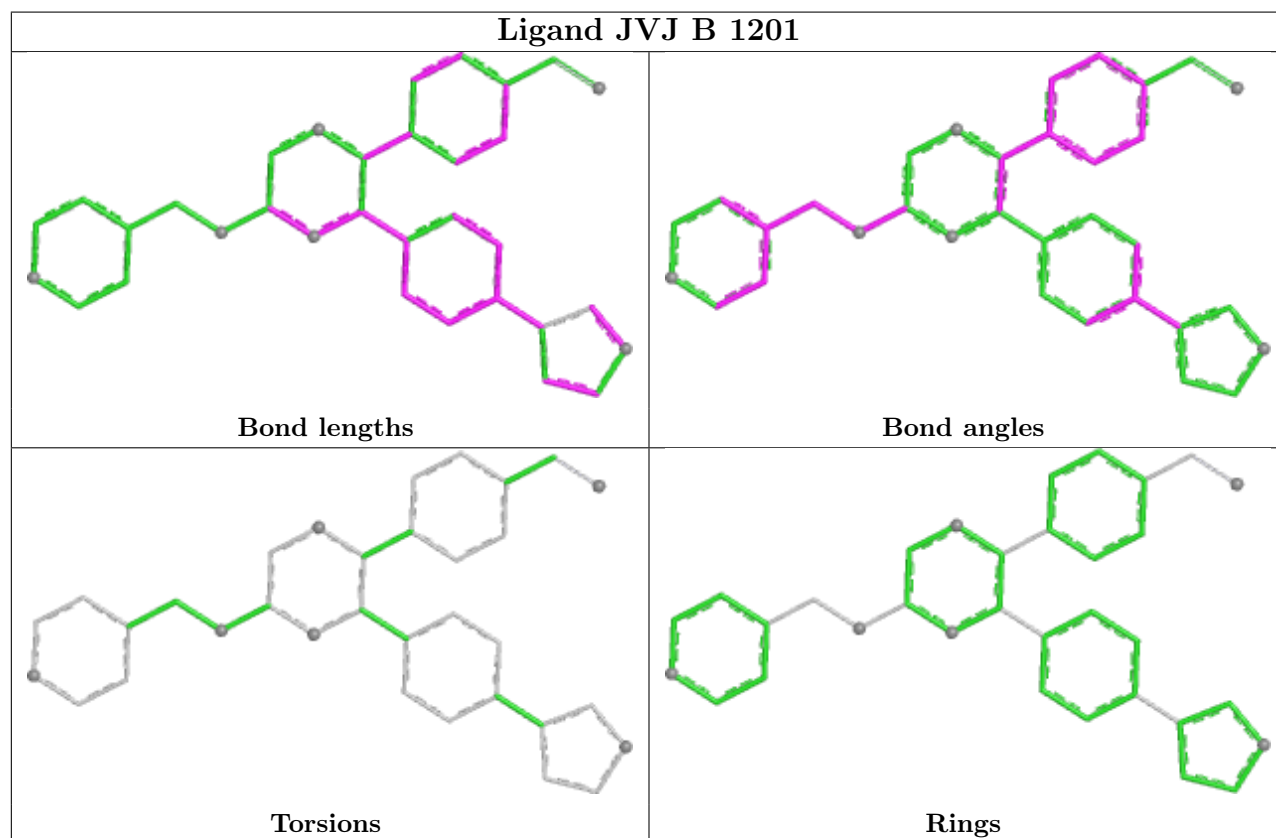
Mol	Chain	Res	Type	Atoms
2	A	1201	JVJ	O11-C12-C13-C18
2	A	1201	JVJ	O11-C12-C13-C14
2	A	1201	JVJ	C7-C20-C21-C22
2	A	1201	JVJ	C30-C24-C25-C29
2	A	1201	JVJ	C7-C20-C21-C31

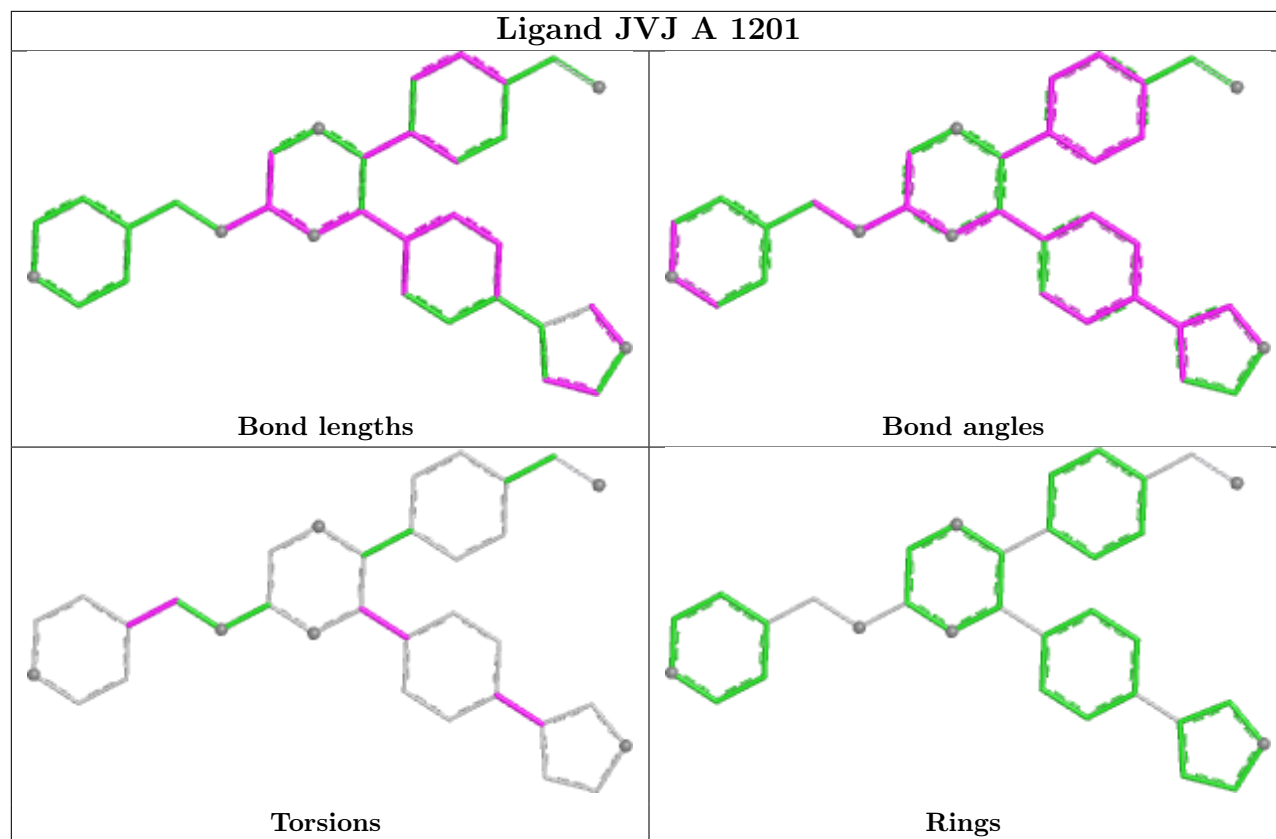
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	JVJ	5	0
2	A	1201	JVJ	3	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	164/247 (66%)	1.72	61 (37%) 1 0	35, 51, 89, 128	0
1	B	164/247 (66%)	1.72	64 (39%) 1 0	33, 50, 99, 115	0
All	All	328/494 (66%)	1.72	125 (38%) 1 0	33, 51, 97, 128	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1169	GLU	11.8
1	B	1030	ILE	6.0
1	A	1033	TYR	5.8
1	B	1167	ASN	5.5
1	B	1100	LEU	5.3
1	A	65	ALA	5.3
1	B	1088	GLU	5.2
1	B	1120	THR	5.1
1	B	1041	TYR	4.9
1	B	1031	LEU	4.8
1	A	1031	LEU	4.7
1	A	1167	ASN	4.7
1	B	1033	TYR	4.5
1	A	1120	THR	4.5
1	B	70	SER	4.3
1	B	53	LEU	4.2
1	A	1091	GLU	4.2
