



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:39 AM UTC

PDB ID : 1VBE / pdb_00001vbe
Title : POLIOVIRUS (TYPE 3, SABIN STRAIN, MUTANT 242-H2) COMPLEXED WITH R78206
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

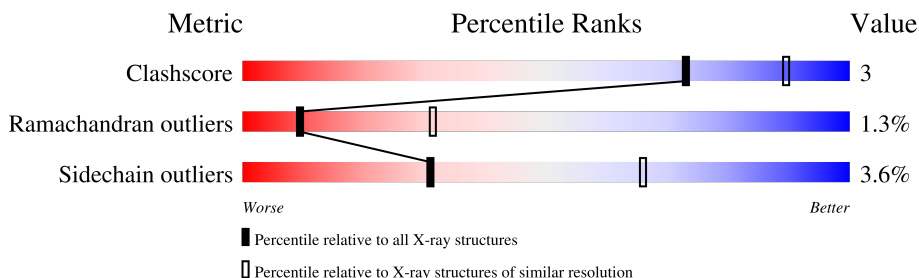
1 Overall quality at a glance

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	100%
2	1	300	68% 21% . . 7%
3	2	271	69% 25% . .
4	3	235	76% 20% .
5	4	68	56% 34% . 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6653 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
			2208	1402	383	416	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	124	LEU	PHE	engineered mutation	UNP P03302
1	134	LEU	PHE	engineered mutation	UNP P03302
1	288	ARG	LYS	conflict	UNP P03302

- 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			

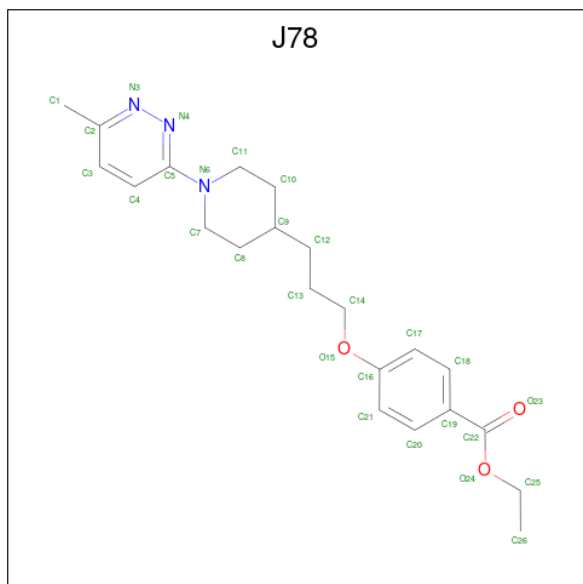
- Molecule 4 is a protein called POLIOVIRUS TYPE 3.

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.

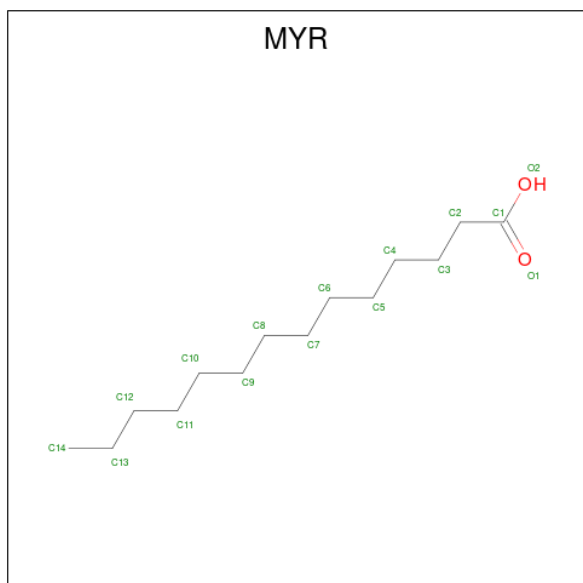
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	4	62	Total	C	N	O	0	0	0
			472	291	79	102			

- Molecule 6 is (METHYLPYRIDAZINE PIPERIDINE PROPYLOXYPHENYL)ETHYLAC ETATE (CCD ID: J78) (formula: $C_{22}H_{29}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	N	O	0	0
			28	22	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. 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.

