



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:09 PM UTC

PDB ID : 1AR9 / pdb_00001ar9
Title : P1/MAHONEY POLIOVIRUS, SINGLE SITE MUTANT H2142Y
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

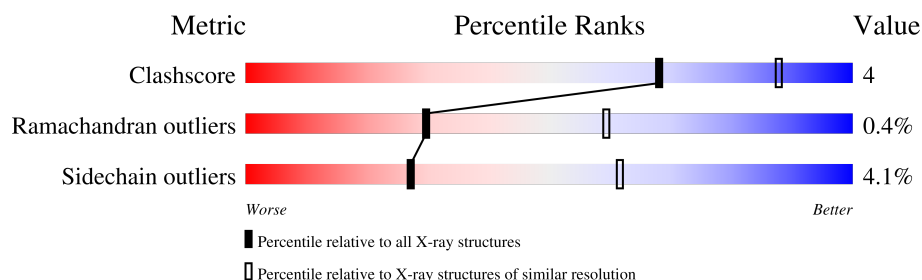
1 Overall quality at a glance

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	5	
2	1	302	
3	2	272	
4	3	238	
5	4	68	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7205 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	5	Total	C	N	O	0	0	0
			29	15	5	9			

- 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
			2222	1416	378	423	5			

- 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
			2087	1320	356	397	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	142	TYR	HIS	engineered mutation	UNP P03300

- 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			

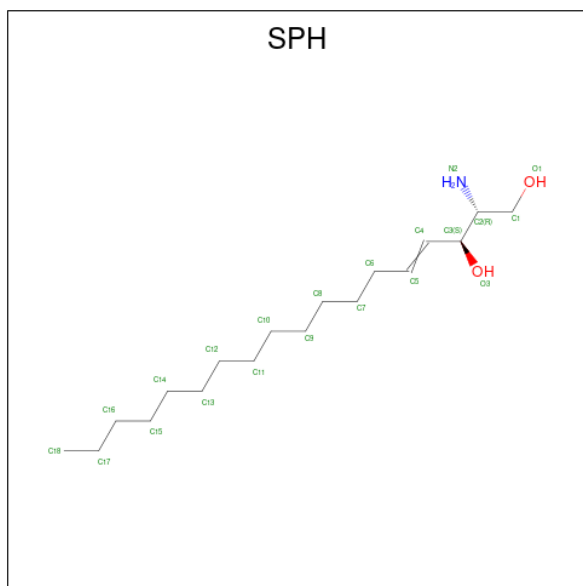
There is a discrepancy between the modelled and reference sequences:

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

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

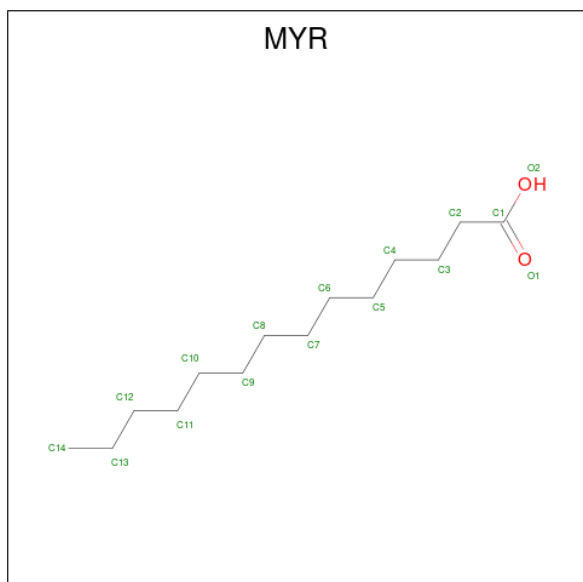
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	60	Total	C	N	O	S	0	0	0
			462	286	78	97	1			

- 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	180	Total	O	0	0
			180	180		
8	2	170	Total	O	0	0
			170	170		
8	3	141	Total	O	0	0
			141	141		
8	4	43	Total	O	0	0
			43	43		

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.

