



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:12 AM UTC

PDB ID : 1VBC / pdb_00001vbc
Title : POLIOVIRUS (TYPE 3, SABIN STRAIN) (P3/SABIN, P3/LEON/12A(1)B)
COMPLEXED WITH R77975
Authors : Grant, R.A.; Hiremath, C.N.; Filman, D.J.; Syed, R.; Andries, K.; Hogle, J.M.
Deposited on : 1996-01-02
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

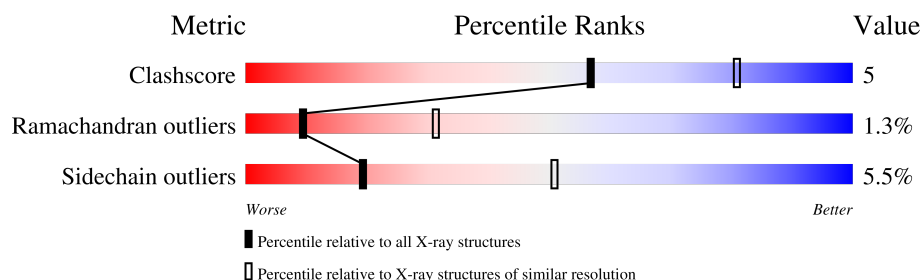
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	4	75% 25%
2	1	300	61% 26% 5% 7%
3	2	271	65% 28% 5% .
4	3	235	69% 27% .
5	4	68	62% 26% . 9%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6658 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 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	0	4	Total	C	N	O	0	0	0
			30	19	4	7			

- Molecule 2 is a protein called POLIOVIRUS TYPE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	279	Total	C	N	O	S	0	0	0
			2214	1408	383	416	7			

- Molecule 3 is a protein called POLIOVIRUS TYPE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	266	Total	C	N	O	S	0	0	0
			2088	1330	354	392	12			

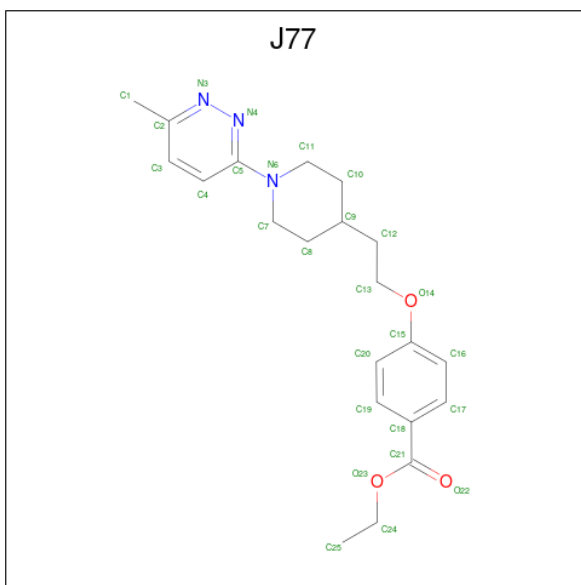
- Molecule 4 is a protein called POLIOVIRUS TYPE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	235	Total	C	N	O	S	0	0	0
			1812	1150	296	348	18			

- Molecule 5 is a protein called POLIOVIRUS TYPE 3.

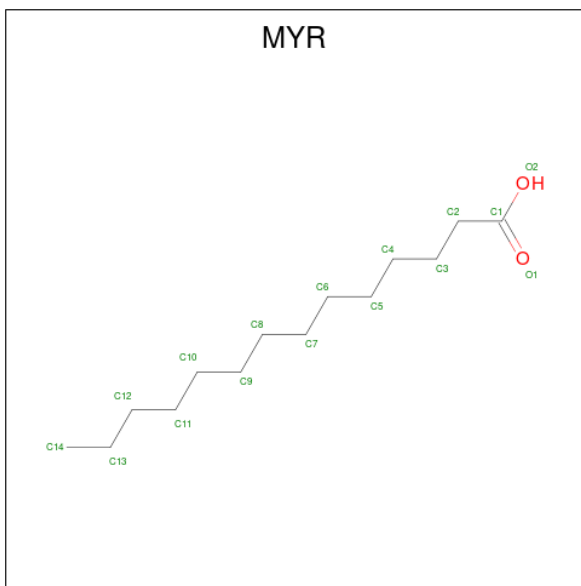
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	4	62	Total	C	N	O	0	0	0
			472	291	79	102			

- Molecule 6 is (METHYLPYRIDAZINE PIPERIDINE ETHYLOXYPHENYL)ETHYLACE TATE (CCD ID: J77) (formula: C₂₁H₂₇N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	N	O	0	0
			27	21	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 [i](#)

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. 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.

Note EDS was not executed.

