



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:03 AM UTC

PDB ID : 1VBB / pdb_00001vbb
Title : POLIOVIRUS (TYPE 3, SABIN STRAIN) (P3/SABIN, P3/LEON/12A(1)B)
COMPLEXED WITH R80633
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)
Xtrriage (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

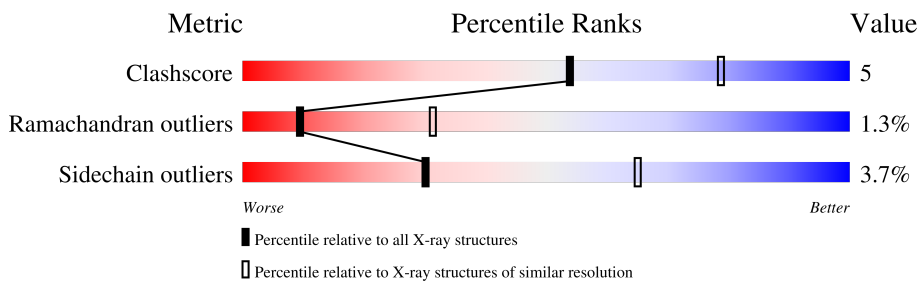
1 Overall quality at a glance

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	
2	1	300	
3	2	271	
4	3	235	
5	4	68	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6660 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
			Total	C	N	O			
1	0	4	30	19	4	7	0	0	0

- Molecule 2 is a protein called POLIOVIRUS TYPE 3.

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

- Molecule 3 is a protein called POLIOVIRUS TYPE 3.

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

- Molecule 4 is a protein called POLIOVIRUS TYPE 3.

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

- Molecule 5 is a protein called POLIOVIRUS TYPE 3.

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

- Molecule 6 is (METHYLPYRIDAZINE PIPERIDINE BUTYLOXYPHENYL)ETHYLACE TATE (CCD ID: J80) (formula: C₂₃H₃₁N₃O₃).

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.

