



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:11 AM UTC

PDB ID : 1AR8 / pdb_00001ar8
Title : P1/MAHONEY POLIOVIRUS, MUTANT P1095S
Authors : Wien, M.W.; Curry, S.; Filman, D.J.; Hogle, J.M.
Deposited on : 1997-08-11
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

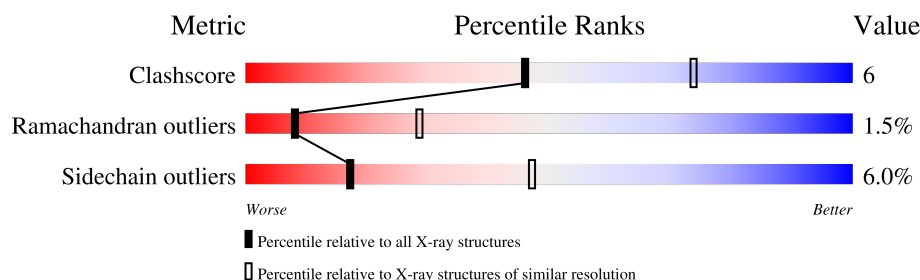
1 Overall quality at a glance

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	8	75% 25%
2	1	302	68% 22% 6%
3	2	272	68% 24% 6%
4	3	238	75% 21% 6%
5	4	68	54% 26% 6% 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7184 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 P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	0	8	Total	C	N	O	0	0	0
			43	24	8	11			

- Molecule 2 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	283	Total	C	N	O	S	0	0	0
			2221	1414	378	424	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	95	SER	PRO	engineered mutation	UNP P03300

- Molecule 3 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	268	Total	C	N	O	S	0	0	0
			2085	1317	358	396	14			

- Molecule 4 is a protein called P1/MAHONEY POLIOVIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	235	Total	C	N	O	S	0	0	0
			1834	1169	299	349	17			

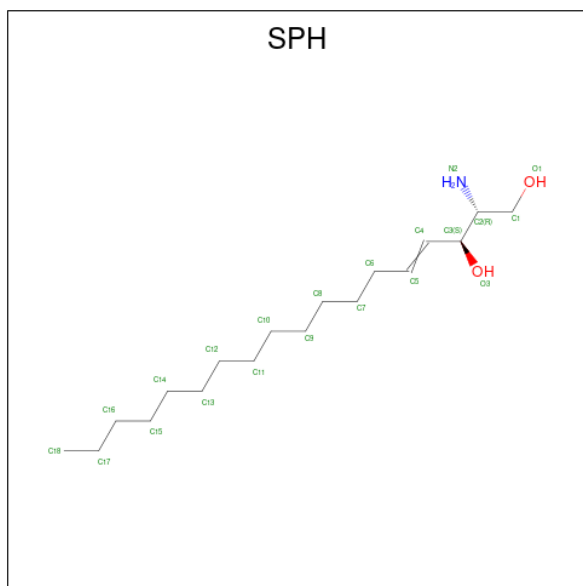
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is a protein called P1/MAHONEY POLIOVIRUS.

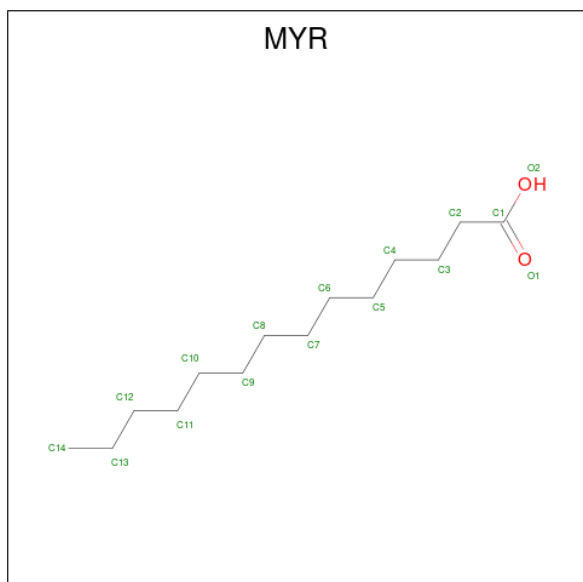
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	60	Total	C	N	O	S	0	0	0
			462	286	78	97	1			

- Molecule 6 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	N	O	0	0
			21	18	1	2		

- 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		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	0	1	Total	O	0	0
			1	1		
8	1	184	Total	O	0	0
			184	184		
8	2	143	Total	O	0	0
			143	143		
8	3	135	Total	O	0	0
			135	135		
8	4	40	Total	O	0	0
			40	40		

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.