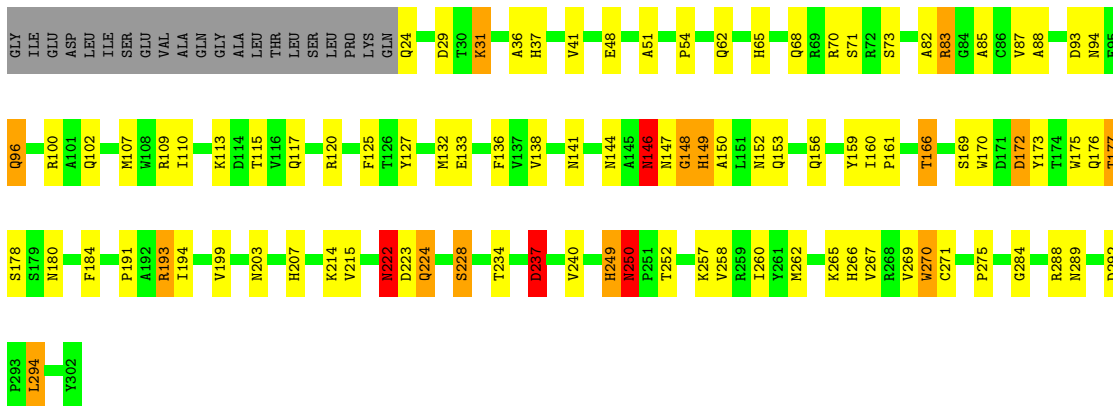
• Molecule 1: POLIOVIRUS TYPE 3

Chain 0:  75% 25%



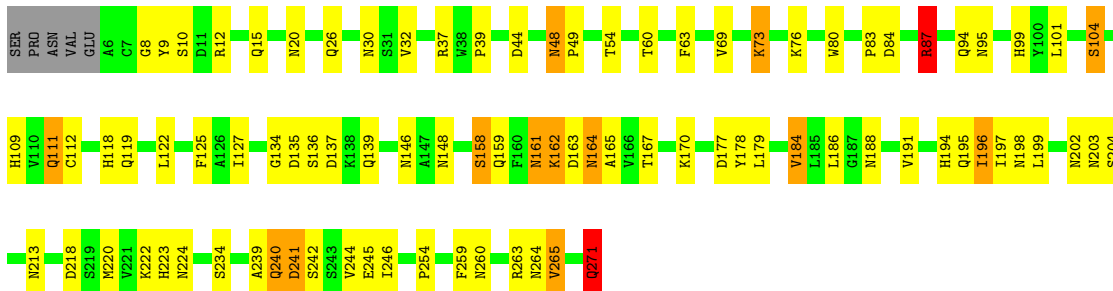
• Molecule 2: POLIOVIRUS TYPE 3

Chain 1:  61% 26% 5% • 7%



• Molecule 3: POLIOVIRUS TYPE 3

Chain 2:  65% 28% 5% • •

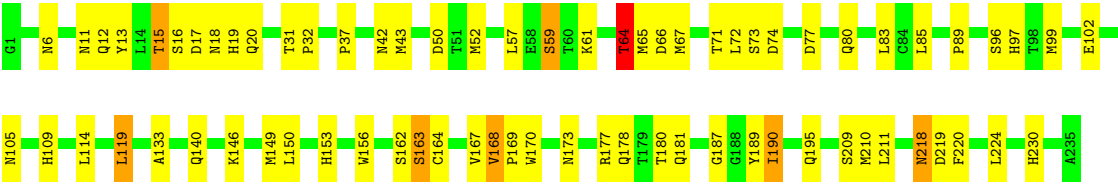


• Molecule 4: POLIOVIRUS TYPE 3

Chain 3:

69%

27%



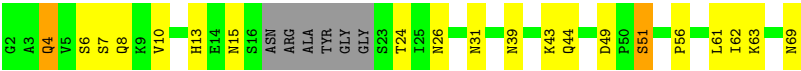
• Molecule 5: POLIOVIRUS TYPE 3

Chain 4:

62%

26%

9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	321.06Å 358.62Å 381.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.289 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6658	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: J77, 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	0.87	0/29	2.00	1/38 (2.6%)
2	1	0.96	9/2278 (0.4%)	1.87	70/3111 (2.3%)
3	2	0.94	7/2146 (0.3%)	1.96	78/2926 (2.7%)
4	3	0.95	5/1857 (0.3%)	1.82	50/2533 (2.0%)
5	4	0.90	1/479 (0.2%)	2.05	22/647 (3.4%)
All	All	0.94	22/6789 (0.3%)	1.90	221/9255 (2.4%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	37	HIS	CD2-NE2	-7.75	1.29	1.37
4	3	97	HIS	CD2-NE2	-7.23	1.29	1.37
4	3	109	HIS	CD2-NE2	-6.94	1.30	1.37
2	1	54	PRO	CA-CB	-6.70	1.48	1.53
3	2	194	HIS	CD2-NE2	-6.68	1.30	1.37
4	3	19	HIS	CD2-NE2	-6.68	1.30	1.37
2	1	65	HIS	CD2-NE2	-6.68	1.30	1.37
3	2	223	HIS	CD2-NE2	-6.68	1.30	1.37
5	4	13	HIS	CD2-NE2	-6.65	1.30	1.37
2	1	249	HIS	CD2-NE2	-6.55	1.30	1.37
3	2	99	HIS	CD2-NE2	-6.23	1.30	1.37
2	1	207	HIS	CD2-NE2	-6.10	1.31	1.37
3	2	109	HIS	CD2-NE2	-5.95	1.31	1.37
3	2	118	HIS	CD2-NE2	-5.92	1.31	1.37
4	3	153	HIS	CD2-NE2	-5.80	1.31	1.37
2	1	266	HIS	CD2-NE2	-5.79	1.31	1.37
3	2	99	HIS	CG-ND1	-5.78	1.31	1.38
2	1	149	HIS	CD2-NE2	-5.48	1.31	1.37
4	3	230	HIS	CD2-NE2	-5.24	1.32	1.37
2	1	266	HIS	CG-ND1	-5.15	1.32	1.38
2	1	161	PRO	CA-CB	-5.12	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	194	HIS	CG-ND1	-5.08	1.32	1.38