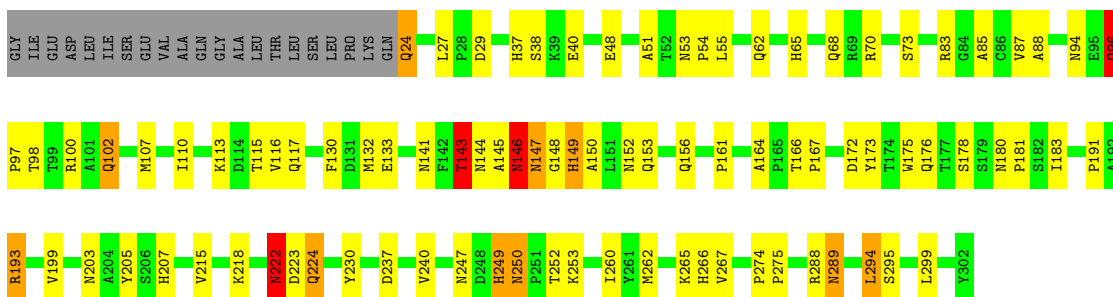
- Molecule 1: POLIOVIRUS TYPE 3

Chain 0: 75% 25%



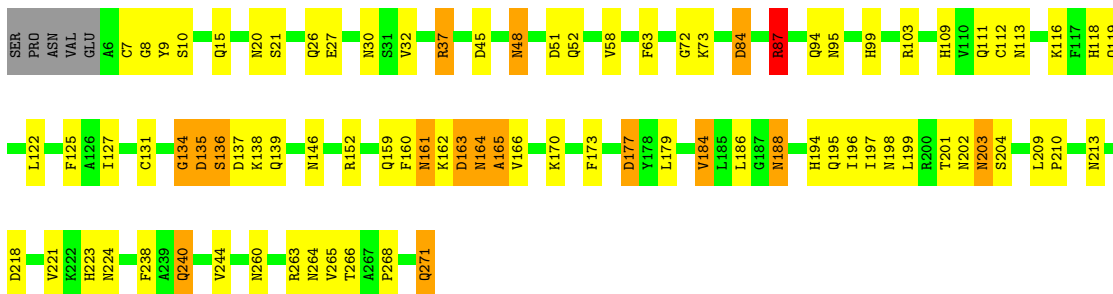
- Molecule 2: POLIOVIRUS TYPE 3

Chain 1: 63% 25% 7%



- Molecule 3: POLIOVIRUS TYPE 3

Chain 2: 66% 26% 6%



- Molecule 4: POLIOVIRUS TYPE 3

Chain 3: 74% 23%





- Molecule 5: POLIOVIRUS TYPE 3



4 Data and refinement statistics

Xtrriage (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}	0.278 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6660	wwPDB-VP
Average B, all atoms (Å ²)	6.0	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: 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	1.06	0/29	1.75	1/38 (2.6%)
2	1	0.93	7/2278 (0.3%)	1.87	66/3111 (2.1%)
3	2	0.95	7/2146 (0.3%)	1.96	73/2926 (2.5%)
4	3	0.96	6/1857 (0.3%)	1.80	44/2533 (1.7%)
5	4	0.90	1/479 (0.2%)	1.97	19/647 (2.9%)
All	All	0.94	21/6789 (0.3%)	1.89	203/9255 (2.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	223	HIS	CD2-NE2	-7.67	1.29	1.37
4	3	153	HIS	CD2-NE2	-7.61	1.29	1.37
4	3	97	HIS	CD2-NE2	-7.35	1.29	1.37
2	1	207	HIS	CD2-NE2	-7.27	1.29	1.37
2	1	266	HIS	CD2-NE2	-7.18	1.29	1.37
4	3	19	HIS	CD2-NE2	-6.92	1.30	1.37
4	3	109	HIS	CD2-NE2	-6.87	1.30	1.37
3	2	194	HIS	CD2-NE2	-6.72	1.30	1.37
3	2	118	HIS	CD2-NE2	-6.61	1.30	1.37
2	1	37	HIS	CD2-NE2	-6.33	1.30	1.37
2	1	65	HIS	CD2-NE2	-6.29	1.30	1.37
3	2	99	HIS	CD2-NE2	-6.14	1.31	1.37
5	4	13	HIS	CD2-NE2	-6.06	1.31	1.37
3	2	223	HIS	CG-ND1	-5.99	1.31	1.38
2	1	266	HIS	CG-ND1	-5.80	1.31	1.38
4	3	153	HIS	CG-ND1	-5.70	1.31	1.38
4	3	230	HIS	CD2-NE2	-5.69	1.31	1.37
3	2	109	HIS	CD2-NE2	-5.54	1.31	1.37
2	1	249	HIS	CD2-NE2	-5.46	1.31	1.37
2	1	149	HIS	CD2-NE2	-5.12	1.32	1.37
3	2	99	HIS	CG-ND1	-5.12	1.32	1.38