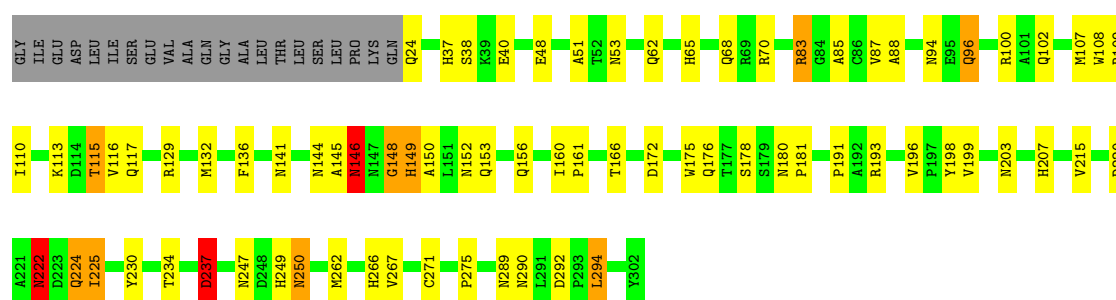
• Molecule 1: POLIOVIRUS TYPE 3

Chain 0:  100%

There are no outlier residues recorded for this chain.

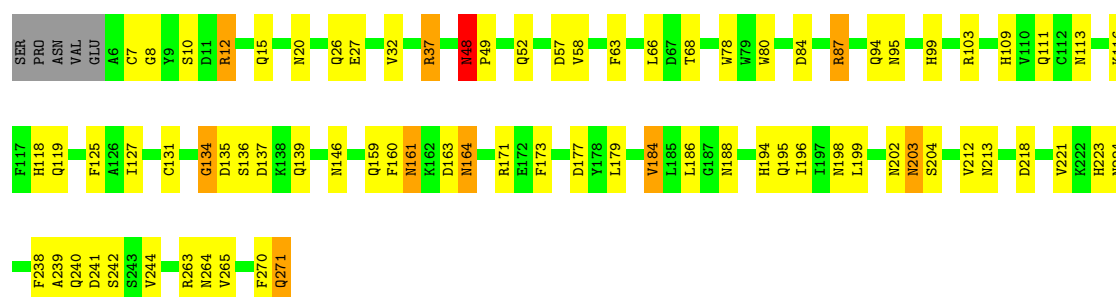
• Molecule 2: POLIOVirus TYPE 3

Chain 1:  68% 21% 7%



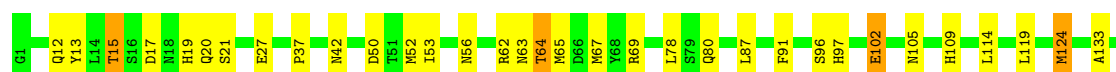
• Molecule 3: POLIOVirus TYPE 3

Chain 2:  69% 25%



• Molecule 4: POLIOVirus TYPE 3

Chain 3:  76% 20%





● Molecule 5: POLIOVIRUS TYPE 3



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 2.1	Depositor
R, R_{free}	0.295 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6653	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: J78, 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	1.58	0/38
2	1	0.89	7/2270 (0.3%)	1.83	63/3101 (2.0%)
3	2	0.91	7/2146 (0.3%)	1.89	66/2926 (2.3%)
4	3	0.90	6/1857 (0.3%)	1.77	41/2533 (1.6%)
5	4	0.89	1/479 (0.2%)	1.98	20/647 (3.1%)
All	All	0.90	21/6781 (0.3%)	1.85	190/9245 (2.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	97	HIS	CD2-NE2	-7.40	1.29	1.37
2	1	37	HIS	CD2-NE2	-6.96	1.30	1.37
2	1	65	HIS	CD2-NE2	-6.65	1.30	1.37
2	1	207	HIS	CD2-NE2	-6.62	1.30	1.37
4	3	109	HIS	CD2-NE2	-6.59	1.30	1.37
3	2	118	HIS	CD2-NE2	-6.51	1.30	1.37
4	3	153	HIS	CD2-NE2	-6.45	1.30	1.37
3	2	223	HIS	CD2-NE2	-6.42	1.30	1.37
3	2	194	HIS	CD2-NE2	-6.40	1.30	1.37
3	2	99	HIS	CD2-NE2	-6.26	1.30	1.37
2	1	266	HIS	CD2-NE2	-6.16	1.31	1.37
4	3	19	HIS	CD2-NE2	-6.13	1.31	1.37
3	2	109	HIS	CD2-NE2	-6.10	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	230	HIS	CD2-NE2	-5.77	1.31	1.37
5	4	13	HIS	CD2-NE2	-5.76	1.31	1.37
3	2	99	HIS	CG-ND1	-5.59	1.32	1.38
2	1	249	HIS	CD2-NE2	-5.51	1.31	1.37
2	1	161	PRO	CA-CB	-5.44	1.49	1.54
2	1	149	HIS	CD2-NE2	-5.39	1.31	1.37
3	2	118	HIS	CG-ND1	-5.39	1.32	1.38
4	3	153	HIS	CG-ND1	-5.21	1.32	1.38

