



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 09:55 PM UTC

PDB ID : 21JX / pdb_000021jx
Title : Crystal structure of compound 1 bound to human Nicotinamide N-methyltransferase
Authors : Yoshida, S.; Kondo, N.; Uehara, S.; Yoshimura, N.; Sako, Y.; Yamamoto, S.; Kitade, M.; Tachibana, Y.
Deposited on : 2025-12-15
Resolution : 2.34 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

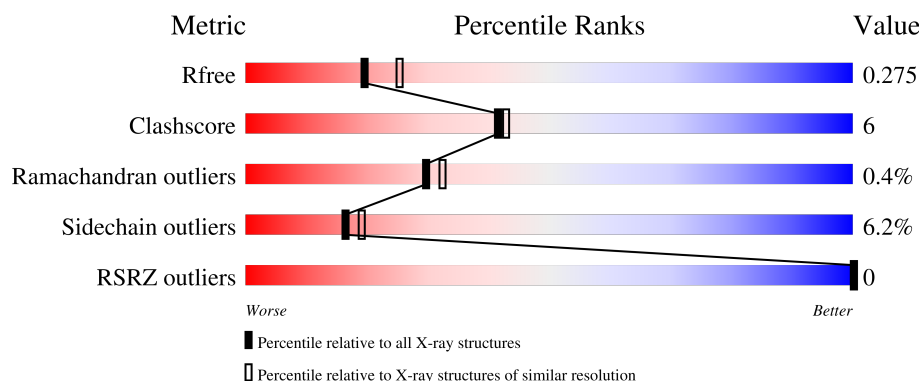
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	276	
1	B	276	
1	C	276	
1	D	276	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8189 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 Nicotinamide N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1982	1276	319	376	11			
1	B	258	Total	C	N	O	S	0	1	0
			1992	1283	319	378	12			
1	C	257	Total	C	N	O	S	0	1	0
			1971	1272	311	376	12			
1	D	257	Total	C	N	O	S	0	1	0
			1973	1273	312	376	12			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P40261
A	-14	GLY	-	expression tag	UNP P40261
A	-13	SER	-	expression tag	UNP P40261
A	-12	SER	-	expression tag	UNP P40261
A	-11	HIS	-	expression tag	UNP P40261
A	-10	HIS	-	expression tag	UNP P40261
A	-9	HIS	-	expression tag	UNP P40261
A	-8	HIS	-	expression tag	UNP P40261
A	-7	HIS	-	expression tag	UNP P40261
A	-6	HIS	-	expression tag	UNP P40261
A	-5	SER	-	expression tag	UNP P40261
A	-4	SER	-	expression tag	UNP P40261
A	-3	GLY	-	expression tag	UNP P40261
A	-2	LEU	-	expression tag	UNP P40261
A	-1	VAL	-	expression tag	UNP P40261
A	0	PRO	-	expression tag	UNP P40261
A	1	ARG	-	expression tag	UNP P40261
A	2	GLY	-	expression tag	UNP P40261
A	103	ALA	GLU	conflict	UNP P40261
B	-15	MET	-	initiating methionine	UNP P40261
B	-14	GLY	-	expression tag	UNP P40261

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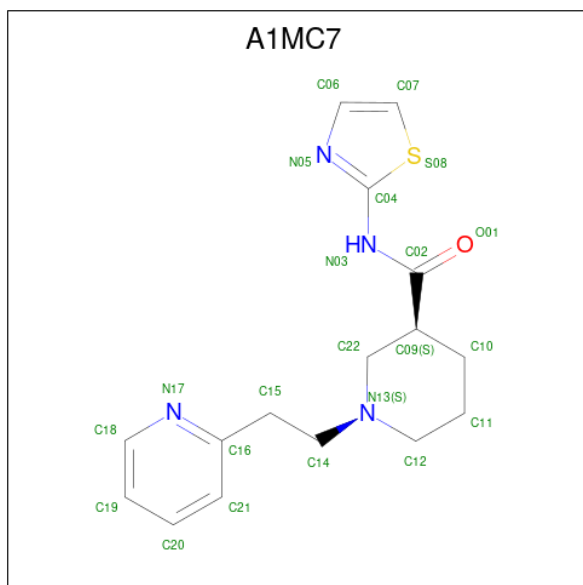
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	expression tag	UNP P40261
B	-12	SER	-	expression tag	UNP P40261
B	-11	HIS	-	expression tag	UNP P40261
B	-10	HIS	-	expression tag	UNP P40261
B	-9	HIS	-	expression tag	UNP P40261
B	-8	HIS	-	expression tag	UNP P40261
B	-7	HIS	-	expression tag	UNP P40261
B	-6	HIS	-	expression tag	UNP P40261
B	-5	SER	-	expression tag	UNP P40261
B	-4	SER	-	expression tag	UNP P40261
B	-3	GLY	-	expression tag	UNP P40261
B	-2	LEU	-	expression tag	UNP P40261
B	-1	VAL	-	expression tag	UNP P40261
B	0	PRO	-	expression tag	UNP P40261
B	1	ARG	-	expression tag	UNP P40261
B	2	GLY	-	expression tag	UNP P40261
B	103	ALA	GLU	conflict	UNP P40261
C	-15	MET	-	initiating methionine	UNP P40261
C	-14	GLY	-	expression tag	UNP P40261
C	-13	SER	-	expression tag	UNP P40261
C	-12	SER	-	expression tag	UNP P40261
C	-11	HIS	-	expression tag	UNP P40261
C	-10	HIS	-	expression tag	UNP P40261
C	-9	HIS	-	expression tag	UNP P40261
C	-8	HIS	-	expression tag	UNP P40261
C	-7	HIS	-	expression tag	UNP P40261
C	-6	HIS	-	expression tag	UNP P40261
C	-5	SER	-	expression tag	UNP P40261
C	-4	SER	-	expression tag	UNP P40261
C	-3	GLY	-	expression tag	UNP P40261
C	-2	LEU	-	expression tag	UNP P40261
C	-1	VAL	-	expression tag	UNP P40261
C	0	PRO	-	expression tag	UNP P40261
C	1	ARG	-	expression tag	UNP P40261
C	2	GLY	-	expression tag	UNP P40261
C	103	ALA	GLU	conflict	UNP P40261
D	-15	MET	-	initiating methionine	UNP P40261
D	-14	GLY	-	expression tag	UNP P40261
D	-13	SER	-	expression tag	UNP P40261
D	-12	SER	-	expression tag	UNP P40261
D	-11	HIS	-	expression tag	UNP P40261
D	-10	HIS	-	expression tag	UNP P40261

