



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:32 AM UTC

PDB ID : 1VBA / pdb_00001vba
Title : POLIOVIRUS (TYPE 3, SABIN STRAIN) (P3/SABIN, P3/LEON/12A(1)B)
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 : 2.90 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)	:	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

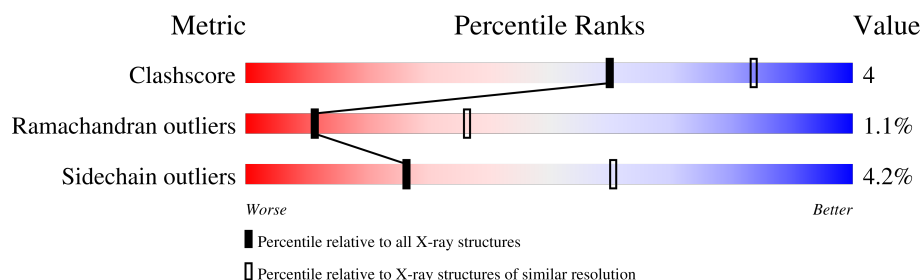
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)

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	66% 21% 6% 7%
3	2	271	66% 26% 5% ..
4	3	235	71% 26% .
5	4	68	57% 31% . 9%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6659 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			

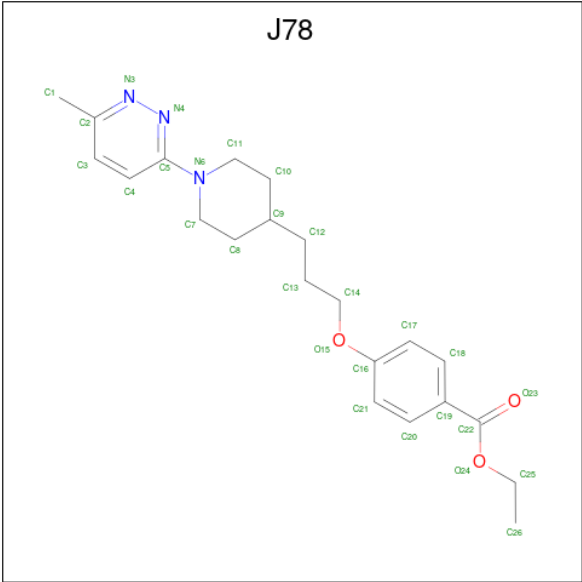
- Molecule 4 is a protein called POLIOVIRUS TYPE 3.

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.

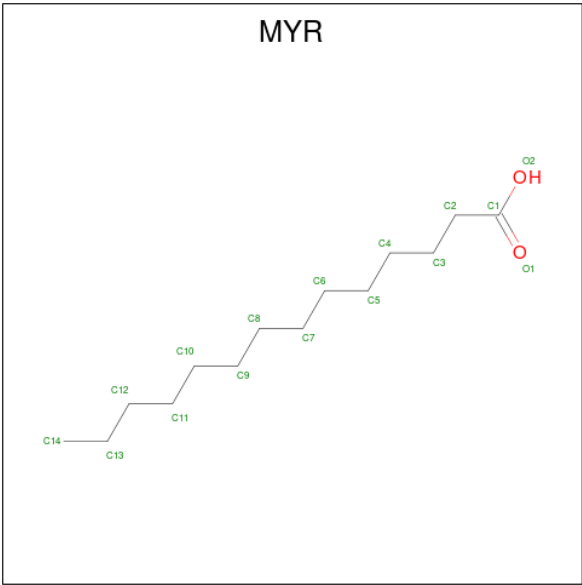
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	4	62	Total	C	N	O	0	0	0
			472	291	79	102			

- Molecule 6 is (METHYLPYRIDAZINE PIPERIDINE PROPYLOXYPHENYL)ETHYLAC ETATE (CCD ID: J78) (formula: C₂₂H₂₉N₃O₃).



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.

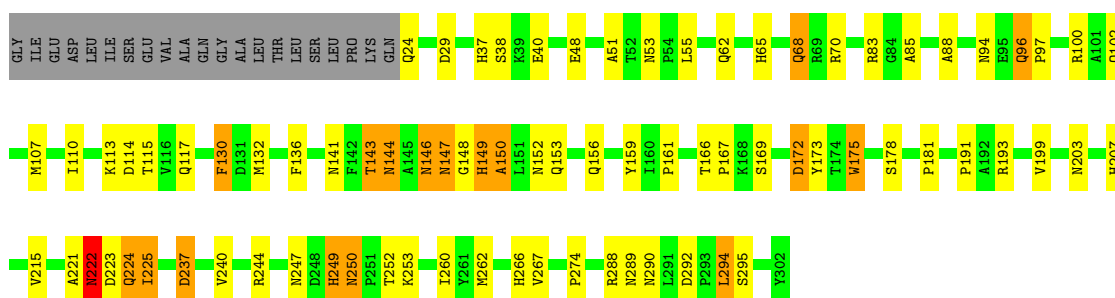
- Molecule 1: POLIOVIRUS TYPE 3

Chain 0:  100%

There are no outlier residues recorded for this chain.

