



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:30 AM UTC

PDB ID : 1PO1 / pdb_00001po1
Title : POLIOVIRUS (TYPE 1, MAHONEY) IN COMPLEX WITH R80633, AN INHIBITOR OF VIRAL REPLICATION
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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

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

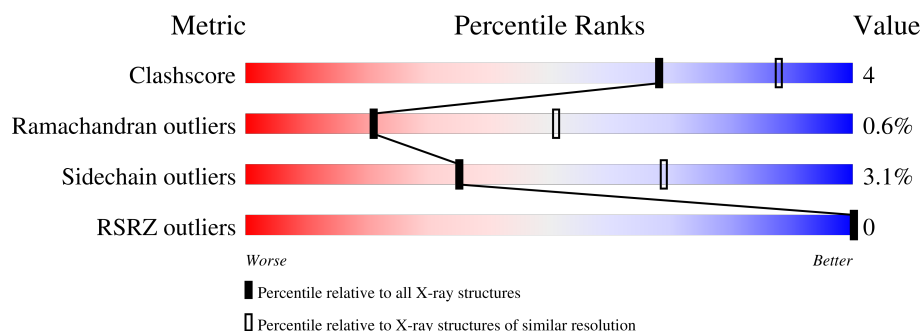
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	0	5	100%
2	1	302	67% 24% 6%
3	2	272	69% 25% . .
4	3	238	74% 23% . .
5	4	68	54% 35% . 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6690 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			

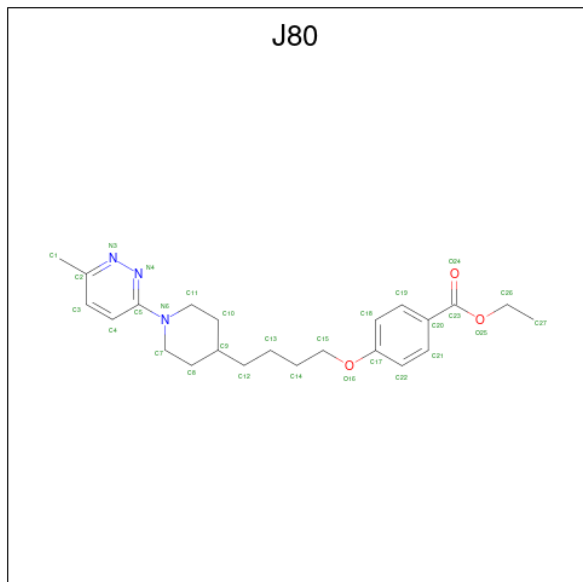
There is a discrepancy between the modelled and reference sequences:

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

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

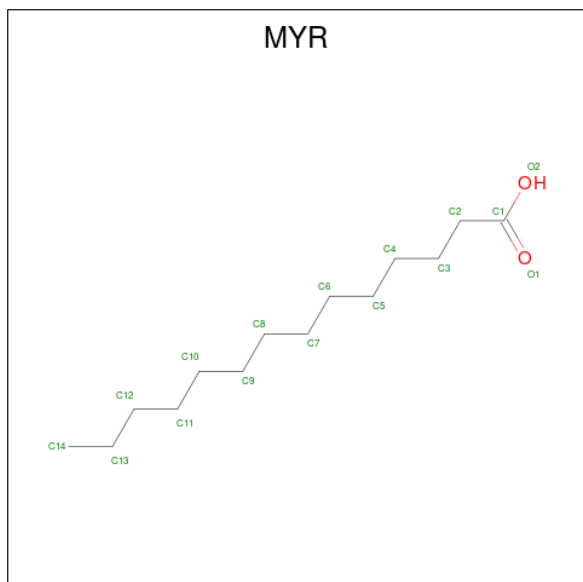
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	62	Total	C	N	O	S	0	0	0
			476	293	81	101	1			

- Molecule 6 is (METHYLPYRIDAZINE PIPERIDINE BUTYLOXYPHENYL)ETHYLACETATE (CCD ID: J80) (formula: $C_{23}H_{31}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	N	O	0	0
			29	23	3	3		

- Molecule 7 is MYRISTIC ACID (CCD ID: 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

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.

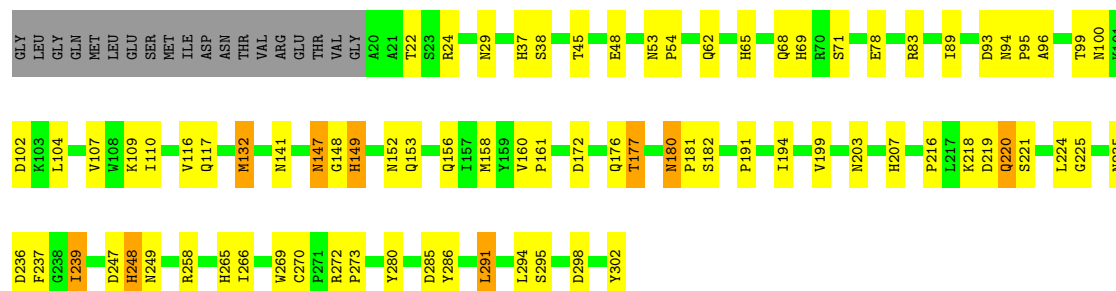
• Molecule 1: POLIOVIRUS TYPE 1 MAHONEY

Chain 0:  100%

There are no outlier residues recorded for this chain.