1	A	1041	TYR	4.1
1	A	53	LEU	4.1
1	B	1018	LEU	4.1
1	A	1057	VAL	4.0
1	B	71	SER	3.9
1	A	1077	ILE	3.8
1	A	70	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	68	SER	3.7
1	A	1018	LEU	3.6
1	A	1165	ILE	3.6
1	B	69	GLY	3.6
1	A	1131	SER	3.6
1	B	1129	ASP	3.5
1	A	49	ALA	3.5
1	A	1070	ALA	3.5
1	B	1061	LYS	3.5
1	A	1032	GLY	3.5
1	A	51	LEU	3.4
1	B	67	ILE	3.4
1	B	1165	ILE	3.4
1	B	1091	GLU	3.4
1	B	1068	SER	3.4
1	A	1111	THR	3.4
1	B	1043	GLU	3.4
1	A	69	GLY	3.3
1	A	1061	LYS	3.3
1	A	1036	ILE	3.3
1	B	1170	LYS	3.3
1	B	1036	ILE	3.2
1	B	1060	HIS	3.2
1	A	1028	LYS	3.2
1	B	1063	LYS	3.2
1	B	63	GLU	3.2
1	A	1053	THR	3.1
1	A	1063	LYS	3.1
1	A	62	GLU	3.1
1	A	1088	GLU	3.1
1	B	1101	GLU	3.1
1	A	1027	GLN	3.1
1	B	1054	ARG	3.1
1	A	1119	ASN	3.1
1	B	1119	ASN	3.1
1	B	1090	LYS	3.0
1	A	1101	GLU	3.0
1	B	1108	ALA	3.0
1	B	1079	TYR	3.0
1	B	1067	PRO	2.9
1	B	1065	ILE	2.9