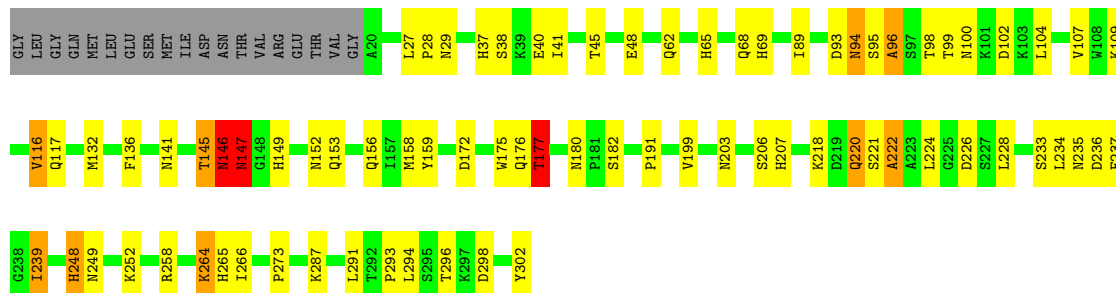
• Molecule 1: P1/MAHONEY POLIOVIRUS

Chain 0:  75% 25%



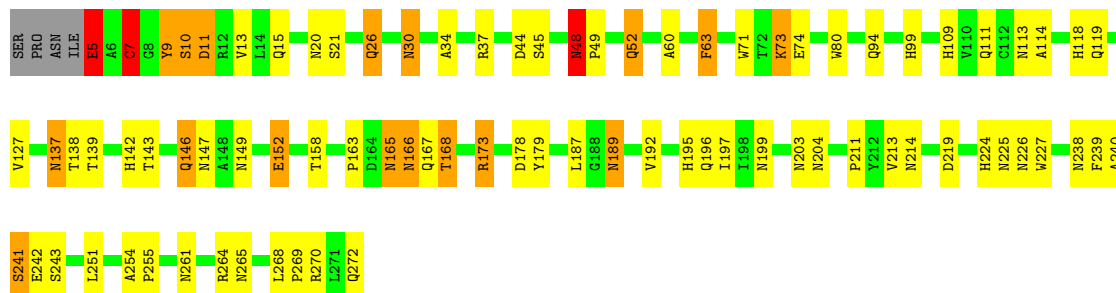
• Molecule 2: P1/MAHONEY POLIOVIRUS

Chain 1:  68% 22% •• 6%



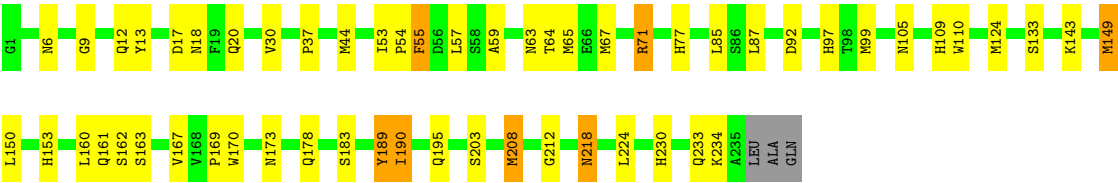
• Molecule 3: P1/MAHONEY POLIOVIRUS

Chain 2:  68% 24% 6% ••

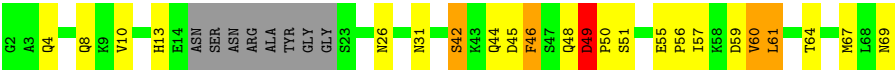


• Molecule 4: P1/MAHONEY POLIOVIRUS

Chain 3:  75% 21% ••



• Molecule 5: P1/MAHONEY POLIOVIRUS



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	323.04Å 358.22Å 380.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.00 – 2.90	Depositor
% Data completeness (in resolution range)	34.0 (11.00-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.270 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7184	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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, SPH