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	135	ASP	N-CA-C	11.05	123.33	111.28
2	1	146	ASN	OD1-CG-ND2	-11.05	111.55	122.60
4	3	218	ASN	OD1-CG-ND2	-10.98	111.62	122.60
3	2	271	GLN	OE1-CD-NE2	-10.83	111.77	122.60
3	2	203	ASN	CA-CB-CG	10.64	123.25	112.60
2	1	117	GLN	OE1-CD-NE2	-10.60	112.00	122.60
2	1	289	ASN	CA-CB-CG	-10.33	102.27	112.60
3	2	240	GLN	OE1-CD-NE2	-9.67	112.93	122.60
4	3	17	ASP	CA-CB-CG	9.56	122.16	112.60
3	2	48	ASN	OD1-CG-ND2	-9.33	113.27	122.60
2	1	289	ASN	N-CA-C	9.21	120.41	108.34
2	1	250	ASN	OD1-CG-ND2	-9.18	113.42	122.60
2	1	96	GLN	OE1-CD-NE2	-8.98	113.62	122.60
3	2	136	SER	N-CA-C	8.87	123.38	109.81
5	4	44	GLN	OE1-CD-NE2	-8.80	113.80	122.60
5	4	69	ASN	OD1-CG-ND2	-8.68	113.92	122.60
2	1	222	ASN	OD1-CG-ND2	-8.66	113.94	122.60
2	1	172	ASP	CA-CB-CG	8.65	121.25	112.60
2	1	24	GLN	OE1-CD-NE2	-8.64	113.96	122.60
3	2	203	ASN	OD1-CG-ND2	-8.60	114.00	122.60
2	1	102	GLN	OE1-CD-NE2	-8.60	114.00	122.60
2	1	94	ASN	OD1-CG-ND2	-8.46	114.14	122.60
3	2	52	GLN	OE1-CD-NE2	-8.46	114.14	122.60
3	2	265	VAL	N-CA-C	8.46	120.79	109.37
3	2	94	GLN	OE1-CD-NE2	-8.35	114.25	122.60
2	1	117	GLN	N-CA-C	8.34	119.99	111.07
2	1	144	ASN	OD1-CG-ND2	-8.28	114.32	122.60
4	3	105	ASN	OD1-CG-ND2	-8.25	114.35	122.60
4	3	133	ALA	N-CA-C	8.24	121.69	109.24
2	1	223	ASP	CA-CB-CG	8.24	120.84	112.60
3	2	164	ASN	N-CA-C	8.24	121.38	111.82
5	4	10	VAL	N-CA-C	8.20	119.11	108.12
4	3	218	ASN	CB-CG-ND2	8.13	128.60	116.40
5	4	8	GLN	OE1-CD-NE2	-8.07	114.53	122.60
2	1	68	GLN	OE1-CD-NE2	-7.97	114.63	122.60
5	4	4	GLN	OE1-CD-NE2	-7.94	114.66	122.60
2	1	153	GLN	OE1-CD-NE2	-7.93	114.67	122.60
3	2	203	ASN	CB-CG-ND2	7.87	128.20	116.40
3	2	202	ASN	OD1-CG-ND2	-7.78	114.82	122.60
2	1	203	ASN	OD1-CG-ND2	-7.75	114.85	122.60
3	2	139	GLN	OE1-CD-NE2	-7.72	114.88	122.60
3	2	218	ASP	CA-CB-CG	7.71	120.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	161	ASN	OD1-CG-ND2	-7.68	114.92	122.60
2	1	152	ASN	OD1-CG-ND2	-7.65	114.95	122.60
4	3	74	ASP	CA-CB-CG	7.62	120.22	112.60
3	2	177	ASP	CA-CB-CG	7.60	120.20	112.60
3	2	271	GLN	CG-CD-NE2	7.58	127.76	116.40
4	3	140	GLN	OE1-CD-NE2	-7.54	115.06	122.60
4	3	53	ILE	N-CA-C	7.53	115.10	108.63
2	1	267	VAL	N-CA-C	7.47	119.38	109.21
3	2	134	GLY	CA-C-N	7.43	130.24	120.28
3	2	134	GLY	C-N-CA	7.43	130.24	120.28
2	1	199	VAL	N-CA-C	7.39	119.45	111.77
2	1	116	VAL	N-CA-C	7.36	118.14	111.81
4	3	173	ASN	OD1-CG-ND2	-7.32	115.28	122.60
2	1	62	GLN	OE1-CD-NE2	-7.28	115.32	122.60
2	1	96	GLN	CG-CD-NE2	7.27	127.31	116.40
3	2	63	PHE	N-CA-C	7.25	119.91	108.67
3	2	213	ASN	OD1-CG-ND2	-7.19	115.41	122.60
5	4	39	ASN	OD1-CG-ND2	-7.19	115.41	122.60
3	2	26	GLN	OE1-CD-NE2	-7.19	115.41	122.60
4	3	233	GLN	OE1-CD-NE2	-7.19	115.41	122.60
3	2	264	ASN	OD1-CG-ND2	-7.17	115.43	122.60
3	2	224	ASN	OD1-CG-ND2	-7.08	115.52	122.60
2	1	224	GLN	OE1-CD-NE2	-7.03	115.57	122.60
4	3	162	SER	N-CA-C	7.03	121.61	112.89