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	146	ASN	OD1-CG-ND2	-12.42	110.18	122.60
5	4	44	GLN	OE1-CD-NE2	-10.32	112.28	122.60
3	2	164	ASN	N-CA-C	10.28	125.08	112.54
3	2	240	GLN	OE1-CD-NE2	-10.24	112.36	122.60
5	4	69	ASN	OD1-CG-ND2	-10.23	112.37	122.60
2	1	250	ASN	OD1-CG-ND2	-10.12	112.48	122.60
3	2	135	ASP	N-CA-C	9.98	123.08	111.11
2	1	156	GLN	OE1-CD-NE2	-9.88	112.72	122.60
2	1	222	ASN	OD1-CG-ND2	-9.87	112.73	122.60
2	1	172	ASP	CA-CB-CG	9.53	122.12	112.60
4	3	218	ASN	OD1-CG-ND2	-9.46	113.14	122.60
3	2	202	ASN	OD1-CG-ND2	-9.39	113.21	122.60
2	1	24	GLN	OE1-CD-NE2	-9.31	113.29	122.60
2	1	117	GLN	OE1-CD-NE2	-9.26	113.34	122.60
2	1	148	GLY	O-C-N	-9.16	114.20	122.90
2	1	117	GLN	N-CA-C	9.10	120.89	110.97
3	2	213	ASN	OD1-CG-ND2	-8.90	113.70	122.60
4	3	178	GLN	OE1-CD-NE2	-8.85	113.75	122.60
4	3	105	ASN	OD1-CG-ND2	-8.83	113.77	122.60
3	2	48	ASN	OD1-CG-ND2	-8.83	113.77	122.60
3	2	127	ILE	N-CA-C	8.76	117.72	107.73
3	2	136	SER	N-CA-C	8.60	122.33	109.95
2	1	224	GLN	OE1-CD-NE2	-8.40	114.20	122.60
2	1	199	VAL	N-CA-C	8.28	119.28	111.91
3	2	139	GLN	OE1-CD-NE2	-8.26	114.34	122.60
4	3	133	ALA	N-CA-C	8.07	121.42	109.24
3	2	26	GLN	OE1-CD-NE2	-7.95	114.66	122.60
4	3	17	ASP	CA-CB-CG	7.94	120.54	112.60
2	1	267	VAL	N-CA-C	7.94	119.37	108.89
2	1	223	ASP	CA-CB-CG	7.85	120.45	112.60
3	2	188	ASN	OD1-CG-ND2	-7.83	114.77	122.60
4	3	50	ASP	CA-CB-CG	7.78	120.38	112.60
5	4	43	LYS	N-CA-C	7.77	122.10	112.47
3	2	94	GLN	OE1-CD-NE2	-7.76	114.84	122.60
4	3	6	ASN	OD1-CG-ND2	-7.75	114.85	122.60
3	2	10	SER	N-CA-C	7.71	120.89	109.24
2	1	144	ASN	OD1-CG-ND2	-7.70	114.90	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	8	GLN	OE1-CD-NE2	-7.67	114.94	122.60
3	2	161	ASN	OD1-CG-ND2	-7.59	115.00	122.60
3	2	204	SER	N-CA-C	7.56	120.23	108.96
2	1	152	ASN	N-CA-C	7.51	121.28	110.24
2	1	102	GLN	OE1-CD-NE2	-7.50	115.10	122.60
3	2	177	ASP	CA-CB-CG	7.49	120.09	112.60
3	2	271	GLN	OE1-CD-NE2	-7.47	115.13	122.60
2	1	153	GLN	OE1-CD-NE2	-7.44	115.16	122.60
5	4	39	ASN	OD1-CG-ND2	-7.39	115.20	122.60
3	2	265	VAL	N-CA-C	7.38	119.33	109.37
4	3	173	ASN	OD1-CG-ND2	-7.38	115.22	122.60
3	2	63	PHE	N-CA-C	7.37	120.90	108.23
4	3	218	ASN	CB-CG-ND2	7.36	127.44	116.40
3	2	184	VAL	O-C-N	-7.35	115.25	122.97
4	3	140	GLN	OE1-CD-NE2	-7.34	115.26	122.60
5	4	15	ASN	OD1-CG-ND2	-7.23	115.37	122.60