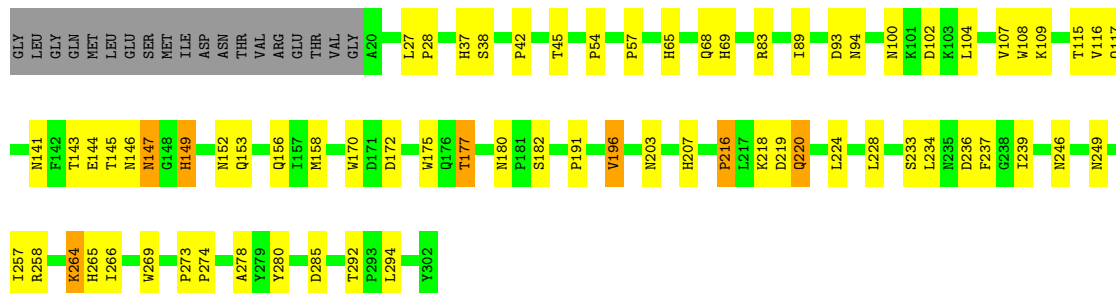
• Molecule 1: P1/MAHONEY POLIOVIRUS

Chain 0: 



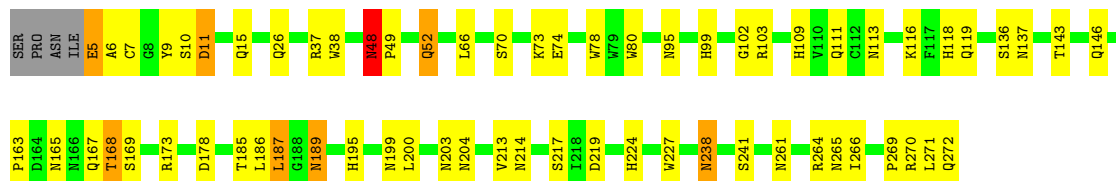
• Molecule 2: P1/MAHONEY POLIOVIRUS

Chain 1: 



• Molecule 3: P1/MAHONEY POLIOVIRUS

Chain 2: 



• Molecule 4: P1/MAHONEY POLIOVIRUS

Chain 3: 





● 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	319.95Å 355.15Å 377.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.00 – 2.90	Depositor
% Data completeness (in resolution range)	81.0 (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}	0.244 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7205	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: SPH, 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	0.96	0/28	1.75	1/36 (2.8%)
2	1	1.04	9/2285 (0.4%)	1.78	49/3124 (1.6%)
3	2	0.94	4/2144 (0.2%)	1.81	55/2931 (1.9%)
4	3	1.00	5/1881 (0.3%)	1.68	33/2562 (1.3%)
5	4	1.05	1/469 (0.2%)	1.92	17/632 (2.7%)
All	All	1.00	19/6807 (0.3%)	1.77	155/9285 (1.7%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	54	PRO	CA-CB	-8.10	1.47	1.53
2	1	149	HIS	CD2-NE2	-7.65	1.29	1.37
2	1	37	HIS	CD2-NE2	-6.94	1.30	1.37
4	3	77	HIS	CD2-NE2	-6.73	1.30	1.37
2	1	265	HIS	CD2-NE2	-6.70	1.30	1.37
4	3	109	HIS	CD2-NE2	-6.67	1.30	1.37
3	2	224	HIS	CD2-NE2	-6.66	1.30	1.37
4	3	230	HIS	CD2-NE2	-6.64	1.30	1.37
2	1	207	HIS	CD2-NE2	-6.63	1.30	1.37
2	1	69	HIS	CD2-NE2	-6.32	1.30	1.37
5	4	13	HIS	CD2-NE2	-6.18	1.31	1.37
3	2	195	HIS	CD2-NE2	-6.12	1.31	1.37
3	2	118	HIS	CD2-NE2	-6.00	1.31	1.37
4	3	97	HIS	CD2-NE2	-5.84	1.31	1.37
2	1	37	HIS	CG-ND1	-5.75	1.31	1.38
3	2	109	HIS	CD2-NE2	-5.37	1.31	1.37
4	3	153	HIS	CD2-NE2	-5.27	1.32	1.37
2	1	65	HIS	CD2-NE2	-5.09	1.32	1.37
2	1	65	HIS	CG-ND1	-5.04	1.32	1.38

