



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:57 pm BST

PDB ID : 1PO2  
Title : POLIOVIRUS (TYPE 1, MAHONEY) IN COMPLEX WITH R77975, AN INHIBITOR OF VIRAL REPLICATION  
Authors : Hiremath, C.N.; Filman, D.J.; Grant, R.A.; Hogle, J.M.  
Deposited on : 1997-01-08  
Resolution : 2.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

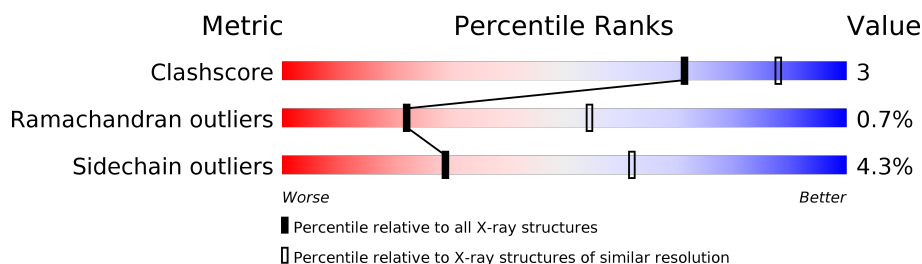
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	5	80% 20%
2	1	302	80% 12% 6%
3	2	272	83% 14% ..
4	3	238	87% 10% ..
5	4	68	74% 15% 9%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6688 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 POLIOVIRUS TYPE 1 MAHONEY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	0	5	Total	C	N	O	0	0	0
			29	15	5	9			

- Molecule 2 is a protein called POLIOVIRUS TYPE 1 MAHONEY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	283	Total	C	N	O	S	0	0	0
			2222	1416	378	423	5			

- Molecule 3 is a protein called POLIOVIRUS TYPE 1 MAHONEY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	268	Total	C	N	O	S	0	0	0
			2085	1317	358	396	14			

- Molecule 4 is a protein called POLIOVIRUS TYPE 1 MAHONEY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	235	Total	C	N	O	S	0	0	0
			1834	1169	299	349	17			

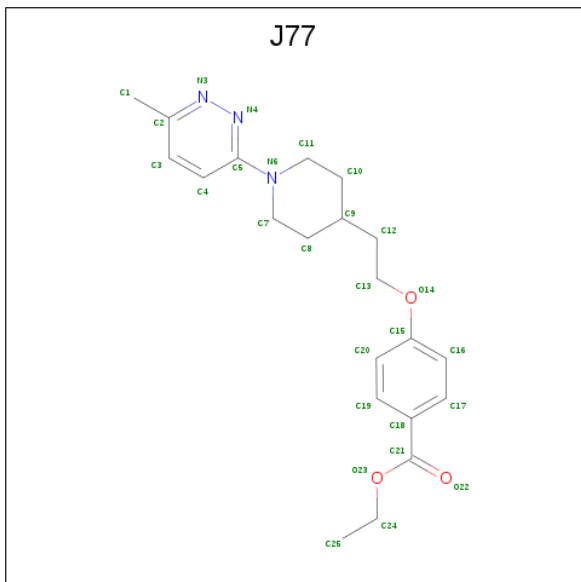
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	CONFLICT	UNP P03300

- Molecule 5 is a protein called POLIOVIRUS TYPE 1 MAHONEY.

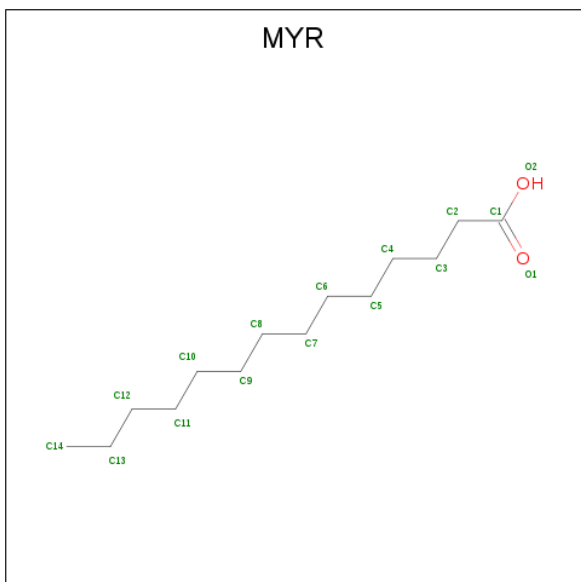
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	62	Total	C	N	O	S	0	0	0
			476	293	81	101	1			