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	HIS	-	expression tag	UNP P40261
D	-8	HIS	-	expression tag	UNP P40261
D	-7	HIS	-	expression tag	UNP P40261
D	-6	HIS	-	expression tag	UNP P40261
D	-5	SER	-	expression tag	UNP P40261
D	-4	SER	-	expression tag	UNP P40261
D	-3	GLY	-	expression tag	UNP P40261
D	-2	LEU	-	expression tag	UNP P40261
D	-1	VAL	-	expression tag	UNP P40261
D	0	PRO	-	expression tag	UNP P40261
D	1	ARG	-	expression tag	UNP P40261
D	2	GLY	-	expression tag	UNP P40261
D	103	ALA	GLU	conflict	UNP P40261

- Molecule 2 is (3 {S})-1-(2-pyridin-2-ylethyl)- {N}-(1,3-thiazol-2-yl)piperidine-3-carboxamid e (CCD ID: A1MC7) (formula: C₁₆H₂₀N₄OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 22	C 16	N 4	O 1	S 1	0	0
2	B	1	Total 22	C 16	N 4	O 1	S 1	0	0
2	C	1	Total 22	C 16	N 4	O 1	S 1	0	0
2	D	1	Total 22	C 16	N 4	O 1	S 1	0	0

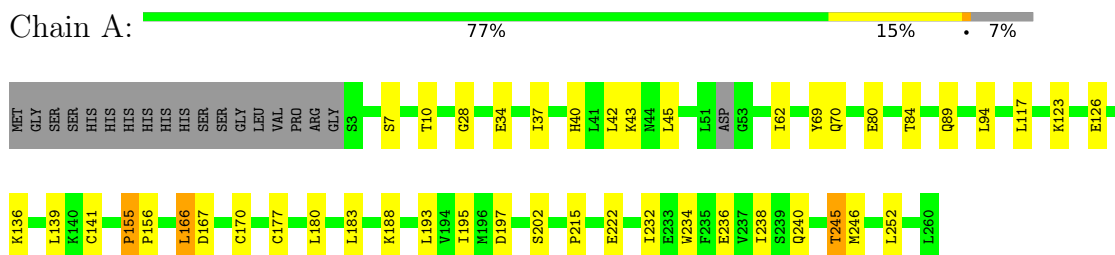
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	67	Total 67	O 67	0	0
3	C	35	Total 35	O 35	0	0
3	D	31	Total 31	O 31	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.

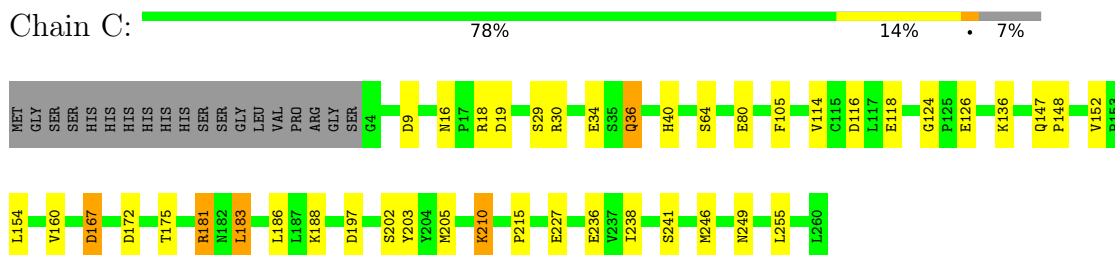
• Molecule 1: Nicotinamide N-methyltransferase



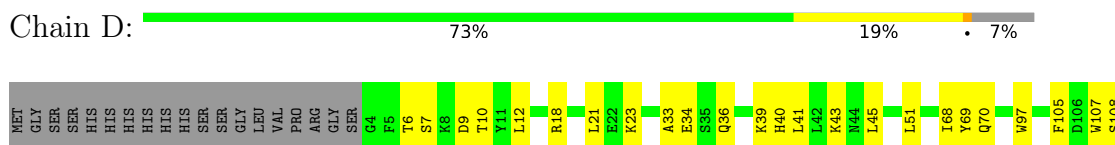
• Molecule 1: Nicotinamide N-methyltransferase

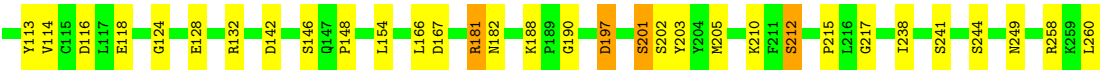


• Molecule 1: Nicotinamide N-methyltransferase



• Molecule 1: Nicotinamide N-methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.58Å 98.83Å 72.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.82 – 2.34 72.82 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.82-2.34) 99.8 (72.82-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.198 , 0.273 0.200 , 0.275	Depositor DCC
R_{free} test set	1915 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 14.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8189	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.79% 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: A1MC7

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	0.95	0/2025	1.15	6/2747 (0.2%)
1	B	0.94	0/2039	1.17	6/2767 (0.2%)
1	C	0.93	0/2018	1.17	4/2742 (0.1%)
1	D	0.91	0/2020	1.11	5/2744 (0.2%)
All	All	0.93	0/8102	1.15	21/11000 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	SER	CA-C-N	7.96	136.03	121.70
1	B	29	SER	C-N-CA	7.96	136.03	121.70
1	C	29	SER	CA-C-N	7.86	135.84	121.70
1	C	29	SER	C-N-CA	7.86	135.84	121.70
1	B	53	GLY	N-CA-C	6.74	121.48	110.77
1	C	29	SER	N-CA-C	-6.73	99.17	109.41
1	A	155	PRO	CA-C-N	-6.02	113.76	119.90
1	A	155	PRO	C-N-CA	-6.02	113.76	119.90
1	C	29	SER	CA-C-O	-5.55	115.15	121.58
1	A	28	GLY	N-CA-C	-5.48	106.15	112.83
1	A	170	CYS	CA-C-N	5.37	124.98	119.56
1	A	170	CYS	C-N-CA	5.37	124.98	119.56
1	A	166	LEU	N-CA-C	5.33	117.51	111.11
1	D	23	LYS	N-CA-C	5.20	117.02	111.36
1	B	166	LEU	N-CA-C	5.15	116.89	111.28
1	D	197	ASP	N-CA-C	5.10	116.05	108.60
1	D	217	GLY	CA-C-N	5.10	128.47	120.82
1	D	217	GLY	C-N-CA	5.10	128.47	120.82
1	B	155	PRO	CA-C-N	-5.10	114.33	119.83
1	B	155	PRO	C-N-CA	-5.10	114.33	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	D	166	LEU	N-CA-C	5.01	117.40	111.33

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	1982	0	1954	25	0
1	B	1992	0	1968	25	0
1	C	1971	0	1928	26	0
1	D	1973	0	1935	28	0
2	A	22	0	0	0	0
2	B	22	0	0	0	0
2	C	22	0	0	0	0
2	D	22	0	0	0	0
3	A	50	0	0	2	0
3	B	67	0	0	2	0
3	C	35	0	0	1	0
3	D	31	0	0	2	0
All	All	8189	0	7785	101	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 6.