5	4	4	GLN	CG-CD-NE2	6.97	126.86	116.40
3	2	20	ASN	OD1-CG-ND2	-6.96	115.64	122.60
2	1	156	GLN	OE1-CD-NE2	-6.93	115.67	122.60
2	1	249	HIS	N-CA-C	6.89	120.37	110.10
4	3	161	GLN	OE1-CD-NE2	-6.78	115.82	122.60
3	2	188	ASN	OD1-CG-ND2	-6.76	115.84	122.60
3	2	164	ASN	CA-CB-CG	-6.74	105.86	112.60
3	2	15	GLN	OE1-CD-NE2	-6.68	115.92	122.60
3	2	177	ASP	N-CA-C	6.67	119.15	111.02
3	2	263	ARG	O-C-N	-6.58	118.18	123.11
5	4	48	GLN	OE1-CD-NE2	-6.56	116.04	122.60
2	1	146	ASN	N-CA-C	6.56	124.77	110.80
5	4	13	HIS	CB-CG-CD2	-6.51	122.73	131.20
3	2	135	ASP	CA-CB-CG	6.51	119.11	112.60
2	1	88	ALA	N-CA-C	6.50	119.03	108.76
2	1	147	ASN	CA-CB-CG	6.49	119.09	112.60
2	1	161	PRO	O-C-N	-6.47	118.11	121.15
3	2	198	ASN	OD1-CG-ND2	-6.47	116.13	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	95	ASN	OD1-CG-ND2	-6.46	116.14	122.60
4	3	181	GLN	OE1-CD-NE2	-6.46	116.14	122.60
3	2	204	SER	N-CA-C	6.45	118.02	108.60
4	3	30	VAL	N-CA-C	6.42	118.04	109.37
2	1	38	SER	N-CA-C	6.42	118.70	109.14
3	2	113	ASN	OD1-CG-ND2	-6.36	116.24	122.60
3	2	240	GLN	CG-CD-NE2	6.34	125.92	116.40
4	3	50	ASP	CA-CB-CG	6.31	118.91	112.60
4	3	180	THR	N-CA-CB	6.31	120.04	110.45
3	2	223	HIS	N-CA-C	6.30	118.72	108.26
3	2	127	ILE	N-CA-C	6.26	114.87	107.73
3	2	184	VAL	O-C-N	-6.26	116.40	122.97
2	1	113	LYS	N-CA-C	6.20	120.85	113.16
4	3	180	THR	CB-CA-C	-6.20	97.43	109.76
2	1	180	ASN	OD1-CG-ND2	-6.19	116.41	122.60
4	3	96	SER	N-CA-C	6.19	119.67	111.75
5	4	63	LYS	N-CA-C	6.17	120.36	112.34
2	1	24	GLN	CG-CD-NE2	6.13	125.60	116.40
3	2	48	ASN	CB-CG-ND2	6.13	125.60	116.40
3	2	260	ASN	OD1-CG-ND2	-6.08	116.52	122.60
2	1	149	HIS	CA-CB-CG	-6.08	107.72	113.80
2	1	222	ASN	CB-CG-ND2	6.07	125.51	116.40
4	3	189	TYR	N-CA-C	6.06	119.01	108.76
4	3	153	HIS	CB-CG-CD2	-6.01	123.39	131.20
2	1	289	ASN	OD1-CG-ND2	-6.00	116.60	122.60
4	3	18	ASN	OD1-CG-ND2	-5.99	116.61	122.60
4	3	150	LEU	N-CA-C	5.97	119.67	112.38
4	3	195	GLN	OE1-CD-NE2	-5.95	116.65	122.60
3	2	164	ASN	OD1-CG-ND2	-5.93	116.67	122.60
4	3	12	GLN	OE1-CD-NE2	-5.93	116.67	122.60
2	1	299	LEU	N-CA-C	5.91	118.48	111.33
5	4	4	GLN	N-CA-CB	-5.90	101.29	110.55
4	3	178	GLN	OE1-CD-NE2	-5.89	116.71	122.60
2	1	85	ALA	N-CA-C	5.88	118.83	109.24
2	1	55	LEU	N-CA-C	5.84	119.60	110.32
3	2	202	ASN	N-CA-C	5.83	118.97	109.06
3	2	160	PHE	N-CA-C	5.81	118.22	108.23
3	2	199	LEU	N-CA-C	5.80	119.89	112.34
3	2	10	SER	N-CA-C	5.79	117.91	108.76
3	2	125	PHE	N-CA-C	5.79	118.34	108.90
2	1	152	ASN	N-CA-C	5.78	118.74	110.24
2	1	51	ALA	N-CA-C	5.76	119.45	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	247	ASN	OD1-CG-ND2	-5.75	116.85	122.60
4	3	77	ASP	CA-CB-CG	5.75	118.35	112.60
3	2	209	LEU	N-CA-C	5.75	117.78	109.04
4	3	56	ASN	OD1-CG-ND2	-5.74	116.86	122.60
3	2	20	ASN	CB-CG-ND2	5.74	125.00	116.40
4	3	15	THR	CA-CB-OG1	-5.72	101.03	109.60
3	2	37	ARG	N-CA-C	5.68	117.78	108.52
3	2	84	ASP	N-CA-C	5.67	120.73	111.37