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	146	ASN	OD1-CG-ND2	-11.93	110.67	122.60
2	1	250	ASN	OD1-CG-ND2	-11.36	111.24	122.60
2	1	117	GLN	OE1-CD-NE2	-11.21	111.39	122.60
3	2	136	SER	N-CA-C	9.57	123.47	109.69
4	3	218	ASN	OD1-CG-ND2	-9.56	113.04	122.60
3	2	203	ASN	CA-CB-CG	9.53	122.13	112.60
5	4	44	GLN	OE1-CD-NE2	-9.50	113.10	122.60
3	2	271	GLN	OE1-CD-NE2	-9.40	113.20	122.60
3	2	135	ASP	N-CA-C	9.32	122.30	111.11
3	2	164	ASN	N-CA-C	9.20	122.50	111.82
5	4	8	GLN	OE1-CD-NE2	-9.06	113.53	122.60
2	1	222	ASN	OD1-CG-ND2	-8.84	113.76	122.60
4	3	17	ASP	CA-CB-CG	8.84	121.44	112.60
3	2	240	GLN	OE1-CD-NE2	-8.80	113.80	122.60
4	3	162	SER	N-CA-C	8.78	121.80	111.71
3	2	48	ASN	OD1-CG-ND2	-8.65	113.95	122.60
4	3	173	ASN	OD1-CG-ND2	-8.64	113.96	122.60
5	4	69	ASN	OD1-CG-ND2	-8.48	114.12	122.60
4	3	140	GLN	OE1-CD-NE2	-8.38	114.22	122.60
2	1	224	GLN	OE1-CD-NE2	-8.34	114.26	122.60
4	3	105	ASN	OD1-CG-ND2	-8.23	114.37	122.60
5	4	39	ASN	OD1-CG-ND2	-8.23	114.37	122.60
2	1	289	ASN	CA-CB-CG	-8.14	104.46	112.60
3	2	10	SER	N-CA-C	8.08	121.76	109.23
3	2	26	GLN	OE1-CD-NE2	-8.07	114.53	122.60
3	2	63	PHE	N-CA-C	8.05	122.08	108.23
4	3	42	ASN	OD1-CG-ND2	-8.01	114.59	122.60
4	3	233	GLN	OE1-CD-NE2	-7.97	114.63	122.60
3	2	139	GLN	OE1-CD-NE2	-7.95	114.65	122.60
3	2	177	ASP	CA-CB-CG	7.95	120.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	265	VAL	N-CA-C	7.84	119.69	109.58
3	2	202	ASN	OD1-CG-ND2	-7.79	114.81	122.60
3	2	164	ASN	CA-CB-CG	-7.64	104.96	112.60
3	2	202	ASN	N-CA-C	7.56	120.86	108.99
2	1	68	GLN	OE1-CD-NE2	-7.56	115.04	122.60
3	2	203	ASN	OD1-CG-ND2	-7.51	115.09	122.60
2	1	249	HIS	N-CA-C	7.45	121.04	110.23
2	1	94	ASN	OD1-CG-ND2	-7.36	115.24	122.60
2	1	88	ALA	N-CA-C	7.34	119.54	108.46
2	1	199	VAL	N-CA-C	7.34	119.19	112.29
2	1	62	GLN	OE1-CD-NE2	-7.32	115.28	122.60
4	3	195	GLN	OE1-CD-NE2	-7.30	115.30	122.60
2	1	144	ASN	OD1-CG-ND2	-7.28	115.32	122.60
3	2	15	GLN	OE1-CD-NE2	-7.26	115.34	122.60
2	1	102	GLN	OE1-CD-NE2	-7.26	115.34	122.60
4	3	53	ILE	N-CA-C	7.25	114.86	108.63
2	1	117	GLN	N-CA-C	7.24	118.86	110.97
4	3	50	ASP	CA-CB-CG	7.24	119.84	112.60
3	2	204	SER	N-CA-C	7.12	119.58	108.96
3	2	271	GLN	CG-CD-NE2	7.07	127.00	116.40
2	1	153	GLN	OE1-CD-NE2	-7.05	115.55	122.60
4	3	133	ALA	N-CA-C	7.04	119.87	109.24
4	3	218	ASN	CB-CG-ND2	7.03	126.94	116.40
2	1	156	GLN	OE1-CD-NE2	-7.02	115.58	122.60
3	2	213	ASN	OD1-CG-ND2	-6.95	115.66	122.60
5	4	10	VAL	N-CA-C	6.90	117.36	108.12
3	2	127	ILE	N-CA-C	6.88	115.58	107.73
2	1	152	ASN	OD1-CG-ND2	-6.88	115.72	122.60
2	1	172	ASP	CA-CB-CG	6.84	119.44	112.60
2	1	149	HIS	CA-CB-CG	-6.83	106.97	113.80
3	2	135	ASP	CA-CB-CG	6.81	119.41	112.60
2	1	146	ASN	N-CA-C	6.73	125.14	110.80