All (101) 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:C:160:VAL:HG11	1:C:183:LEU:CD2	1.86	1.04
1:C:160:VAL:HG11	1:C:183:LEU:HD21	1.05	1.02
1:C:160:VAL:CG1	1:C:183:LEU:HD21	1.89	1.01
1:D:203:TYR:CD1	1:D:205:MET:HE3	1.97	0.99
1:C:202:SER:HB3	1:C:215:PRO:HG3	1.62	0.81
1:B:123:LYS:HE3	1:B:126:GLU:HB2	1.63	0.79
1:A:193:LEU:HD21	1:A:195:ILE:HD11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:TYR:HD1	1:D:205:MET:HE3	1.50	0.77
1:A:40:HIS:CE1	1:A:238:ILE:HG21	2.23	0.73
1:A:156:PRO:HB2	1:A:188:LYS:HG3	1.72	0.72
1:B:244:SER:HB3	3:B:464:HOH:O	1.90	0.71
1:B:29:SER:HA	1:B:30:ARG:HB2	1.70	0.71
1:D:205:MET:HE1	1:D:210:LYS:HG3	1.72	0.71
1:B:40:HIS:NE2	1:B:238:ILE:HG21	2.08	0.69
1:A:238:ILE:HD12	1:A:240:GLN:HB3	1.76	0.67
1:A:84:THR:HB	1:A:141:CYS:HB3	1.78	0.65
1:A:34:GLU:OE2	1:A:246:MET:HG3	1.98	0.64
1:D:201:SER:HB2	1:D:249:ASN:HB3	1.81	0.63
1:D:205:MET:HE1	1:D:210:LYS:CG	2.28	0.62
1:B:238:ILE:HD12	1:B:240:GLN:HB3	1.81	0.62
1:D:7:SER:OG	1:D:10:THR:HG22	1.99	0.61
1:B:7:SER:HB3	1:B:10:THR:H	1.67	0.60
1:B:181:ARG:HG2	1:B:181:ARG:HH11	1.66	0.60
1:B:47:LYS:CB	3:D:431:HOH:O	2.49	0.60
1:D:18:ARG:HH12	1:D:105:PHE:N	1.99	0.59
1:B:29:SER:HA	1:B:30:ARG:CB	2.33	0.59
1:D:34:GLU:HB2	3:D:403:HOH:O	2.04	0.57
1:A:45:LEU:HD13	1:A:70:GLN:HA	1.86	0.57
1:A:202:SER:HB3	1:A:215:PRO:HG3	1.86	0.57
1:B:156:PRO:HB2	1:B:188:LYS:HG3	1.86	0.57
1:C:181:ARG:CG	1:C:181:ARG:HH11	2.18	0.56
1:D:40:HIS:CE1	1:D:238:ILE:HG21	2.41	0.56
1:B:40:HIS:CD2	1:B:238:ILE:HG21	2.41	0.55
1:C:181:ARG:HH11	1:C:181:ARG:HG3	1.71	0.55
1:C:16:ASN:ND2	1:C:19:ASP:H	2.05	0.55
1:A:222:GLU:HG2	1:A:232:ILE:CD1	2.37	0.54
1:D:181:ARG:HG3	1:D:181:ARG:HH11	1.72	0.54
1:A:245:THR:HB	1:A:246:MET:HE2	1.90	0.54
1:B:202:SER:HB3	1:B:215:PRO:HG3	1.90	0.54
1:C:114:VAL:O	1:C:118:GLU:HG3	2.07	0.54
1:D:181:ARG:HH11	1:D:181:ARG:CG	2.22	0.53
1:C:181:ARG:HG3	1:C:181:ARG:NH1	2.23	0.53
1:D:201:SER:HB2	1:D:249:ASN:CB	2.39	0.53
1:A:167:ASP:HB2	3:A:413:HOH:O	2.09	0.53
1:C:40:HIS:CE1	1:C:238:ILE:HG21	2.44	0.53
1:D:205:MET:CE	1:D:210:LYS:HG3	2.40	0.52
1:D:203:TYR:CE1	1:D:205:MET:HE3	2.42	0.52
1:B:45:LEU:HD13	1:B:70:GLN:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:VAL:O	1:D:118:GLU:HG3	2.11	0.51
1:A:177:CYS:HB3	3:A:448:HOH:O	2.11	0.51
1:B:181:ARG:HH11	1:B:181:ARG:CG	2.25	0.51
1:C:241:SER:OG	1:C:249:ASN:O	2.27	0.51
1:C:172:ASP:HB2	1:C:175:THR:OG1	2.11	0.50
1:A:7:SER:HB3	1:A:10:THR:H	1.77	0.49
1:C:34:GLU:HB3	3:C:433:HOH:O	2.13	0.49
1:D:181:ARG:HG3	1:D:181:ARG:NH1	2.26	0.49
1:A:222:GLU:HG2	1:A:232:ILE:HD12	1.95	0.49
1:A:234:TRP:HB3	1:C:238:ILE:HG22	1.94	0.48
1:C:203:TYR:CD2	1:C:205:MET:HE2	2.48	0.48
1:D:33:ALA:HB1	1:D:241:SER:O	2.14	0.48
1:C:80:GLU:HG3	1:C:136:LYS:HB2	1.96	0.47
1:D:128:GLU:HB3	1:D:132:ARG:NH1	2.29	0.47
1:A:193:LEU:HD21	1:A:195:ILE:CD1	2.43	0.47
1:B:27:PHE:HA	1:B:35:SER:OG	2.15	0.46
1:C:188:LYS:HB3	1:C:188:LYS:HE2	1.78	0.46
1:A:84:THR:HA	1:A:139:LEU:O	2.15	0.46
1:B:51:LEU:HD13	1:D:43:LYS:HG2	1.97	0.46
1:C:16:ASN:HD22	1:C:19:ASP:H	1.61	0.46
1:A:155:PRO:O	1:A:156:PRO:C	2.55	0.45
1:D:68:ILE:O	1:D:69:TYR:C	2.59	0.45
1:D:142:ASP:O	1:D:148:PRO:HA	2.16	0.45
1:D:202:SER:HB3	1:D:215:PRO:HG3	1.98	0.45
1:A:62:ILE:HG21	1:A:183:LEU:HD11	1.97	0.44
1:D:97:TRP:CD1	1:D:107:TRP:HD1	2.35	0.44
1:B:30:ARG:H	1:B:35:SER:CB	2.30	0.44
1:B:148:PRO:HG3	1:B:182:ASN:HB3	2.00	0.44
1:B:222:GLU:HG3	1:B:232:ILE:CD1	2.48	0.44
1:D:190:GLY:O	1:D:258:ARG:HD3	2.16	0.44
1:D:39:LYS:HG2	1:D:113:TYR:CZ	2.53	0.43
1:C:255:LEU:C	1:C:255:LEU:HD12	2.43	0.43
1:C:205:MET:HE1	1:C:210:LYS:HG3	2.01	0.43
1:C:148:PRO:HG2	1:C:186:LEU:HD11	2.00	0.43
1:C:181:ARG:CG	1:C:181:ARG:NH1	2.80	0.42
1:D:146:SER:HA	1:D:182:ASN:ND2	2.34	0.42
1:D:6:THR:H	1:D:212:SER:HB2	1.84	0.42
1:B:30:ARG:HD3	1:B:30:ARG:HA	1.76	0.42
1:B:122:VAL:HG21	3:B:415:HOH:O	2.20	0.42
1:A:238:ILE:HD11	1:A:252:LEU:HD13	2.02	0.41
1:A:80:GLU:HG3	1:A:136:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ASP:HB2	1:C:197:ASP:CG	2.45	0.41
1:A:45:LEU:CD1	1:A:70:GLN:HA	2.50	0.41
1:A:123:LYS:NZ	1:A:126:GLU:HB2	2.35	0.41
1:C:36:GLN:HE21	1:C:36:GLN:HB2	1.68	0.41
1:A:42:LEU:HD21	1:A:69:TYR:HB2	2.02	0.41
1:A:236:GLU:HB2	1:C:236:GLU:HG3	2.02	0.41
1:B:181:ARG:CG	1:B:181:ARG:NH1	2.82	0.41
1:C:18:ARG:NH2	1:C:105:PHE:HD1	2.19	0.41
1:B:118:GLU:OE1	1:B:127:LYS:NZ	2.46	0.40
1:B:45:LEU:HG	1:B:196:MET:HE1	2.02	0.40
1:B:18:ARG:NH1	1:B:103:ALA:O	2.50	0.40
1:D:45:LEU:HD13	1:D:70:GLN:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/276 (92%)	245 (97%)	8 (3%)	0	100	100
1	B	257/276 (93%)	248 (96%)	8 (3%)	1 (0%)	30	32
1	C	256/276 (93%)	243 (95%)	11 (4%)	2 (1%)	16	16
1	D	256/276 (93%)	242 (94%)	13 (5%)	1 (0%)	30	32
All	All	1022/1104 (93%)	978 (96%)	40 (4%)	4 (0%)	30	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	ARG
1	C	30	ARG
1	C	124	GLY