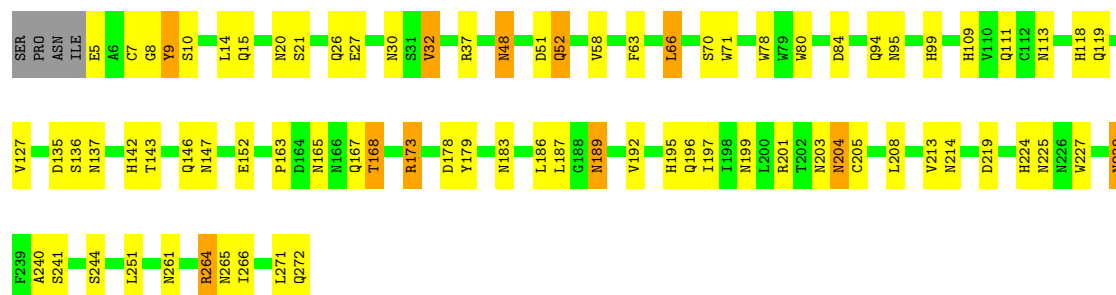
• Molecule 2: POLIOVirus TYPE 1 MAHONEY

Chain 1:  67% 24% 6%



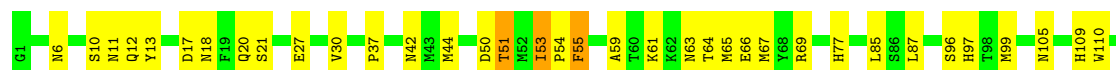
• Molecule 3: POLIOVirus TYPE 1 MAHONEY

Chain 2:  69% 25% 6%



• Molecule 4: POLIOVirus TYPE 1 MAHONEY

Chain 3:  74% 23% 3%





● Molecule 5: POLIOVIRUS TYPE 1 MAHONEY



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	322.94Å 358.04Å 380.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 200.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 27.1 (200.00-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.85Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.241 , (Not available) 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.28	EDS
Total number of atoms	6690	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: J80, MYR

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	1.03	0/28	2.09	0/36
2	1	0.97	8/2285 (0.4%)	1.79	50/3124 (1.6%)
3	2	0.95	7/2142 (0.3%)	1.90	75/2928 (2.6%)
4	3	0.94	6/1881 (0.3%)	1.72	45/2562 (1.8%)
5	4	1.00	1/483 (0.2%)	2.05	20/651 (3.1%)
All	All	0.96	22/6819 (0.3%)	1.83	190/9301 (2.0%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	77	HIS	CD2-NE2	-7.27	1.29	1.37
4	3	97	HIS	CD2-NE2	-7.09	1.30	1.37
2	1	37	HIS	CD2-NE2	-6.87	1.30	1.37
2	1	69	HIS	CD2-NE2	-6.86	1.30	1.37
3	2	224	HIS	CD2-NE2	-6.86	1.30	1.37
2	1	54	PRO	CA-CB	-6.66	1.48	1.53
4	3	109	HIS	CD2-NE2	-6.40	1.30	1.37
3	2	195	HIS	CD2-NE2	-6.16	1.31	1.37
2	1	207	HIS	CD2-NE2	-6.02	1.31	1.37
3	2	142	HIS	CD2-NE2	-6.02	1.31	1.37
4	3	230	HIS	CD2-NE2	-5.62	1.31	1.37
2	1	65	HIS	CD2-NE2	-5.62	1.31	1.37
2	1	265	HIS	CD2-NE2	-5.56	1.31	1.37
3	2	99	HIS	CD2-NE2	-5.56	1.31	1.37
2	1	149	HIS	CD2-NE2	-5.55	1.31	1.37
2	1	248	HIS	CD2-NE2	-5.47	1.31	1.37
5	4	13	HIS	CD2-NE2	-5.44	1.31	1.37
4	3	153	HIS	CD2-NE2	-5.30	1.32	1.37
3	2	109	HIS	CD2-NE2	-5.29	1.32	1.37
3	2	224	HIS	CG-ND1	-5.24	1.32	1.38
3	2	118	HIS	CD2-NE2	-5.22	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	77	HIS	CG-ND1	-5.09	1.32	1.38

