



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:22 PM UTC

PDB ID : 1POV / pdb_00001pov
Title : ROLE AND MECHANISM OF THE MATURATION CLEAVAGE OF VP0
IN POLIOVIRUS ASSEMBLY: STRUCTURE OF THE EMPTY CAPSID
ASSEMBLY INTERMEDIATE AT 2.9 ANGSTROMS RESOLUTION
Authors : Basavappa, R.; Filman, D.J.; Hogle, J.M.
Deposited on : 1995-08-10
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

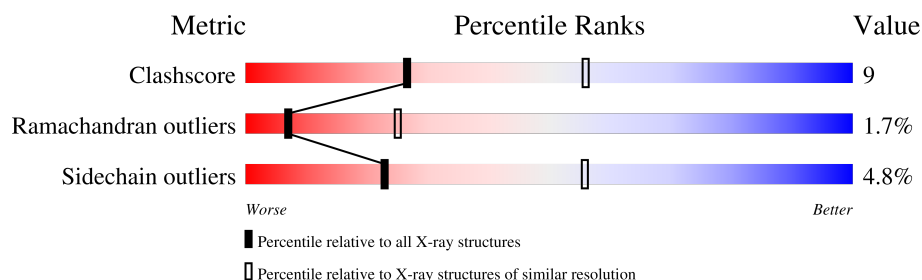
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	340	
2	1	302	
3	3	238	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SPH	1	0	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6281 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 NATIVE EMPTY CAPSID (TYPE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	300	Total	C	N	O	S	0	0	0
			2312	1460	401	436	15			

- Molecule 2 is a protein called POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	235	Total	C	N	O	S	0	0	0
			1874	1204	315	350	5			

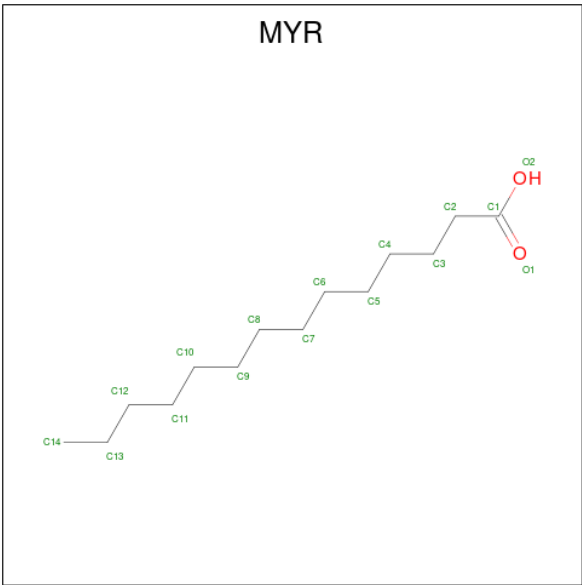
- Molecule 3 is a protein called POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	238	Total	C	N	O	S	0	0	0
			1849	1177	302	353	17			

There is a discrepancy between the modelled and reference sequences:

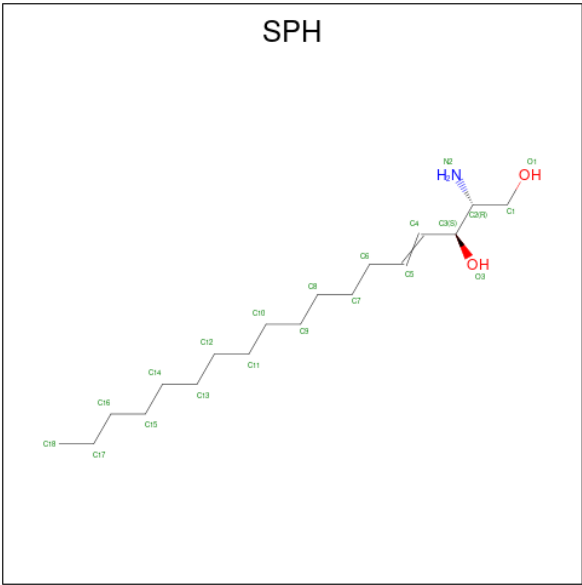
Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	conflict	UNP P03300

- Molecule 4 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	0	1	Total	C	O	0	0
			15	14	1		

- Molecule 5 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 6 is water.

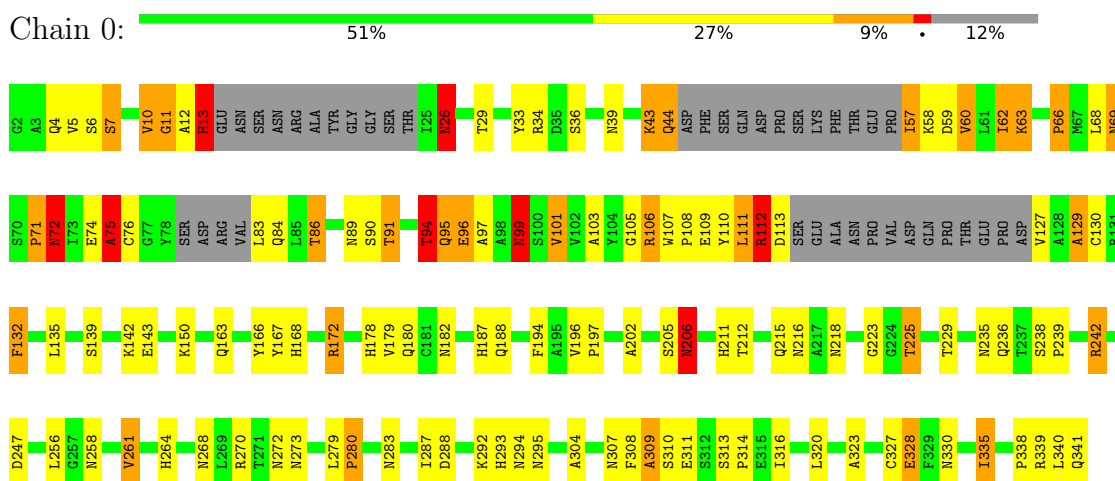
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	0	73	Total 73	O 73	0	0
6	1	75	Total 75	O 75	0	0
6	3	62	Total 62	O 62	0	0