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	0.64	0/41	1.83	0/53
2	1	1.03	8/2283 (0.4%)	1.75	49/3120 (1.6%)
3	2	1.04	8/2142 (0.4%)	1.82	60/2928 (2.0%)
4	3	1.01	6/1881 (0.3%)	1.67	33/2562 (1.3%)
5	4	0.97	1/469 (0.2%)	1.95	15/632 (2.4%)
All	All	1.02	23/6816 (0.3%)	1.77	157/9295 (1.7%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	149	HIS	CD2-NE2	-8.52	1.28	1.37
2	1	207	HIS	CD2-NE2	-7.69	1.29	1.37
4	3	77	HIS	CD2-NE2	-7.67	1.29	1.37
4	3	97	HIS	CD2-NE2	-7.28	1.29	1.37
3	2	195	HIS	CD2-NE2	-7.12	1.30	1.37
3	2	118	HIS	CD2-NE2	-7.05	1.30	1.37
3	2	224	HIS	CD2-NE2	-7.04	1.30	1.37
4	3	230	HIS	CD2-NE2	-6.97	1.30	1.37
3	2	99	HIS	CD2-NE2	-6.54	1.30	1.37
2	1	265	HIS	CD2-NE2	-6.51	1.30	1.37
4	3	153	HIS	CD2-NE2	-6.45	1.30	1.37
3	2	109	HIS	CD2-NE2	-6.38	1.30	1.37
5	4	13	HIS	CD2-NE2	-6.32	1.30	1.37
2	1	69	HIS	CD2-NE2	-6.32	1.30	1.37
2	1	37	HIS	CD2-NE2	-6.15	1.31	1.37
4	3	109	HIS	CD2-NE2	-6.05	1.31	1.37
2	1	149	HIS	CE1-NE2	-6.02	1.26	1.32
4	3	77	HIS	CG-ND1	-5.95	1.31	1.38
2	1	65	HIS	CD2-NE2	-5.72	1.31	1.37
3	2	224	HIS	CG-ND1	-5.41	1.32	1.38
3	2	142	HIS	CD2-NE2	-5.30	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	195	HIS	CG-ND1	-5.13	1.32	1.38
2	1	265	HIS	CG-ND1	-5.07	1.32	1.38