2	1	68	GLN	OE1-CD-NE2	-7.18	115.42	122.60
5	4	4	GLN	OE1-CD-NE2	-7.12	115.48	122.60
3	2	240	GLN	CG-CD-NE2	7.12	127.08	116.40
3	2	264	ASN	OD1-CG-ND2	-7.04	115.56	122.60
3	2	218	ASP	CA-CB-CG	7.03	119.63	112.60
2	1	289	ASN	OD1-CG-ND2	-6.95	115.65	122.60
5	4	26	ASN	OD1-CG-ND2	-6.95	115.66	122.60
2	1	203	ASN	OD1-CG-ND2	-6.93	115.67	122.60
4	3	17	ASP	N-CA-C	6.92	119.89	110.55
2	1	146	ASN	N-CA-C	6.87	125.43	110.80
4	3	153	HIS	N-CA-C	6.87	119.61	108.76
3	2	134	GLY	CA-C-N	6.85	129.78	120.54
3	2	134	GLY	C-N-CA	6.85	129.78	120.54
3	2	125	PHE	N-CA-C	6.84	120.09	109.07
4	3	42	ASN	OD1-CG-ND2	-6.83	115.77	122.60
5	4	13	HIS	CB-CG-CD2	-6.83	122.33	131.20
2	1	62	GLN	OE1-CD-NE2	-6.81	115.79	122.60
2	1	93	ASP	CA-CB-CG	6.78	119.38	112.60
3	2	202	ASN	N-CA-C	6.71	120.23	108.75
2	1	141	ASN	OD1-CG-ND2	-6.68	115.92	122.60
2	1	94	ASN	OD1-CG-ND2	-6.67	115.93	122.60
4	3	109	HIS	CA-CB-CG	6.60	120.40	113.80
3	2	135	ASP	CA-CB-CG	6.59	119.19	112.60
4	3	74	ASP	CA-CB-CG	6.58	119.18	112.60
3	2	15	GLN	OE1-CD-NE2	-6.55	116.05	122.60
3	2	95	ASN	OD1-CG-ND2	-6.50	116.10	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	241	ASP	CA-CB-CG	6.49	119.09	112.60
3	2	167	THR	N-CA-C	6.42	118.81	111.11
2	1	73	SER	N-CA-C	6.41	118.26	111.28
3	2	164	ASN	CA-CB-CG	-6.40	106.20	112.60
2	1	180	ASN	OD1-CG-ND2	-6.40	116.20	122.60
4	3	71	THR	N-CA-C	6.38	119.02	109.25
2	1	289	ASN	N-CA-C	6.29	118.52	109.14
2	1	222	ASN	CB-CG-ND2	6.25	125.78	116.40
5	4	61	LEU	N-CA-C	6.25	120.11	110.42
3	2	165	ALA	N-CA-C	6.24	119.71	108.17
5	4	10	VAL	N-CA-C	6.23	117.34	108.93
4	3	195	GLN	OE1-CD-NE2	-6.21	116.39	122.60
2	1	153	GLN	N-CA-C	6.20	119.76	109.46
4	3	150	LEU	N-CA-C	6.18	120.38	112.34
5	4	24	THR	N-CA-C	6.18	118.71	109.25
4	3	32	PRO	N-CA-C	6.12	116.34	110.47
2	1	249	HIS	N-CA-C	6.10	119.20	110.10
4	3	12	GLN	OE1-CD-NE2	-6.08	116.53	122.60
3	2	20	ASN	OD1-CG-ND2	-6.07	116.53	122.60
3	2	73	LYS	N-CA-C	6.06	119.51	111.75
5	4	69	ASN	CB-CG-ND2	6.05	125.47	116.40
4	3	180	THR	N-CA-CB	5.99	119.56	110.45
4	3	163	SER	N-CA-C	5.99	118.96	109.50
2	1	152	ASN	OD1-CG-ND2	-5.97	116.63	122.60
2	1	149	HIS	CA-CB-CG	-5.95	107.85	113.80
3	2	263	ARG	O-C-N	-5.94	118.65	123.11
3	2	224	ASN	OD1-CG-ND2	-5.94	116.66	122.60
5	4	51	SER	N-CA-C	5.90	123.38	110.80
4	3	96	SER	N-CA-C	5.88	119.28	111.75
2	1	29	ASP	CA-CB-CG	5.86	118.45	112.60