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	147	ASN	OD1-CG-ND2	-11.53	111.07	122.60
4	3	233	GLN	OE1-CD-NE2	-11.14	111.46	122.60
4	3	218	ASN	OD1-CG-ND2	-10.77	111.83	122.60
3	2	48	ASN	OD1-CG-ND2	-10.57	112.03	122.60
2	1	117	GLN	OE1-CD-NE2	-10.15	112.45	122.60
5	4	31	ASN	OD1-CG-ND2	-10.10	112.50	122.60
4	3	173	ASN	OD1-CG-ND2	-9.74	112.86	122.60
2	1	266	ILE	N-CA-C	9.45	122.06	109.21
3	2	204	ASN	CA-CB-CG	9.39	121.99	112.60
2	1	220	GLN	OE1-CD-NE2	-9.37	113.23	122.60
5	4	4	GLN	OE1-CD-NE2	-9.27	113.33	122.60
5	4	39	ASN	OD1-CG-ND2	-9.24	113.36	122.60
3	2	203	ASN	OD1-CG-ND2	-8.98	113.62	122.60
4	3	17	ASP	CA-CB-CG	8.79	121.39	112.60
2	1	153	GLN	OE1-CD-NE2	-8.68	113.92	122.60
3	2	178	ASP	CA-CB-CG	8.46	121.06	112.60
4	3	162	SER	N-CA-C	8.40	121.37	111.71
3	2	52	GLN	OE1-CD-NE2	-8.35	114.25	122.60
3	2	178	ASP	N-CA-C	8.35	121.12	111.11
3	2	94	GLN	OE1-CD-NE2	-8.29	114.31	122.60
3	2	26	GLN	OE1-CD-NE2	-8.28	114.32	122.60
4	3	53	ILE	N-CA-C	8.25	115.72	108.63
3	2	8	GLY	N-CA-C	8.20	126.23	115.40
2	1	236	ASP	N-CA-C	8.15	120.08	111.03
5	4	69	ASN	OD1-CG-ND2	-8.10	114.50	122.60
2	1	100	ASN	OD1-CG-ND2	-8.09	114.51	122.60
3	2	146	GLN	OE1-CD-NE2	-8.09	114.51	122.60
4	3	105	ASN	OD1-CG-ND2	-8.09	114.51	122.60
4	3	218	ASN	CB-CG-ND2	8.05	128.47	116.40
2	1	219	ASP	CA-CB-CG	7.99	120.59	112.60
4	3	178	GLN	OE1-CD-NE2	-7.88	114.72	122.60
5	4	8	GLN	OE1-CD-NE2	-7.77	114.83	122.60
3	2	189	ASN	OD1-CG-ND2	-7.75	114.85	122.60
3	2	265	ASN	OD1-CG-ND2	-7.67	114.93	122.60
3	2	214	ASN	OD1-CG-ND2	-7.63	114.97	122.60
2	1	94	ASN	OD1-CG-ND2	-7.62	114.98	122.60
5	4	10	VAL	N-CA-C	7.59	119.44	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	10	SER	N-CA-C	7.57	120.96	109.23
2	1	93	ASP	CA-CB-CG	7.55	120.15	112.60
3	2	15	GLN	OE1-CD-NE2	-7.47	115.13	122.60
2	1	147	ASN	CB-CG-ND2	7.45	127.57	116.40
2	1	176	GLN	OE1-CD-NE2	-7.44	115.16	122.60
3	2	272	GLN	OE1-CD-NE2	-7.41	115.19	122.60
2	1	203	ASN	OD1-CG-ND2	-7.33	115.27	122.60
4	3	20	GLN	OE1-CD-NE2	-7.30	115.30	122.60
3	2	219	ASP	CA-CB-CG	7.28	119.88	112.60
2	1	199	VAL	N-CA-C	7.19	119.05	112.29
2	1	117	GLN	N-CA-C	7.17	118.78	110.97
3	2	224	HIS	N-CA-C	7.15	120.13	108.26
2	1	104	LEU	N-CA-C	7.12	119.40	109.15
5	4	4	GLN	CG-CD-NE2	7.11	127.06	116.40
3	2	167	GLN	OE1-CD-NE2	-7.05	115.55	122.60
2	1	68	GLN	OE1-CD-NE2	-7.04	115.56	122.60
2	1	29	ASN	OD1-CG-ND2	-7.01	115.59	122.60
5	4	15	ASN	OD1-CG-ND2	-6.98	115.62	122.60
4	3	42	ASN	OD1-CG-ND2	-6.94	115.66	122.60
3	2	199	ASN	OD1-CG-ND2	-6.91	115.69	122.60
3	2	261	ASN	OD1-CG-ND2	-6.90	115.70	122.60
3	2	266	ILE	N-CA-C	6.79	118.34	109.58
2	1	172	ASP	CA-CB-CG	6.77	119.37	112.60
3	2	119	GLN	OE1-CD-NE2	-6.77	115.83	122.60
3	2	8	GLY	O-C-N	-6.70	113.64	122.28