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	147	ASN	OD1-CG-ND2	-13.39	109.21	122.60
4	3	6	ASN	OD1-CG-ND2	-11.34	111.26	122.60
2	1	149	HIS	CB-CG-CD2	-11.02	116.88	131.20
2	1	117	GLN	OE1-CD-NE2	-10.61	111.99	122.60
2	1	226	ASP	N-CA-C	10.25	124.95	110.50
2	1	249	ASN	OD1-CG-ND2	-10.03	112.57	122.60
4	3	218	ASN	OD1-CG-ND2	-9.63	112.97	122.60
5	4	10	VAL	N-CA-C	9.13	121.26	108.93
3	2	26	GLN	OE1-CD-NE2	-9.04	113.56	122.60
2	1	94	ASN	OD1-CG-ND2	-9.02	113.58	122.60
4	3	105	ASN	OD1-CG-ND2	-8.92	113.68	122.60
3	2	165	ASN	OD1-CG-ND2	-8.68	113.92	122.60
2	1	220	GLN	OE1-CD-NE2	-8.51	114.09	122.60
4	3	20	GLN	OE1-CD-NE2	-8.46	114.14	122.60
5	4	69	ASN	OD1-CG-ND2	-8.39	114.20	122.60
3	2	272	GLN	OE1-CD-NE2	-8.33	114.27	122.60
2	1	147	ASN	CB-CG-ND2	8.31	128.87	116.40
5	4	31	ASN	OD1-CG-ND2	-8.22	114.38	122.60
3	2	137	ASN	OD1-CG-ND2	-7.88	114.72	122.60
3	2	166	ASN	OD1-CG-ND2	-7.81	114.79	122.60
3	2	9	TYR	N-CA-C	7.75	121.21	110.35
4	3	173	ASN	OD1-CG-ND2	-7.73	114.87	122.60
2	1	149	HIS	CB-CG-ND1	7.66	134.19	122.70
2	1	298	ASP	N-CA-C	7.63	121.57	110.28
4	3	18	ASN	OD1-CG-ND2	-7.62	114.98	122.60
5	4	44	GLN	OE1-CD-NE2	-7.61	114.99	122.60
2	1	104	LEU	N-CA-C	7.61	120.47	108.67
4	3	17	ASP	CA-CB-CG	7.55	120.15	112.60
3	2	48	ASN	OD1-CG-ND2	-7.49	115.11	122.60
5	4	4	GLN	OE1-CD-NE2	-7.48	115.12	122.60
3	2	203	ASN	OD1-CG-ND2	-7.45	115.15	122.60
3	2	165	ASN	N-CA-C	7.40	123.44	113.97
3	2	165	ASN	CA-CB-CG	-7.37	105.23	112.60
5	4	48	GLN	OE1-CD-NE2	-7.21	115.39	122.60
3	2	15	GLN	OE1-CD-NE2	-7.14	115.46	122.60
3	2	146	GLN	OE1-CD-NE2	-7.13	115.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	94	GLN	OE1-CD-NE2	-7.04	115.56	122.60
2	1	149	HIS	ND1-CE1-NE2	6.90	115.30	108.40
4	3	53	ILE	N-CA-C	6.82	114.50	108.63
2	1	141	ASN	OD1-CG-ND2	-6.80	115.80	122.60
2	1	203	ASN	OD1-CG-ND2	-6.70	115.90	122.60
3	2	147	ASN	OD1-CG-ND2	-6.66	115.94	122.60
3	2	167	GLN	OE1-CD-NE2	-6.65	115.95	122.60
4	3	178	GLN	OE1-CD-NE2	-6.59	116.01	122.60
4	3	97	HIS	CB-CG-CD2	-6.53	122.71	131.20
4	3	59	ALA	N-CA-C	6.50	119.19	111.33
4	3	195	GLN	OE1-CD-NE2	-6.50	116.10	122.60
2	1	199	VAL	N-CA-C	6.50	118.40	112.29
5	4	42	SER	N-CA-C	6.48	119.16	111.71
2	1	156	GLN	OE1-CD-NE2	-6.47	116.13	122.60
2	1	117	GLN	N-CA-C	6.43	117.98	110.97
3	2	204	ASN	OD1-CG-ND2	-6.42	116.18	122.60
2	1	172	ASP	CA-CB-CG	6.41	119.01	112.60
3	2	52	GLN	OE1-CD-NE2	-6.41	116.19	122.60
3	2	219	ASP	CA-CB-CG	6.37	118.97	112.60
3	2	137	ASN	CB-CG-ND2	6.36	125.93	116.40
2	1	176	GLN	OE1-CD-NE2	-6.35	116.25	122.60
2	1	69	HIS	CB-CG-CD2	-6.34	122.96	131.20
3	2	265	ASN	OD1-CG-ND2	-6.33	116.27	122.60
3	2	119	GLN	OE1-CD-NE2	-6.30	116.30	122.60
3	2	269	PRO	N-CA-CB	6.29	109.19	103.34
5	4	46	PHE	CA-CB-CG	-6.26	107.54	113.80
2	1	266	ILE	N-CA-C	6.25	118.38	108.87
2	1	177	THR	CB-CA-C	-6.21	102.64	111.95
3	2	11	ASP	N-CA-C	6.20	119.69	111.75
5	4	45	ASP	N-CA-C	6.20	120.15	110.17
3	2	168	THR	CA-CB-OG1	-6.20	100.30	109.60
4	3	161	GLN	OE1-CD-NE2	-6.20	116.40	122.60
5	4	8	GLN	OE1-CD-NE2	-6.18	116.42	122.60
4	3	183	SER	N-CA-C	6.17	118.80	111.33
3	2	261	ASN	OD1-CG-ND2	-6.15	116.45	122.60
4	3	63	ASN	OD1-CG-ND2	-6.15	116.45	122.60
2	1	248	HIS	CB-CG-CD2	-6.11	123.25	131.20
4	3	162	SER	N-CA-C	6.10	118.73	111.71
3	2	113	ASN	OD1-CG-ND2	-6.08	116.53	122.60
3	2	189	ASN	OD1-CG-ND2	-6.08	116.53	122.60
3	2	149	ASN	OD1-CG-ND2	-6.06	116.54	122.60