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Mol	Chain	Res	Type
1	D	124	GLY

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	215/240 (90%)	206 (96%)	9 (4%)	26	34
1	B	217/240 (90%)	204 (94%)	13 (6%)	17	20
1	C	212/240 (88%)	198 (93%)	14 (7%)	15	17
1	D	213/240 (89%)	196 (92%)	17 (8%)	11	12
All	All	857/960 (89%)	804 (94%)	53 (6%)	16	19

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	43	LYS
1	A	89	GLN
1	A	94	LEU
1	A	117	LEU
1	A	166	LEU
1	A	180	LEU
1	A	197	ASP
1	A	245	THR
1	B	3	SER
1	B	12	LEU
1	B	37	ILE
1	B	77	SER
1	B	88	ASP
1	B	98	LEU
1	B	117	LEU
1	B	146	SER
1	B	180	LEU
1	B	181	ARG
1	B	197	ASP

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Mol	Chain	Res	Type
1	B	243	SER
1	B	245	THR
1	C	9	ASP
1	C	36	GLN
1	C	64	SER
1	C	116	ASP
1	C	126	GLU
1	C	147	GLN
1	C	152	VAL
1	C	154	LEU
1	C	167	ASP
1	C	181	ARG
1	C	183	LEU
1	C	210	LYS
1	C	227	GLU
1	C	246	MET
1	D	9	ASP
1	D	12	LEU
1	D	21	LEU
1	D	36	GLN
1	D	41	LEU
1	D	51	LEU
1	D	108	SER
1	D	116	ASP
1	D	154	LEU
1	D	167	ASP
1	D	181	ARG
1	D	188	LYS
1	D	197	ASP
1	D	201	SER
1	D	212	SER
1	D	244	SER
1	D	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	92	GLN
1	A	120	ASN
1	B	89	GLN
1	B	120	ASN

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Mol	Chain	Res	Type
1	B	145	GLN
1	B	182	ASN
1	C	14	HIS
1	C	16	ASN
1	C	36	GLN
1	C	40	HIS
1	C	137	GLN
1	C	145	GLN
1	C	209	GLN
1	C	240	GLN
1	D	36	GLN
1	D	40	HIS
1	D	145	GLN
1	D	182	ASN
1	D	240	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A1MC7	D	301	-	24,24,24	3.66	9 (37%)	31,31,31	2.26	8 (25%)
2	A1MC7	C	301	-	24,24,24	3.59	10 (41%)	31,31,31	2.20	10 (32%)
2	A1MC7	B	301	-	24,24,24	3.32	11 (45%)	31,31,31	2.06	7 (22%)
2	A1MC7	A	301	-	24,24,24	3.37	10 (41%)	31,31,31	1.91	7 (22%)