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	117	GLN	OE1-CD-NE2	-11.27	111.33	122.60
2	1	149	HIS	CB-CG-CD2	-10.46	117.61	131.20
4	3	6	ASN	CB-CG-ND2	10.02	131.43	116.40
2	1	219	ASP	CA-CB-CG	9.96	122.56	112.60
2	1	220	GLN	OE1-CD-NE2	-9.96	112.64	122.60
3	2	165	ASN	OD1-CG-ND2	-9.92	112.68	122.60
2	1	147	ASN	OD1-CG-ND2	-9.44	113.17	122.60
5	4	31	ASN	OD1-CG-ND2	-9.41	113.19	122.60
3	2	168	THR	CA-CB-OG1	-9.19	95.81	109.60
4	3	218	ASN	OD1-CG-ND2	-9.17	113.43	122.60
3	2	137	ASN	OD1-CG-ND2	-8.82	113.78	122.60
3	2	265	ASN	OD1-CG-ND2	-8.71	113.89	122.60
2	1	68	GLN	OE1-CD-NE2	-8.66	113.94	122.60
4	3	20	GLN	OE1-CD-NE2	-8.50	114.10	122.60
2	1	100	ASN	OD1-CG-ND2	-8.42	114.18	122.60
4	3	53	ILE	N-CA-C	8.38	115.84	108.63
5	4	69	ASN	OD1-CG-ND2	-8.33	114.27	122.60
3	2	52	GLN	OE1-CD-NE2	-8.28	114.33	122.60
2	1	149	HIS	CB-CG-ND1	7.89	134.53	122.70
2	1	152	ASN	OD1-CG-ND2	-7.76	114.84	122.60
5	4	44	GLN	OE1-CD-NE2	-7.75	114.85	122.60
2	1	172	ASP	CA-CB-CG	7.75	120.34	112.60
3	2	146	GLN	OE1-CD-NE2	-7.68	114.92	122.60
3	2	48	ASN	OD1-CG-ND2	-7.66	114.94	122.60
2	1	220	GLN	CG-CD-NE2	7.54	127.71	116.40
4	3	18	ASN	OD1-CG-ND2	-7.53	115.07	122.60
2	1	141	ASN	OD1-CG-ND2	-7.50	115.11	122.60
3	2	165	ASN	CA-CB-CG	-7.45	105.15	112.60
2	1	266	ILE	N-CA-C	7.44	119.79	108.71
3	2	52	GLN	CG-CD-NE2	7.40	127.50	116.40
3	2	199	ASN	OD1-CG-ND2	-7.33	115.27	122.60
4	3	105	ASN	OD1-CG-ND2	-7.33	115.27	122.60
3	2	167	GLN	OE1-CD-NE2	-7.20	115.40	122.60
3	2	203	ASN	OD1-CG-ND2	-7.15	115.45	122.60
2	1	94	ASN	OD1-CG-ND2	-7.15	115.45	122.60
3	2	178	ASP	N-CA-C	7.14	119.74	111.02
5	4	46	PHE	CA-CB-CG	-7.06	106.74	113.80
5	4	49	ASP	CA-CB-CG	7.03	119.63	112.60
3	2	219	ASP	CA-CB-CG	6.92	119.53	112.60
2	1	246	ASN	OD1-CG-ND2	-6.85	115.75	122.60
3	2	95	ASN	CA-CB-CG	-6.79	105.81	112.60
4	3	173	ASN	OD1-CG-ND2	-6.77	115.83	122.60
3	2	168	THR	CA-CB-CG2	6.75	121.97	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	272	GLN	OE1-CD-NE2	-6.74	115.86	122.60
3	2	238	ASN	CA-CB-CG	-6.68	105.92	112.60
2	1	104	LEU	N-CA-C	6.66	118.74	109.15
3	2	26	GLN	OE1-CD-NE2	-6.66	115.94	122.60
4	3	6	ASN	CB-CG-OD1	-6.63	107.55	120.80
4	3	189	TYR	N-CA-C	6.63	119.21	108.41
5	4	4	GLN	OE1-CD-NE2	-6.61	115.99	122.60
5	4	8	GLN	OE1-CD-NE2	-6.60	116.00	122.60
3	2	261	ASN	OD1-CG-ND2	-6.59	116.01	122.60
4	3	63	ASN	OD1-CG-ND2	-6.52	116.08	122.60