3	2	9	TYR	N-CA-C	6.69	120.18	110.28
3	2	203	ASN	N-CA-C	6.61	119.48	109.23
5	4	45	ASP	N-CA-C	6.60	120.80	110.17
2	1	291	LEU	N-CA-C	6.60	120.94	113.02
3	2	147	ASN	OD1-CG-ND2	-6.58	116.02	122.60
4	3	133	SER	N-CA-C	6.58	120.24	109.72
5	4	42	SER	N-CA-C	6.55	119.26	111.33
3	2	111	GLN	OE1-CD-NE2	-6.55	116.05	122.60
4	3	18	ASN	OD1-CG-ND2	-6.54	116.06	122.60
3	2	238	ASN	CA-CB-CG	-6.52	106.08	112.60
3	2	136	SER	N-CA-C	6.50	119.54	109.07
3	2	205	CYS	N-CA-C	6.49	118.64	108.96
3	2	137	ASN	OD1-CG-ND2	-6.47	116.13	122.60
3	2	204	ASN	OD1-CG-ND2	-6.46	116.14	122.60
3	2	264	ARG	O-C-N	-6.41	118.30	123.11
2	1	220	GLN	CG-CD-NE2	6.41	126.01	116.40
2	1	236	ASP	CA-CB-CG	6.40	119.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	195	GLN	OE1-CD-NE2	-6.40	116.20	122.60
3	2	63	PHE	N-CA-C	6.38	118.56	108.67
2	1	156	GLN	OE1-CD-NE2	-6.37	116.23	122.60
3	2	165	ASN	CA-CB-CG	-6.35	106.25	112.60
3	2	48	ASN	CB-CG-ND2	6.33	125.89	116.40
3	2	165	ASN	OD1-CG-ND2	-6.31	116.29	122.60
2	1	62	GLN	OE1-CD-NE2	-6.31	116.29	122.60
3	2	113	ASN	OD1-CG-ND2	-6.24	116.36	122.60
2	1	69	HIS	CB-CG-CD2	-6.23	123.10	131.20
5	4	48	GLN	OE1-CD-NE2	-6.21	116.39	122.60
3	2	204	ASN	CB-CA-C	-6.21	97.60	109.95
2	1	153	GLN	CG-CD-NE2	6.19	125.68	116.40
4	3	97	HIS	CA-CB-CG	-6.17	107.63	113.80
2	1	110	ILE	N-CA-C	6.17	117.26	108.93
2	1	152	ASN	OD1-CG-ND2	-6.16	116.44	122.60
5	4	31	ASN	CB-CG-ND2	6.10	125.56	116.40
3	2	225	ASN	OD1-CG-ND2	-6.09	116.51	122.60
5	4	44	GLN	OE1-CD-NE2	-6.09	116.51	122.60
5	4	39	ASN	CB-CG-ND2	6.08	125.53	116.40
4	3	30	VAL	N-CA-C	6.06	116.88	109.30
3	2	109	HIS	CB-CG-CD2	-6.06	123.33	131.20
4	3	11	ASN	OD1-CG-ND2	-6.04	116.56	122.60
4	3	189	TYR	N-CA-C	6.03	118.95	108.76
4	3	63	ASN	OD1-CG-ND2	-6.02	116.58	122.60
2	1	149	HIS	CB-CG-CD2	-5.98	123.42	131.20
3	2	20	ASN	OD1-CG-ND2	-5.95	116.65	122.60
4	3	6	ASN	OD1-CG-ND2	-5.92	116.68	122.60
3	2	165	ASN	N-CA-C	5.91	120.33	113.18
5	4	49	ASP	CA-CB-CG	5.90	118.50	112.60
4	3	96	SER	N-CA-C	5.88	119.99	112.34
4	3	27	GLU	N-CA-C	5.88	119.76	112.47
5	4	63	LYS	N-CA-C	5.86	119.25	111.75
4	3	233	GLN	CG-CD-NE2	5.84	125.16	116.40
4	3	161	GLN	OE1-CD-NE2	-5.82	116.78	122.60
4	3	54	PRO	N-CA-CB	5.82	106.48	102.35
4	3	136	PRO	O-C-N	-5.81	118.64	121.31
3	2	183	ASN	OD1-CG-ND2	-5.81	116.79	122.60
2	1	141	ASN	OD1-CG-ND2	-5.75	116.85	122.60
2	1	235	ASN	OD1-CG-ND2	-5.73	116.87	122.60
2	1	116	VAL	N-CA-C	5.67	120.34	112.35
4	3	12	GLN	OE1-CD-NE2	-5.62	116.98	122.60
4	3	77	HIS	CB-CG-CD2	-5.61	123.90	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	119	GLN	CG-CD-NE2	5.61	124.82	116.40
3	2	142	HIS	CB-CG-CD2	-5.60	123.92	131.20
2	1	298	ASP	N-CA-C	5.59	119.03	110.20
3	2	127	VAL	N-CA-C	5.59	114.03	107.77