3	2	178	ASP	N-CA-C	6.06	118.39	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	189	TYR	N-CA-C	6.05	118.26	108.34
5	4	13	HIS	CB-CG-CD2	-6.04	123.34	131.20
2	1	249	ASN	CB-CG-ND2	5.96	125.35	116.40
3	2	199	ASN	OD1-CG-ND2	-5.96	116.64	122.60
3	2	225	ASN	OD1-CG-ND2	-5.93	116.67	122.60
2	1	153	GLN	N-CA-C	5.90	119.53	110.20
2	1	152	ASN	OD1-CG-ND2	-5.90	116.70	122.60
5	4	26	ASN	OD1-CG-ND2	-5.90	116.70	122.60
2	1	62	GLN	OE1-CD-NE2	-5.88	116.72	122.60
4	3	153	HIS	CB-CG-CD2	-5.87	123.57	131.20
4	3	54	PRO	N-CA-CB	5.82	106.33	102.25
4	3	30	VAL	N-CA-C	5.82	116.57	109.30
2	1	29	ASN	OD1-CG-ND2	-5.79	116.81	122.60
2	1	146	ASN	N-CA-CB	-5.75	100.77	110.49
3	2	127	VAL	N-CA-C	5.75	114.28	107.73
3	2	63	PHE	N-CA-C	5.74	117.56	108.67
2	1	68	GLN	N-CA-C	5.72	118.00	109.25
3	2	44	ASP	N-CA-C	5.72	117.51	111.28
4	3	12	GLN	OE1-CD-NE2	-5.71	116.89	122.60
3	2	152	GLU	N-CA-C	5.69	118.25	111.71
3	2	118	HIS	CB-CG-CD2	-5.68	123.81	131.20
5	4	69	ASN	CB-CG-ND2	5.68	124.92	116.40
3	2	196	GLN	OE1-CD-NE2	-5.67	116.93	122.60
3	2	111	GLN	OE1-CD-NE2	-5.67	116.94	122.60
3	2	224	HIS	N-CA-C	5.66	118.32	108.76
2	1	248	HIS	CA-CB-CG	-5.65	108.15	113.80
4	3	203	SER	CA-C-O	5.65	125.82	119.78
2	1	94	ASN	CB-CG-ND2	5.63	124.85	116.40
4	3	218	ASN	CB-CG-ND2	5.63	124.84	116.40
4	3	133	SER	N-CA-C	5.62	118.72	109.72
3	2	178	ASP	CA-CB-CG	5.56	118.16	112.60
3	2	173	ARG	N-CA-C	5.56	118.13	109.52
2	1	248	HIS	N-CA-C	5.55	118.49	110.28
2	1	38	SER	N-CA-C	5.52	115.41	108.45
5	4	13	HIS	CA-CB-CG	-5.52	108.28	113.80
3	2	165	ASN	CB-CG-ND2	5.52	124.68	116.40
4	3	55	PHE	N-CA-C	5.51	118.00	111.33
2	1	222	ALA	N-CA-C	5.51	116.96	111.07
3	2	168	THR	CA-CB-CG2	5.47	119.79	110.50
3	2	142	HIS	CB-CG-CD2	-5.43	124.14	131.20
3	2	20	ASN	OD1-CG-ND2	-5.42	117.17	122.60
3	2	7	CYS	O-C-N	-5.42	115.38	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	175	TRP	CG-CD2-CE3	5.42	139.32	133.90
2	1	116	VAL	N-CA-C	5.37	118.33	112.96
4	3	97	HIS	CA-CB-CG	-5.33	108.47	113.80
3	2	163	PRO	N-CA-CB	5.31	108.04	103.36
3	2	71	TRP	CE2-CD2-CG	-5.31	100.83	107.20
3	2	214	ASN	OD1-CG-ND2	-5.28	117.32	122.60
2	1	175	TRP	CE2-CD2-CG	-5.26	100.89	107.20
4	3	170	TRP	CE2-CD2-CG	-5.25	100.90	107.20
4	3	105	ASN	CB-CG-ND2	5.22	124.23	116.40
4	3	9	GLY	CA-C-O	5.21	124.91	119.07
3	2	10	SER	N-CA-C	5.21	117.17	108.99
4	3	92	ASP	CA-C-N	5.21	125.51	119.47
4	3	92	ASP	C-N-CA	5.21	125.51	119.47
3	2	80	TRP	CE2-CD2-CG	-5.18	100.98	107.20
2	1	96	ALA	N-CA-C	5.18	116.61	109.15
2	1	264	LYS	CA-CB-CG	5.16	124.42	114.10
3	2	99	HIS	CB-CG-CD2	-5.15	124.51	131.20
5	4	49	ASP	N-CA-CB	-5.14	103.81	110.03
2	1	93	ASP	CA-CB-CG	5.13	117.73	112.60
3	2	227	TRP	CE2-CD2-CG	-5.12	101.06	107.20
3	2	21	SER	N-CA-C	5.11	117.23	108.90
4	3	97	HIS	CB-CG-ND1	5.10	130.35	122.70
4	3	110	TRP	CE2-CD2-CG	-5.10	101.08	107.20
2	1	228	LEU	N-CA-C	5.09	117.62	110.23
3	2	226	ASN	OD1-CG-ND2	-5.09	117.51	122.60
2	1	153	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	1	235	ASN	OD1-CG-ND2	-5.07	117.53	122.60
3	2	268	LEU	CA-C-N	5.07	124.83	119.76
3	2	268	LEU	C-N-CA	5.07	124.83	119.76
2	1	145	THR	CA-C-N	5.07	131.22	121.54
2	1	145	THR	C-N-CA	5.07	131.22	121.54
2	1	117	GLN	CG-CD-NE2	5.07	124.00	116.40
2	1	136	PHE	N-CA-C	5.05	116.75	108.52
3	2	5	GLU	OE1-CD-OE2	-5.04	110.79	122.90
3	2	30	ASN	OD1-CG-ND2	-5.04	117.56	122.60
2	1	100	ASN	CA-CB-CG	5.03	117.63	112.60
3	2	227	TRP	CG-CD2-CE3	5.01	138.91	133.90