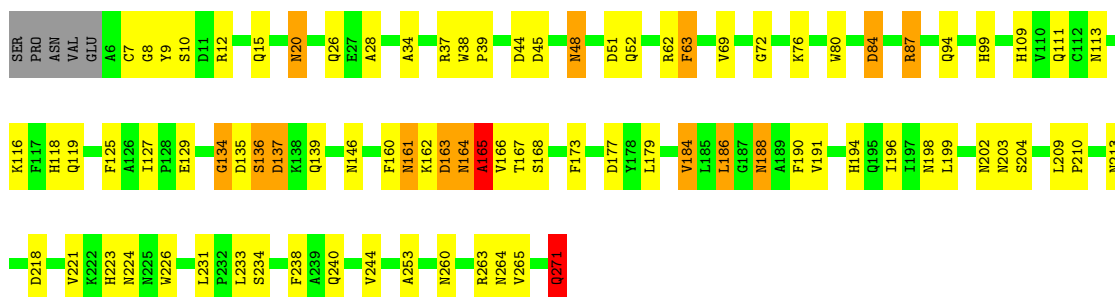
- Molecule 2: POLIOVirus TYPE 3

Chain 1:  66% 21% 6% 7%



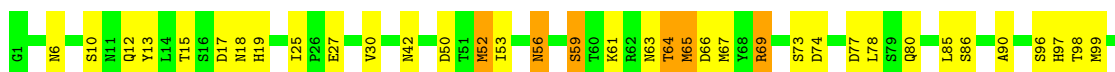
- Molecule 3: POLIOVirus TYPE 3

Chain 2:  66% 26% 5% ..



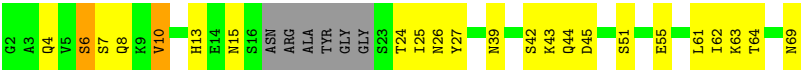
- Molecule 4: POLIOVirus TYPE 3

Chain 3:  71% 26% .





● 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) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.297 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6659	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, J78

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	0.79	0/29	1.83	0/38
2	1	0.95	8/2278 (0.4%)	1.83	61/3111 (2.0%)
3	2	0.93	6/2146 (0.3%)	1.95	77/2926 (2.6%)
4	3	0.95	6/1857 (0.3%)	1.80	55/2533 (2.2%)
5	4	0.97	1/479 (0.2%)	2.06	24/647 (3.7%)
All	All	0.95	21/6789 (0.3%)	1.88	217/9255 (2.3%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	97	HIS	CD2-NE2	-7.61	1.29	1.37
3	2	223	HIS	CD2-NE2	-7.55	1.29	1.37
2	1	65	HIS	CD2-NE2	-7.12	1.30	1.37
3	2	99	HIS	CD2-NE2	-6.88	1.30	1.37
4	3	19	HIS	CD2-NE2	-6.71	1.30	1.37
2	1	207	HIS	CD2-NE2	-6.55	1.30	1.37
2	1	149	HIS	CD2-NE2	-6.44	1.30	1.37
2	1	266	HIS	CD2-NE2	-6.37	1.30	1.37
4	3	153	HIS	CD2-NE2	-6.37	1.30	1.37
4	3	109	HIS	CD2-NE2	-6.35	1.30	1.37
5	4	13	HIS	CD2-NE2	-6.18	1.31	1.37
3	2	118	HIS	CD2-NE2	-6.16	1.31	1.37
2	1	37	HIS	CD2-NE2	-6.13	1.31	1.37
2	1	249	HIS	CD2-NE2	-6.11	1.31	1.37
4	3	230	HIS	CD2-NE2	-5.99	1.31	1.37
3	2	223	HIS	CG-ND1	-5.94	1.31	1.38
3	2	194	HIS	CD2-NE2	-5.83	1.31	1.37
2	1	266	HIS	CG-ND1	-5.05	1.32	1.38
2	1	161	PRO	CA-CB	-5.02	1.49	1.54
3	2	109	HIS	CD2-NE2	-5.01	1.32	1.37
4	3	153	HIS	CG-ND1	-5.01	1.32	1.38