3	2	21	SER	N-CA-C	5.57	118.18	108.76
3	2	168	THR	CA-CB-OG1	-5.57	101.24	109.60
5	4	26	ASN	OD1-CG-ND2	-5.57	117.03	122.60
3	2	118	HIS	CB-CG-CD2	-5.56	123.97	131.20
4	3	6	ASN	N-CA-C	5.56	117.77	109.59
2	1	247	ASP	CA-CB-CG	5.56	118.16	112.60
5	4	13	HIS	CB-CG-CD2	-5.56	123.98	131.20
4	3	153	HIS	CB-CG-CD2	-5.54	124.00	131.20
3	2	163	PRO	N-CA-CB	5.53	108.25	103.27
4	3	173	ASN	CB-CG-ND2	5.53	124.69	116.40
4	3	178	GLN	CG-CD-NE2	5.52	124.68	116.40
2	1	272	ARG	O-C-N	-5.52	117.96	121.88
4	3	21	SER	O-C-N	-5.52	117.99	121.85
2	1	161	PRO	O-C-N	-5.51	118.56	121.15
2	1	294	LEU	N-CA-C	5.50	118.89	110.20
4	3	10	SER	N-CA-C	5.49	118.31	110.24
4	3	97	HIS	CB-CG-CD2	-5.47	124.08	131.20
4	3	59	ALA	N-CA-C	5.42	118.69	111.75
4	3	55	PHE	N-CA-C	5.42	117.19	111.28
3	2	142	HIS	N-CA-C	5.41	119.19	112.59
3	2	244	SER	N-CA-C	5.41	118.47	108.94
4	3	69	ARG	N-CA-C	5.41	117.45	108.20
2	1	148	GLY	O-C-N	-5.40	115.68	122.70
3	2	271	LEU	N-CA-C	5.39	119.85	113.16
5	4	69	ASN	CB-CG-ND2	5.38	124.48	116.40
2	1	224	LEU	N-CA-C	5.37	117.22	111.36
3	2	173	ARG	N-CA-C	5.36	117.55	109.41
2	1	53	ASN	OD1-CG-ND2	-5.34	117.25	122.60
3	2	196	GLN	OE1-CD-NE2	-5.34	117.26	122.60
4	3	218	ASN	N-CA-C	5.33	122.15	110.80
3	2	70	SER	N-CA-C	5.32	117.09	108.41
2	1	180	ASN	OD1-CG-ND2	-5.32	117.28	122.60
2	1	38	SER	N-CA-C	5.31	117.49	109.41
2	1	102	ASP	N-CA-C	5.30	117.56	110.35
3	2	95	ASN	CA-CB-CG	-5.30	107.30	112.60
3	2	204	ASN	CB-CG-ND2	5.29	124.34	116.40
3	2	95	ASN	OD1-CG-ND2	-5.28	117.32	122.60
2	1	269	TRP	CE2-CD2-CG	-5.28	100.87	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	51	ASP	CA-CB-CG	5.26	117.86	112.60
4	3	170	TRP	CG-CD2-CE3	5.26	139.16	133.90
4	3	110	TRP	CE2-CD2-CG	-5.24	100.92	107.20
3	2	80	TRP	CE2-CD2-CG	-5.23	100.93	107.20
2	1	78	GLU	CB-CA-C	-5.22	102.62	110.92
3	2	204	ASN	N-CA-CB	5.22	119.17	110.41
2	1	65	HIS	CB-CG-CD2	-5.21	124.43	131.20
3	2	52	GLN	CG-CD-NE2	5.20	124.20	116.40
4	3	170	TRP	CE2-CD2-CG	-5.19	100.97	107.20
3	2	227	TRP	CE2-CD2-CG	-5.19	100.97	107.20
3	2	84	ASP	N-CA-C	5.17	119.89	111.37
3	2	32	VAL	N-CA-C	5.14	115.71	108.36
2	1	221	SER	N-CA-C	5.13	117.78	110.24
3	2	58	VAL	N-CA-C	5.11	118.23	111.17
3	2	71	TRP	CE2-CD2-CG	-5.09	101.09	107.20
3	2	152	GLU	N-CA-C	5.08	117.48	111.33
4	3	105	ASN	CB-CG-ND2	5.07	124.01	116.40
2	1	132	MET	N-CA-C	5.07	117.16	108.90
3	2	14	LEU	N-CA-C	5.06	117.50	109.50
3	2	78	TRP	CE2-CD2-CG	-5.06	101.13	107.20
2	1	269	TRP	CB-CG-CD1	-5.06	119.31	126.90
3	2	186	LEU	N-CA-C	5.05	117.79	109.76
2	1	153	GLN	N-CA-C	5.05	118.17	110.20
3	2	135	ASP	CA-CB-CG	5.05	117.65	112.60
4	3	50	ASP	CA-CB-CG	5.03	117.63	112.60
4	3	153	HIS	N-CA-C	5.02	116.71	109.07
5	4	51	SER	N-CA-C	5.01	121.48	110.80