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	43	0	39	0	0
2	1	2221	0	2171	34	0
3	2	2085	0	2000	30	0
4	3	1834	0	1816	23	0
5	4	462	0	446	7	0
6	1	21	0	37	7	0
7	4	15	0	27	1	0
8	0	1	0	0	0	0
8	1	184	0	0	3	0
8	2	143	0	0	2	0
8	3	135	0	0	2	0
8	4	40	0	0	0	0
All	All	7184	0	6536	76	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 6.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:187:LEU:HD22	4:3:65:MET:HE1	1.48	0.95
2:1:158:MET:SD	2:1:177:THR:HG23	2.16	0.84
3:2:5:GLU:OE2	3:2:7:CYS:HB3	1.78	0.83
4:3:124:MET:HG3	8:3:277:HOH:O	1.81	0.80
4:3:149:MET:HE2	4:3:150:LEU:HG	1.69	0.73
2:1:177:THR:HG22	2:1:180:ASN:HB2	1.69	0.73
2:1:40:GLU:HB3	5:4:64:THR:HB	1.71	0.73
3:2:5:GLU:HG2	3:2:9:TYR:HD2	1.57	0.70
2:1:287:LYS:HA	3:2:137:ASN:HD21	1.55	0.70
2:1:218:LYS:HD2	8:2:405:HOH:O	1.93	0.68
2:1:107:VAL:HG13	2:1:239:ILE:HD13	1.75	0.67
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.78	0.65
2:1:236:ASP:HB3	2:1:237:PHE:CD2	2.32	0.64
3:2:5:GLU:OE2	3:2:7:CYS:CB	2.46	0.63
2:1:218:LYS:HA	3:2:270:ARG:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:192:VAL:HG11	4:3:99:MET:HE2	1.81	0.63
3:2:143:THR:HG23	3:2:173:ARG:HA	1.80	0.61
3:2:187:LEU:HD22	4:3:65:MET:CE	2.29	0.60
3:2:213:VAL:HG22	4:3:37:PRO:HG2	1.86	0.58
2:1:177:THR:HG21	2:1:182:SER:OG	2.04	0.57
5:4:57:ILE:HD11	5:4:61:LEU:HB3	1.87	0.57
6:1:0:SPH:H4	8:1:448:HOH:O	2.04	0.56
3:2:179:TYR:HA	4:3:65:MET:CE	2.36	0.56
2:1:159:TYR:HB2	6:1:0:SPH:H162	1.87	0.55
3:2:146:GLN:NE2	3:2:270:ARG:HD2	2.22	0.55
2:1:48:GLU:HA	3:2:197:ILE:HB	1.89	0.55
3:2:179:TYR:HA	4:3:65:MET:HE2	1.89	0.55
2:1:287:LYS:HA	3:2:137:ASN:ND2	2.21	0.54
2:1:89:ILE:HG12	2:1:258:ARG:HG2	1.90	0.53
3:2:48:ASN:HB3	3:2:49:PRO:HD3	1.92	0.52
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.92	0.52
2:1:45:THR:OG1	5:4:67:MET:HE2	2.10	0.51
2:1:222:ALA:HA	8:1:336:HOH:O	2.09	0.51
8:3:317:HOH:O	5:4:46:PHE:HB2	2.10	0.51
4:3:167:VAL:O	4:3:169:PRO:HD3	2.11	0.50
2:1:96:ALA:HB2	2:1:248:HIS:CD2	2.47	0.50
2:1:27:LEU:HB3	2:1:28:PRO:HD2	1.94	0.50
4:3:208:MET:HE2	4:3:208:MET:N	2.27	0.49
3:2:30:ASN:HD21	5:4:59:ASP:HB2	1.76	0.49
4:3:55:PHE:HE2	4:3:212:GLY:HA3	1.78	0.49
3:2:5:GLU:CD	3:2:7:CYS:H	2.20	0.49
4:3:64:THR:O	4:3:67:MET:HG2	2.14	0.48
2:1:302:TYR:CE1	4:3:189:TYR:HB3	2.49	0.47
3:2:60:ALA:O	3:2:255:PRO:HG2	2.15	0.47
3:2:73:LYS:HE2	3:2:243:SER:O	2.15	0.47
4:3:87:LEU:HD13	4:3:190:ILE:HD11	1.97	0.47
2:1:206:SER:O	6:1:0:SPH:H11	2.14	0.47
2:1:273:PRO:HB3	3:2:189:ASN:HB2	1.97	0.46
2:1:132:MET:HE1	6:1:0:SPH:H81	1.97	0.46
2:1:294:LEU:HD12	4:3:67:MET:SD	2.56	0.46
2:1:94:ASN:ND2	2:1:248:HIS:HA	2.31	0.46
2:1:132:MET:HE1	6:1:0:SPH:C8	2.46	0.45
3:2:34:ALA:HB3	3:2:211:PRO:HD2	1.99	0.45
2:1:132:MET:HE1	6:1:0:SPH:C9	2.47	0.45
2:1:296:THR:HA	4:3:57:LEU:O	2.17	0.44
5:4:49:ASP:HA	5:4:50:PRO:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:63:PHE:CD1	3:2:254:ALA:HB2	2.53	0.43
3:2:37:ARG:HG3	4:3:37:PRO:HB3	2.00	0.43
2:1:96:ALA:O	2:1:98:THR:HG23	2.19	0.43
3:2:138:THR:HG23	8:2:395:HOH:O	2.19	0.42
2:1:291:LEU:C	2:1:293:PRO:HD3	2.45	0.42
4:3:71:ARG:CZ	4:3:71:ARG:HB2	2.49	0.42
5:4:55:GLU:N	5:4:56:PRO:HD3	2.34	0.42
2:1:237:PHE:CD2	6:1:0:SPH:H71	2.55	0.42
4:3:143:LYS:HA	4:3:143:LYS:HD3	1.75	0.42
4:3:44:MET:HE2	4:3:44:MET:HA	2.01	0.41
3:2:146:GLN:HE21	3:2:270:ARG:HD2	1.85	0.41
3:2:13:VAL:HG22	3:2:26:GLN:HA	2.03	0.41
3:2:5:GLU:CD	3:2:7:CYS:HB3	2.45	0.41
2:1:96:ALA:HB2	2:1:248:HIS:NE2	2.35	0.41
2:1:102:ASP:N	8:1:456:HOH:O	2.51	0.41
2:1:116:VAL:CG2	4:3:233:GLN:HB2	2.50	0.41
3:2:37:ARG:O	3:2:211:PRO:HG3	2.20	0.41
4:3:149:MET:CE	4:3:150:LEU:HG	2.46	0.41
7:4:1:MYR:H71	7:4:1:MYR:H101	1.80	0.40
3:2:239:PHE:O	3:2:241:SER:N	2.54	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	4/8 (50%)	3 (75%)	0	1 (25%)	0	0
2	1	281/302 (93%)	256 (91%)	21 (8%)	4 (1%)	9	30
3	2	266/272 (98%)	246 (92%)	15 (6%)	5 (2%)	6	23
4	3	233/238 (98%)	222 (95%)	10 (4%)	1 (0%)	30	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	56/68 (82%)	51 (91%)	3 (5%)	2 (4%)	2	11
All	All	840/888 (95%)	778 (93%)	49 (6%)	13 (2%)	8	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	99	THR
3	2	166	ASN
1	0	4	ALA
2	1	147	ASN
2	1	234	LEU
3	2	240	ALA
5	4	60	VAL
2	1	146	ASN
3	2	48	ASN
4	3	234	LYS
3	2	7	CYS
3	2	114	ALA
5	4	51	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%)	3 (75%)	1 (25%)	0	2
2	1	245/261 (94%)	232 (95%)	13 (5%)	20	52
3	2	228/232 (98%)	211 (92%)	17 (8%)	12	37
4	3	210/212 (99%)	201 (96%)	9 (4%)	26	60
5	4	52/57 (91%)	48 (92%)	4 (8%)	12	35
All	All	739/766 (96%)	695 (94%)	44 (6%)	17	47