4	3	178	GLN	OE1-CD-NE2	-6.71	115.89	122.60
5	4	63	LYS	N-CA-C	6.65	120.99	112.34
3	2	188	ASN	OD1-CG-ND2	-6.64	115.96	122.60
3	2	203	ASN	CB-CG-ND2	6.63	126.35	116.40
3	2	134	GLY	CA-C-N	6.62	129.48	120.54
3	2	134	GLY	C-N-CA	6.62	129.48	120.54
3	2	111	GLN	OE1-CD-NE2	-6.61	115.99	122.60
3	2	203	ASN	CB-CA-C	-6.55	97.03	110.38
2	1	203	ASN	OD1-CG-ND2	-6.52	116.08	122.60
3	2	218	ASP	CA-CB-CG	6.49	119.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	184	VAL	O-C-N	-6.46	116.18	122.97
2	1	289	ASN	N-CA-C	6.45	119.21	109.41
2	1	222	ASN	CB-CG-ND2	6.39	125.99	116.40
2	1	24	GLN	OE1-CD-NE2	-6.32	116.28	122.60
2	1	96	GLN	OE1-CD-NE2	-6.32	116.28	122.60
2	1	53	ASN	OD1-CG-ND2	-6.31	116.29	122.60
5	4	69	ASN	CB-CG-ND2	6.31	125.86	116.40
4	3	96	SER	N-CA-C	6.30	119.81	111.75
3	2	177	ASP	N-CA-C	6.28	118.64	111.11
3	2	146	ASN	OD1-CG-ND2	-6.27	116.33	122.60
4	3	181	GLN	OE1-CD-NE2	-6.26	116.33	122.60
4	3	56	ASN	OD1-CG-ND2	-6.26	116.34	122.60
3	2	161	ASN	OD1-CG-ND2	-6.25	116.35	122.60
2	1	247	ASN	OD1-CG-ND2	-6.25	116.36	122.60
2	1	267	VAL	N-CA-C	6.18	117.62	109.21
5	4	13	HIS	CB-CG-CD2	-6.15	123.20	131.20
3	2	263	ARG	O-C-N	-6.15	118.50	123.11
2	1	148	GLY	O-C-N	-6.15	115.91	122.67
3	2	223	HIS	CA-CB-CG	6.13	119.93	113.80
5	4	45	ASP	N-CA-C	6.10	119.34	109.40
2	1	38	SER	N-CA-C	6.10	118.22	109.14
4	3	219	ASP	CA-CB-CG	6.08	118.68	112.60
3	2	198	ASN	OD1-CG-ND2	-6.07	116.53	122.60
4	3	12	GLN	OE1-CD-NE2	-6.06	116.54	122.60
4	3	233	GLN	CG-CD-NE2	6.05	125.48	116.40
2	1	117	GLN	CG-CD-NE2	6.04	125.46	116.40
5	4	4	GLN	OE1-CD-NE2	-6.03	116.57	122.60
3	2	264	ASN	OD1-CG-ND2	-6.03	116.57	122.60
3	2	113	ASN	OD1-CG-ND2	-5.97	116.63	122.60
2	1	289	ASN	OD1-CG-ND2	-5.96	116.64	122.60
4	3	153	HIS	CB-CG-CD2	-5.94	123.47	131.20
5	4	8	GLN	CG-CD-NE2	5.93	125.29	116.40
3	2	270	PHE	N-CA-C	5.92	119.56	112.93
4	3	69	ARG	N-CA-C	5.92	118.17	108.52
3	2	119	GLN	OE1-CD-NE2	-5.90	116.70	122.60
2	1	108	TRP	CG-CD2-CE3	5.89	139.79	133.90
3	2	20	ASN	OD1-CG-ND2	-5.86	116.74	122.60
2	1	113	LYS	N-CA-C	5.86	120.42	113.16
2	1	85	ALA	N-CA-C	5.83	118.75	109.24
5	4	26	ASN	N-CA-C	5.81	119.14	110.14
2	1	294	LEU	N-CA-C	5.79	119.06	109.46
5	4	51	SER	N-CA-C	5.77	120.89	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	64	THR	CA-CB-OG1	-5.76	100.96	109.60
4	3	153	HIS	N-CA-C	5.74	117.79	109.07
2	1	224	GLN	CG-CD-NE2	5.70	124.95	116.40
4	3	15	THR	CA-CB-OG1	-5.67	101.09	109.60
2	1	115	THR	CA-CB-OG1	-5.67	101.09	109.60
2	1	178	SER	N-CA-C	5.67	119.29	112.38
3	2	87	ARG	N-CA-C	5.63	118.96	111.75
4	3	27	GLU	N-CA-C	5.61	119.43	112.47
2	1	68	GLN	N-CA-C	5.59	117.81	109.59
5	4	44	GLN	CG-CD-NE2	5.57	124.76	116.40
3	2	118	HIS	CB-CG-CD2	-5.56	123.98	131.20
3	2	52	GLN	OE1-CD-NE2	-5.55	117.05	122.60