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	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	2085	0	2000	15	0
4	3	1834	0	1816	17	0
5	4	476	0	457	5	0
6	1	29	0	31	2	0
7	4	15	0	27	1	0
All	All	6690	0	6528	47	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 4.

All (47) 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)
3:2:187:LEU:HD22	4:3:65:MET:HE1	1.67	0.75
2:1:158:MET:SD	2:1:177:THR:HG23	2.29	0.71
2:1:177:THR:HG22	2:1:180:ASN:HB2	1.74	0.70
4:3:51:THR:HG21	4:3:99:MET:H	1.61	0.64
3:2:143:THR:HG23	3:2:173:ARG:HA	1.82	0.60
3:2:37:ARG:HG3	4:3:37:PRO:HB3	1.85	0.58
2:1:177:THR:HG21	2:1:182:SER:OG	2.04	0.57
3:2:179:TYR:HA	4:3:65:MET:HE2	1.87	0.57
3:2:213:VAL:HG22	4:3:37:PRO:HG2	1.86	0.56
3:2:30:ASN:HD21	5:4:59:ASP:HB2	1.70	0.55
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.90	0.53
2:1:22:THR:HG22	2:1:24:ARG:H	1.75	0.52
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.91	0.52
5:4:10:VAL:HG21	5:4:25:ILE:HD12	1.91	0.51
2:1:107:VAL:HG13	2:1:239:ILE:HD13	1.92	0.51
2:1:45:THR:OG1	5:4:67:MET:HE2	2.11	0.51
4:3:87:LEU:HD11	4:3:114:LEU:HD12	1.93	0.49
4:3:167:VAL:O	4:3:169:PRO:HD3	2.12	0.49
2:1:48:GLU:HA	3:2:197:ILE:HB	1.94	0.49
4:3:120:PHE:HA	4:3:210:ILE:HG22	1.94	0.49
3:2:5:GLU:HB3	3:2:9:TYR:H	1.78	0.48
2:1:273:PRO:HB3	3:2:189:ASN:HB2	1.96	0.48
5:4:30:ILE:HD13	7:4:1:MYR:H72	1.95	0.48
5:4:57:ILE:HD11	5:4:61:LEU:HB3	1.96	0.48
2:1:237:PHE:HB3	6:1:0:J80:H132	1.95	0.47
2:1:96:ALA:HA	2:1:249:ASN:O	2.14	0.47
3:2:192:VAL:HG11	4:3:99:MET:HE2	1.97	0.46
4:3:61:LYS:HD3	4:3:66:GLU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:55:PHE:HE2	4:3:212:GLY:HA3	1.82	0.45
3:2:5:GLU:HG3	3:2:7:CYS:H	1.81	0.45
4:3:149:MET:HE2	4:3:150:LEU:HG	1.98	0.45
3:2:32:VAL:HB	3:2:208:LEU:HD23	2.00	0.44
4:3:53:ILE:HD11	4:3:214:VAL:HB	1.99	0.44
2:1:181:PRO:HB2	6:1:0:J80:H3	1.98	0.44
3:2:27:GLU:HB2	3:2:204:ASN:OD1	2.18	0.43
2:1:160:VAL:HB	2:1:239:ILE:HG13	2.01	0.42
4:3:44:MET:HE2	4:3:44:MET:HA	2.01	0.42
4:3:64:THR:O	4:3:67:MET:HG2	2.19	0.42
2:1:216:PRO:HA	2:1:225:GLY:HA3	2.02	0.42
2:1:24:ARG:HA	2:1:71:SER:OG	2.20	0.42
2:1:286:TYR:HB2	2:1:291:LEU:HD21	2.02	0.41
2:1:302:TYR:CE1	4:3:189:TYR:HB3	2.55	0.41
3:2:66:LEU:HD12	3:2:251:LEU:HD23	2.02	0.41
2:1:89:ILE:HG12	2:1:258:ARG:HG2	2.02	0.41
2:1:95:PRO:O	2:1:248:HIS:HB3	2.21	0.41
2:1:280:TYR:HB3	2:1:285:ASP:O	2.22	0.40
3:2:201:ARG:HH11	3:2:201:ARG:HD3	1.77	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	0	3/5 (60%)	3 (100%)	0	0	100	100
2	1	281/302 (93%)	268 (95%)	12 (4%)	1 (0%)	30	59
3	2	266/272 (98%)	248 (93%)	16 (6%)	2 (1%)	16	44
4	3	233/238 (98%)	220 (94%)	13 (6%)	0	100	100
5	4	58/68 (85%)	52 (90%)	4 (7%)	2 (3%)	3	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	841/885 (95%)	791 (94%)	45 (5%)	5 (1%)	21 51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	240	ALA
3	2	48	ASN
5	4	11	GLY
2	1	270	CYS
5	4	60	VAL