3	2	136	SER	N-CA-C	6.31	119.75	109.59
3	2	178	ASP	CA-CB-CG	6.31	118.91	112.60
4	3	17	ASP	CA-CB-CG	6.31	118.91	112.60
5	4	13	HIS	CB-CG-CD2	-6.26	123.06	131.20
3	2	137	ASN	CB-CG-ND2	6.22	125.74	116.40
3	2	224	HIS	CA-CB-CG	6.22	120.02	113.80
2	1	156	GLN	OE1-CD-NE2	-6.21	116.39	122.60
3	2	99	HIS	CB-CG-CD2	-6.19	123.15	131.20
3	2	200	LEU	N-CA-C	6.18	118.81	111.33
5	4	63	LYS	N-CA-C	6.17	119.91	112.38
3	2	271	LEU	N-CA-C	6.16	120.95	113.38
4	3	161	GLN	OE1-CD-NE2	-6.15	116.45	122.60
5	4	45	ASP	N-CA-C	6.08	119.62	109.95
4	3	153	HIS	CB-CG-CD2	-6.07	123.31	131.20
2	1	116	VAL	N-CA-C	6.06	119.02	112.96
4	3	133	SER	N-CA-C	6.05	119.27	109.40
4	3	162	SER	N-CA-C	6.05	118.67	111.71
2	1	153	GLN	N-CA-C	6.02	119.72	110.20
2	1	93	ASP	CA-CB-CG	6.00	118.61	112.60
2	1	38	SER	N-CA-C	6.00	117.02	108.74
3	2	204	ASN	OD1-CG-ND2	-5.98	116.62	122.60
4	3	195	GLN	OE1-CD-NE2	-5.94	116.66	122.60
3	2	214	ASN	OD1-CG-ND2	-5.91	116.69	122.60
4	3	96	SER	N-CA-C	5.89	119.56	112.38
2	1	216	PRO	N-CA-CB	5.88	108.00	103.30
2	1	69	HIS	CB-CG-CD2	-5.87	123.56	131.20
4	3	54	PRO	N-CA-CB	5.85	106.51	102.35
3	2	113	ASN	OD1-CG-ND2	-5.85	116.75	122.60
5	4	49	ASP	N-CA-CB	-5.85	101.89	110.14
4	3	97	HIS	CB-CG-CD2	-5.82	123.64	131.20
4	3	21	SER	O-C-N	-5.78	117.43	121.65
3	2	118	HIS	CB-CG-CD2	-5.77	123.70	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	54	PRO	N-CA-CB	5.76	106.59	102.79
4	3	183	SER	N-CA-C	5.76	118.30	111.33
3	2	102	GLY	O-C-N	-5.76	118.89	123.27
5	4	10	VAL	N-CA-C	5.76	116.44	108.84
4	3	178	GLN	OE1-CD-NE2	-5.75	116.86	122.60
3	2	189	ASN	OD1-CG-ND2	-5.73	116.87	122.60
5	4	42	SER	N-CA-C	5.71	118.45	111.82
4	3	42	ASN	OD1-CG-ND2	-5.70	116.90	122.60
2	1	228	LEU	N-CA-C	5.70	118.72	110.28
5	4	13	HIS	CB-CG-ND1	5.70	131.25	122.70
4	3	27	GLU	N-CA-C	5.66	119.48	112.47
5	4	31	ASN	CB-CG-ND2	5.65	124.87	116.40
2	1	264	LYS	CB-CA-C	-5.64	99.96	109.83
4	3	233	GLN	OE1-CD-NE2	-5.64	116.96	122.60
2	1	68	GLN	CG-CD-NE2	5.63	124.84	116.40
3	2	266	ILE	N-CA-C	5.62	116.85	109.21
3	2	10	SER	N-CA-C	5.61	117.92	109.23
2	1	278	ALA	N-CA-C	5.60	118.19	110.35
2	1	83	ARG	NE-CZ-NH2	-5.57	114.18	119.20
5	4	48	GLN	OE1-CD-NE2	-5.55	117.05	122.60
3	2	186	LEU	N-CA-C	5.55	118.28	109.96
3	2	70	SER	N-CA-C	5.54	117.94	108.90
4	3	77	HIS	CB-CG-CD2	-5.53	124.01	131.20
2	1	264	LYS	CB-CG-CD	-5.52	98.61	111.30
2	1	65	HIS	CB-CG-CD2	-5.46	124.10	131.20
4	3	153	HIS	N-CA-C	5.46	117.14	108.79