- Molecule 6 is (METHYLPYRIDAZINE PIPERIDINE ETHYLOXYPHENYL)ETHYLACETATE (three-letter code: J77) (formula:  $C_{21}H_{27}N_3O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	N	O	0	0
			27	21	3	3		

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	4	1	Total	C	O	0	0
			15	14	1		

### 3 Residue-property plots [i](#)

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

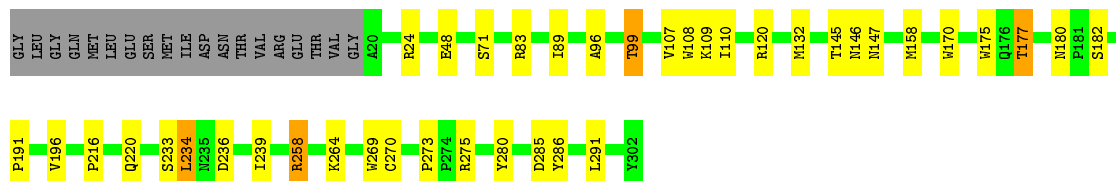
#### • Molecule 1: POLIOVIRUS TYPE 1 MAHONEY

Chain 0: 




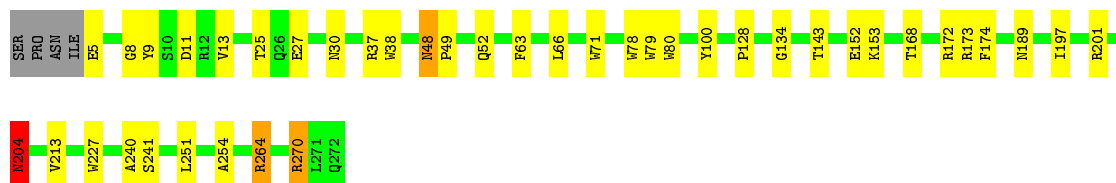
#### • Molecule 2: POLIOVirus TYPE 1 MAHONEY

Chain 1: 



#### • Molecule 3: POLIOVirus TYPE 1 MAHONEY

Chain 2: 



#### • Molecule 4: POLIOVirus TYPE 1 MAHONEY

Chain 3: 



#### • Molecule 5: POLIOVirus TYPE 1 MAHONEY

Chain 4: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	322.94Å 358.04Å 380.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 30.75 – 2.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 18.9 (30.75-2.87)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.67 (at 2.85Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.249 , (Not available) 0.220 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 1.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.21	EDS
Total number of atoms	6688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MYR, J77