3	2	224	ASN	OD1-CG-ND2	-5.54	117.06	122.60
3	2	37	ARG	N-CA-C	5.54	117.45	108.41
5	4	5	VAL	N-CA-C	5.53	115.86	108.11
5	4	39	ASN	CB-CG-ND2	5.52	124.68	116.40
4	3	180	THR	N-CA-CB	5.50	118.23	110.36
2	1	37	HIS	CA-CB-CG	5.50	119.30	113.80
5	4	26	ASN	OD1-CG-ND2	-5.50	117.10	122.60
4	3	140	GLN	CG-CD-NE2	5.49	124.64	116.40
3	2	94	GLN	OE1-CD-NE2	-5.49	117.11	122.60
3	2	48	ASN	CB-CG-ND2	5.47	124.61	116.40
2	1	141	ASN	N-CA-C	5.47	116.58	108.60
3	2	57	ASP	N-CA-C	5.47	116.62	108.31
2	1	290	ASN	OD1-CG-ND2	-5.46	117.14	122.60
4	3	109	HIS	CA-CB-CG	5.45	119.25	113.80
4	3	161	GLN	OE1-CD-NE2	-5.44	117.16	122.60
2	1	250	ASN	CB-CG-ND2	5.42	124.53	116.40
3	2	125	PHE	N-CA-C	5.42	117.74	108.90
5	4	62	ILE	N-CA-C	5.41	116.06	109.30
2	1	108	TRP	CE2-CD2-CG	-5.40	100.72	107.20
2	1	160	ILE	CA-C-N	5.40	123.55	119.66
2	1	160	ILE	C-N-CA	5.40	123.55	119.66
2	1	132	MET	N-CA-C	5.38	117.67	108.90
3	2	95	ASN	CA-CB-CG	-5.38	107.22	112.60
5	4	48	GLN	OE1-CD-NE2	-5.37	117.23	122.60
2	1	225	ILE	CB-CA-C	-5.35	105.03	112.04
3	2	163	ASP	CA-CB-CG	5.34	117.94	112.60
4	3	21	SER	O-C-N	-5.33	117.67	121.83
4	3	80	GLN	OE1-CD-NE2	-5.31	117.29	122.60
4	3	180	THR	CB-CA-C	-5.31	98.80	109.68
4	3	170	TRP	CG-CD2-CE3	5.29	139.19	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	171	ARG	N-CA-C	5.29	118.69	111.39
2	1	51	ALA	N-CA-C	5.29	118.69	110.17
3	2	80	TRP	CE2-CD2-CG	-5.29	100.85	107.20
3	2	68	THR	N-CA-C	5.24	117.82	110.23
4	3	78	LEU	N-CA-C	5.23	118.77	112.38
3	2	199	LEU	N-CA-C	5.23	118.44	111.75
2	1	153	GLN	N-CA-C	5.22	118.74	109.96
4	3	102	GLU	N-CA-C	5.22	116.66	111.07
3	2	109	HIS	CB-CG-CD2	-5.22	124.41	131.20
2	1	161	PRO	O-C-N	-5.22	118.70	121.15
2	1	152	ASN	N-CA-C	5.21	117.91	110.24
4	3	209	SER	N-CA-C	5.21	118.55	110.17
5	4	13	HIS	CB-CG-ND1	5.21	130.51	122.70
2	1	65	HIS	CB-CG-CD2	-5.17	124.47	131.20
2	1	176	GLN	OE1-CD-NE2	-5.17	117.44	122.60
3	2	195	GLN	OE1-CD-NE2	-5.15	117.45	122.60
4	3	183	SER	N-CA-C	5.15	117.56	111.33
2	1	292	ASP	CA-C-N	5.15	124.94	119.28
2	1	292	ASP	C-N-CA	5.15	124.94	119.28
3	2	159	GLN	OE1-CD-NE2	-5.14	117.46	122.60
3	2	223	HIS	N-CA-C	5.14	117.80	108.69
2	1	193	ARG	N-CA-C	5.14	117.73	108.48
3	2	203	ASN	N-CA-CB	5.14	118.21	110.30
3	2	84	ASP	N-CA-C	5.13	119.83	111.37
4	3	15	THR	CA-CB-CG2	5.12	119.20	110.50
3	2	58	VAL	N-CA-C	5.11	118.22	111.17
3	2	78	TRP	CE2-CD2-CG	-5.11	101.07	107.20
2	1	175	TRP	CE2-CD2-CG	-5.09	101.09	107.20
4	3	170	TRP	CB-CG-CD1	-5.08	119.28	126.90
2	1	180	ASN	OD1-CG-ND2	-5.07	117.53	122.60
3	2	160	PHE	N-CA-C	5.07	116.52	108.67
4	3	20	GLN	OE1-CD-NE2	-5.01	117.59	122.60
2	1	136	PHE	N-CA-C	5.00	116.85	107.99
2	1	116	VAL	N-CA-C	5.00	116.11	111.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	198	TYR	Sidechain