4	3	173	ASN	CB-CG-ND2	5.45	124.58	116.40
2	1	83	ARG	CA-CB-CG	5.45	125.00	114.10
3	2	15	GLN	OE1-CD-NE2	-5.44	117.16	122.60
4	3	80	ASP	N-CA-C	5.40	116.88	110.07
3	2	80	TRP	CE2-CD2-CG	-5.39	100.73	107.20
4	3	218	ASN	CB-CG-ND2	5.39	124.49	116.40
1	0	7	SER	CB-CA-C	-5.38	102.39	110.24
3	2	163	PRO	N-CA-CB	5.37	108.08	103.36
3	2	6	ALA	N-CA-C	5.37	118.93	112.38
3	2	11	ASP	CA-C-O	5.36	126.20	120.20
2	1	147	ASN	CB-CG-ND2	5.31	124.36	116.40
3	2	111	GLN	OE1-CD-NE2	-5.31	117.29	122.60
3	2	6	ALA	CA-C-O	5.29	125.90	119.49
2	1	220	GLN	CA-CB-CG	5.24	124.58	114.10
3	2	5	GLU	CB-CG-CD	5.24	121.50	112.60
2	1	102	ASP	N-CA-C	5.23	117.47	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	83	ARG	CG-CD-NE	-5.22	100.52	112.00
2	1	175	TRP	CG-CD2-CE3	5.21	139.11	133.90
4	3	156	TRP	CE2-CD2-CG	-5.21	100.95	107.20
3	2	48	ASN	CB-CG-ND2	5.20	124.19	116.40
3	2	78	TRP	CE2-CD2-CG	-5.19	100.97	107.20
5	4	51	SER	N-CA-C	5.17	121.81	110.80
4	3	232	GLU	CA-CB-CG	5.16	124.43	114.10
2	1	117	GLN	N-CA-C	5.16	116.71	111.14
2	1	269	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	1	203	ASN	OD1-CG-ND2	-5.14	117.46	122.60
2	1	249	ASN	CA-C-N	5.12	124.57	119.24
2	1	249	ASN	C-N-CA	5.12	124.57	119.24
2	1	108	TRP	CE2-CD2-CG	-5.12	101.06	107.20
2	1	292	THR	CA-C-N	5.12	124.29	118.97
2	1	292	THR	C-N-CA	5.12	124.29	118.97
2	1	175	TRP	CE2-CD2-CG	-5.09	101.09	107.20
3	2	269	PRO	N-CA-CB	5.09	108.08	103.15
3	2	38	TRP	CE2-CD2-CG	-5.08	101.10	107.20
2	1	170	TRP	CE2-CD2-CG	-5.07	101.12	107.20
3	2	119	GLN	OE1-CD-NE2	-5.07	117.53	122.60
3	2	227	TRP	CE2-CD2-CG	-5.05	101.14	107.20
3	2	10	SER	CA-C-N	5.04	127.73	120.38
3	2	10	SER	C-N-CA	5.04	127.73	120.38
2	1	236	ASP	CA-CB-CG	5.03	117.63	112.60
3	2	109	HIS	CB-CG-CD2	-5.02	124.67	131.20
3	2	185	THR	O-C-N	-5.02	117.07	123.24
4	3	170	TRP	CE2-CD2-CG	-5.01	101.19	107.20
2	1	108	TRP	CG-CD2-CE3	5.00	138.90	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	29	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	2222	0	2173	27	0
3	2	2087	0	2002	13	0
4	3	1834	0	1816	15	0
5	4	462	0	446	7	0
6	1	21	0	37	4	0
7	4	15	0	27	0	0
8	0	1	0	0	0	0
8	1	180	0	0	2	0
8	2	170	0	0	1	0
8	3	141	0	0	1	0
8	4	43	0	0	0	0
All	All	7205	0	6525	47	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 (47) 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	1.58	0.85
2:1:177:THR:HG22	2:1:180:ASN:HB2	1.62	0.80