3	2	135	ASP	CB-CA-C	-5.66	101.39	110.79
2	1	141	ASN	OD1-CG-ND2	-5.66	116.94	122.60
2	1	178	SER	N-CA-C	5.66	118.22	111.71
5	4	69	ASN	CB-CG-ND2	5.64	124.86	116.40
2	1	53	ASN	OD1-CG-ND2	-5.63	116.97	122.60
3	2	45	ASP	CA-CB-CG	5.62	118.22	112.60
4	3	64	THR	O-C-N	-5.61	116.85	123.25
5	4	15	ASN	OD1-CG-ND2	-5.61	116.99	122.60
4	3	27	GLU	N-CA-C	5.59	119.41	112.47
4	3	219	ASP	CA-CB-CG	5.58	118.18	112.60
5	4	5	VAL	N-CA-C	5.57	115.89	107.75
3	2	152	ARG	CB-CA-C	-5.53	100.39	110.63
4	3	42	ASN	OD1-CG-ND2	-5.50	117.10	122.60
4	3	6	ASN	OD1-CG-ND2	-5.48	117.12	122.60
2	1	222	ASN	O-C-N	-5.48	116.77	122.96
2	1	294	LEU	N-CA-C	5.47	118.16	109.24
3	2	9	TYR	N-CA-C	5.47	117.75	110.53
4	3	80	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	1	29	ASP	CA-CB-CG	5.40	118.00	112.60
2	1	260	ILE	N-CA-C	5.39	115.86	107.99
3	2	165	ALA	N-CA-C	5.39	122.28	110.80
4	3	20	GLN	OE1-CD-NE2	-5.38	117.22	122.60
3	2	30	ASN	OD1-CG-ND2	-5.36	117.24	122.60
2	1	153	GLN	N-CA-C	5.36	118.54	109.76
2	1	143	THR	CA-CB-OG1	-5.35	101.57	109.60
4	3	153	HIS	N-CA-C	5.34	116.96	108.79
4	3	140	GLN	CG-CD-NE2	5.32	124.39	116.40
3	2	73	LYS	N-CA-C	5.32	118.56	111.75
3	2	146	ASN	OD1-CG-ND2	-5.31	117.29	122.60
2	1	117	GLN	CG-CD-NE2	5.31	124.36	116.40
5	4	24	THR	N-CA-C	5.31	118.27	109.46
3	2	194	HIS	N-CA-C	5.31	116.35	108.60
4	3	97	HIS	CB-CG-CD2	-5.30	124.31	131.20
5	4	45	ASP	N-CA-C	5.30	117.36	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	240	VAL	N-CA-C	5.29	117.68	108.95
1	0	8	GLU	CA-CB-CG	5.29	124.68	114.10
3	2	21	SER	N-CA-C	5.28	117.51	108.90
5	4	42	SER	N-CA-C	5.28	118.51	111.75
2	1	73	SER	N-CA-C	5.26	117.01	111.28
2	1	146	ASN	CB-CG-ND2	5.25	124.28	116.40
3	2	51	ASP	CA-CB-CG	5.24	117.83	112.60
2	1	37	HIS	CA-CB-CG	5.22	119.02	113.80
3	2	111	GLN	OE1-CD-NE2	-5.22	117.38	122.60
2	1	149	HIS	N-CA-C	5.21	115.26	108.07
4	3	69	ARG	N-CA-C	5.19	116.98	108.52
4	3	11	ASN	OD1-CG-ND2	-5.18	117.42	122.60
4	3	234	SER	N-CA-C	5.18	117.80	110.50
2	1	147	ASN	CB-CA-C	-5.17	104.45	111.95
3	2	203	ASN	CB-CA-C	-5.17	99.51	110.31
2	1	295	SER	N-CA-C	5.16	117.34	110.53
2	1	289	ASN	CB-CG-ND2	5.15	124.12	116.40
2	1	149	HIS	CB-CG-CD2	-5.14	124.52	131.20
3	2	159	GLN	OE1-CD-NE2	-5.14	117.46	122.60
4	3	148	ALA	N-CA-C	5.13	116.88	111.28
3	2	72	GLY	O-C-N	-5.13	119.14	123.60
5	4	13	HIS	CB-CG-ND1	5.11	130.36	122.70
2	1	164	ALA	N-CA-C	5.10	116.31	109.83
2	1	175	TRP	CE2-CD2-CG	-5.10	101.08	107.20
3	2	119	GLN	N-CA-CB	-5.10	102.04	111.52
3	2	194	HIS	CB-CG-CD2	-5.10	124.57	131.20
3	2	195	GLN	OE1-CD-NE2	-5.09	117.51	122.60
3	2	112	CYS	O-C-N	-5.08	118.82	123.50
4	3	15	THR	CA-CB-CG2	5.06	119.10	110.50
3	2	58	VAL	N-CA-C	5.05	118.14	111.17
5	4	44	GLN	CG-CD-NE2	5.05	123.97	116.40
2	1	94	ASN	CB-CG-ND2	5.04	123.95	116.40
3	2	87	ARG	N-CA-C	5.04	118.20	111.75
4	3	64	THR	CA-CB-OG1	-5.02	102.07	109.60
2	1	65	HIS	CB-CG-CD2	-5.01	124.69	131.20