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	A1MC7	D	301	-	-	0/13/23/23	0/3/3/3
2	A1MC7	C	301	-	-	0/13/23/23	0/3/3/3
2	A1MC7	B	301	-	-	0/13/23/23	0/3/3/3
2	A1MC7	A	301	-	-	0/13/23/23	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	A1MC7	C14-N13	-11.36	1.21	1.47
2	C	301	A1MC7	C14-N13	-10.59	1.23	1.47
2	A	301	A1MC7	C14-N13	-9.83	1.25	1.47
2	B	301	A1MC7	C14-N13	-9.80	1.25	1.47
2	C	301	A1MC7	C04-S08	-7.60	1.63	1.74
2	D	301	A1MC7	C04-S08	-6.89	1.64	1.74
2	B	301	A1MC7	C04-S08	-6.57	1.65	1.74
2	D	301	A1MC7	C02-N03	5.62	1.46	1.36
2	A	301	A1MC7	C04-S08	-5.56	1.66	1.74
2	A	301	A1MC7	C06-N05	5.49	1.48	1.38
2	B	301	A1MC7	C06-N05	5.30	1.48	1.38
2	A	301	A1MC7	C04-N05	5.25	1.39	1.31
2	D	301	A1MC7	C04-N03	5.21	1.45	1.38
2	C	301	A1MC7	C02-N03	5.12	1.45	1.36
2	C	301	A1MC7	C06-N05	5.04	1.47	1.38
2	D	301	A1MC7	C04-N05	4.93	1.39	1.31
2	B	301	A1MC7	C04-N05	4.75	1.39	1.31
2	A	301	A1MC7	C02-N03	4.71	1.45	1.36
2	C	301	A1MC7	C04-N03	4.69	1.45	1.38
2	C	301	A1MC7	C04-N05	4.54	1.38	1.31
2	D	301	A1MC7	C06-N05	4.52	1.46	1.38
2	A	301	A1MC7	C06-C07	4.36	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	A1MC7	C02-N03	4.26	1.44	1.36
2	B	301	A1MC7	C06-C07	4.10	1.43	1.34
2	D	301	A1MC7	C06-C07	3.35	1.42	1.34
2	D	301	A1MC7	C11-C10	-3.29	1.44	1.53
2	C	301	A1MC7	C11-C10	-3.28	1.45	1.53
2	C	301	A1MC7	C06-C07	3.28	1.41	1.34
2	A	301	A1MC7	C11-C10	-3.26	1.45	1.53
2	C	301	A1MC7	C10-C09	-3.06	1.45	1.53
2	D	301	A1MC7	C10-C09	-3.04	1.45	1.53
2	A	301	A1MC7	C10-C09	-2.95	1.45	1.53
2	A	301	A1MC7	O01-C02	-2.94	1.17	1.23
2	B	301	A1MC7	C04-N03	2.79	1.42	1.38
2	B	301	A1MC7	C11-C10	-2.75	1.46	1.53
2	A	301	A1MC7	C04-N03	2.74	1.42	1.38
2	B	301	A1MC7	O01-C02	-2.67	1.18	1.23
2	B	301	A1MC7	C10-C09	-2.61	1.46	1.53
2	B	301	A1MC7	C07-S08	-2.04	1.61	1.70
2	C	301	A1MC7	C07-S08	-2.03	1.61	1.70

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	A1MC7	C07-S08-C04	6.49	97.50	90.07
2	D	301	A1MC7	C07-S08-C04	6.19	97.16	90.07
2	B	301	A1MC7	C07-S08-C04	5.94	96.88	90.07
2	D	301	A1MC7	C07-C06-N05	-5.00	108.90	116.12
2	C	301	A1MC7	C07-C06-N05	-4.97	108.95	116.12
2	A	301	A1MC7	C07-S08-C04	4.92	95.71	90.07
2	D	301	A1MC7	C12-N13-C22	4.52	117.06	109.53
2	B	301	A1MC7	C12-N13-C22	4.40	116.85	109.53
2	D	301	A1MC7	C18-N17-C16	3.91	122.90	117.41
2	A	301	A1MC7	C18-N17-C16	3.88	122.86	117.41
2	B	301	A1MC7	C07-C06-N05	-3.87	110.53	116.12
2	A	301	A1MC7	C12-N13-C22	3.84	115.93	109.53
2	C	301	A1MC7	C12-N13-C22	3.70	115.68	109.53
2	A	301	A1MC7	C07-C06-N05	-3.55	111.00	116.12
2	B	301	A1MC7	C10-C11-C12	3.05	114.76	110.75
2	B	301	A1MC7	C18-N17-C16	3.02	121.65	117.41
2	D	301	A1MC7	C19-C18-N17	-3.02	118.64	123.42
2	C	301	A1MC7	C18-N17-C16	3.01	121.63	117.41
2	D	301	A1MC7	C10-C11-C12	2.82	114.45	110.75
2	B	301	A1MC7	C11-C12-N13	2.67	115.45	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	A1MC7	S08-C04-N03	2.48	127.71	123.29
2	A	301	A1MC7	C11-C12-N13	2.35	114.95	111.30
2	C	301	A1MC7	C14-C15-C16	2.35	115.75	111.70
2	D	301	A1MC7	S08-C04-N05	-2.34	110.18	114.59
2	C	301	A1MC7	C19-C20-C21	-2.33	117.37	120.24
2	A	301	A1MC7	C10-C11-C12	2.28	113.75	110.75
2	A	301	A1MC7	S08-C04-N03	2.22	127.25	123.29
2	C	301	A1MC7	C10-C11-C12	2.21	113.66	110.75
2	C	301	A1MC7	C15-C16-N17	2.20	121.39	116.86
2	B	301	A1MC7	S08-C04-N03	2.16	127.15	123.29
2	C	301	A1MC7	S08-C04-N05	-2.11	110.62	114.59
2	C	301	A1MC7	C19-C18-N17	-2.00	120.25	123.42

There are no chirality outliers.