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	THR
2	1	41	ILE
2	1	95	SER
2	1	145	THR
2	1	146	ASN
2	1	147	ASN
2	1	177	THR
2	1	220	GLN
2	1	221	SER
2	1	224	LEU
2	1	233	SER
2	1	239	ILE
2	1	252	LYS
2	1	264	LYS
3	2	5	GLU
3	2	10	SER
3	2	11	ASP
3	2	45	SER
3	2	52	GLN
3	2	73	LYS
3	2	74	GLU
3	2	139	THR
3	2	152	GLU
3	2	158	THR
3	2	165	ASN
3	2	168	THR
3	2	238	ASN
3	2	241	SER
3	2	242	GLU
3	2	251	LEU
3	2	264	ARG
4	3	71	ARG
4	3	85	LEU
4	3	149	MET
4	3	160	LEU
4	3	163	SER
4	3	190	ILE
4	3	208	MET
4	3	218	ASN
4	3	224	LEU
5	4	42	SER
5	4	49	ASP
5	4	60	VAL

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Mol	Chain	Res	Type
5	4	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	180	ASN
3	2	95	ASN
3	2	149	ASN
3	2	165	ASN
3	2	225	ASN
3	2	272	GLN
4	3	218	ASN
5	4	4	GLN
5	4	13	HIS
5	4	26	ASN
5	4	31	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	0.47	0	12,13,15	0.90	0
6	SPH	1	0	-	19,20,20	0.43	0	18,21,21	2.07	4 (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	-	5/12/12/13	-
6	SPH	1	0	-	-	4/21/21/21	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	0	SPH	O3-C3-C4	-4.83	98.39	110.88
6	1	0	SPH	O3-C3-C2	-4.63	99.53	107.31
6	1	0	SPH	C1-C2-C3	-3.53	105.70	113.00
6	1	0	SPH	O1-C1-C2	3.24	118.58	111.55