3 Residue-property plots

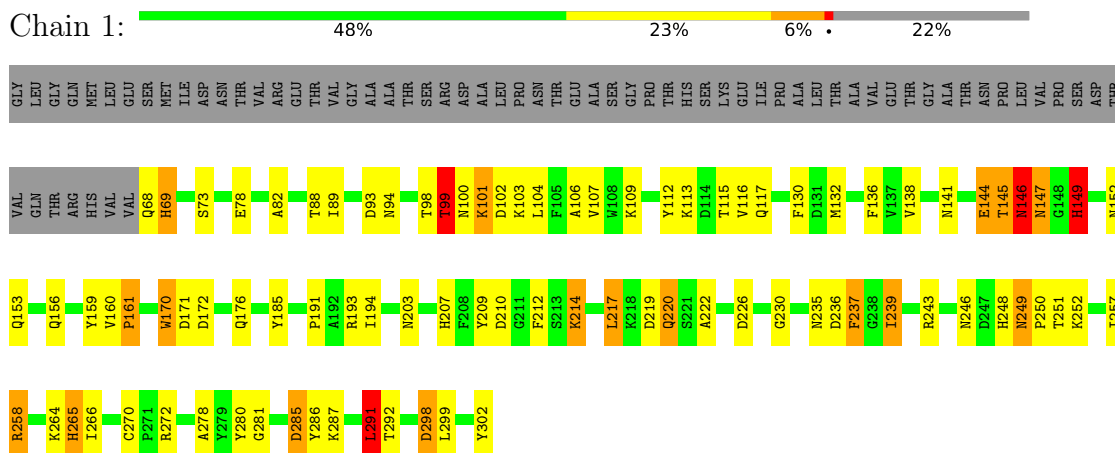
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 NATIVE EMPTY CAPSID (TYPE 1)

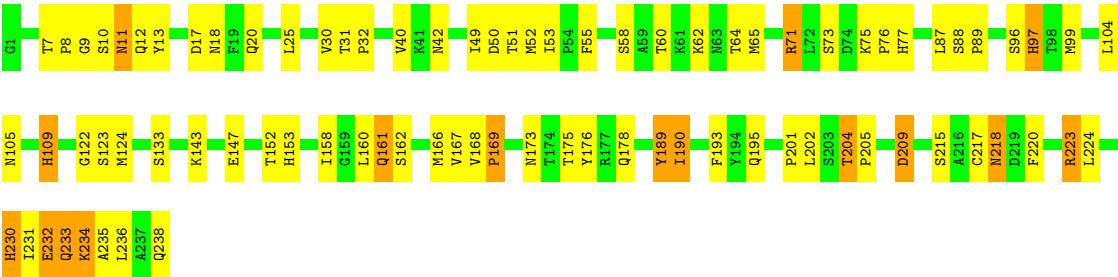


- Molecule 2: POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1)



- Molecule 3: POLIOVIRUS NATIVE EMPTY CAPSID (TYPE 1)





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	322.90Å 358.00Å 380.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.281 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6281	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	1.18	11/2367 (0.5%)	2.06	101/3225 (3.1%)
2	1	1.10	6/1930 (0.3%)	1.91	74/2634 (2.8%)
3	3	1.20	11/1896 (0.6%)	1.87	47/2584 (1.8%)
All	All	1.16	28/6193 (0.5%)	1.95	222/8443 (2.6%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	293	HIS	CD2-NE2	-7.73	1.29	1.37
2	1	207	HIS	CD2-NE2	-7.60	1.29	1.37
3	3	77	HIS	CD2-NE2	-7.21	1.29	1.37
3	3	230	HIS	CD2-NE2	-7.16	1.29	1.37
1	0	264	HIS	CD2-NE2	-7.09	1.30	1.37
3	3	153	HIS	CD2-NE2	-7.04	1.30	1.37
1	0	187	HIS	CD2-NE2	-6.75	1.30	1.37
2	1	265	HIS	CD2-NE2	-6.61	1.30	1.37
3	3	153	HIS	CG-ND1	-6.52	1.31	1.38
3	3	97	HIS	CD2-NE2	-6.45	1.30	1.37
1	0	168	HIS	CD2-NE2	-6.43	1.30	1.37
3	3	109	HIS	CD2-NE2	-6.28	1.30	1.37
1	0	293	HIS	CG-ND1	-6.17	1.31	1.38
1	0	187	HIS	CG-ND1	-5.88	1.31	1.38
1	0	168	HIS	CG-ND1	-5.74	1.31	1.38
3	3	109	HIS	CG-ND1	-5.65	1.32	1.38
1	0	211	HIS	CD2-NE2	-5.62	1.31	1.37
3	3	230	HIS	CG-ND1	-5.61	1.32	1.38
1	0	264	HIS	CG-ND1	-5.42	1.32	1.38
2	1	265	HIS	CG-ND1	-5.42	1.32	1.38
1	0	280	PRO	CA-CB	-5.33	1.46	1.53
2	1	248	HIS	CD2-NE2	-5.33	1.31	1.37
3	3	77	HIS	CG-ND1	-5.32	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	147	GLU	CA-CB	-5.29	1.45	1.53
2	1	161	PRO	CA-CB	-5.28	1.49	1.54
3	3	169	PRO	CA-CB	-5.15	1.46	1.53
1	0	178	HIS	CD2-NE2	-5.13	1.32	1.37
2	1	207	HIS	CG-ND1	-5.01	1.32	1.38