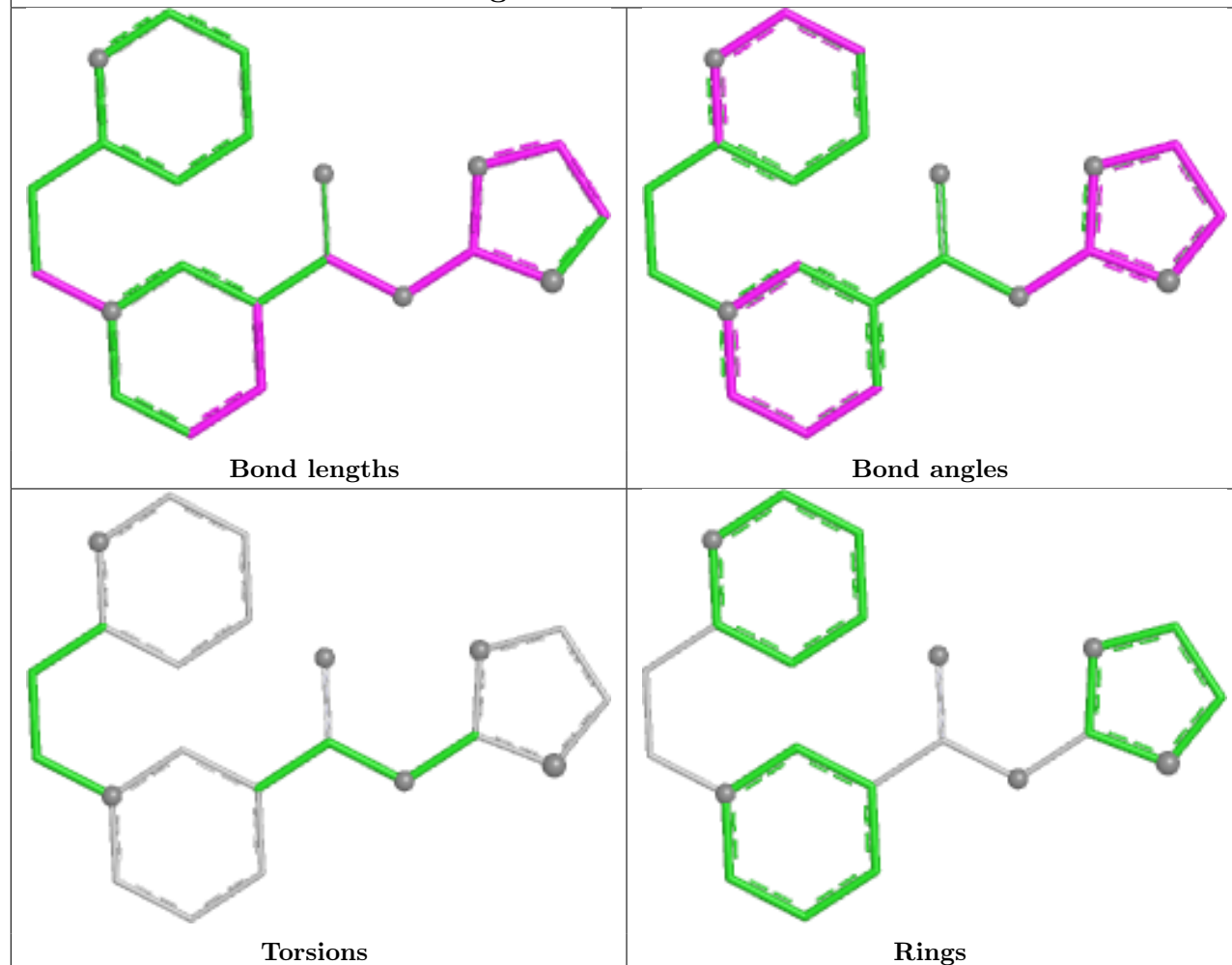
There are no torsion outliers.

There are no ring outliers.

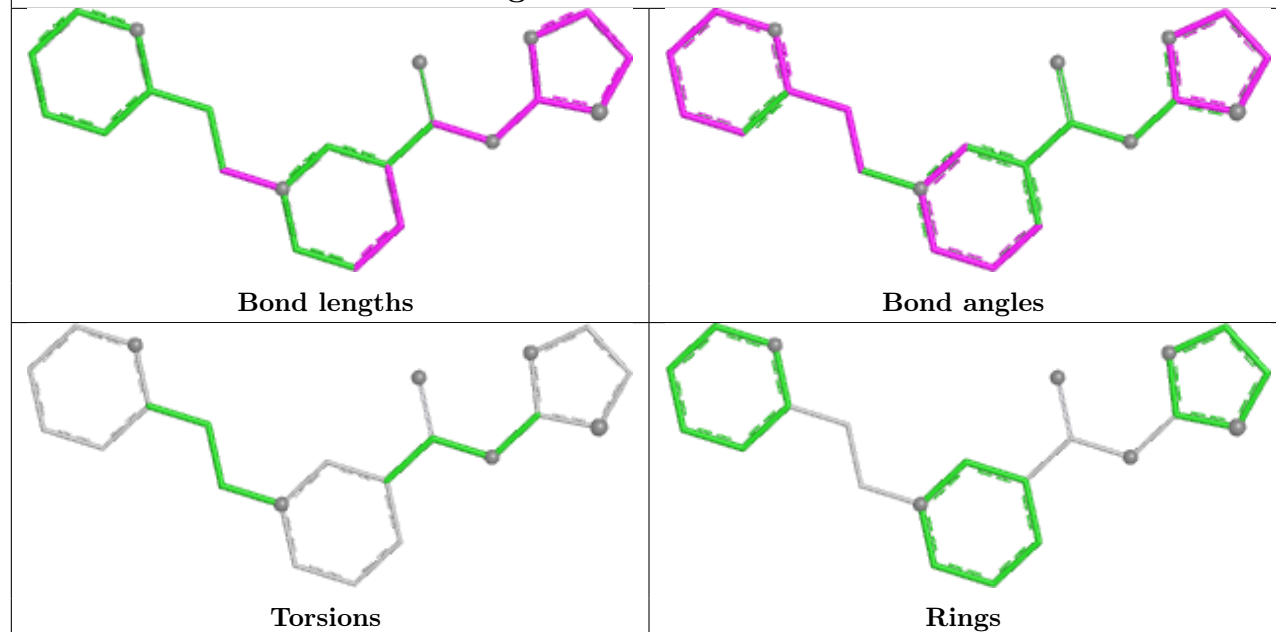
No monomer is involved in short contacts.

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.