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	0	0.70	0/28	1.53	0/36
2	1	0.74	0/2285	1.39	15/3124 (0.5%)
3	2	0.75	0/2142	1.44	22/2928 (0.8%)
4	3	0.73	0/1881	1.33	16/2562 (0.6%)
5	4	0.73	0/483	1.41	1/651 (0.2%)
All	All	0.74	0/6819	1.39	54/9301 (0.6%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	38	TRP	CD1-CG-CD2	8.93	113.44	106.30
3	2	227	TRP	CD1-CG-CD2	8.86	113.39	106.30
4	3	110	TRP	CD1-CG-CD2	8.43	113.04	106.30
3	2	79	TRP	CD1-CG-CD2	8.20	112.86	106.30
3	2	80	TRP	CD1-CG-CD2	8.10	112.78	106.30
4	3	110	TRP	CE2-CD2-CG	-8.08	100.84	107.30
3	2	78	TRP	CD1-CG-CD2	8.07	112.75	106.30
4	3	170	TRP	CE2-CD2-CG	-8.02	100.89	107.30
3	2	227	TRP	CE2-CD2-CG	-7.99	100.91	107.30
2	1	175	TRP	CD1-CG-CD2	7.98	112.68	106.30
3	2	80	TRP	CE2-CD2-CG	-7.95	100.94	107.30
2	1	269	TRP	CD1-CG-CD2	7.94	112.65	106.30
4	3	170	TRP	CD1-CG-CD2	7.89	112.61	106.30
3	2	71	TRP	CD1-CG-CD2	7.83	112.56	106.30
2	1	83	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	1	170	TRP	CD1-CG-CD2	7.65	112.42	106.30
2	1	83	ARG	NE-CZ-NH2	-7.63	116.49	120.30
3	2	38	TRP	CE2-CD2-CG	-7.51	101.29	107.30
2	1	175	TRP	CE2-CD2-CG	-7.45	101.34	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	71	TRP	CE2-CD2-CG	-7.31	101.45	107.30
2	1	269	TRP	CE2-CD2-CG	-7.30	101.46	107.30
2	1	108	TRP	CD1-CG-CD2	7.30	112.14	106.30
2	1	170	TRP	CE2-CD2-CG	-7.27	101.48	107.30
3	2	79	TRP	CE2-CD2-CG	-7.27	101.48	107.30
2	1	108	TRP	CE2-CD2-CG	-7.16	101.57	107.30
3	2	100	TYR	CB-CG-CD2	-7.14	116.72	121.00
3	2	78	TRP	CE2-CD2-CG	-7.07	101.64	107.30
4	3	226	ARG	NE-CZ-NH1	6.72	123.66	120.30
4	3	170	TRP	CG-CD2-CE3	6.47	139.72	133.90
4	3	156	TRP	CE2-CD2-CG	-6.42	102.17	107.30
4	3	156	TRP	CD1-CG-CD2	6.36	111.39	106.30
4	3	223	ARG	NE-CZ-NH2	-6.20	117.20	120.30
4	3	170	TRP	CB-CG-CD1	-5.95	119.26	127.00
4	3	206	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	2	79	TRP	CB-CG-CD1	-5.81	119.44	127.00
4	3	226	ARG	NE-CZ-NH2	-5.68	117.46	120.30
3	2	227	TRP	CG-CD1-NE1	-5.65	104.45	110.10
5	4	32	TYR	CB-CG-CD2	-5.59	117.64	121.00
2	1	258	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	1	269	TRP	CB-CG-CD1	-5.52	119.83	127.00
2	1	108	TRP	CG-CD2-CE3	5.48	138.83	133.90
3	2	227	TRP	CG-CD2-CE3	5.41	138.77	133.90
3	2	8	GLY	N-CA-C	5.37	126.53	113.10
3	2	38	TRP	CG-CD1-NE1	-5.37	104.73	110.10
3	2	79	TRP	CG-CD2-CE3	5.34	138.70	133.90
3	2	204	ASN	CB-CA-C	-5.31	99.78	110.40
3	2	172	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	1	120	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	1	275	ARG	NE-CZ-NH1	5.23	122.91	120.30
4	3	110	TRP	CG-CD2-CE3	5.17	138.56	133.90
4	3	110	TRP	CG-CD1-NE1	-5.14	104.96	110.10
4	3	85	LEU	CA-CB-CG	5.11	127.06	115.30
3	2	264	ARG	NE-CZ-NH1	5.10	122.85	120.30
4	3	233	GLN	OE1-CD-NE2	-5.05	110.28	121.90