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	240	GLN	OE1-CD-NE2	-11.61	110.99	122.60
3	2	203	ASN	CA-CB-CG	11.29	123.89	112.60
2	1	250	ASN	OD1-CG-ND2	-10.60	112.00	122.60
2	1	222	ASN	OD1-CG-ND2	-10.17	112.43	122.60
2	1	117	GLN	OE1-CD-NE2	-10.09	112.51	122.60
5	4	44	GLN	OE1-CD-NE2	-10.08	112.52	122.60
3	2	136	SER	N-CA-C	9.89	125.47	109.85
3	2	164	ASN	N-CA-C	9.51	122.65	111.71
3	2	203	ASN	OD1-CG-ND2	-9.44	113.16	122.60
2	1	223	ASP	CA-CB-CG	9.16	121.76	112.60
5	4	4	GLN	OE1-CD-NE2	-9.15	113.45	122.60
2	1	146	ASN	OD1-CG-ND2	-9.07	113.53	122.60
2	1	172	ASP	CA-CB-CG	9.05	121.65	112.60
4	3	218	ASN	OD1-CG-ND2	-9.02	113.58	122.60
3	2	203	ASN	CB-CG-ND2	8.92	129.78	116.40
3	2	271	GLN	OE1-CD-NE2	-8.85	113.75	122.60
4	3	140	GLN	OE1-CD-NE2	-8.64	113.96	122.60
5	4	69	ASN	OD1-CG-ND2	-8.60	114.00	122.60
4	3	233	GLN	OE1-CD-NE2	-8.58	114.02	122.60
2	1	94	ASN	OD1-CG-ND2	-8.56	114.04	122.60
2	1	224	GLN	OE1-CD-NE2	-8.46	114.14	122.60
3	2	177	ASP	CA-CB-CG	8.46	121.06	112.60
3	2	161	ASN	OD1-CG-ND2	-8.37	114.23	122.60
2	1	153	GLN	OE1-CD-NE2	-8.33	114.27	122.60
3	2	26	GLN	OE1-CD-NE2	-8.22	114.38	122.60
3	2	218	ASP	CA-CB-CG	8.14	120.74	112.60
2	1	144	ASN	OD1-CG-ND2	-8.06	114.54	122.60
2	1	146	ASN	N-CA-C	8.04	127.93	110.80
2	1	152	ASN	OD1-CG-ND2	-8.03	114.57	122.60
2	1	203	ASN	OD1-CG-ND2	-8.02	114.58	122.60
5	4	8	GLN	OE1-CD-NE2	-8.02	114.58	122.60
4	3	133	ALA	N-CA-C	7.84	121.08	109.24
3	2	213	ASN	OD1-CG-ND2	-7.83	114.77	122.60
3	2	164	ASN	CA-CB-CG	-7.75	104.86	112.60
3	2	135	ASP	CA-CB-CG	7.69	120.29	112.60
2	1	247	ASN	OD1-CG-ND2	-7.68	114.92	122.60
3	2	48	ASN	OD1-CG-ND2	-7.64	114.96	122.60
4	3	173	ASN	OD1-CG-ND2	-7.62	114.98	122.60
4	3	30	VAL	N-CA-C	7.61	118.81	109.30
3	2	202	ASN	N-CA-C	7.57	120.87	108.99
2	1	117	GLN	N-CA-C	7.44	119.08	110.97
2	1	199	VAL	N-CA-C	7.43	119.23	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	53	ILE	N-CA-C	7.36	114.96	108.63
3	2	139	GLN	OE1-CD-NE2	-7.34	115.26	122.60
3	2	202	ASN	OD1-CG-ND2	-7.27	115.33	122.60
3	2	94	GLN	OE1-CD-NE2	-7.18	115.42	122.60
3	2	20	ASN	OD1-CG-ND2	-7.10	115.50	122.60
3	2	265	VAL	N-CA-C	7.06	118.12	109.30
3	2	224	ASN	OD1-CG-ND2	-7.05	115.55	122.60
3	2	240	GLN	CG-CD-NE2	7.01	126.92	116.40
2	1	222	ASN	CB-CG-ND2	6.99	126.89	116.40
4	3	105	ASN	OD1-CG-ND2	-6.99	115.61	122.60
3	2	188	ASN	OD1-CG-ND2	-6.98	115.62	122.60
3	2	127	ILE	N-CA-C	6.95	115.65	107.73
5	4	15	ASN	OD1-CG-ND2	-6.94	115.66	122.60
3	2	20	ASN	CB-CG-ND2	6.93	126.80	116.40
4	3	74	ASP	CA-CB-CG	6.91	119.51	112.60
2	1	289	ASN	OD1-CG-ND2	-6.91	115.69	122.60
2	1	267	VAL	N-CA-C	6.89	118.58	109.21
2	1	294	LEU	N-CA-C	6.84	120.82	109.46
2	1	62	GLN	OE1-CD-NE2	-6.83	115.77	122.60
3	2	52	GLN	OE1-CD-NE2	-6.82	115.78	122.60
5	4	63	LYS	N-CA-C	6.81	121.20	112.34
4	3	96	SER	N-CA-C	6.81	120.46	111.75
4	3	178	GLN	OE1-CD-NE2	-6.77	115.83	122.60
5	4	10	VAL	N-CA-C	6.72	117.12	108.12
3	2	271	GLN	CG-CD-NE2	6.71	126.46	116.40
2	1	156	GLN	OE1-CD-NE2	-6.68	115.92	122.60
4	3	195	GLN	OE1-CD-NE2	-6.68	115.92	122.60
3	2	135	ASP	N-CA-C	6.68	125.02	110.80