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	2208	0	2154	21	0
3	2	2088	0	2005	16	0
4	3	1812	0	1792	15	0
5	4	472	0	453	5	0
6	1	28	0	29	4	0
7	4	15	0	27	0	0
All	All	6653	0	6490	42	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 (42) 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)
3:2:186:LEU:HD22	4:3:65:MET:HE1	1.65	0.78
3:2:116:LYS:HD2	4:3:124:MET:SD	2.27	0.75
2:1:40:GLU:HB3	5:4:64:THR:HB	1.74	0.69
2:1:107:MET:HE1	2:1:166:THR:HB	1.74	0.69
2:1:181:PRO:HB2	6:1:500:J78:H3	1.76	0.68
3:2:238:PHE:HB3	3:2:244:VAL:HG21	1.76	0.67
3:2:212:VAL:HG22	4:3:37:PRO:HG2	1.85	0.58
2:1:294:LEU:HD13	4:3:67:MET:SD	2.46	0.56
2:1:222:ASN:HD22	2:1:224:GLN:HB2	1.70	0.56
2:1:215:VAL:HG21	3:2:221:VAL:HG12	1.89	0.55
2:1:83:ARG:HG3	4:3:15:THR:HG22	1.89	0.54
4:3:52:MET:HE2	4:3:211:LEU:HD13	1.89	0.54
3:2:179:LEU:HA	3:2:184:VAL:O	2.08	0.53
4:3:167:VAL:O	4:3:169:PRO:HD3	2.09	0.52
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.92	0.51
3:2:271:GLN:NE2	3:2:271:GLN:HA	2.26	0.49
4:3:87:LEU:HD11	4:3:114:LEU:HD12	1.96	0.48
2:1:220:ASP:HB3	2:1:225:ILE:HD12	1.96	0.48
3:2:238:PHE:HB3	3:2:244:VAL:CG2	2.43	0.47
3:2:134:GLY:HA2	3:2:173:PHE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:234:THR:OG1	2:1:237:ASP:HA	2.16	0.46
4:3:91:PHE:CD2	4:3:181:GLN:HB2	2.50	0.46
3:2:27:GLU:HB2	3:2:203:ASN:OD1	2.16	0.46
4:3:62:ARG:HH11	4:3:63:ASN:ND2	2.14	0.46
2:1:145:ALA:O	2:1:146:ASN:HB2	2.15	0.46
2:1:148:GLY:O	2:1:149:HIS:ND1	2.49	0.45
2:1:196:VAL:HG11	6:1:500:J78:H9	1.97	0.44
4:3:119:LEU:HD23	4:3:211:LEU:HD12	1.98	0.44
5:4:6:SER:HB2	5:4:27:TYR:CE1	2.52	0.44
2:1:70:ARG:NH2	4:3:219:ASP:O	2.50	0.44
3:2:48:ASN:HB3	3:2:49:PRO:HD3	2.00	0.44
2:1:87:VAL:HG11	2:1:262:MET:HG2	1.99	0.44
2:1:110:ILE:HG21	6:1:500:J78:H101	2.00	0.43
2:1:110:ILE:HG21	6:1:500:J78:H131	2.00	0.43
5:4:3:ALA:HA	5:4:30:ILE:HG12	2.00	0.43
3:2:12:ARG:HH21	5:4:68:LEU:HD13	1.83	0.43
3:2:37:ARG:HG3	4:3:37:PRO:HB3	2.00	0.42
3:2:32:VAL:HG13	5:4:56:PRO:HB2	2.01	0.42
2:1:230:TYR:OH	3:2:131:CYS:HA	2.20	0.42
2:1:150:ALA:HA	2:1:250:ASN:ND2	2.35	0.41
2:1:48:GLU:HA	3:2:196:ILE:HB	2.03	0.40
2:1:275:PRO:HG2	4:3:102:GLU:HG3	2.03	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	2/4 (50%)	2 (100%)	0	0	100	100
2	1	277/300 (92%)	255 (92%)	19 (7%)	3 (1%)	11	36
3	2	264/271 (97%)	242 (92%)	16 (6%)	6 (2%)	5	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	233/235 (99%)	219 (94%)	14 (6%)	0	100	100
5	4	58/68 (85%)	53 (91%)	3 (5%)	2 (3%)	3	11
All	All	834/878 (95%)	771 (92%)	52 (6%)	11 (1%)	9	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	237	ASP
3	2	7	CYS
3	2	242	SER
2	1	146	ASN
3	2	8	GLY
3	2	48	ASN
3	2	239	ALA
3	2	241	ASP
5	4	43	LYS
2	1	271	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%)	4 (100%)	0	100	100
2	1	241/258 (93%)	232 (96%)	9 (4%)	30	65
3	2	224/229 (98%)	217 (97%)	7 (3%)	35	70
4	3	210/210 (100%)	202 (96%)	8 (4%)	29	64
5	4	53/56 (95%)	51 (96%)	2 (4%)	29	64
All	All	732/757 (97%)	706 (96%)	26 (4%)	31	66