2:1:158:MET:SD	2:1:177:THR:HG23	2.24	0.76
2:1:107:VAL:HG13	2:1:239:ILE:HD13	1.76	0.67
3:2:5:GLU:HG2	3:2:9:TYR:HD2	1.62	0.63
3:2:37:ARG:HG3	4:3:37:PRO:HB3	1.83	0.61
4:3:167:VAL:O	4:3:169:PRO:HD3	2.04	0.57
2:1:177:THR:HG21	2:1:182:SER:OG	2.04	0.57
5:4:55:GLU:HG2	5:4:61:LEU:HD23	1.88	0.56
2:1:45:THR:OG1	5:4:67:MET:HE2	2.05	0.56
2:1:273:PRO:HB3	3:2:189:ASN:HB2	1.89	0.55
4:3:87:LEU:HD11	4:3:114:LEU:HD12	1.90	0.54
2:1:191:PRO:HG2	4:3:13:TYR:HB2	1.89	0.53
2:1:144:GLU:HG3	2:1:146:ASN:HD22	1.74	0.53
2:1:144:GLU:HG2	8:1:444:HOH:O	2.09	0.52
2:1:274:PRO:HG2	4:3:102:GLU:HG3	1.91	0.52
3:2:5:GLU:HG3	3:2:7:CYS:H	1.75	0.52
3:2:5:GLU:HG2	3:2:9:TYR:CD2	2.45	0.52
3:2:213:VAL:HG22	4:3:37:PRO:HG2	1.92	0.52
2:1:42:PRO:HA	5:4:63:LYS:O	2.09	0.51
2:1:216:PRO:HB2	3:2:270:ARG:HB3	1.92	0.51
6:1:0:SPH:H4	8:1:400:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:57:PRO:HB3	4:3:169:PRO:HB3	1.94	0.49
2:1:237:PHE:CG	6:1:0:SPH:H91	2.47	0.49
3:2:143:THR:HG23	3:2:173:ARG:HA	1.97	0.46
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.96	0.46
2:1:115:THR:HA	4:3:233:GLN:HE22	1.81	0.45
4:3:120:PHE:HA	4:3:210:ILE:HG22	1.98	0.45
3:2:48:ASN:HB3	3:2:49:PRO:HD3	1.99	0.45
2:1:196:VAL:HG21	6:1:0:SPH:H141	1.98	0.44
3:2:103:ARG:HD2	3:2:217:SER:O	2.17	0.44
3:2:116:LYS:HE3	4:3:124:MET:SD	2.58	0.43
8:3:322:HOH:O	5:4:46:PHE:HB2	2.19	0.43
2:1:264:LYS:NZ	5:4:37:ALA:O	2.51	0.43
2:1:273:PRO:HB3	3:2:189:ASN:CB	2.49	0.43
4:3:55:PHE:HE2	4:3:212:GLY:HA3	1.84	0.42
5:4:49:ASP:HA	5:4:50:PRO:HD3	1.92	0.42
2:1:218:LYS:HD2	8:2:411:HOH:O	2.18	0.42
2:1:280:TYR:HB3	2:1:285:ASP:O	2.20	0.42
5:4:10:VAL:HG21	5:4:25:ILE:HD12	2.01	0.42
2:1:27:LEU:HB3	2:1:28:PRO:HD2	2.03	0.41
2:1:89:ILE:HG12	2:1:258:ARG:HG2	2.03	0.41
2:1:294:LEU:CD1	4:3:67:MET:SD	3.09	0.41
4:3:64:THR:O	4:3:67:MET:HG2	2.21	0.41
2:1:237:PHE:CZ	6:1:0:SPH:H3	2.56	0.40
2:1:294:LEU:HD13	4:3:67:MET:SD	2.62	0.40
2:1:257:ILE:HD12	2:1:257:ILE:N	2.36	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	3/5 (60%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	281/302 (93%)	266 (95%)	14 (5%)	1 (0%)	30	59
3	2	266/272 (98%)	250 (94%)	15 (6%)	1 (0%)	30	59
4	3	233/238 (98%)	223 (96%)	10 (4%)	0	100	100
5	4	56/68 (82%)	52 (93%)	3 (5%)	1 (2%)	6	25
All	All	839/885 (95%)	794 (95%)	42 (5%)	3 (0%)	30	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	234	LEU
3	2	48	ASN
5	4	60	VAL