1	B	48	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	68	SER	2.9
1	B	1098	LEU	2.9
1	B	1032	GLY	2.8
1	A	1093	GLU	2.8
1	A	1166	ALA	2.8
1	B	1057	VAL	2.8
1	B	1132	PRO	2.7
1	A	1030	ILE	2.7
1	B	1066	GLU	2.7
1	A	67	ILE	2.7
1	A	1019	GLU	2.7
1	B	1059	MET	2.7
1	A	1100	LEU	2.6
1	B	1103	GLY	2.6
1	B	1028	LYS	2.6
1	B	1062	GLY	2.6
1	B	1025	ILE	2.6
1	B	1019	GLU	2.6
1	B	1116	PHE	2.6
1	A	66	GLU	2.5
1	B	1169	GLU	2.5
1	A	1068	SER	2.5
1	A	1067	PRO	2.5
1	A	57	ALA	2.5
1	B	1027	GLN	2.4
1	A	1029	GLY	2.4
1	A	64	GLN	2.4
1	B	1109	VAL	2.4
1	B	51	LEU	2.4
1	B	1082	GLY	2.4
1	B	1022	ALA	2.4
1	B	1053	THR	2.4
1	B	50	ASP	2.4
1	A	1107	ARG	2.4
1	A	1055	GLY	2.3
1	A	1064	ARG	2.3
1	A	1073	LYS	2.3
1	A	1127	SER	2.3
1	B	1080	GLY	2.3
1	B	56	ALA	2.3
1	A	1118	THR	2.3
1	B	1038	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1108	ALA	2.2
1	B	66	GLU	2.2
1	A	1060	HIS	2.2
1	A	1116	PHE	2.2
1	A	54	GLU	2.2
1	A	1079	TYR	2.2