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	235	ASN	OD1-CG-ND2	-12.29	110.31	122.60
3	3	53	ILE	N-CA-C	10.97	118.07	108.63
2	1	172	ASP	N-CA-C	10.84	123.63	110.19
1	0	99	ASN	CA-CB-CG	-10.80	101.80	112.60
1	0	94	THR	N-CA-C	10.70	125.86	108.41
1	0	330	ASN	OD1-CG-ND2	-10.03	112.57	122.60
3	3	195	GLN	OE1-CD-NE2	-9.55	113.05	122.60
1	0	273	ASN	OD1-CG-ND2	-9.39	113.20	122.60
2	1	171	ASP	N-CA-C	9.39	122.72	111.82
2	1	102	ASP	N-CA-C	9.29	122.32	110.24
1	0	26	ASN	N-CA-C	9.21	121.45	108.74
1	0	69	ASN	N-CA-C	8.92	122.43	112.97
1	0	112	ARG	N-CA-C	8.79	124.31	110.17
1	0	215	GLN	OE1-CD-NE2	-8.75	113.85	122.60
2	1	117	GLN	OE1-CD-NE2	-8.69	113.91	122.60
2	1	104	LEU	N-CA-C	8.60	122.00	108.67
3	3	20	GLN	OE1-CD-NE2	-8.59	114.01	122.60
1	0	129	ALA	N-CA-C	-8.51	103.03	113.41
1	0	283	ASN	OD1-CG-ND2	-8.39	114.21	122.60
2	1	176	GLN	OE1-CD-NE2	-8.34	114.26	122.60
1	0	99	ASN	N-CA-C	8.14	122.58	113.21
2	1	149	HIS	N-CA-C	8.13	120.72	109.18
1	0	335	ILE	N-CA-C	8.13	120.07	109.58
3	3	55	PHE	N-CA-C	7.95	120.65	111.11
1	0	84	GLN	OE1-CD-NE2	-7.93	114.67	122.60
1	0	163	GLN	OE1-CD-NE2	-7.89	114.71	122.60
3	3	218	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	0	180	GLN	OE1-CD-NE2	-7.75	114.85	122.60
1	0	196	VAL	N-CA-C	7.74	116.43	107.77
2	1	266	ILE	N-CA-C	7.73	120.61	108.87
3	3	193	PHE	N-CA-C	7.71	120.88	109.24
3	3	17	ASP	CA-CB-CG	7.70	120.30	112.60
1	0	62	ILE	N-CA-C	7.70	118.92	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	272	ASN	OD1-CG-ND2	-7.69	114.91	122.60
2	1	252	LYS	N-CA-C	7.59	122.20	110.20
3	3	18	ASN	OD1-CG-ND2	-7.54	115.06	122.60
3	3	238	GLN	OE1-CD-NE2	-7.54	115.06	122.60
2	1	146	ASN	N-CA-C	7.46	126.70	110.80
1	0	60	VAL	N-CA-C	7.37	119.02	110.62
1	0	106	ARG	N-CA-C	7.35	120.38	108.41
1	0	330	ASN	N-CA-C	7.34	119.55	108.46
3	3	161	GLN	N-CA-C	7.33	121.15	108.76
3	3	223	ARG	N-CA-C	7.28	119.99	109.14
1	0	194	PHE	N-CA-C	7.25	120.34	108.52
1	0	188	GLN	OE1-CD-NE2	-7.24	115.36	122.60
2	1	172	ASP	CA-CB-CG	7.22	119.82	112.60
1	0	91	THR	CB-CA-C	-7.18	99.76	110.24
2	1	156	GLN	OE1-CD-NE2	-7.14	115.46	122.60
3	3	223	ARG	CA-CB-CG	7.13	128.36	114.10
3	3	162	SER	N-CA-C	7.12	120.87	111.75
3	3	232	GLU	N-CA-C	7.09	119.34	108.42
3	3	173	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	0	235	ASN	CB-CG-ND2	7.02	126.93	116.40
1	0	247	ASP	CA-CB-CG	6.98	119.58	112.60
1	0	113	ASP	CA-CB-CG	-6.92	105.68	112.60
3	3	133	SER	N-CA-C	6.90	120.76	109.24
2	1	130	PHE	N-CA-C	6.89	119.71	108.55
3	3	30	VAL	N-CA-C	6.89	119.55	109.63
1	0	86	THR	N-CA-C	6.88	120.38	108.76
1	0	60	VAL	CB-CA-C	-6.84	103.08	112.04
2	1	222	ALA	N-CA-C	6.81	119.57	111.33
1	0	74	GLU	N-CA-C	6.77	118.35	110.97
1	0	139	SER	N-CA-C	6.76	119.54	108.52
2	1	136	PHE	N-CA-C	6.72	119.88	107.99
3	3	96	SER	N-CA-C	6.69	120.31	111.75
1	0	242	ARG	N-CA-C	6.69	119.11	109.14
2	1	292	THR	CA-C-N	6.69	125.93	118.97
2	1	292	THR	C-N-CA	6.69	125.93	118.97
1	0	132	PHE	N-CA-C	6.69	119.04	108.67
1	0	89	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	0	279	LEU	CA-C-N	6.60	126.56	120.03
1	0	279	LEU	C-N-CA	6.60	126.56	120.03
1	0	328	GLU	N-CA-C	6.58	120.25	109.06
3	3	105	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	0	106	ARG	CA-C-O	6.56	127.32	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	220	GLN	OE1-CD-NE2	-6.55	116.05	122.60
2	1	141	ASN	OD1-CG-ND2	-6.55	116.05	122.60
2	1	73	SER	N-CA-C	6.50	118.92	111.11
3	3	189	TYR	N-CA-C	6.50	119.74	108.76
3	3	73	SER	N-CA-C	6.48	118.62	108.96
2	1	100	ASN	OD1-CG-ND2	-6.44	116.16	122.60
2	1	226	ASP	N-CA-C	6.43	119.99	110.48
1	0	63	LYS	N-CA-C	6.42	119.03	109.59
2	1	144	GLU	N-CA-C	6.42	120.37	110.42
2	1	285	ASP	N-CA-C	6.41	119.07	110.35
1	0	72	ASN	CB-CA-C	-6.41	99.23	109.80
3	3	233	GLN	OE1-CD-NE2	-6.38	116.22	122.60
2	1	116	VAL	N-CA-C	6.38	121.35	112.35
2	1	239	ILE	N-CA-C	6.38	119.48	108.90
2	1	203	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	0	236	GLN	OE1-CD-NE2	-6.33	116.27	122.60
2	1	270	CYS	CA-C-N	6.29	126.25	119.78
2	1	270	CYS	C-N-CA	6.29	126.25	119.78
1	0	39	ASN	OD1-CG-ND2	-6.25	116.35	122.60
3	3	161	GLN	OE1-CD-NE2	-6.24	116.36	122.60
3	3	31	THR	CA-C-N	6.19	126.76	120.38
3	3	31	THR	C-N-CA	6.19	126.76	120.38
1	0	316	ILE	CA-C-N	6.18	126.10	119.85
1	0	316	ILE	C-N-CA	6.18	126.10	119.85
1	0	6	SER	N-CA-C	6.17	118.50	108.76
1	0	295	ASN	N-CA-C	6.16	118.91	111.40
1	0	99	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	0	13	HIS	CA-CB-CG	-6.14	107.66	113.80
2	1	236	ASP	N-CA-C	6.12	118.49	111.02
2	1	246	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	0	182	ASN	N-CA-C	6.10	120.00	110.17
1	0	258	ASN	OD1-CG-ND2	-6.10	116.50	122.60
2	1	113	LYS	N-CA-C	6.10	120.72	113.16
1	0	205	SER	N-CA-C	6.09	119.75	109.76
2	1	217	LEU	N-CA-C	6.04	118.56	108.96