5	4	6	SER	N-CA-C	5.85	117.96	109.07
3	2	203	ASN	CA-CB-CG	5.83	118.43	112.60
5	4	49	ASP	CA-CB-CG	5.83	118.43	112.60
3	2	158	SER	N-CA-C	5.81	120.09	112.89
1	0	8	GLU	N-CA-C	5.78	118.09	108.20
3	2	198	ASN	OD1-CG-ND2	-5.78	116.82	122.60
3	2	76	LYS	N-CA-C	5.76	120.38	113.23
2	1	184	PHE	CA-CB-CG	-5.76	108.04	113.80
2	1	51	ALA	N-CA-C	5.71	118.98	110.52
3	2	109	HIS	CB-CG-CD2	-5.71	123.78	131.20
3	2	203	ASN	CB-CA-C	-5.71	98.06	109.99
2	1	156	GLN	CG-CD-NE2	5.70	124.95	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	178	SER	N-CA-C	5.70	119.33	112.38
2	1	161	PRO	O-C-N	-5.68	118.48	121.15
4	3	153	HIS	CB-CG-CD2	-5.67	123.82	131.20
3	2	111	GLN	N-CA-C	5.66	117.75	108.52
2	1	113	LYS	N-CA-C	5.64	120.16	113.28
2	1	289	ASN	CA-CB-CG	-5.63	106.97	112.60
2	1	228	SER	N-CA-C	5.63	117.73	109.24
3	2	111	GLN	OE1-CD-NE2	-5.62	116.97	122.60
3	2	119	GLN	OE1-CD-NE2	-5.62	116.98	122.60
2	1	176	GLN	OE1-CD-NE2	-5.61	116.99	122.60
3	2	69	VAL	O-C-N	-5.61	117.15	122.98
4	3	80	GLN	N-CA-C	5.61	118.43	110.24
5	4	7	SER	N-CA-C	5.60	118.36	109.96
3	2	223	HIS	CA-CB-CG	5.59	119.39	113.80
2	1	224	GLN	CG-CD-NE2	5.58	124.77	116.40
4	3	20	GLN	OE1-CD-NE2	-5.57	117.03	122.60
4	3	105	ASN	CB-CG-ND2	5.57	124.75	116.40
5	4	31	ASN	OD1-CG-ND2	-5.57	117.03	122.60
3	2	39	PRO	N-CA-C	5.56	119.94	111.15
4	3	64	THR	O-C-N	-5.56	115.96	122.96
2	1	36	ALA	N-CA-C	5.55	118.52	109.24
3	2	87	ARG	N-CA-C	5.55	118.85	111.75
3	2	242	SER	N-CA-C	5.55	119.15	112.38
3	2	9	TYR	N-CA-C	5.53	117.83	110.53
4	3	230	HIS	N-CA-C	5.53	119.57	113.21
3	2	223	HIS	N-CA-C	5.51	118.39	108.48
2	1	173	TYR	N-CA-C	5.50	118.03	111.71
3	2	259	PHE	N-CA-C	5.47	118.31	109.40
2	1	269	VAL	N-CA-C	5.46	117.76	108.86
3	2	118	HIS	CB-CG-CD2	-5.45	124.12	131.20
3	2	30	ASN	OD1-CG-ND2	-5.42	117.18	122.60
2	1	31	LYS	N-CA-C	5.42	119.07	109.96
4	3	180	THR	CB-CA-C	-5.42	98.98	109.76
2	1	68	GLN	N-CA-C	5.41	117.52	109.25
2	1	260	ILE	N-CA-C	5.41	115.88	107.99
2	1	292	ASP	CA-CB-CG	5.41	118.01	112.60
2	1	161	PRO	N-CA-CB	5.40	106.03	103.22
3	2	137	ASP	CA-C-O	5.38	126.17	120.10
4	3	64	THR	CA-CB-OG1	-5.35	101.57	109.60
3	2	194	HIS	N-CA-C	5.34	116.92	108.96
3	2	162	LYS	N-CA-C	5.32	118.03	110.10
2	1	141	ASN	N-CA-C	5.27	116.30	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	63	LYS	N-CA-C	5.27	119.19	112.34
3	2	245	GLU	N-CA-C	5.26	116.65	107.49