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%)	4 (100%)	0	100 100
2	1	245/261 (94%)	234 (96%)	11 (4%)	24 58
3	2	228/232 (98%)	222 (97%)	6 (3%)	40 73
4	3	210/212 (99%)	205 (98%)	5 (2%)	43 75
5	4	54/57 (95%)	53 (98%)	1 (2%)	50 79
All	All	741/766 (97%)	718 (97%)	23 (3%)	35 69

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	83	ARG
2	1	99	THR
2	1	132	MET
2	1	147	ASN
2	1	149	HIS
2	1	177	THR
2	1	194	ILE
2	1	218	LYS
2	1	220	GLN

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Mol	Chain	Res	Type
2	1	239	ILE
2	1	295	SER
3	2	52	GLN
3	2	66	LEU
3	2	168	THR
3	2	238	ASN
3	2	241	SER
3	2	264	ARG
4	3	51	THR
4	3	85	LEU
4	3	163	SER
4	3	208	MET
4	3	218	ASN
5	4	16	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	100	ASN
2	1	180	ASN
2	1	203	ASN
3	2	95	ASN
3	2	238	ASN
3	2	261	ASN
4	3	6	ASN
4	3	218	ASN
5	4	26	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 oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	J80	1	0	-	31,31,31	1.51	3 (9%)	38,40,40	2.12	10 (26%)
7	MYR	4	1	5	13,14,15	0.38	0	12,13,15	0.57	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	J80	1	0	-	-	5/19/29/29	0/3/3/3
7	MYR	4	1	5	-	5/12/12/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	0	J80	O25-C23	5.23	1.46	1.33
6	1	0	J80	C20-C23	-4.97	1.38	1.50
6	1	0	J80	O25-C26	-2.12	1.40	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	0	J80	C1-C2-N3	5.17	119.17	116.13
6	1	0	J80	C4-C5-N4	-4.93	116.61	123.84
6	1	0	J80	O25-C26-C27	4.86	125.83	108.40
6	1	0	J80	C11-N6-C7	4.69	122.12	111.57
6	1	0	J80	C5-N4-N3	4.44	123.45	118.97
6	1	0	J80	C7-C8-C9	3.04	119.40	111.92
6	1	0	J80	O25-C23-C20	2.99	117.16	112.15
6	1	0	J80	C13-C14-C15	-2.54	102.43	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	0	J80	C8-C7-N6	2.52	116.63	110.92
6	1	0	J80	C3-C4-C5	2.25	120.76	117.65

There are no chirality outliers.

All (10) torsion outliers are listed below:

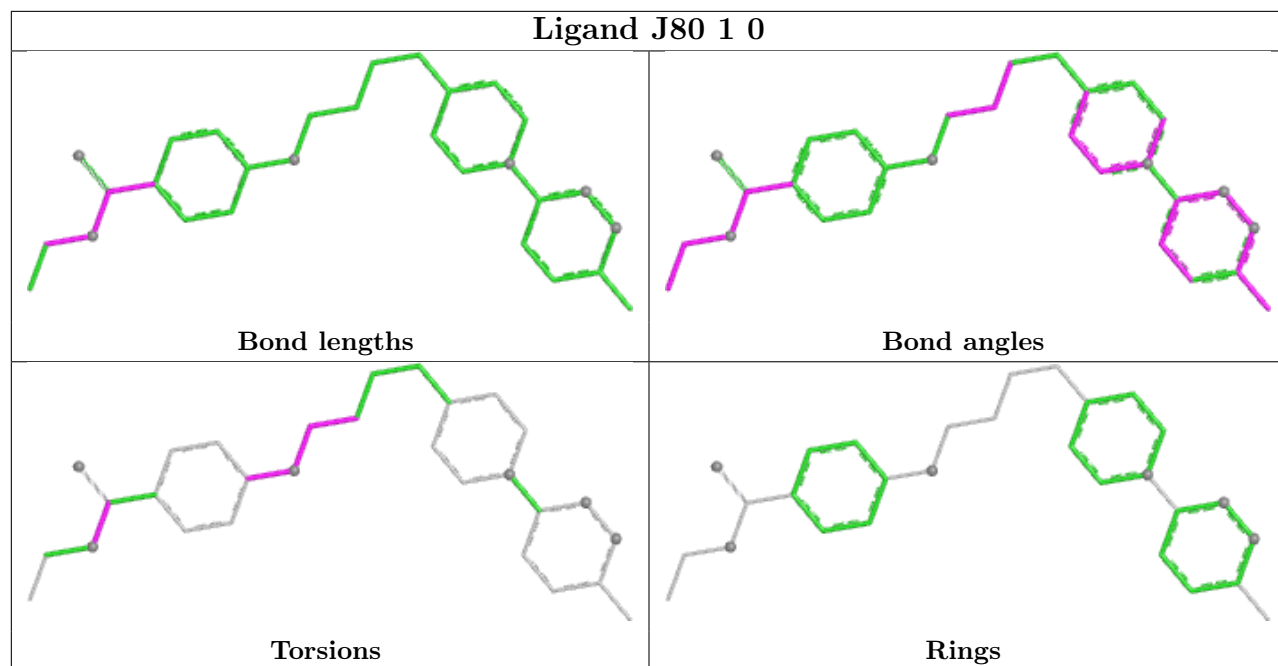
Mol	Chain	Res	Type	Atoms
7	4	1	MYR	O1-C1-C2-C3
6	1	0	J80	C18-C17-O16-C15
7	4	1	MYR	C6-C7-C8-C9
6	1	0	J80	C22-C17-O16-C15
7	4	1	MYR	C11-C12-C13-C14
6	1	0	J80	O24-C23-O25-C26
7	4	1	MYR	C10-C11-C12-C13
6	1	0	J80	C14-C15-O16-C17
6	1	0	J80	C13-C14-C15-O16
7	4	1	MYR	C5-C6-C7-C8