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%)	236 (96%)	9 (4%)	30	64
3	2	228/232 (98%)	217 (95%)	11 (5%)	23	55
4	3	210/212 (99%)	204 (97%)	6 (3%)	37	71
5	4	52/57 (91%)	49 (94%)	3 (6%)	18	49
All	All	739/766 (96%)	709 (96%)	30 (4%)	27	61

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	THR
2	1	143	THR
2	1	145	THR
2	1	147	ASN
2	1	149	HIS

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Mol	Chain	Res	Type
2	1	177	THR
2	1	196	VAL
2	1	220	GLN
2	1	224	LEU
2	1	233	SER
3	2	11	ASP
3	2	52	GLN
3	2	66	LEU
3	2	73	LYS
3	2	74	GLU
3	2	168	THR
3	2	169	SER
3	2	187	LEU
3	2	238	ASN
3	2	241	SER
3	2	264	ARG
4	3	71	ARG
4	3	85	LEU
4	3	178	GLN
4	3	208	MET
4	3	218	ASN
4	3	224	LEU
5	4	49	ASP
5	4	60	VAL
5	4	61	LEU

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	65	HIS
2	1	153	GLN
3	2	94	GLN
3	2	119	GLN
3	2	238	ASN
3	2	261	ASN
4	3	105	ASN
4	3	218	ASN
5	4	4	GLN
5	4	8	GLN
5	4	26	ASN
5	4	31	ASN
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$
7	MYR	4	1	5	13,14,15	0.40	0	12,13,15	0.78	0
6	SPH	1	0	-	19,20,20	0.90	1 (5%)	18,21,21	2.51	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	-	6/12/12/13	-
6	SPH	1	0	-	-	8/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	0	SPH	C1-C2	3.43	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	0	SPH	O3-C3-C2	-6.30	96.72	107.31
6	1	0	SPH	O1-C1-C2	5.37	123.20	111.55
6	1	0	SPH	O3-C3-C4	-4.97	98.03	110.88
6	1	0	SPH	C1-C2-C3	-3.47	105.82	113.00

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	0	SPH	O3-C3-C4-C5
6	1	0	SPH	C3-C4-C5-C6
7	4	1	MYR	O1-C1-C2-C3
6	1	0	SPH	C10-C11-C12-C13
7	4	1	MYR	C5-C6-C7-C8
6	1	0	SPH	O1-C1-C2-N2
7	4	1	MYR	C6-C7-C8-C9
6	1	0	SPH	O1-C1-C2-C3
7	4	1	MYR	C10-C11-C12-C13
6	1	0	SPH	C1-C2-C3-O3
6	1	0	SPH	N2-C2-C3-O3
7	4	1	MYR	C11-C12-C13-C14
6	1	0	SPH	C2-C3-C4-C5
7	4	1	MYR	C7-C8-C9-C10

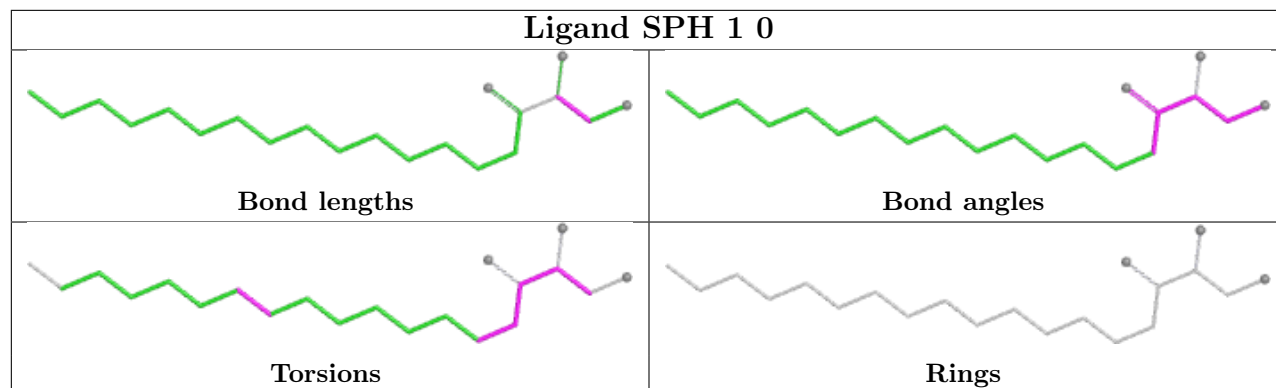
There are no ring outliers.

1 monomer is involved in 4 short contacts:

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