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	83	ARG
2	1	96	GLN
2	1	100	ARG
2	1	109	ARG
2	1	115	THR
2	1	129	ARG
2	1	146	ASN
2	1	222	ASN
2	1	237	ASP
3	2	12	ARG
3	2	66	LEU
3	2	87	ARG
3	2	103	ARG
3	2	137	ASP
3	2	161	ASN
3	2	164	ASN
4	3	64	THR
4	3	124	MET
4	3	149	MET
4	3	163	SER
4	3	180	THR
4	3	206	LYS
4	3	218	ASN
4	3	224	LEU
5	4	7	SER
5	4	62	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	180	ASN
2	1	203	ASN
2	1	222	ASN
2	1	250	ASN
3	2	94	GLN
3	2	95	ASN
3	2	139	GLN
3	2	271	GLN
4	3	6	ASN
4	3	80	GLN
4	3	230	HIS
5	4	8	GLN
5	4	13	HIS

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	J78	1	500	-	30,30,30	1.50	3 (10%)	37,39,39	2.11	10 (27%)
7	MYR	4	1	5	13,14,15	0.34	0	12,13,15	0.79	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	J78	1	500	-	-	6/18/28/28	0/3/3/3
7	MYR	4	1	5	-	1/12/12/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	500	J78	C19-C22	-5.17	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	500	J78	O24-C22	5.03	1.45	1.33
6	1	500	J78	O24-C25	-2.27	1.39	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	500	J78	C11-N6-C7	4.96	122.73	111.57
6	1	500	J78	O24-C25-C26	4.95	126.15	108.40
6	1	500	J78	C5-N4-N3	4.54	123.55	118.97
6	1	500	J78	C4-C5-N4	-4.21	117.67	123.84
6	1	500	J78	C1-C2-N3	4.15	118.57	116.13
6	1	500	J78	C11-C10-C9	3.15	119.68	111.92
6	1	500	J78	O24-C22-C19	3.14	117.42	112.15
6	1	500	J78	C12-C9-C8	-2.62	105.45	112.05
6	1	500	J78	C10-C11-N6	2.60	116.81	110.92
6	1	500	J78	C2-N3-N4	-2.06	118.73	119.97