1	A	56	ALA	2.2
1	B	1092	GLY	2.2
1	A	1095	VAL	2.2
1	A	1143	LYS	2.1
1	B	1121	GLY	2.1
1	A	1038	ALA	2.1
1	B	57	ALA	2.1
1	A	1170	LYS	2.1
1	B	49	ALA	2.1
1	A	1058	LEU	2.0
1	B	1147	VAL	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](#)

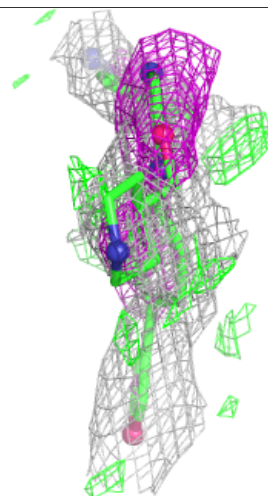
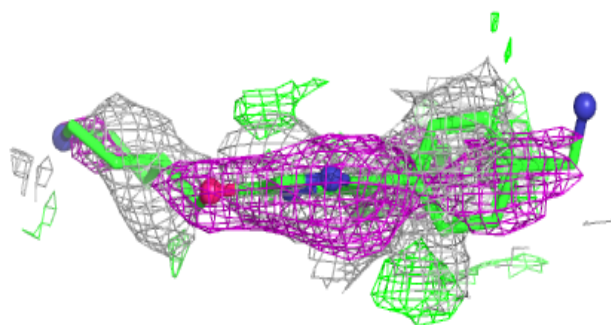
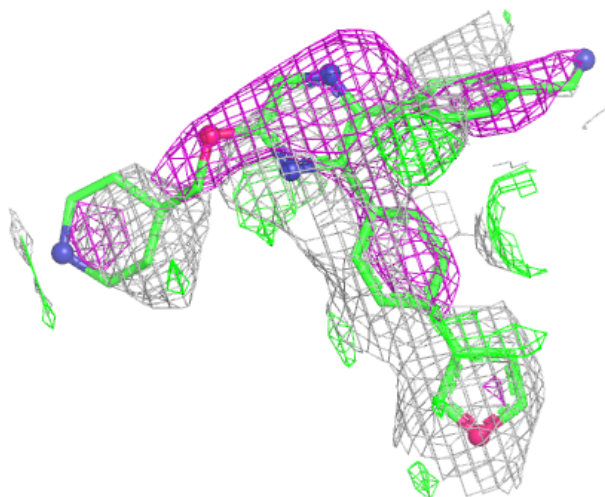
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	JVJ	B	1201	33/33	0.34	0.27	33,46,54,73	0
2	JVJ	A	1201	33/33	0.35	0.23	37,45,52,56	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.

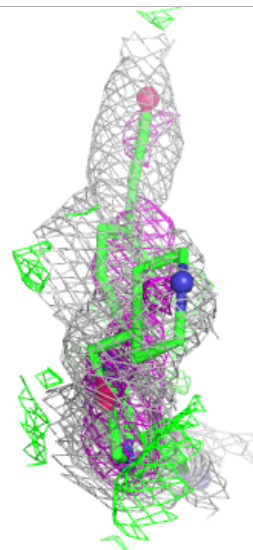
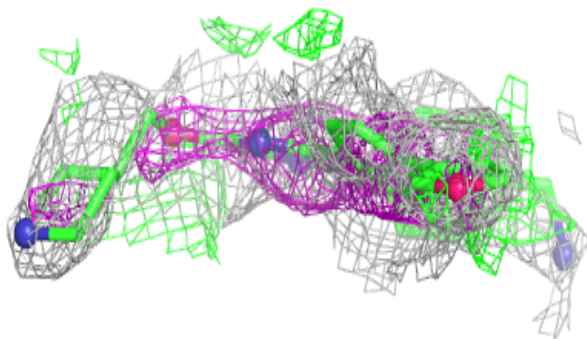
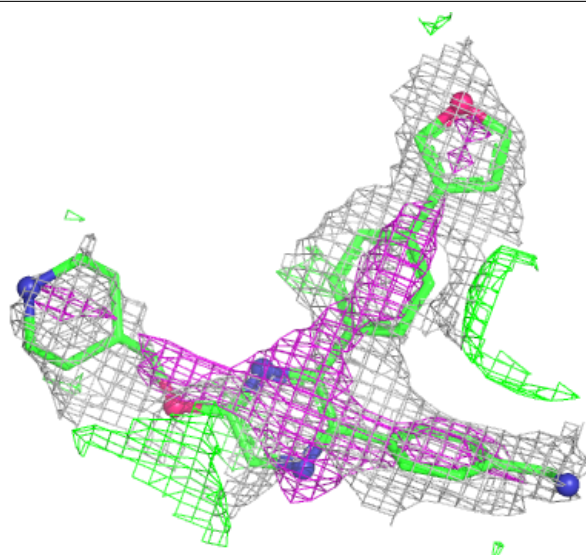
Electron density around JVJ B 1201:

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



Electron density around JVJ A 1201:

$2mF_o-DF_c$ (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.