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	36	0
3	2	2088	0	2005	26	0
4	3	1812	0	1792	17	0
5	4	472	0	453	6	0
6	1	29	0	31	4	0
7	4	15	0	27	0	0
All	All	6660	0	6488	65	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 (65) 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	1.57	0.84
2:1:143:THR:HG21	2:1:253:LYS:HD3	1.62	0.80
2:1:87:VAL:HG21	2:1:262:MET:HE3	1.70	0.74
2:1:288:ARG:HE	3:2:162:LYS:HZ2	1.36	0.73
2:1:288:ARG:HE	3:2:162:LYS:NZ	1.93	0.66
3:2:238:PHE:HB3	3:2:244:VAL:HG21	1.80	0.63
3:2:271:GLN:NE2	3:2:271:GLN:HA	2.16	0.61
3:2:271:GLN:HA	3:2:271:GLN:HE21	1.65	0.61
2:1:132:MET:SD	2:1:262:MET:HG2	2.41	0.59
2:1:222:ASN:HD22	2:1:224:GLN:HB2	1.68	0.59
3:2:116:LYS:HD3	4:3:124:MET:SD	2.44	0.58
3:2:179:LEU:HA	3:2:184:VAL:O	2.05	0.57
2:1:294:LEU:HD13	4:3:67:MET:SD	2.45	0.56
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.88	0.56
2:1:96:GLN:HG2	2:1:249:HIS:CE1	2.43	0.54
4:3:66:ASP:HA	4:3:69:ARG:HD2	1.90	0.53
2:1:107:MET:HE1	2:1:166:THR:HB	1.90	0.53
4:3:194:TYR:HE1	4:3:198:ILE:HD13	1.75	0.52
2:1:181:PRO:HB2	6:1:500:J80:H3	1.93	0.51
3:2:136:SER:HB3	3:2:138:LYS:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:183:ILE:HG13	6:1:500:J80:H12	1.92	0.51
2:1:110:ILE:HD13	6:1:500:J80:H9	1.92	0.51
2:1:145:ALA:O	2:1:146:ASN:HB2	2.10	0.51
2:1:40:GLU:HB3	5:4:64:THR:HB	1.93	0.51
4:3:167:VAL:O	4:3:169:PRO:HD3	2.12	0.50
3:2:177:ASP:HB2	4:3:65:MET:HE3	1.92	0.50
2:1:230:TYR:OH	3:2:131:CYS:HA	2.11	0.49
4:3:87:LEU:HD11	4:3:114:LEU:HD12	1.94	0.49
3:2:135:ASP:HB3	3:2:163:ASP:HB3	1.95	0.49
2:1:148:GLY:O	2:1:149:HIS:ND1	2.47	0.48
2:1:70:ARG:NH2	4:3:219:ASP:O	2.47	0.48
3:2:27:GLU:HB2	3:2:203:ASN:OD1	2.14	0.47
3:2:32:VAL:HG13	5:4:56:PRO:HB2	1.95	0.47
2:1:27:LEU:HD11	4:3:221:SER:HB3	1.96	0.47
2:1:150:ALA:HA	2:1:250:ASN:ND2	2.30	0.47
2:1:215:VAL:HG21	3:2:221:VAL:HG12	1.96	0.46
3:2:186:LEU:HD22	4:3:65:MET:CE	2.38	0.46
2:1:133:GLU:HB2	2:1:265:LYS:HE2	1.98	0.46
2:1:146:ASN:HD22	2:1:147:ASN:N	2.14	0.46
3:2:37:ARG:O	3:2:210:PRO:HG3	2.15	0.46
4:3:44:MET:HE3	4:3:47:ALA:HB3	1.97	0.46
2:1:205:TYR:CZ	6:1:500:J80:H22	2.51	0.46
2:1:130:PHE:HE1	2:1:132:MET:HE2	1.81	0.46
5:4:10:VAL:HG21	5:4:25:ILE:HD12	1.98	0.46
2:1:132:MET:HE3	2:1:262:MET:SD	2.56	0.46
2:1:97:PRO:HD3	2:1:249:HIS:CD2	2.51	0.45
3:2:201:THR:HG23	5:4:68:LEU:HD11	1.98	0.45
3:2:238:PHE:HB3	3:2:244:VAL:CG2	2.45	0.45
5:4:6:SER:HB2	5:4:27:TYR:CE1	2.52	0.44
3:2:266:THR:HG22	3:2:268:PRO:HD3	2.00	0.44
2:1:193:ARG:HG2	4:3:21:SER:HB3	2.00	0.43
2:1:48:GLU:HA	3:2:196:ILE:HB	2.01	0.43
3:2:134:GLY:HA2	3:2:173:PHE:HA	2.01	0.43
3:2:84:ASP:O	3:2:87:ARG:HG2	2.19	0.42
2:1:275:PRO:HG2	4:3:102:GLU:HG3	2.01	0.42
3:2:122:LEU:HB2	3:2:197:ILE:HB	2.01	0.42
2:1:107:MET:HE3	2:1:167:PRO:HD2	2.01	0.42
2:1:98:THR:N	2:1:102:GLN:HE22	2.17	0.42
3:2:137:ASP:N	3:2:162:LYS:HE2	2.34	0.42
4:3:64:THR:O	4:3:67:MET:HG2	2.20	0.41
2:1:173:TYR:O	2:1:176:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:194:TYR:CE1	4:3:198:ILE:HD13	2.54	0.41
2:1:146:ASN:HD22	2:1:147:ASN:H	1.69	0.40
2:1:54:PRO:HG3	5:4:55:GLU:OE2	2.22	0.40
2:1:274:PRO:HB3	3:2:188:ASN:HB2	2.04	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%)	1 (50%)	0	1 (50%)	0	0
2	1	277/300 (92%)	251 (91%)	24 (9%)	2 (1%)	18	47
3	2	264/271 (97%)	243 (92%)	15 (6%)	6 (2%)	5	18
4	3	233/235 (99%)	226 (97%)	7 (3%)	0	100	100
5	4	58/68 (85%)	48 (83%)	8 (14%)	2 (3%)	3	11
All	All	834/878 (95%)	769 (92%)	54 (6%)	11 (1%)	9	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	7	CYS
3	2	166	VAL
5	4	15	ASN
3	2	165	ALA
2	1	146	ASN
3	2	8	GLY
3	2	163	ASP
1	0	8	GLU
3	2	48	ASN
2	1	237	ASP