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	0	SPH	C2-C3-C4-C5
6	1	0	SPH	O3-C3-C4-C5
6	1	0	SPH	C3-C4-C5-C6
7	4	1	MYR	O1-C1-C2-C3
7	4	1	MYR	C6-C7-C8-C9
7	4	1	MYR	C10-C11-C12-C13
6	1	0	SPH	C11-C10-C9-C8
7	4	1	MYR	C5-C6-C7-C8
7	4	1	MYR	C7-C8-C9-C10

There are no ring outliers.

2 monomers are involved in 8 short contacts:

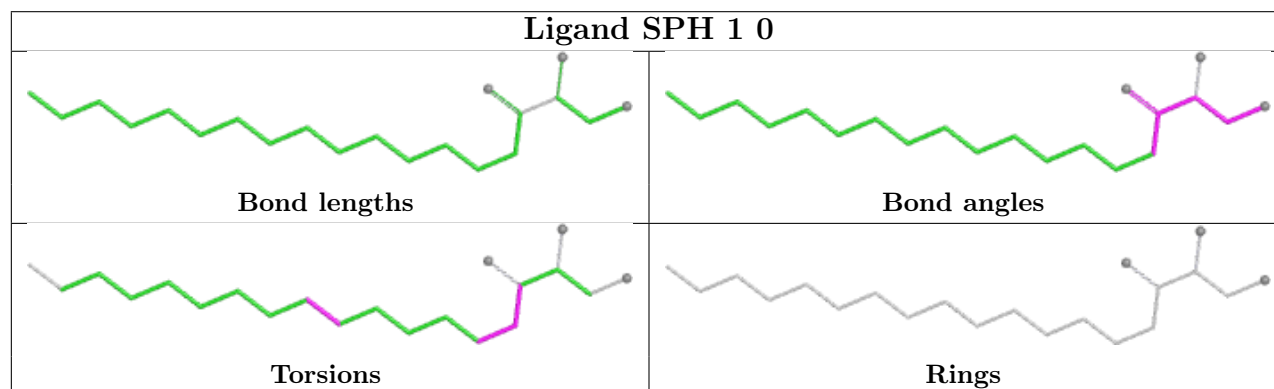
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	4	1	MYR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	0	SPH	7	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.