5	4	43	LYS	N-CA-C	6.66	120.72	112.47
2	1	178	SER	N-CA-C	6.65	119.36	111.71
4	3	80	GLN	OE1-CD-NE2	-6.64	115.96	122.60
5	4	39	ASN	OD1-CG-ND2	-6.63	115.97	122.60
3	2	113	ASN	OD1-CG-ND2	-6.60	116.00	122.60
3	2	72	GLY	O-C-N	-6.59	118.87	123.95
4	3	181	GLN	OE1-CD-NE2	-6.58	116.02	122.60
2	1	289	ASN	CA-CB-CG	-6.56	106.04	112.60
2	1	249	HIS	N-CA-C	6.55	119.86	110.10
4	3	218	ASN	CB-CG-ND2	6.55	126.22	116.40
5	4	13	HIS	CB-CG-CD2	-6.53	122.71	131.20
3	2	119	GLN	OE1-CD-NE2	-6.49	116.11	122.60
2	1	260	ILE	N-CA-C	6.49	117.46	107.99
2	1	113	LYS	N-CA-C	6.48	121.33	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	18	ASN	OD1-CG-ND2	-6.47	116.13	122.60
4	3	17	ASP	CA-CB-CG	6.46	119.06	112.60
2	1	289	ASN	N-CA-C	6.45	117.95	108.86
2	1	141	ASN	OD1-CG-ND2	-6.39	116.21	122.60
3	2	264	ASN	OD1-CG-ND2	-6.38	116.22	122.60
4	3	233	GLN	CG-CD-NE2	6.36	125.94	116.40
2	1	24	GLN	OE1-CD-NE2	-6.31	116.29	122.60
4	3	56	ASN	OD1-CG-ND2	-6.29	116.31	122.60
2	1	38	SER	N-CA-C	6.26	118.29	108.96
3	2	184	VAL	O-C-N	-6.23	116.43	122.97
5	4	4	GLN	CG-CD-NE2	6.22	125.74	116.40
2	1	290	ASN	OD1-CG-ND2	-6.21	116.39	122.60
5	4	26	ASN	N-CA-C	6.17	119.71	110.14
4	3	180	THR	N-CA-CB	6.17	119.26	110.44
4	3	12	GLN	OE1-CD-NE2	-6.15	116.45	122.60
3	2	263	ARG	O-C-N	-6.14	118.50	123.11
3	2	15	GLN	OE1-CD-NE2	-6.11	116.49	122.60
2	1	152	ASN	N-CA-C	6.04	119.12	110.24
5	4	44	GLN	CG-CD-NE2	6.02	125.43	116.40
4	3	162	SER	N-CA-C	6.00	119.87	112.54
3	2	204	SER	N-CA-C	5.99	117.96	108.79
4	3	27	GLU	N-CA-C	5.99	119.90	112.47
3	2	198	ASN	OD1-CG-ND2	-5.97	116.62	122.60
3	2	146	ASN	OD1-CG-ND2	-5.97	116.63	122.60
3	2	165	ALA	N-CA-C	5.96	123.48	110.80
4	3	42	ASN	OD1-CG-ND2	-5.94	116.66	122.60
3	2	134	GLY	N-CA-C	5.93	121.91	112.06
5	4	51	SER	N-CA-C	5.91	121.12	111.37
3	2	260	ASN	OD1-CG-ND2	-5.90	116.70	122.60
3	2	177	ASP	N-CA-C	5.89	118.21	111.02
3	2	111	GLN	OE1-CD-NE2	-5.89	116.71	122.60
3	2	37	ARG	N-CA-C	5.88	118.10	108.52
2	1	102	GLN	OE1-CD-NE2	-5.88	116.72	122.60
4	3	140	GLN	CG-CD-NE2	5.86	125.19	116.40
5	4	45	ASP	N-CA-C	5.84	119.00	109.59
2	1	88	ALA	N-CA-C	5.84	118.00	108.55
5	4	24	THR	N-CA-C	5.82	118.21	108.96
3	2	63	PHE	N-CA-C	5.81	117.68	108.67
5	4	55	GLU	N-CA-C	5.80	117.94	109.30
2	1	29	ASP	CA-CB-CG	5.79	118.39	112.60
2	1	149	HIS	N-CA-C	5.79	115.92	108.34
5	4	26	ASN	OD1-CG-ND2	-5.79	116.81	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	153	HIS	CB-CG-CD2	-5.78	123.69	131.20
3	2	84	ASP	N-CA-C	5.74	120.84	111.37
2	1	147	ASN	CA-CB-CG	5.73	118.33	112.60
4	3	183	SER	N-CA-C	5.72	118.25	111.33
5	4	39	ASN	N-CA-C	5.70	118.54	110.50
4	3	64	THR	O-C-N	-5.69	116.76	123.25
4	3	64	THR	CA-CB-OG1	-5.68	101.08	109.60
4	3	218	ASN	N-CA-C	5.65	122.83	110.80
2	1	55	LEU	N-CA-C	5.63	118.82	110.48
4	3	217	CYS	O-C-N	-5.63	116.37	122.79
3	2	28	ALA	N-CA-C	5.63	117.79	110.53
3	2	163	ASP	CA-CB-CG	5.62	118.22	112.60
2	1	51	ALA	N-CA-C	5.61	119.20	110.17
3	2	87	ARG	N-CA-C	5.61	118.93	111.75
4	3	15	THR	CA-CB-OG1	-5.60	101.20	109.60
2	1	53	ASN	OD1-CG-ND2	-5.59	117.01	122.60
2	1	224	GLN	CG-CD-NE2	5.59	124.79	116.40