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Mol	Chain	Res	Type
5	4	11	GLY

5.3.2 Protein sidechains [i](#)

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	241/258 (93%)	229 (95%)	12 (5%)	22	54
3	2	224/229 (98%)	218 (97%)	6 (3%)	39	74
4	3	210/210 (100%)	204 (97%)	6 (3%)	37	73
5	4	53/56 (95%)	51 (96%)	2 (4%)	29	64
All	All	732/757 (97%)	705 (96%)	27 (4%)	30	65

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	8	GLU
2	1	24	GLN
2	1	83	ARG
2	1	96	GLN
2	1	100	ARG
2	1	115	THR
2	1	143	THR
2	1	146	ASN
2	1	193	ARG
2	1	218	LYS
2	1	222	ASN
2	1	252	THR
2	1	289	ASN
3	2	87	ARG
3	2	103	ARG
3	2	161	ASN
3	2	164	ASN
3	2	170	LYS

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Mol	Chain	Res	Type
3	2	240	GLN
4	3	44	MET
4	3	64	THR
4	3	149	MET
4	3	207	SER
4	3	218	ASN
4	3	224	LEU
5	4	15	ASN
5	4	62	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	102	GLN
2	1	144	ASN
2	1	146	ASN
2	1	152	ASN
2	1	180	ASN
2	1	203	ASN
2	1	249	HIS
2	1	250	ASN
3	2	94	GLN
3	2	95	ASN
3	2	119	GLN
3	2	139	GLN
3	2	260	ASN
3	2	271	GLN
4	3	6	ASN
4	3	80	GLN
4	3	97	HIS
4	3	230	HIS
5	4	13	HIS

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	0.45	0	12,13,15	0.77	0
6	J80	1	500	-	31,31,31	1.52	3 (9%)	38,40,40	2.46	10 (26%)