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	0	29	0	24	0	0
2	1	2222	0	2173	22	0
3	2	2085	0	2000	15	0
4	3	1834	0	1816	11	0
5	4	476	0	457	6	0
6	1	27	0	27	5	0
7	4	15	0	27	2	0
All	All	6688	0	6524	46	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 3.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:110:ILE:HG21	6:1:0:J77:H101	1.59	0.84
2:1:132:MET:HE3	6:1:0:J77:H102	1.65	0.79
2:1:177:THR:HG22	2:1:180:ASN:HB2	1.68	0.76
2:1:158:MET:SD	2:1:177:THR:HG23	2.29	0.72
3:2:37:ARG:HG3	4:3:37:PRO:HB3	1.72	0.71
5:4:30:ILE:HD13	7:4:1:MYR:H72	1.79	0.64
4:3:87:LEU:HD11	4:3:114:LEU:HD12	1.81	0.62
3:2:5:GLU:HB3	3:2:9:TYR:HB2	1.81	0.61
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.83	0.60
4:3:51:THR:HG21	4:3:99:MET:H	1.67	0.59
2:1:110:ILE:HD13	6:1:0:J77:H112	1.84	0.59
3:2:30:ASN:HD21	5:4:59:ASP:HB2	1.69	0.58
2:1:132:MET:CE	6:1:0:J77:H102	2.34	0.57
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.88	0.56
2:1:280:TYR:HB3	2:1:285:ASP:O	2.07	0.55
2:1:286:TYR:HB2	2:1:291:LEU:HD21	1.91	0.52
4:3:55:PHE:HE2	4:3:212:GLY:HA3	1.74	0.52
4:3:167:VAL:O	4:3:169:PRO:HD3	2.09	0.52
2:1:107:VAL:HG13	2:1:239:ILE:HD13	1.92	0.51
5:4:57:ILE:HD11	5:4:61:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:66:LEU:HD12	3:2:251:LEU:HD23	1.92	0.51
3:2:143:THR:HG23	3:2:173:ARG:HA	1.92	0.50
2:1:273:PRO:HB3	3:2:189:ASN:HB2	1.94	0.50
2:1:196:VAL:HG11	6:1:0:J77:H82	1.94	0.48
2:1:177:THR:HG21	2:1:182:SER:OG	2.13	0.48
3:2:134:GLY:HA2	3:2:174:PHE:HA	1.97	0.47
2:1:216:PRO:HB2	3:2:270:ARG:HB3	1.97	0.47
5:4:32:TYR:HD1	7:4:1:MYR:H131	1.79	0.47
2:1:48:GLU:HA	3:2:197:ILE:HB	1.98	0.46
4:3:61:LYS:HD2	4:3:66:GLU:HB3	1.97	0.46
2:1:96:ALA:O	2:1:99:THR:HG23	2.15	0.46
2:1:89:ILE:HG12	2:1:258:ARG:HG2	1.98	0.45
4:3:70:VAL:HB	4:3:210:ILE:HG13	1.98	0.45
3:2:213:VAL:HG22	4:3:37:PRO:HG2	1.98	0.45
3:2:48:ASN:HB3	3:2:49:PRO:HD3	2.00	0.44
2:1:264:LYS:HE3	5:4:37:ALA:O	2.17	0.44
2:1:24:ARG:HA	2:1:71:SER:OG	2.18	0.44
2:1:158:MET:SD	2:1:177:THR:CG2	3.05	0.43
3:2:5:GLU:HG2	3:2:9:TYR:HD2	1.83	0.42
3:2:63:PHE:CD1	3:2:254:ALA:HB2	2.54	0.42
5:4:49:ASP:HA	5:4:50:PRO:HD3	1.98	0.42
4:3:120:PHE:HA	4:3:210:ILE:HG22	2.02	0.42
2:1:132:MET:HB3	2:1:132:MET:HE2	1.85	0.41
3:2:13:VAL:HA	3:2:25:THR:O	2.20	0.41
4:3:143:LYS:HD3	4:3:143:LYS:HA	1.85	0.40
3:2:27:GLU:HB2	3:2:204:ASN:OD1	2.22	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	0	3/5 (60%)	3 (100%)	0	0	100	100
2	1	281/302 (93%)	268 (95%)	10 (4%)	3 (1%)	14	42
3	2	266/272 (98%)	250 (94%)	14 (5%)	2 (1%)	19	51
4	3	233/238 (98%)	219 (94%)	14 (6%)	0	100	100
5	4	58/68 (85%)	52 (90%)	5 (9%)	1 (2%)	9	31
All	All	841/885 (95%)	792 (94%)	43 (5%)	6 (1%)	22	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	146	ASN
3	2	48	ASN
3	2	240	ALA
2	1	234	LEU
2	1	270	CYS
5	4	11	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	0	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	1	245/261 (94%)	237 (97%)	8 (3%)	38	72
3	2	228/232 (98%)	217 (95%)	11 (5%)	25	58
4	3	210/212 (99%)	202 (96%)	8 (4%)	33	67
5	4	54/57 (95%)	50 (93%)	4 (7%)	13	38
All	All	741/766 (97%)	709 (96%)	32 (4%)	29	62