2	1	94	ASN	CB-CG-ND2	5.57	124.76	116.40
4	3	186	GLU	N-CA-C	5.57	118.35	110.50
3	2	137	ASP	CA-C-O	5.56	126.38	120.10
4	3	78	LEU	N-CA-C	5.56	118.11	111.71
3	2	203	ASN	CB-CA-C	-5.54	98.73	110.31
5	4	42	SER	N-CA-C	5.54	118.08	111.71
4	3	19	HIS	CB-CG-CD2	-5.52	124.03	131.20
2	1	117	GLN	CG-CD-NE2	5.51	124.67	116.40
2	1	65	HIS	CB-CG-CD2	-5.51	124.03	131.20
5	4	69	ASN	CB-CG-ND2	5.51	124.66	116.40
3	2	113	ASN	CB-CG-ND2	5.50	124.65	116.40
5	4	13	HIS	CB-CG-ND1	5.49	130.93	122.70
3	2	160	PHE	N-CA-C	5.45	117.61	108.23
4	3	77	ASP	CA-CB-CG	5.45	118.05	112.60
3	2	109	HIS	CB-CG-CD2	-5.45	124.12	131.20
4	3	180	THR	CB-CA-C	-5.44	99.14	110.40
4	3	25	ILE	CA-C-N	5.43	125.37	119.78
4	3	25	ILE	C-N-CA	5.43	125.37	119.78
2	1	289	ASN	CB-CG-ND2	5.41	124.52	116.40
3	2	125	PHE	N-CA-C	5.40	117.70	108.90
3	2	69	VAL	O-C-N	-5.38	117.66	123.14
5	4	7	SER	N-CA-C	5.38	118.99	109.96
4	3	69	ARG	N-CA-C	5.37	117.28	108.52
2	1	68	GLN	N-CA-C	5.34	117.96	109.96
2	1	68	GLN	OE1-CD-NE2	-5.33	117.27	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	129	GLU	N-CA-C	5.33	118.55	111.30
3	2	194	HIS	CB-CG-CD2	-5.33	124.27	131.20
4	3	161	GLN	OE1-CD-NE2	-5.33	117.27	122.60
2	1	173	TYR	N-CA-C	5.33	117.84	111.71
2	1	292	ASP	CA-CB-CG	5.32	117.92	112.60
4	3	98	THR	O-C-N	-5.32	116.73	122.79
3	2	223	HIS	N-CA-C	5.31	118.09	108.69
4	3	10	SER	N-CA-C	5.28	118.00	110.24
2	1	152	ASN	CB-CG-ND2	5.28	124.31	116.40
4	3	212	GLY	O-C-N	-5.26	118.51	123.25
4	3	109	HIS	CB-CG-CD2	-5.26	124.36	131.20
4	3	86	SER	N-CA-C	5.25	118.77	109.96
3	2	10	SER	N-CA-C	5.25	117.22	108.99
3	2	51	ASP	CA-CB-CG	5.24	117.84	112.60
3	2	223	HIS	CA-CB-CG	5.22	119.03	113.80
2	1	85	ALA	N-CA-C	5.22	118.00	109.59
3	2	163	ASP	CA-C-O	5.20	127.94	120.51
4	3	17	ASP	N-CA-C	5.19	118.12	110.59
2	1	136	PHE	N-CA-C	5.17	117.15	107.99
4	3	59	SER	N-CA-C	5.17	121.80	110.80
4	3	19	HIS	N-CA-C	5.16	117.52	109.52
2	1	114	ASP	CA-C-O	5.16	125.32	119.18
3	2	118	HIS	CB-CG-CD2	-5.16	124.49	131.20
2	1	250	ASN	CB-CG-ND2	5.15	124.12	116.40
3	2	226	TRP	CE2-CD2-CG	-5.14	101.03	107.20
4	3	6	ASN	OD1-CG-ND2	-5.14	117.46	122.60
4	3	150	LEU	N-CA-C	5.11	119.14	113.01
4	3	63	ASN	OD1-CG-ND2	-5.11	117.49	122.60
5	4	61	LEU	N-CA-C	5.11	117.81	109.59
2	1	161	PRO	O-C-N	-5.09	118.76	121.15
2	1	150	ALA	N-CA-C	5.08	117.35	108.76
2	1	247	ASN	CB-CG-ND2	5.08	124.02	116.40
3	2	48	ASN	CB-CG-ND2	5.08	124.02	116.40
3	2	199	LEU	N-CA-C	5.08	118.25	111.75
2	1	130	PHE	N-CA-C	5.08	116.56	108.79
2	1	295	SER	N-CA-C	5.07	117.22	110.53
3	2	45	ASP	CA-CB-CG	5.06	117.66	112.60
4	3	110	TRP	CE2-CD2-CG	-5.05	101.14	107.20
4	3	219	ASP	CA-CB-CG	5.05	117.65	112.60
3	2	209	LEU	CA-C-N	5.04	125.02	120.03
3	2	209	LEU	C-N-CA	5.04	125.02	120.03
3	2	9	TYR	N-CA-C	5.03	117.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	44	ASP	N-CA-C	5.02	118.17	111.75
4	3	50	ASP	CA-CB-CG	5.02	117.62	112.60
2	1	175	TRP	CE2-CD2-CG	-5.01	101.18	107.20
3	2	80	TRP	CE2-CD2-CG	-5.01	101.19	107.20
3	2	234	SER	CA-C-N	5.01	124.94	119.78
3	2	234	SER	C-N-CA	5.01	124.94	119.78
3	2	139	GLN	N-CA-C	5.00	118.11	110.20