2	1	281	GLY	CA-C-N	5.99	125.61	119.56
2	1	281	GLY	C-N-CA	5.99	125.61	119.56
2	1	88	THR	N-CA-C	5.98	117.62	108.42
2	1	170	TRP	CA-C-N	5.97	129.39	120.31
2	1	170	TRP	C-N-CA	5.97	129.39	120.31
1	0	293	HIS	CA-CB-CG	5.96	119.76	113.80
1	0	71	PRO	N-CA-C	5.96	119.56	111.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	9	GLY	CA-C-O	5.95	124.74	119.56
1	0	182	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	0	4	GLN	OE1-CD-NE2	-5.87	116.73	122.60
1	0	279	LEU	N-CA-C	5.85	117.93	109.04
1	0	268	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	0	247	ASP	N-CA-C	5.80	118.09	111.02
1	0	330	ASN	CB-CG-ND2	5.80	125.09	116.40
2	1	291	LEU	N-CA-C	5.77	119.95	113.02
3	3	52	MET	N-CA-C	5.76	118.92	109.76
1	0	293	HIS	N-CA-C	5.74	118.47	108.76
1	0	341	GLN	OE1-CD-NE2	-5.74	116.86	122.60
2	1	117	GLN	N-CA-C	5.74	117.40	111.03
2	1	147	ASN	N-CA-CB	-5.73	107.63	114.17
2	1	299	LEU	N-CA-C	5.73	120.82	111.37
3	3	209	ASP	N-CA-C	5.72	118.80	109.59
1	0	106	ARG	CA-CB-CG	-5.72	102.67	114.10
1	0	101	VAL	N-CA-C	5.70	115.88	108.35
1	0	130	CYS	CA-CB-SG	-5.70	101.30	114.40
1	0	75	ALA	N-CA-C	5.68	122.89	110.80
1	0	218	ASN	CA-C-N	5.67	125.77	119.87
1	0	218	ASN	C-N-CA	5.67	125.77	119.87
1	0	239	PRO	N-CA-C	5.67	119.76	111.03
2	1	94	ASN	OD1-CG-ND2	-5.66	116.94	122.60
3	3	11	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	0	129	ALA	CA-C-O	5.63	125.78	119.41
1	0	327	CYS	N-CA-C	5.62	118.97	109.76
3	3	168	VAL	CA-C-N	5.62	125.54	119.76
3	3	168	VAL	C-N-CA	5.62	125.54	119.76
3	3	160	LEU	CA-C-N	-5.60	114.12	122.74
3	3	160	LEU	C-N-CA	-5.60	114.12	122.74
1	0	109	GLU	N-CA-C	5.59	117.76	108.99
2	1	141	ASN	N-CA-C	5.58	116.75	108.60
1	0	95	GLN	CB-CG-CD	5.58	122.08	112.60
1	0	196	VAL	CA-C-N	5.57	125.49	119.76
1	0	196	VAL	C-N-CA	5.57	125.49	119.76
2	1	249	ASN	CA-C-N	5.54	126.77	119.84
2	1	249	ASN	C-N-CA	5.54	126.77	119.84
1	0	206	ASN	OD1-CG-ND2	-5.54	117.06	122.60
2	1	298	ASP	CA-CB-CG	5.54	118.14	112.60
2	1	249	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	0	39	ASN	N-CA-C	5.52	118.23	110.23
1	0	91	THR	N-CA-C	5.51	117.60	108.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	42	ASN	OD1-CG-ND2	-5.51	117.09	122.60
2	1	99	THR	N-CA-C	5.50	122.52	110.80
2	1	278	ALA	N-CA-C	5.49	118.43	110.42
1	0	225	THR	N-CA-C	5.48	118.16	109.50
2	1	214	LYS	N-CA-C	5.47	117.57	108.99
1	0	236	GLN	N-CA-C	5.45	122.42	110.80
1	0	7	SER	N-CA-C	5.44	118.69	110.64
3	3	71	ARG	N-CA-C	5.43	118.40	109.76
1	0	294	ASN	OD1-CG-ND2	-5.43	117.17	122.60
2	1	258	ARG	NE-CZ-NH2	5.43	124.08	119.20
1	0	10	VAL	N-CA-C	5.42	117.61	109.20
1	0	143	GLU	N-CA-C	5.42	120.58	112.94
3	3	153	HIS	N-CA-C	5.42	117.31	109.07
3	3	32	PRO	N-CA-C	5.41	117.30	110.70
2	1	235	ASN	N-CA-C	5.39	119.05	107.67
1	0	238	SER	CA-C-N	5.39	125.65	119.83
1	0	238	SER	C-N-CA	5.39	125.65	119.83
1	0	94	THR	O-C-N	-5.39	117.02	123.27
1	0	313	SER	N-CA-C	5.38	120.81	108.81
2	1	138	VAL	N-CA-C	5.38	115.60	107.80
3	3	220	PHE	N-CA-C	5.37	118.97	109.96
1	0	264	HIS	N-CA-C	5.36	116.14	108.74
2	1	147	ASN	OD1-CG-ND2	-5.36	117.24	122.60
2	1	93	ASP	CA-CB-CG	5.35	117.95	112.60
1	0	304	ALA	CA-C-N	5.35	125.27	119.76
1	0	304	ALA	C-N-CA	5.35	125.27	119.76
2	1	153	GLN	N-CA-C	5.32	118.89	109.96
3	3	122	GLY	O-C-N	-5.31	118.24	122.81
1	0	229	THR	N-CA-C	5.30	117.81	108.75
1	0	5	VAL	N-CA-C	5.29	115.93	108.36
2	1	160	VAL	CA-C-N	5.28	123.46	119.66
2	1	160	VAL	C-N-CA	5.28	123.46	119.66
1	0	202	ALA	N-CA-C	5.27	117.93	110.50
2	1	93	ASP	N-CA-C	5.25	116.78	108.96
2	1	94	ASN	CA-C-N	5.24	125.71	120.52
2	1	94	ASN	C-N-CA	5.24	125.71	120.52
2	1	193	ARG	N-CA-C	5.23	116.89	108.32
2	1	101	LYS	N-CA-C	5.22	118.45	110.20
3	3	25	LEU	CA-C-N	5.22	125.16	119.78
3	3	25	LEU	C-N-CA	5.22	125.16	119.78
3	3	143	LYS	CA-C-O	5.21	124.78	119.05
2	1	152	ASN	OD1-CG-ND2	-5.20	117.41	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	105	ASN	N-CA-C	5.18	119.45	113.18
1	0	33	TYR	N-CA-C	5.18	118.17	110.14
2	1	146	ASN	CB-CA-C	-5.16	100.15	110.42
1	0	112	ARG	O-C-N	5.15	129.02	123.10
1	0	216	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	0	12	ALA	N-CA-C	5.15	119.03	109.56
2	1	185	TYR	N-CA-C	5.14	117.63	109.24
2	1	212	PHE	N-CA-C	5.14	117.95	109.72
3	3	88	SER	CA-C-N	5.14	125.18	119.32
3	3	88	SER	C-N-CA	5.14	125.18	119.32
2	1	264	LYS	CB-CA-C	-5.13	101.34	109.80
1	0	288	ASP	CA-CB-CG	5.12	117.72	112.60
2	1	106	ALA	N-CA-C	5.12	118.56	109.96
2	1	171	ASP	CA-CB-CG	5.11	117.71	112.60
1	0	273	ASN	N-CA-C	5.09	119.19	112.92
2	1	243	ARG	N-CA-C	5.09	116.98	108.99
3	3	12	GLN	OE1-CD-NE2	-5.08	117.52	122.60
3	3	178	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	1	171	ASP	CB-CA-C	-5.06	100.95	110.67
2	1	237	PHE	CA-CB-CG	-5.03	108.77	113.80
1	0	44	GLN	OE1-CD-NE2	-5.01	117.59	122.60