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	4	1	MYR	O1-C1-C2-C3
6	1	500	J78	C19-C22-O24-C25
6	1	500	J78	O23-C22-O24-C25
6	1	500	J78	C26-C25-O24-C22
6	1	500	J78	C21-C16-O15-C14
6	1	500	J78	C12-C13-C14-O15
6	1	500	J78	C17-C16-O15-C14

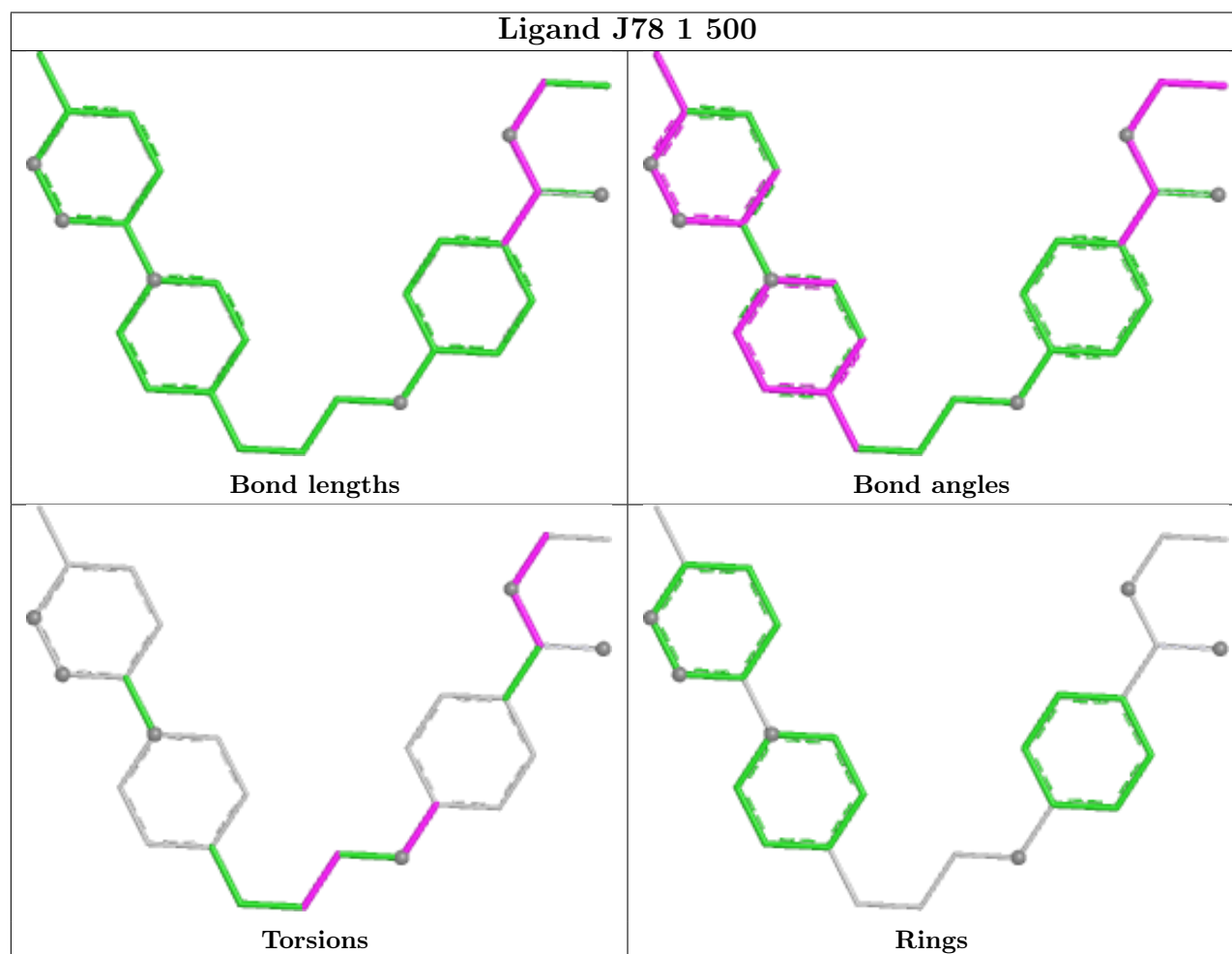
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	500	J78	4	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

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.