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	0	J80	2	0
7	4	1	MYR	1	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 [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	0	5/5 (100%)	0.48	0 100 100	87, 88, 89, 91	0
2	1	283/302 (93%)	-1.07	0 100 100	3, 12, 51, 83	0
3	2	268/272 (98%)	-1.09	0 100 100	3, 9, 48, 95	0
4	3	235/238 (98%)	-1.16	0 100 100	4, 9, 22, 66	0
5	4	62/68 (91%)	-0.87	0 100 100	7, 28, 74, 96	0
All	All	853/885 (96%)	-1.08	0 100 100	3, 10, 52, 96	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](#)

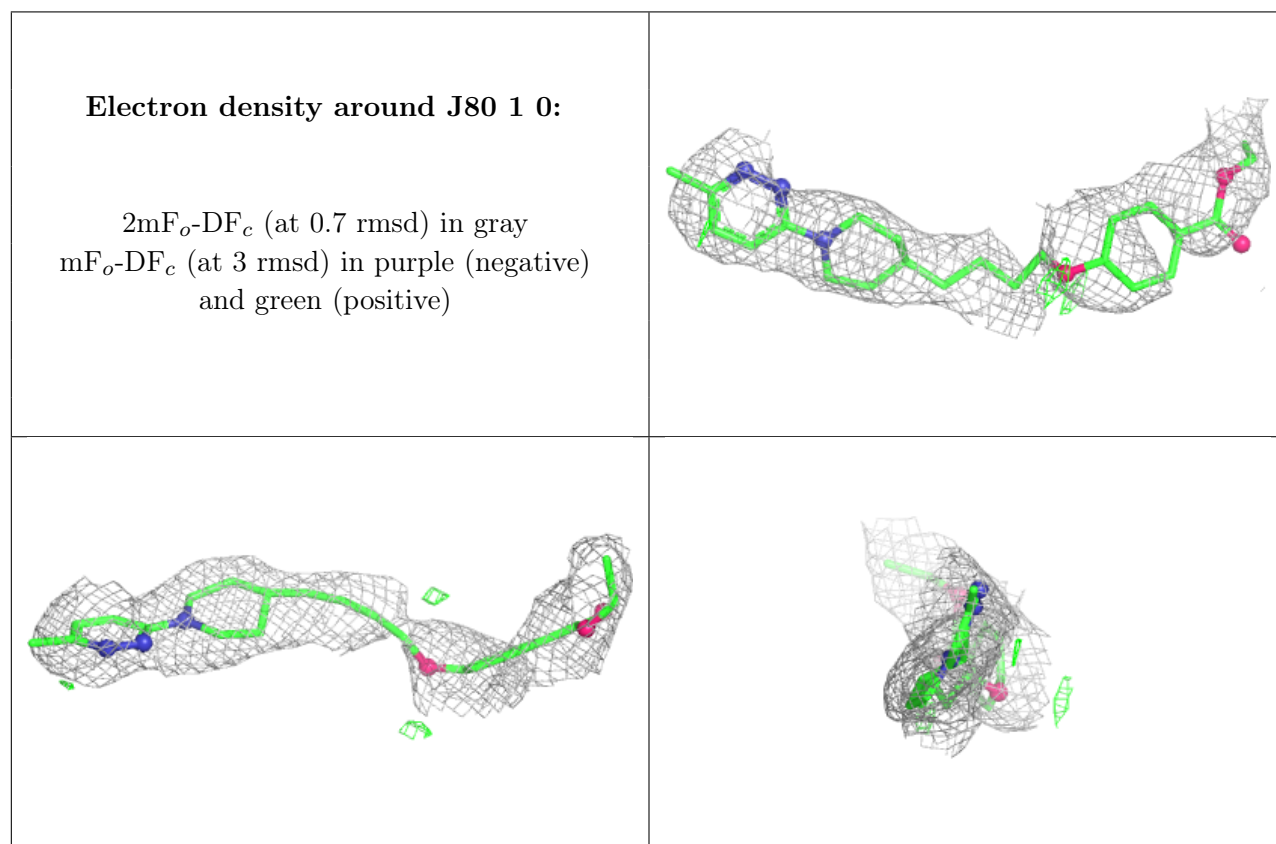
There are no oligosaccharides in this entry.

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
6	J80	1	0	29/29	0.99	0.06	23,28,58,62	0
7	MYR	4	1	15/16	0.99	0.08	34,49,60,61	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.