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	2312	0	2230	56	0
2	1	1874	0	1822	36	0
3	3	1849	0	1820	34	0
4	0	15	0	27	0	0
5	1	21	0	36	5	0
6	0	73	0	0	3	0
6	1	75	0	0	1	0
6	3	62	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6281	0	5935	112	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 9.

All (112) 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)
1:0:95:GLN:HG3	1:0:96:GLU:N	1.83	0.94
1:0:256:LEU:HD22	3:3:65:MET:SD	2.17	0.85
2:1:217:LEU:H	2:1:220:GLN:NE2	1.74	0.84
2:1:109:LYS:HA	2:1:239:ILE:HG22	1.63	0.79
2:1:217:LEU:H	2:1:220:GLN:HE21	1.30	0.79
1:0:292:LYS:HE2	2:1:214:LYS:HA	1.63	0.79
2:1:132:MET:HE1	5:1:0:SPH:H101	1.69	0.74
3:3:232:GLU:HG2	6:3:272:HOH:O	1.89	0.72
1:0:127:VAL:HG12	1:0:129:ALA:H	1.56	0.71
3:3:175:THR:HG22	3:3:176:TYR:CD1	2.27	0.69
2:1:191:PRO:HG2	3:3:13:TYR:HB2	1.75	0.69
1:0:212:THR:HG23	1:0:242:ARG:HA	1.74	0.69
2:1:68:GLN:O	2:1:69:HIS:HB2	1.92	0.69
3:3:167:VAL:O	3:3:169:PRO:HD3	1.93	0.67
3:3:124:MET:HG3	6:3:275:HOH:O	1.95	0.66
1:0:311:GLU:HG3	6:0:405:HOH:O	1.97	0.64
1:0:112:ARG:NE	1:0:112:ARG:HA	2.14	0.63
2:1:132:MET:CE	5:1:0:SPH:H101	2.27	0.63
3:3:109:HIS:ND1	3:3:223:ARG:NH1	2.47	0.62
1:0:112:ARG:HA	1:0:112:ARG:HE	1.64	0.62
2:1:115:THR:HA	3:3:233:GLN:HE22	1.64	0.61
1:0:63:LYS:HE3	1:0:69:ASN:ND2	2.15	0.60
1:0:111:LEU:C	1:0:112:ARG:HE	2.11	0.59
1:0:106:ARG:O	1:0:280:PRO:HG3	2.03	0.58
2:1:249:ASN:CG	2:1:250:PRO:HD2	2.29	0.58
1:0:206:ASN:HD21	2:1:287:LYS:HA	1.68	0.58
2:1:217:LEU:N	2:1:220:GLN:HE21	1.98	0.58
3:3:50:ASP:HA	3:3:215:SER:HB3	1.87	0.57
3:3:201:PRO:O	3:3:204:THR:HG23	2.05	0.57
1:0:7:SER:HA	1:0:26:ASN:HB3	1.87	0.57
1:0:90:SER:HB2	1:0:132:PHE:HB2	1.87	0.57
1:0:150:LYS:HE3	2:1:210:ASP:OD2	2.05	0.57
3:3:202:LEU:O	3:3:204:THR:HG22	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:83:LEU:HB2	1:0:94:THR:O	2.07	0.55
1:0:112:ARG:HE	1:0:112:ARG:CA	2.20	0.55
2:1:217:LEU:O	2:1:220:GLN:HG2	2.07	0.55
1:0:167:TYR:CE2	1:0:335:ILE:HD12	2.42	0.54
1:0:142:LYS:HE3	1:0:314:PRO:HD2	1.88	0.54
1:0:197:PRO:O	2:1:272:ARG:NH2	2.42	0.52
1:0:111:LEU:HB2	1:0:172:ARG:HD3	1.90	0.52
3:3:75:LYS:HB2	3:3:76:PRO:HD2	1.91	0.52
1:0:72:ASN:H	1:0:75:ALA:HB3	1.74	0.51
1:0:95:GLN:HG3	1:0:96:GLU:H	1.73	0.51
1:0:71:PRO:O	1:0:101:VAL:HA	2.11	0.51
1:0:60:VAL:HA	3:3:218:ASN:OD1	2.10	0.51
1:0:107:TRP:CG	1:0:108:PRO:HD2	2.45	0.50
1:0:103:ALA:HB3	1:0:280:PRO:HD2	1.94	0.49
2:1:146:ASN:O	2:1:147:ASN:HB3	2.12	0.49
1:0:110:TYR:O	1:0:112:ARG:N	2.46	0.49
2:1:103:LYS:HD3	2:1:170:TRP:CG	2.47	0.49
1:0:107:TRP:CD1	1:0:108:PRO:HD2	2.47	0.49
2:1:99:THR:HG22	2:1:101:LYS:N	2.28	0.49
1:0:57:ILE:HG12	1:0:58:LYS:H	1.77	0.49
3:3:231:ILE:HG13	3:3:232:GLU:N	2.28	0.48
2:1:98:THR:OG1	2:1:99:THR:N	2.47	0.48
1:0:59:ASP:HB3	1:0:62:ILE:HD12	1.95	0.48
1:0:34:ARG:O	1:0:34:ARG:HG2	2.13	0.48