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	7	SER
2	1	99	THR

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Mol	Chain	Res	Type
2	1	145	THR
2	1	147	ASN
2	1	177	THR
2	1	220	GLN
2	1	233	SER
2	1	234	LEU
2	1	236	ASP
3	2	11	ASP
3	2	52	GLN
3	2	128	PRO
3	2	152	GLU
3	2	153	LYS
3	2	168	THR
3	2	201	ARG
3	2	204	ASN
3	2	241	SER
3	2	264	ARG
3	2	270	ARG
4	3	51	THR
4	3	85	LEU
4	3	99	MET
4	3	163	SER
4	3	169	PRO
4	3	208	MET
4	3	218	ASN
4	3	224	LEU
5	4	16	SER
5	4	42	SER
5	4	49	ASP
5	4	69	ASN

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

Mol	Chain	Res	Type
2	1	100	ASN
4	3	6	ASN
4	3	97	HIS
4	3	218	ASN

### 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 carbohydrates 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$
6	J77	1	0	-	29,29,29	1.46	3 (10%)	37,38,38	2.18	7 (18%)
7	MYR	4	1	5	14,14,15	0.31	0	13,13,15	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	J77	1	0	-	-	4/17/27/27	0/3/3/3
7	MYR	4	1	5	-	2/11/12/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	0	J77	C18-C21	-4.90	1.38	1.50

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	0	J77	O23-C21	4.28	1.44	1.33
6	1	0	J77	O23-C24	-2.02	1.40	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	0	J77	C13-C12-C9	6.08	121.57	113.88
6	1	0	J77	C11-N6-C7	5.25	123.11	111.52
6	1	0	J77	O23-C24-C25	4.68	125.61	108.42
6	1	0	J77	C4-C5-N4	-4.35	117.36	123.86
6	1	0	J77	C5-N4-N3	4.11	123.18	118.97
6	1	0	J77	O23-C21-C18	3.74	118.66	112.14
6	1	0	J77	C10-C11-N6	2.43	116.11	111.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	0	J77	C25-C24-O23-C21
6	1	0	J77	C16-C15-O14-C13
6	1	0	J77	C20-C15-O14-C13
6	1	0	J77	C12-C13-O14-C15
7	4	1	MYR	C6-C7-C8-C9
7	4	1	MYR	C5-C6-C7-C8

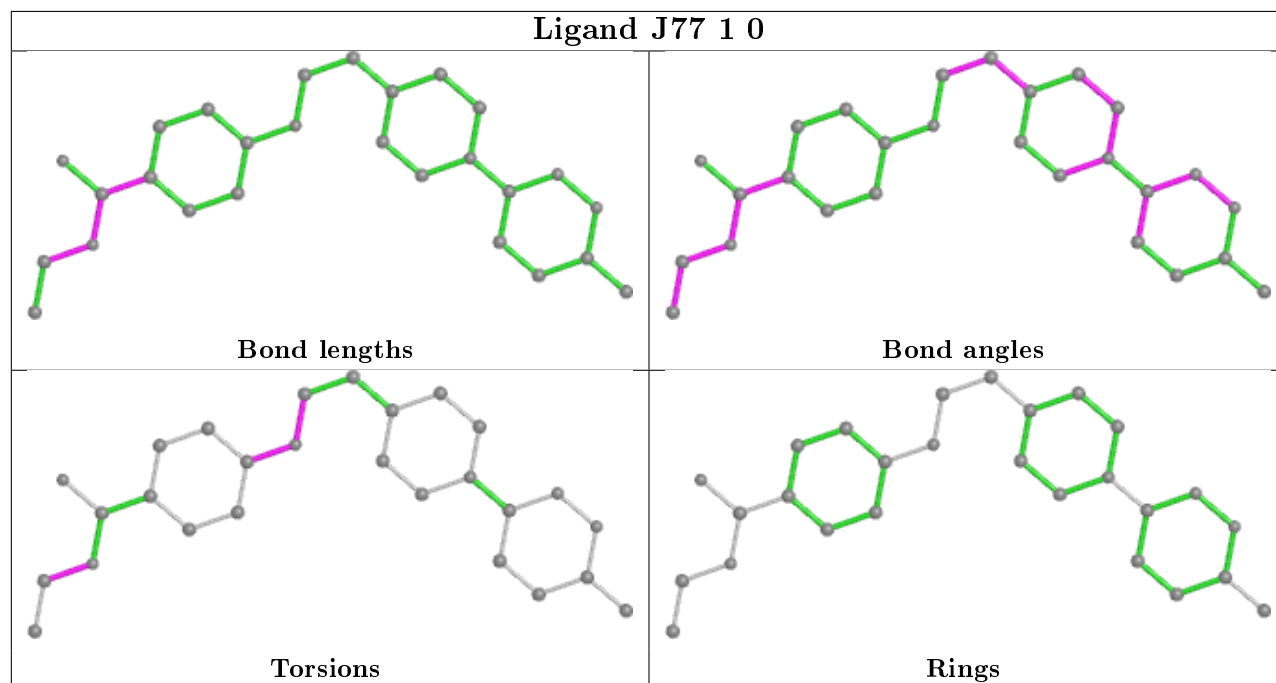
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	0	J77	5	0
7	4	1	MYR	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