2	1	294	LEU	N-CA-C	5.26	118.80	109.96
2	1	136	PHE	N-CA-C	5.26	117.29	107.99
2	1	160	ILE	CA-C-N	5.25	123.44	119.66
2	1	160	ILE	C-N-CA	5.25	123.44	119.66
2	1	54	PRO	N-CA-CB	5.23	106.24	102.79
2	1	88	ALA	N-CA-C	5.23	117.03	108.76
2	1	149	HIS	CB-CG-CD2	-5.22	124.41	131.20
4	3	189	TYR	N-CA-C	5.22	117.91	109.40
4	3	209	SER	N-CA-C	5.21	118.57	110.17
4	3	168	VAL	CA-C-O	5.21	122.04	119.12
3	2	80	TRP	CE2-CD2-CG	-5.21	100.95	107.20
4	3	181	GLN	OE1-CD-NE2	-5.20	117.40	122.60
3	2	164	ASN	OD1-CG-ND2	-5.20	117.40	122.60
3	2	146	ASN	OD1-CG-ND2	-5.20	117.40	122.60
3	2	177	ASP	N-CA-C	5.20	119.89	111.37
2	1	166	THR	CA-C-N	5.19	125.49	119.93
2	1	166	THR	C-N-CA	5.19	125.49	119.93
3	2	99	HIS	CB-CG-CD2	-5.19	124.45	131.20
4	3	119	LEU	N-CA-C	5.19	116.98	108.52
4	3	31	THR	CA-C-N	5.19	123.45	119.66
4	3	31	THR	C-N-CA	5.19	123.45	119.66
3	2	260	ASN	OD1-CG-ND2	-5.18	117.42	122.60
2	1	284	GLY	O-C-N	-5.17	118.22	122.92
3	2	195	GLN	OE1-CD-NE2	-5.15	117.45	122.60
2	1	24	GLN	CG-CD-NE2	5.15	124.12	116.40
3	2	104	SER	N-CA-C	5.14	116.89	108.55
4	3	15	THR	CA-CB-OG1	-5.14	101.89	109.60
4	3	59	SER	N-CA-C	5.14	121.75	110.80
2	1	85	ALA	N-CA-C	5.14	117.61	109.24
3	2	159	GLN	OE1-CD-NE2	-5.13	117.47	122.60
4	3	218	ASN	N-CA-C	5.13	121.72	110.80
4	3	77	ASP	CA-CB-CG	5.12	117.72	112.60
2	1	170	TRP	CE2-CD2-CG	-5.12	101.06	107.20
4	3	18	ASN	OD1-CG-ND2	-5.10	117.50	122.60
4	3	42	ASN	CB-CG-ND2	5.10	124.05	116.40
4	3	97	HIS	CB-CG-CD2	-5.10	124.57	131.20
5	4	44	GLN	CG-CD-NE2	5.10	124.05	116.40
2	1	257	LYS	N-CA-C	5.08	116.68	108.34
3	2	234	SER	CA-C-N	5.08	125.01	119.78
3	2	234	SER	C-N-CA	5.08	125.01	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	54	THR	CB-CA-C	-5.08	101.38	109.75
4	3	162	SER	N-CA-C	5.08	121.61	110.80
3	2	48	ASN	CB-CG-ND2	5.07	124.00	116.40
2	1	177	THR	N-CA-C	5.07	118.43	111.54
2	1	175	TRP	CE2-CD2-CG	-5.06	101.12	107.20
5	4	13	HIS	CB-CG-ND1	5.06	130.29	122.70
3	2	203	ASN	N-CA-CB	5.05	118.63	110.40
4	3	11	ASN	OD1-CG-ND2	-5.05	117.55	122.60
5	4	4	GLN	CG-CD-NE2	5.04	123.96	116.40
3	2	84	ASP	N-CA-C	5.04	119.69	111.37
4	3	6	ASN	CB-CG-ND2	5.04	123.95	116.40
3	2	44	ASP	CA-CB-CG	5.02	117.62	112.60
3	2	199	LEU	N-CA-C	5.02	118.87	112.34
4	3	220	PHE	N-CA-C	5.02	117.73	109.76
2	1	270	TRP	CE2-CD2-CG	-5.01	101.19	107.20
4	3	15	THR	CA-CB-CG2	5.00	119.01	110.50