2:1:103:LYS:HD3	2:1:170:TRP:CD2	2.49	0.47
3:3:233:GLN:HB3	3:3:236:LEU:CB	2.44	0.47
2:1:159:TYR:O	2:1:161:PRO:HD3	2.14	0.47
2:1:280:TYR:HB3	2:1:285:ASP:O	2.14	0.47
1:0:71:PRO:HG2	1:0:105:GLY:HA2	1.96	0.47
3:3:232:GLU:HG3	3:3:234:LYS:H	1.79	0.47
1:0:179:VAL:HG22	1:0:320:LEU:CD2	2.45	0.47
1:0:308:PHE:O	1:0:310:SER:N	2.48	0.46
1:0:86:THR:OG1	1:0:91:THR:HG23	2.16	0.46
3:3:51:THR:HG21	3:3:99:MET:HB2	1.97	0.46
1:0:132:PHE:CD1	1:0:323:ALA:HB2	2.51	0.46
2:1:112:TYR:HD2	5:1:0:SPH:H5	1.80	0.46
1:0:112:ARG:NH2	1:0:328:GLU:OE1	2.49	0.46
1:0:223:GLY:HA3	6:0:364:HOH:O	2.17	0.46
3:3:7:THR:HB	3:3:8:PRO:HD2	1.98	0.45
1:0:97:ALA:C	1:0:99:ASN:N	2.73	0.45
1:0:112:ARG:NE	1:0:112:ARG:CA	2.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:270:ARG:NH1	3:3:123:SER:O	2.50	0.45
1:0:83:LEU:O	1:0:94:THR:N	2.51	0.44
2:1:145:THR:O	2:1:147:ASN:N	2.51	0.44
2:1:107:VAL:HG13	2:1:239:ILE:HD13	1.99	0.44
1:0:66:PRO:O	1:0:69:ASN:N	2.48	0.44
1:0:261:VAL:HA	3:3:49:ILE:HG21	2.00	0.44
3:3:97:HIS:CE1	3:3:230:HIS:ND1	2.86	0.44
2:1:302:TYR:CE1	3:3:189:TYR:HB3	2.54	0.43
1:0:13:HIS:N	1:0:13:HIS:ND1	2.65	0.43
1:0:309:ALA:HA	3:3:205:PRO:HD3	2.00	0.43
2:1:144:GLU:HB2	2:1:146:ASN:ND2	2.34	0.42
1:0:10:VAL:HG12	1:0:11:GLY:O	2.20	0.42
1:0:338:PRO:HB2	1:0:340:LEU:HG	2.00	0.42
1:0:311:GLU:HB3	6:0:346:HOH:O	2.19	0.42
2:1:149:HIS:CD2	6:1:307:HOH:O	2.73	0.42
3:3:89:PRO:HB2	3:3:104:LEU:CD1	2.50	0.42
2:1:89:ILE:HG12	2:1:258:ARG:HG2	2.02	0.42
2:1:237:PHE:CZ	5:1:0:SPH:H4	2.55	0.41
3:3:89:PRO:HB2	3:3:104:LEU:HD12	2.01	0.41
1:0:172:ARG:HB3	1:0:287:ILE:HG13	2.01	0.41
3:3:71:ARG:NH1	3:3:209:ASP:OD1	2.49	0.41
3:3:233:GLN:O	3:3:236:LEU:N	2.53	0.41
1:0:68:LEU:HD11	3:3:40:VAL:HG22	2.02	0.41
2:1:209:TYR:O	2:1:230:GLY:HA2	2.20	0.41
2:1:257:ILE:HD12	2:1:257:ILE:N	2.36	0.41
3:3:97:HIS:CE1	3:3:230:HIS:CE1	3.08	0.41
1:0:60:VAL:HB	3:3:217:CYS:HB3	2.02	0.41
2:1:144:GLU:HB2	2:1:146:ASN:HD22	1.86	0.41
1:0:103:ALA:HB3	1:0:280:PRO:CD	2.50	0.41
3:3:87:LEU:HD13	3:3:190:ILE:HD11	2.03	0.41
3:3:10:SER:O	3:3:11:ASN:HB2	2.21	0.40
3:3:62:LYS:O	3:3:64:THR:HG23	2.21	0.40
3:3:152:THR:HG22	3:3:166:MET:HE2	2.03	0.40
1:0:43:LYS:HD3	1:0:43:LYS:HA	1.76	0.40
2:1:78:GLU:OE2	2:1:265:HIS:N	2.54	0.40
2:1:286:TYR:HB2	2:1:291:LEU:HD11	2.03	0.40
1:0:166:TYR:CE1	1:0:338:PRO:HG3	2.57	0.40
2:1:112:TYR:CD2	5:1:0:SPH:H5	2.56	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	290/340 (85%)	258 (89%)	26 (9%)	6 (2%)	5	20
2	1	233/302 (77%)	213 (91%)	15 (6%)	5 (2%)	5	20
3	3	236/238 (99%)	218 (92%)	16 (7%)	2 (1%)	16	44
All	All	759/880 (86%)	689 (91%)	57 (8%)	13 (2%)	7	25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	111	LEU
1	0	309	ALA
2	1	146	ASN
3	3	234	LYS
3	3	235	ALA
1	0	11	GLY
1	0	43	LYS
2	1	99	THR
1	0	75	ALA
2	1	82	ALA
2	1	219	ASP
1	0	66	PRO
2	1	69	HIS