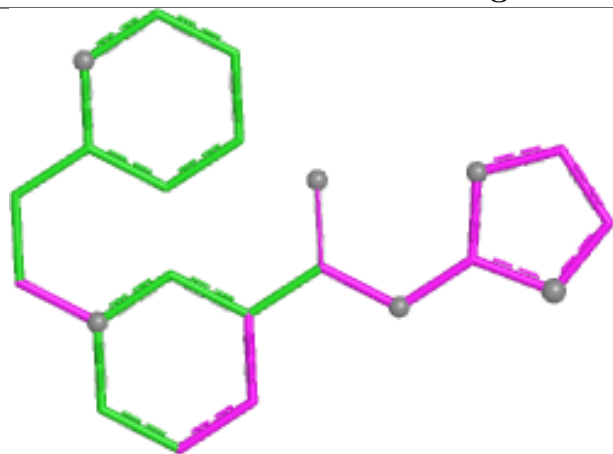
Ligand A1MC7 D 301



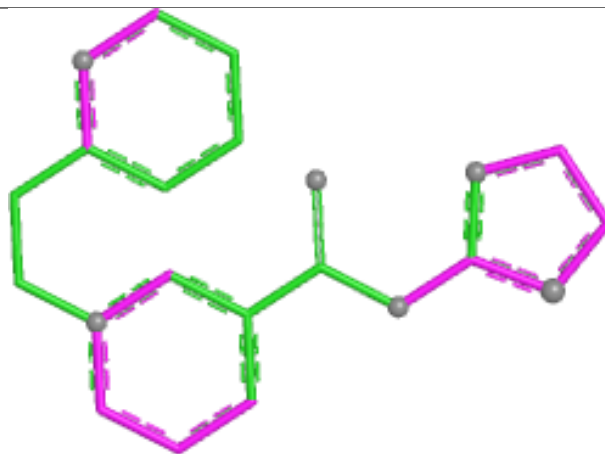
Ligand A1MC7 C 301



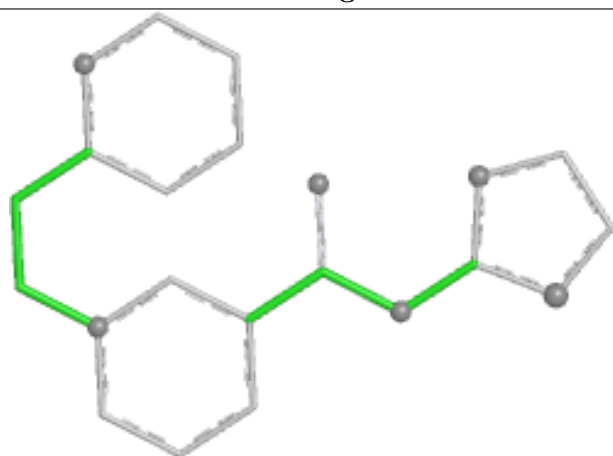
Ligand A1MC7 B 301



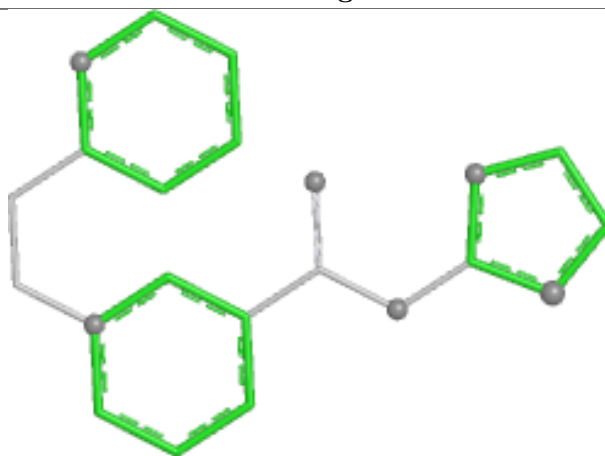
Bond lengths



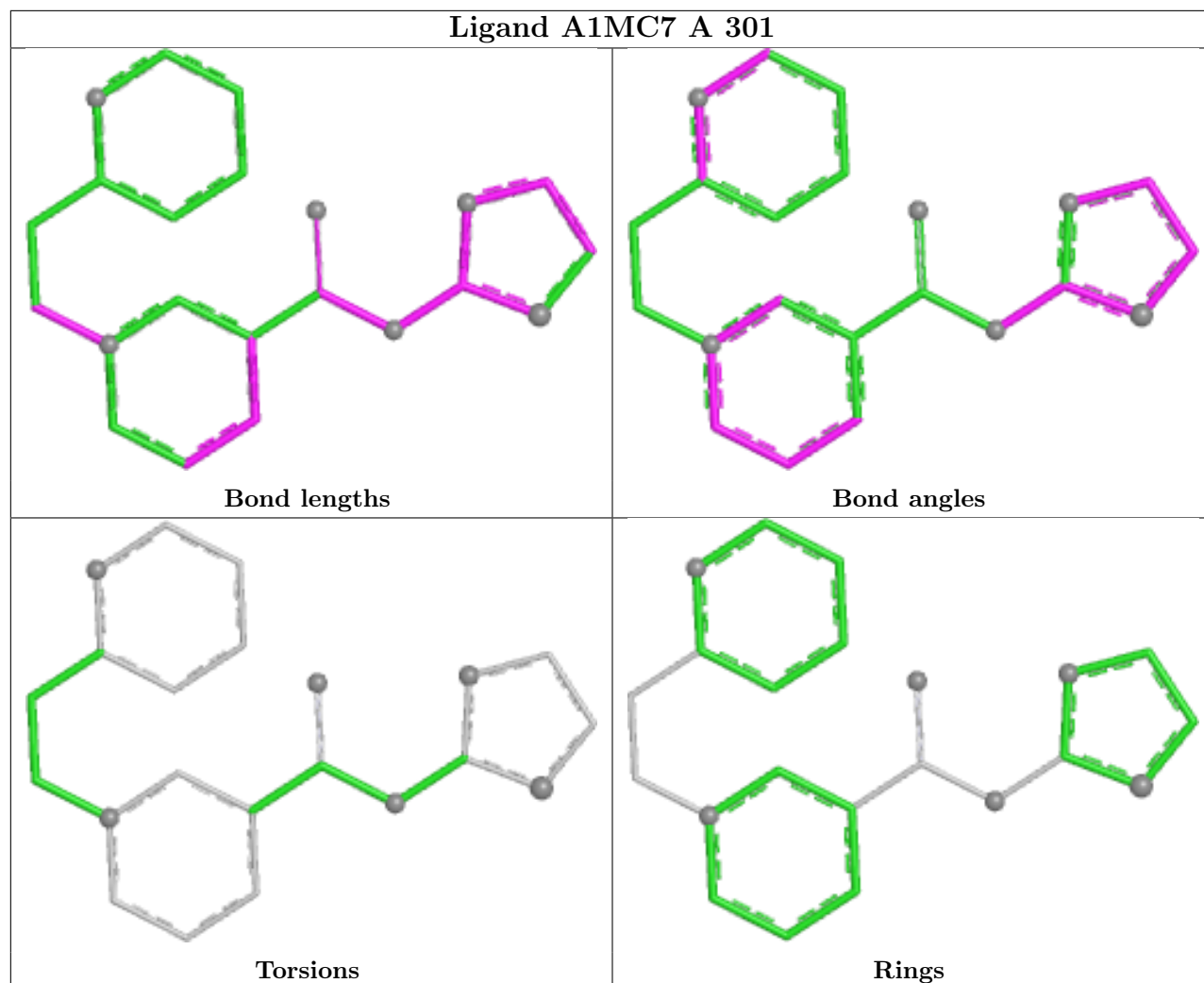
Bond angles



Torsions



Rings



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	257/276 (93%)	-1.31	0 100 100	20, 31, 53, 79	0
1	B	258/276 (93%)	-1.32	0 100 100	19, 31, 57, 76	1 (0%)
1	C	257/276 (93%)	-1.15	0 100 100	24, 40, 61, 88	1 (0%)
1	D	257/276 (93%)	-1.16	0 100 100	22, 40, 60, 87	1 (0%)
All	All	1029/1104 (93%)	-1.23	0 100 100	19, 35, 59, 88	3 (0%)

There are no RSRZ outliers to report.