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	30	0
3	2	2088	0	2005	25	0
4	3	1812	0	1792	14	0
5	4	472	0	453	3	0
6	1	28	0	29	4	0
7	4	15	0	27	0	0
All	All	6659	0	6486	56	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 (56) 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:HD13	6:1:500:J78:H101	1.67	0.77
3:2:116:LYS:HD2	4:3:124:MET:SD	2.28	0.72
2:1:40:GLU:HB3	5:4:64:THR:HB	1.73	0.70
3:2:238:PHE:HB3	3:2:244:VAL:HG21	1.75	0.68
2:1:143:THR:HG21	2:1:253:LYS:HD3	1.79	0.64
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:132:MET:SD	2:1:262:MET:HG2	2.39	0.63
3:2:233:LEU:HD22	4:3:52:MET:HE1	1.81	0.62
2:1:288:ARG:HE	3:2:162:LYS:HZ2	1.48	0.62
2:1:181:PRO:HB2	6:1:500:J78:H3	1.82	0.61
3:2:271:GLN:NE2	3:2:271:GLN:HA	2.18	0.57
2:1:222:ASN:HD22	2:1:224:GLN:HB2	1.70	0.56
3:2:191:VAL:HG11	4:3:99:MET:HE3	1.86	0.56
2:1:169:SER:HB3	2:1:172:ASP:HB3	1.87	0.56
2:1:147:ASN:HB2	2:1:252:THR:HB	1.88	0.55
4:3:90:ALA:HB2	4:3:104:LEU:HB3	1.93	0.51
2:1:215:VAL:HG21	3:2:221:VAL:HG12	1.94	0.49
2:1:159:TYR:CZ	6:1:500:J78:H81	2.47	0.49
3:2:186:LEU:HD22	4:3:65:MET:HE1	1.93	0.49
2:1:107:MET:HE1	2:1:166:THR:HB	1.93	0.48
3:2:34:ALA:HB3	3:2:210:PRO:HD2	1.96	0.48
3:2:179:LEU:HA	3:2:184:VAL:O	2.14	0.48
2:1:150:ALA:HA	2:1:250:ASN:ND2	2.29	0.48
2:1:288:ARG:NE	3:2:162:LYS:HZ2	2.11	0.48
3:2:84:ASP:O	3:2:87:ARG:HG2	2.13	0.48
4:3:156:TRP:CD1	4:3:164:CYS:HB2	2.48	0.48
5:4:10:VAL:HG21	5:4:25:ILE:HD12	1.97	0.47
3:2:186:LEU:HD13	3:2:231:LEU:HD22	1.96	0.47
4:3:167:VAL:O	4:3:169:PRO:HD3	2.15	0.46
2:1:110:ILE:HG21	6:1:500:J78:H131	1.98	0.46
2:1:222:ASN:ND2	2:1:225:ILE:HG12	2.30	0.46
2:1:294:LEU:HD13	4:3:67:MET:SD	2.55	0.46
2:1:288:ARG:NE	3:2:162:LYS:NZ	2.64	0.46
3:2:38:TRP:CD1	3:2:39:PRO:HD2	2.51	0.45
3:2:190:PHE:CE2	4:3:52:MET:HE3	2.52	0.44
3:2:63:PHE:CD1	3:2:253:ALA:HB2	2.52	0.44
3:2:134:GLY:HA2	3:2:173:PHE:HA	1.99	0.44
2:1:148:GLY:O	2:1:149:HIS:ND1	2.51	0.43
5:4:6:SER:HB2	5:4:27:TYR:CE1	2.54	0.43
4:3:66:ASP:HA	4:3:69:ARG:HD2	2.01	0.43
2:1:96:GLN:HG3	2:1:249:HIS:CE1	2.54	0.43
3:2:238:PHE:HB3	3:2:244:VAL:CG2	2.46	0.43
2:1:274:PRO:HB3	3:2:188:ASN:HB2	2.00	0.43
3:2:186:LEU:HD22	4:3:65:MET:CE	2.49	0.42
3:2:20:ASN:OD1	3:2:62:ARG:NH1	2.51	0.42
3:2:165:ALA:O	3:2:167:THR:N	2.53	0.42
2:1:96:GLN:HA	2:1:97:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:107:MET:HE3	2:1:167:PRO:HD2	2.03	0.41
4:3:56:ASN:ND2	4:3:61:LYS:HG3	2.36	0.41
2:1:143:THR:HG22	2:1:144:ASN:CG	2.46	0.41
3:2:186:LEU:HD13	4:3:65:MET:HE1	2.03	0.41
2:1:48:GLU:HA	3:2:196:ILE:HB	2.03	0.40
2:1:68:GLN:HE22	2:1:70:ARG:NH1	2.18	0.40
2:1:107:MET:HE2	2:1:240:VAL:HG21	2.03	0.40
2:1:130:PHE:HE1	2:1:132:MET:HE2	1.85	0.40
2:1:175:TRP:CZ3	2:1:244:ARG:HG2	2.57	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%)	261 (94%)	14 (5%)	2 (1%)	18	48
3	2	264/271 (97%)	243 (92%)	15 (6%)	6 (2%)	5	19
4	3	233/235 (99%)	221 (95%)	11 (5%)	1 (0%)	30	59
5	4	58/68 (85%)	53 (91%)	5 (9%)	0	100	100
All	All	834/878 (95%)	780 (94%)	45 (5%)	9 (1%)	11	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	165	ALA
3	2	166	VAL
2	1	237	ASP
3	2	7	CYS
3	2	8	GLY