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	250/289 (86%)	231 (92%)	19 (8%)	12	36
2	1	205/261 (78%)	199 (97%)	6 (3%)	37	73
3	3	210/212 (99%)	203 (97%)	7 (3%)	33	69
All	All	665/762 (87%)	633 (95%)	32 (5%)	23	56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	13	HIS
1	0	26	ASN
1	0	29	THR
1	0	36	SER
1	0	44	GLN
1	0	57	ILE
1	0	72	ASN
1	0	76	CYS
1	0	94	THR
1	0	96	GLU
1	0	99	ASN
1	0	112	ARG
1	0	135	LEU
1	0	172	ARG
1	0	206	ASN
1	0	225	THR
1	0	261	VAL
1	0	307	ASN
1	0	339	ARG
2	1	145	THR
2	1	149	HIS
2	1	194	ILE
2	1	251	THR
2	1	291	LEU
2	1	298	ASP
3	3	58	SER
3	3	60	THR
3	3	158	ILE
3	3	161	GLN
3	3	190	ILE
3	3	204	THR
3	3	224	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	0	4	GLN
1	0	69	ASN
1	0	180	GLN
1	0	188	GLN
1	0	235	ASN
1	0	330	ASN
1	0	341	GLN
2	1	100	ASN
2	1	146	ASN
2	1	203	ASN
2	1	220	GLN
3	3	97	HIS
3	3	233	GLN