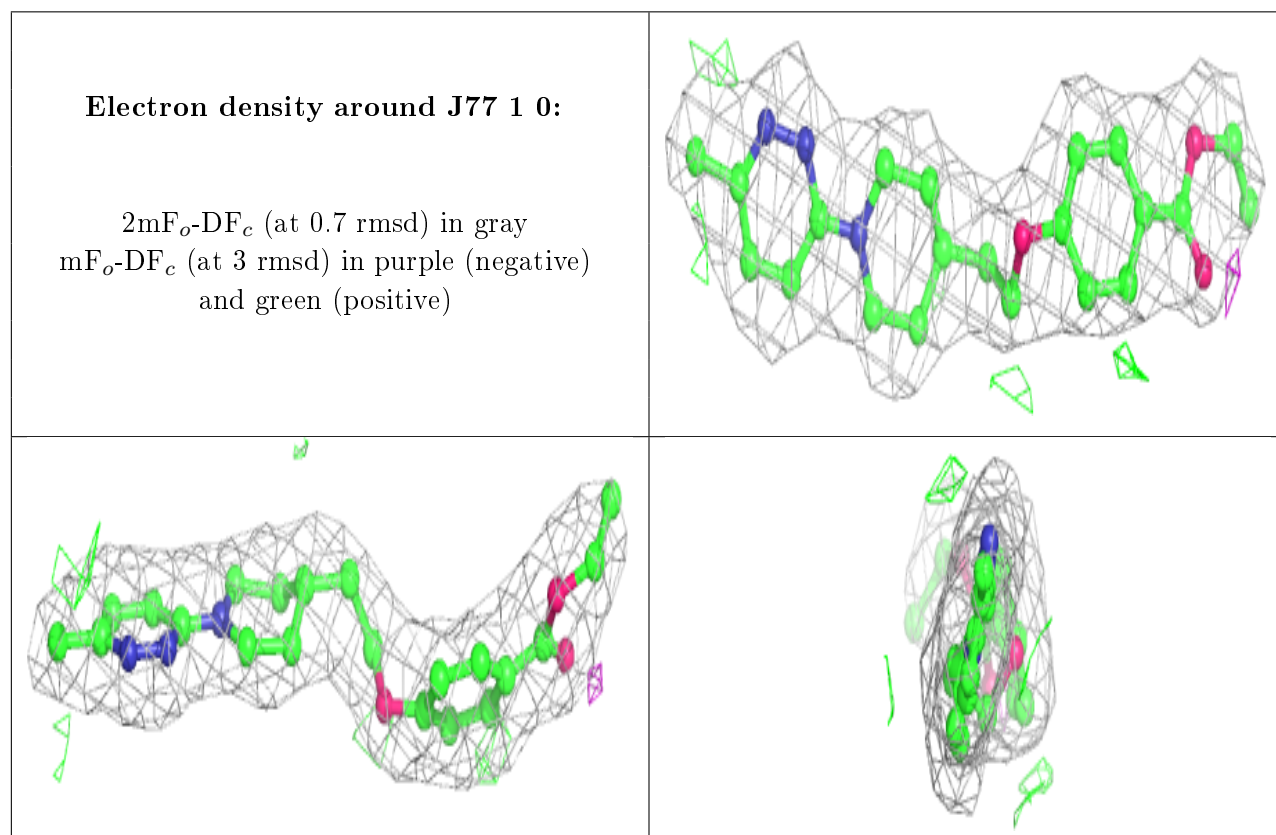
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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





## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.