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](#)

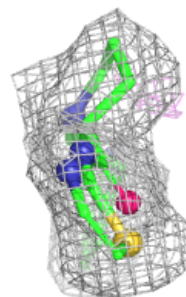
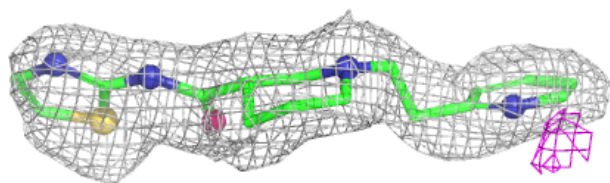
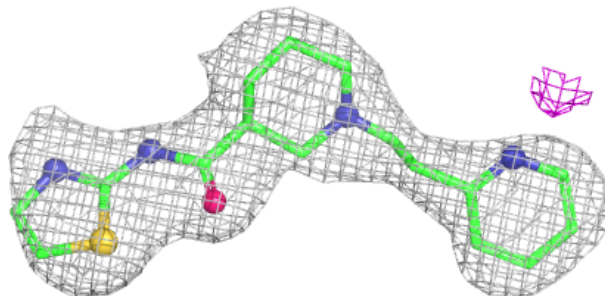
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1MC7	A	301	22/22	0.99	0.03	25,28,33,34	0
2	A1MC7	B	301	22/22	0.99	0.03	24,29,34,35	0
2	A1MC7	C	301	22/22	0.99	0.03	31,34,37,38	0
2	A1MC7	D	301	22/22	0.99	0.03	32,35,40,43	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.

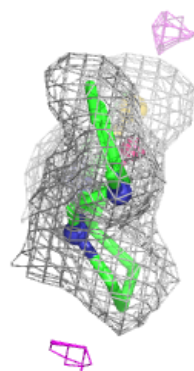
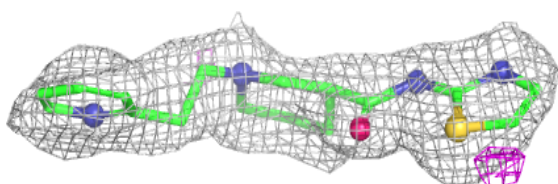
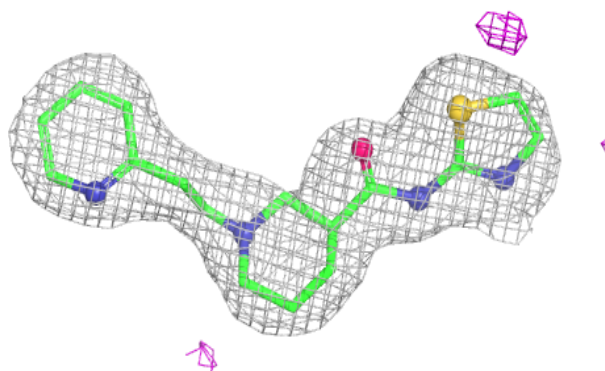
Electron density around A1MC7 A 301:

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

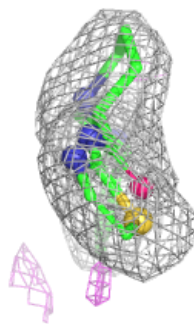
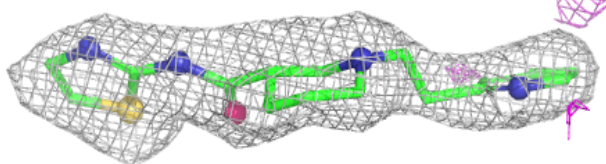
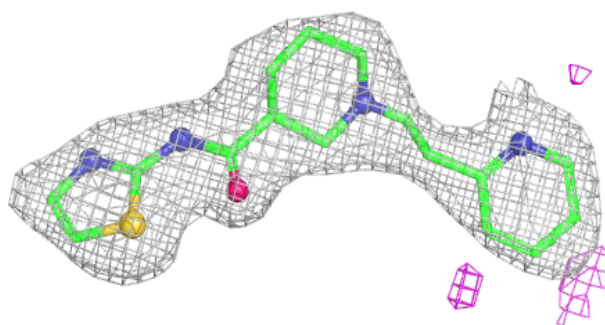


Electron density around A1MC7 B 301:

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

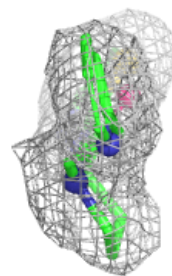
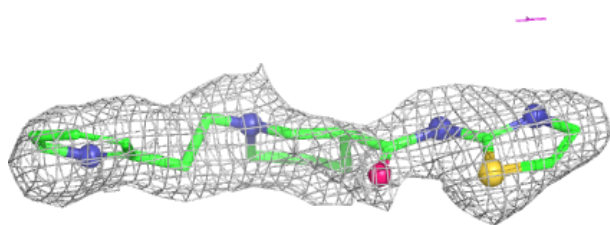
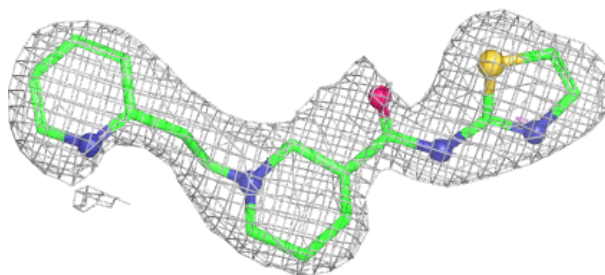
**Electron density around A1MC7 C 301:**

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



Electron density around A1MC7 D 301:

$2mF_o-DF_c$ (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.