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
4	MYR	0	1	1	13,14,15	0.56	0	12,13,15	0.88	0
5	SPH	1	0	-	19,20,20	0.89	1 (5%)	18,21,21	3.50	6 (33%)

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
4	MYR	0	1	1	-	6/12/12/13	-
5	SPH	1	0	-	2/2/2/4	8/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	0	SPH	O3-C3	3.13	1.49	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	0	SPH	O3-C3-C2	-9.63	91.11	107.31
5	1	0	SPH	O1-C1-C2	8.88	130.80	111.55
5	1	0	SPH	O3-C3-C4	-4.21	99.99	110.88
5	1	0	SPH	C3-C4-C5	-3.49	117.45	124.69
5	1	0	SPH	C6-C5-C4	-3.15	111.41	125.47
5	1	0	SPH	C1-C2-C3	2.26	117.67	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	1	0	SPH	C3
5	1	0	SPH	C2

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	0	1	MYR	O1-C1-C2-C3
5	1	0	SPH	O1-C1-C2-C3
5	1	0	SPH	N2-C2-C3-O3
5	1	0	SPH	N2-C2-C3-C4
5	1	0	SPH	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

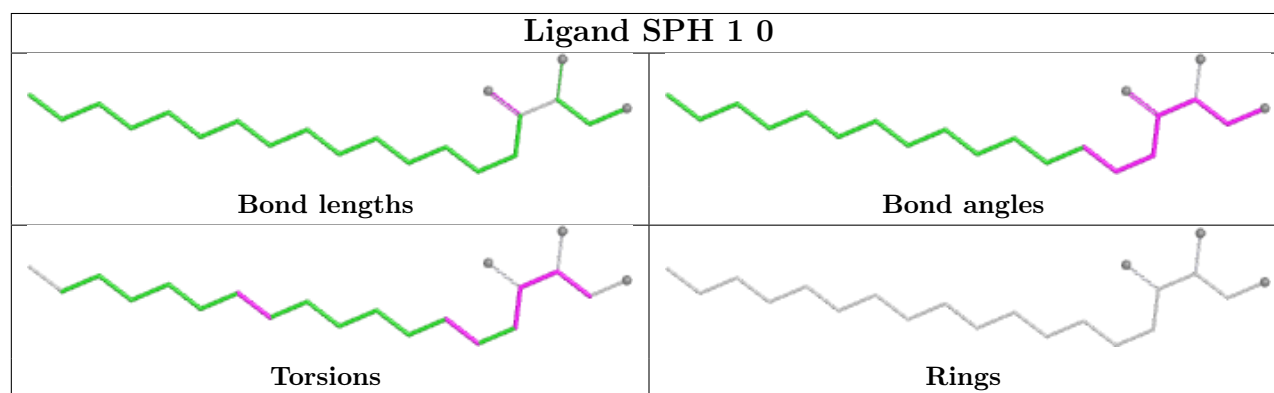
Mol	Chain	Res	Type	Atoms
5	1	0	SPH	O3-C3-C4-C5
4	0	1	MYR	C4-C5-C6-C7
5	1	0	SPH	C4-C5-C6-C7
4	0	1	MYR	C9-C10-C11-C12
4	0	1	MYR	C3-C4-C5-C6
4	0	1	MYR	C6-C7-C8-C9
4	0	1	MYR	C11-C12-C13-C14
5	1	0	SPH	O1-C1-C2-N2
5	1	0	SPH	C10-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	0	SPH	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.