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Mol	Chain	Res	Type
3	2	48	ASN
3	2	163	ASP
2	1	221	ALA
4	3	59	SER

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%)	231 (96%)	10 (4%)	27	61
3	2	224/229 (98%)	215 (96%)	9 (4%)	28	62
4	3	210/210 (100%)	200 (95%)	10 (5%)	23	55
5	4	53/56 (95%)	51 (96%)	2 (4%)	29	64
All	All	732/757 (97%)	701 (96%)	31 (4%)	26	60

All (31) 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	115	THR
2	1	143	THR
2	1	146	ASN
2	1	193	ARG
2	1	222	ASN
2	1	225	ILE
2	1	237	ASP
3	2	12	ARG
3	2	76	LYS
3	2	136	SER
3	2	137	ASP
3	2	161	ASN

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Mol	Chain	Res	Type
3	2	164	ASN
3	2	168	SER
3	2	186	LEU
3	2	271	GLN
4	3	52	MET
4	3	64	THR
4	3	65	MET
4	3	73	SER
4	3	85	LEU
4	3	149	MET
4	3	206	LYS
4	3	207	SER
4	3	218	ASN
4	3	224	LEU
5	4	6	SER
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	102	GLN
2	1	117	GLN
2	1	146	ASN
2	1	147	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	260	ASN
3	2	271	GLN
4	3	56	ASN
4	3	218	ASN
5	4	13	HIS
5	4	26	ASN
5	4	44	GLN
5	4	69	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	J78	1	500	-	30,30,30	1.48	3 (10%)	37,39,39	2.18	7 (18%)
7	MYR	4	1	5	13,14,15	0.25	0	12,13,15	0.84	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	-	-	5/18/28/28	0/3/3/3
7	MYR	4	1	5	-	3/12/12/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	500	J78	O24-C22	5.21	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	500	J78	C19-C22	-4.54	1.39	1.50
6	1	500	J78	O24-C25	-2.32	1.39	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	500	J78	C1-C2-N3	6.82	120.15	116.13
6	1	500	J78	O24-C25-C26	5.07	126.58	108.40
6	1	500	J78	C11-N6-C7	4.84	122.46	111.57
6	1	500	J78	O24-C22-C19	4.02	118.89	112.15
6	1	500	J78	C4-C5-N4	-3.84	118.22	123.84
6	1	500	J78	C5-N4-N3	3.73	122.73	118.97
6	1	500	J78	C7-C8-C9	2.04	116.95	111.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	4	1	MYR	O1-C1-C2-C3
6	1	500	J78	C26-C25-O24-C22
6	1	500	J78	C17-C16-O15-C14
6	1	500	J78	C21-C16-O15-C14
7	4	1	MYR	C11-C10-C9-C8
6	1	500	J78	O23-C22-O24-C25
6	1	500	J78	C13-C14-O15-C16
7	4	1	MYR	C5-C6-C7-C8