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	-	3/12/12/13	-
6	J80	1	500	-	-	6/19/29/29	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	J80	C20-C23	-5.04	1.38	1.50
6	1	500	J80	O25-C23	4.98	1.45	1.33
6	1	500	J80	O25-C26	-2.48	1.39	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	500	J80	C1-C2-N3	10.19	122.13	116.13
6	1	500	J80	C11-N6-C7	5.02	122.86	111.57
6	1	500	J80	O25-C26-C27	4.15	123.28	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	500	J80	C4-C5-N4	-3.99	117.99	123.84
6	1	500	J80	C5-N4-N3	3.37	122.36	118.97
6	1	500	J80	C1-C2-C3	-3.22	115.41	121.61
6	1	500	J80	C10-C11-N6	2.94	117.60	110.92
6	1	500	J80	C4-C5-N6	-2.86	116.79	121.73
6	1	500	J80	O25-C23-C20	2.42	116.21	112.15
6	1	500	J80	C4-C3-C2	-2.23	117.71	119.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

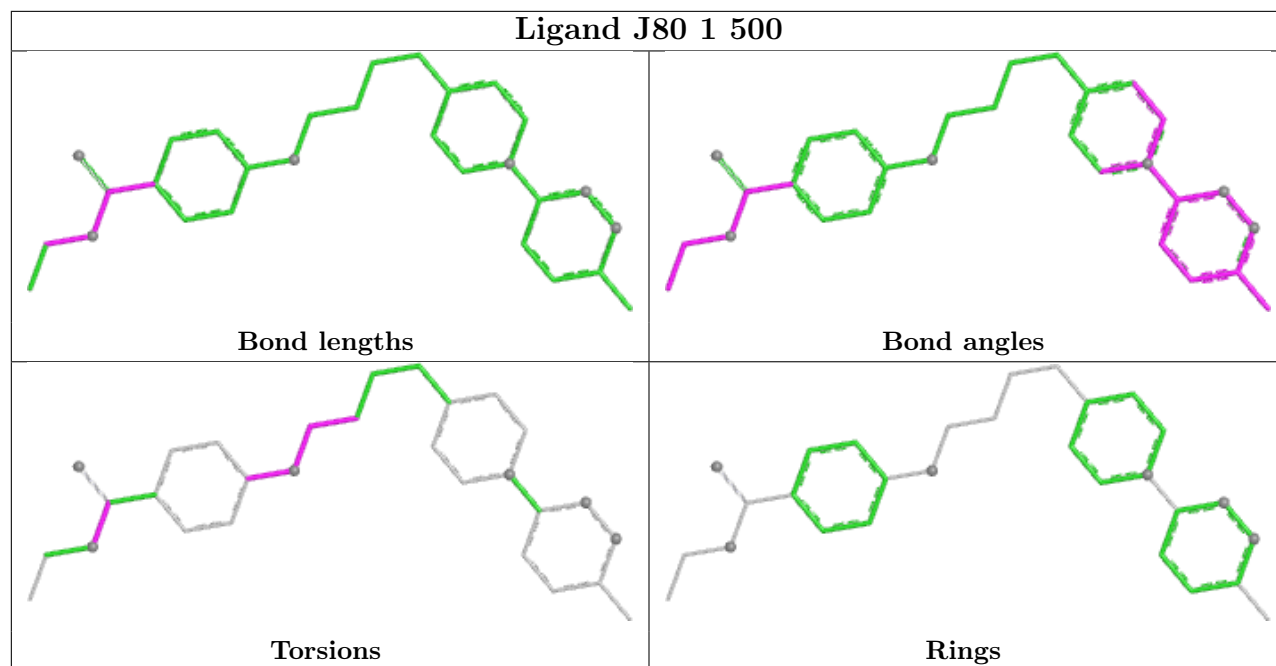
Mol	Chain	Res	Type	Atoms
7	4	1	MYR	O1-C1-C2-C3
6	1	500	J80	C20-C23-O25-C26
6	1	500	J80	O24-C23-O25-C26
6	1	500	J80	C22-C17-O16-C15
6	1	500	J80	C13-C14-C15-O16
6	1	500	J80	C18-C17-O16-C15
6	1	500	J80	C14-C15-O16-C17
7	4	1	MYR	C9-C10-C11-C12
7	4	1	MYR	C7-C8-C9-C10

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	500	J80	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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.