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	30	0	30	0	0
2	1	2214	0	2150	34	0
3	2	2088	0	2005	19	0
4	3	1812	0	1792	23	0
5	4	472	0	453	1	0
6	1	27	0	27	3	0
7	4	15	0	27	0	0
All	All	6658	0	6484	60	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 5.

All (60) 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	6:1:500:J77:H82	1.69	0.73
2:1:110:ILE:HD13	6:1:500:J77:H72	1.70	0.71
3:2:186:LEU:HD22	4:3:65:MET:HE1	1.72	0.70
3:2:271:GLN:NE2	3:2:271:GLN:HA	2.13	0.62
2:1:288:ARG:HE	3:2:162:LYS:NZ	2.01	0.58
3:2:191:VAL:HG11	4:3:99:MET:HE2	1.86	0.57
3:2:178:TYR:HA	4:3:65:MET:HE3	1.86	0.57
4:3:61:LYS:O	4:3:64:THR:HG22	2.06	0.56
2:1:169:SER:HB3	2:1:172:ASP:HB3	1.88	0.55
3:2:112:CYS:SG	3:2:246:ILE:HD12	2.47	0.55
2:1:147:ASN:HB2	2:1:252:THR:HB	1.88	0.55
2:1:138:VAL:HG22	2:1:258:VAL:HG22	1.88	0.55
2:1:48:GLU:HA	3:2:196:ILE:HB	1.90	0.54
2:1:146:ASN:HD22	2:1:147:ASN:N	2.05	0.54
2:1:294:LEU:HD13	4:3:67:MET:SD	2.48	0.53
2:1:234:THR:OG1	2:1:237:ASP:HA	2.08	0.53
3:2:37:ARG:HG3	4:3:37:PRO:HB3	1.91	0.52
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.91	0.52
4:3:64:THR:O	4:3:67:MET:HG2	2.10	0.52
4:3:89:PRO:HG3	4:3:114:LEU:HD11	1.92	0.51
3:2:122:LEU:HB2	3:2:197:ILE:HB	1.92	0.51
2:1:132:MET:SD	2:1:262:MET:HG2	2.51	0.51
4:3:167:VAL:O	4:3:169:PRO:HD3	2.11	0.51
2:1:96:GLN:HG3	2:1:249:HIS:CE1	2.46	0.50
3:2:32:VAL:HG13	5:4:56:PRO:HB2	1.93	0.50
4:3:64:THR:HG23	4:3:66:ASP:H	1.77	0.49
2:1:133:GLU:HB2	2:1:265:LYS:HE2	1.94	0.49
2:1:288:ARG:HE	3:2:162:LYS:HZ2	1.61	0.48
3:2:49:PRO:HG3	3:2:101:LEU:HD13	1.94	0.48
3:2:60:THR:O	3:2:254:PRO:HG2	2.14	0.47
4:3:168:VAL:HG21	4:3:190:ILE:HD11	1.97	0.47
2:1:120:ARG:NH2	2:1:275:PRO:HB2	2.30	0.47
3:2:271:GLN:HA	3:2:271:GLN:HE21	1.79	0.46
2:1:125:PHE:HZ	4:3:43:MET:SD	2.39	0.46
3:2:179:LEU:HA	3:2:184:VAL:O	2.16	0.46
4:3:177:ARG:CZ	4:3:187:GLY:HA2	2.46	0.46
2:1:133:GLU:CD	2:1:193:ARG:HD2	2.41	0.46
2:1:159:TYR:CE2	6:1:500:J77:H111	2.51	0.45
2:1:127:TYR:HB2	2:1:270:TRP:HB2	1.98	0.45
4:3:146:LYS:O	4:3:149:MET:HE2	2.17	0.44
2:1:150:ALA:HA	2:1:250:ASN:ND2	2.32	0.44
2:1:87:VAL:HG21	2:1:262:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:109:ARG:HA	2:1:240:VAL:HG12	1.99	0.43
2:1:70:ARG:NH2	4:3:219:ASP:O	2.51	0.43
2:1:148:GLY:O	2:1:149:HIS:ND1	2.52	0.43
4:3:72:LEU:HD11	4:3:210:MET:HB2	2.00	0.43
2:1:222:ASN:HD22	2:1:224:GLN:HB2	1.83	0.43
3:2:178:TYR:CA	4:3:65:MET:HE3	2.48	0.42
4:3:119:LEU:HD23	4:3:211:LEU:HD12	2.01	0.42
2:1:107:MET:HE2	2:1:240:VAL:HG21	2.01	0.42
2:1:215:VAL:HG23	3:2:222:LYS:HG2	2.02	0.42
3:2:87:ARG:NH2	3:2:148:ASN:O	2.53	0.42
2:1:31:LYS:HD2	2:1:31:LYS:HA	1.79	0.42
2:1:294:LEU:HD22	4:3:57:LEU:HD21	2.02	0.41
2:1:83:ARG:CG	4:3:15:THR:HG22	2.51	0.41
2:1:275:PRO:HG2	4:3:102:GLU:HG3	2.03	0.41
2:1:107:MET:HE1	2:1:166:THR:HB	2.04	0.40
4:3:156:TRP:CD1	4:3:164:CYS:HB2	2.56	0.40
2:1:214:LYS:HG3	2:1:228:SER:OG	2.21	0.40
3:2:83:PRO:HG3	3:2:220:MET:HB3	2.04	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	2/4 (50%)	2 (100%)	0	0	100	100
2	1	277/300 (92%)	252 (91%)	21 (8%)	4 (1%)	9	30
3	2	264/271 (97%)	243 (92%)	17 (6%)	4 (2%)	8	28
4	3	233/235 (99%)	220 (94%)	11 (5%)	2 (1%)	14	41
5	4	58/68 (85%)	49 (84%)	8 (14%)	1 (2%)	7	25
All	All	834/878 (95%)	766 (92%)	57 (7%)	11 (1%)	9	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	237	ASP
3	2	48	ASN
4	3	59	SER
4	3	170	TRP
3	2	239	ALA
5	4	51	SER
2	1	146	ASN
3	2	163	ASP
2	1	82	ALA
2	1	271	CYS
3	2	8	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%)	4 (100%)	0	100	100
2	1	241/258 (93%)	228 (95%)	13 (5%)	20	51
3	2	224/229 (98%)	209 (93%)	15 (7%)	15	42
4	3	210/210 (100%)	200 (95%)	10 (5%)	23	56
5	4	53/56 (95%)	51 (96%)	2 (4%)	29	64
All	All	732/757 (97%)	692 (94%)	40 (6%)	19	51