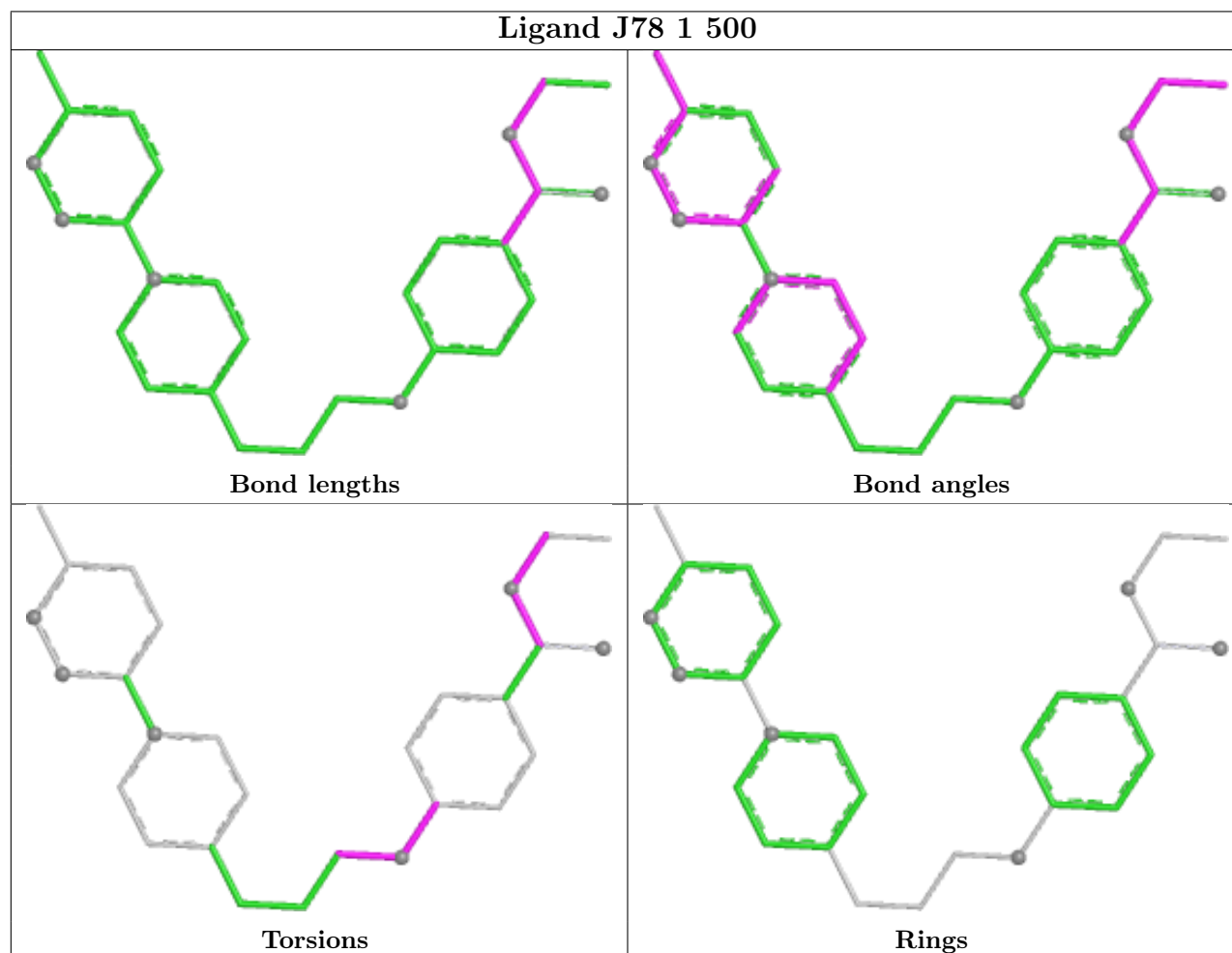
There are no ring outliers.

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.