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	41	VAL
2	1	71	SER
2	1	83	ARG
2	1	96	GLN
2	1	100	ARG
2	1	115	THR
2	1	146	ASN

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Mol	Chain	Res	Type
2	1	177	THR
2	1	193	ARG
2	1	194	ILE
2	1	222	ASN
2	1	237	ASP
2	1	250	ASN
3	2	12	ARG
3	2	73	LYS
3	2	87	ARG
3	2	104	SER
3	2	111	GLN
3	2	158	SER
3	2	161	ASN
3	2	164	ASN
3	2	170	LYS
3	2	196	ILE
3	2	240	GLN
3	2	241	ASP
3	2	244	VAL
3	2	265	VAL
3	2	271	GLN
4	3	16	SER
4	3	52	MET
4	3	64	THR
4	3	73	SER
4	3	83	LEU
4	3	85	LEU
4	3	163	SER
4	3	190	ILE
4	3	218	ASN
4	3	224	LEU
5	4	4	GLN
5	4	62	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	24	GLN
2	1	94	ASN
2	1	146	ASN
2	1	149	HIS
2	1	153	GLN

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Mol	Chain	Res	Type
2	1	203	ASN
2	1	250	ASN
3	2	95	ASN
3	2	139	GLN
3	2	271	GLN
4	3	6	ASN
4	3	56	ASN
4	3	218	ASN
5	4	13	HIS
5	4	15	ASN
5	4	44	GLN
5	4	48	GLN
5	4	69	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	$\# Z > 2$
7	MYR	4	1	5	13,14,15	0.29	0	12,13,15	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	J77	1	500	-	29,29,29	1.40	3 (10%)	35,38,38	2.12	8 (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
7	MYR	4	1	5	-	2/12/12/13	-
6	J77	1	500	-	-	8/17/27/27	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	500	J77	C18-C21	-4.94	1.38	1.50
6	1	500	J77	O23-C21	3.75	1.42	1.33
6	1	500	J77	O23-C24	-2.07	1.40	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	500	J77	C5-N4-N3	4.67	123.68	118.97
6	1	500	J77	O23-C24-C25	4.65	125.07	108.40
6	1	500	J77	C4-C5-N4	-4.60	117.10	123.84
6	1	500	J77	O23-C21-C18	4.40	119.52	112.15
6	1	500	J77	C11-N6-C7	4.18	120.96	111.57
6	1	500	J77	C1-C2-N3	3.32	118.08	116.13
6	1	500	J77	C11-C10-C9	2.98	119.27	111.92
6	1	500	J77	C10-C11-N6	2.81	117.31	110.92

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	500	J77	C16-C15-O14-C13
6	1	500	J77	C20-C15-O14-C13
6	1	500	J77	C13-C12-C9-C8
6	1	500	J77	C13-C12-C9-C10
6	1	500	J77	C19-C18-C21-O23

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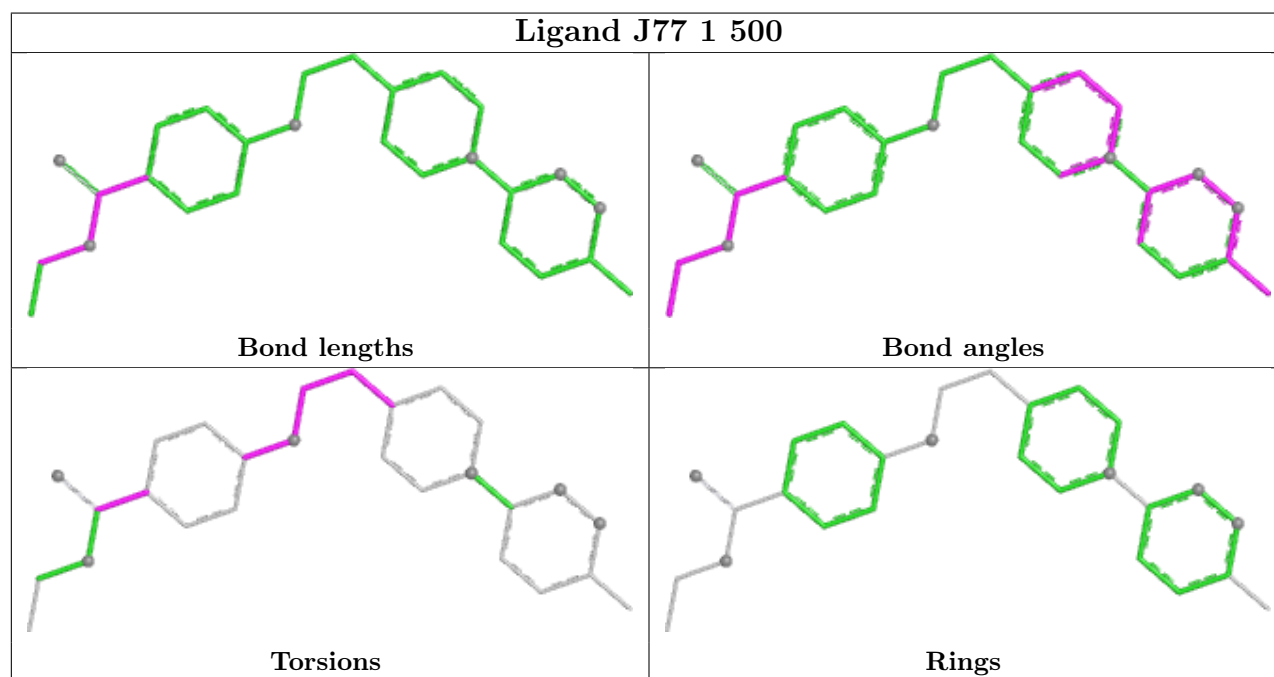
Mol	Chain	Res	Type	Atoms
6	1	500	J77	C9-C12-C13-O14
7	4	1	MYR	C9-C10-C11-C12
6	1	500	J77	C12-C13-O14-C15
6	1	500	J77	C19-C18-C21-O22

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	500	J77	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.