



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:01 PM UTC

PDB ID : 1HXS / pdb_00001hxs
Title : CRYSTAL STRUCTURE OF MAHONEY STRAIN OF POLIOVIRUS AT 2.2A RESOLUTION
Authors : Miller, S.T.; Hogle, J.M.; Filman, D.J.
Deposited on : 2001-01-16
Resolution : 2.20 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

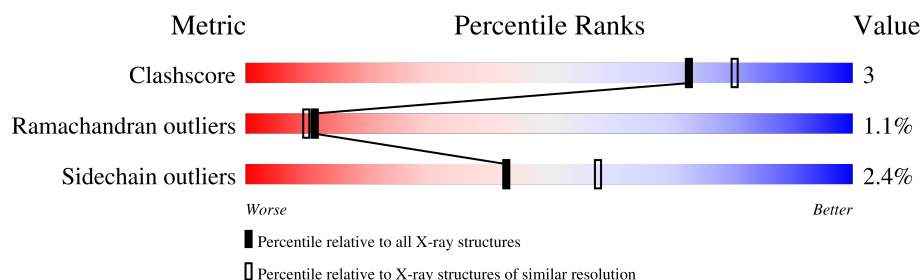
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	1	302	 76% 17% • 5%
2	2	272	 78% 18% ••
3	3	237	 78% 18% ••
4	4	68	 56% 38% ••

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7256 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 GENOME POLYPROTEIN, COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	288	Total	C	N	O	S	0	0	0
			2250	1431	383	431	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	6	GLY	LEU	SEE REMARK 999	UNP P03300
1	7	SER	GLU	SEE REMARK 999	UNP P03300
1	9	SER	MET	SEE REMARK 999	UNP P03300
1	10	THR	ILE	SEE REMARK 999	UNP P03300

- Molecule 2 is a protein called GENOME POLYPROTEIN, COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	267	Total	C	N	O	S	0	0	0
			2075	1312	357	392	14			

- Molecule 3 is a protein called GENOME POLYPROTEIN, COAT PROTEIN VP3.

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

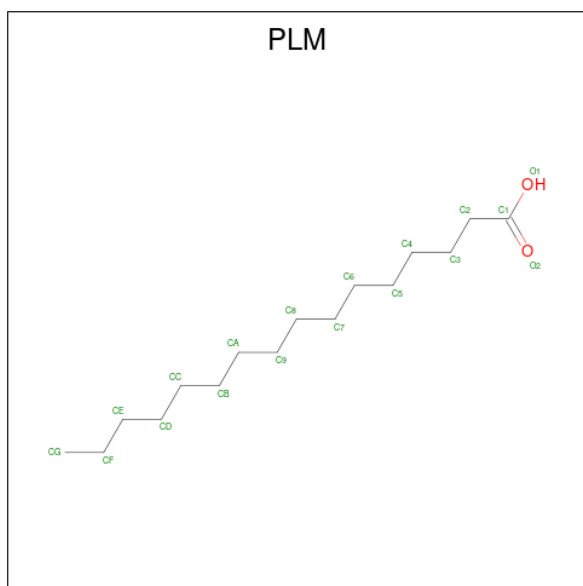
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	SEE REMARK 999	UNP P03300

- Molecule 4 is a protein called GENOME POLYPROTEIN, COAT PROTEIN VP4.

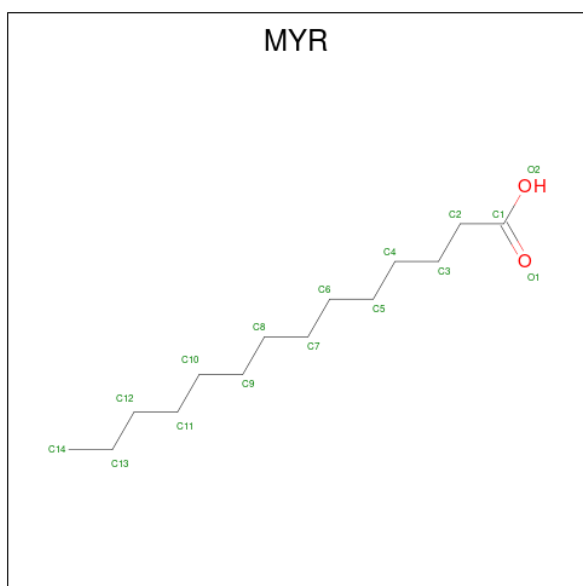
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	68	Total	C	N	O	S	0	0	0
			519	319	91	108	1			

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	1	1	Total	C	O	0	0
			18	16	2		

- Molecule 6 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	4	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is water.

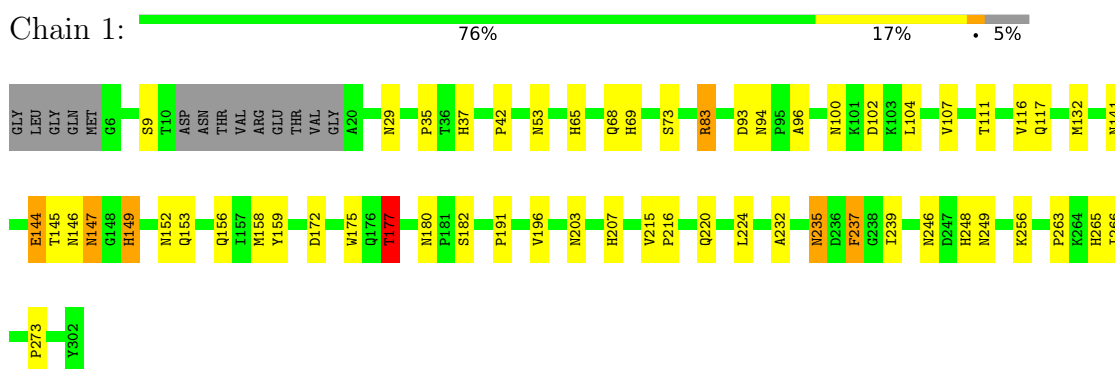
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	213	Total	O	0	0
			213	213		
7	2	136	Total	O	0	0
			136	136		
7	3	144	Total	O	0	0
			144	144		
7	4	52	Total	O	0	0
			52	52		

3 Residue-property plots

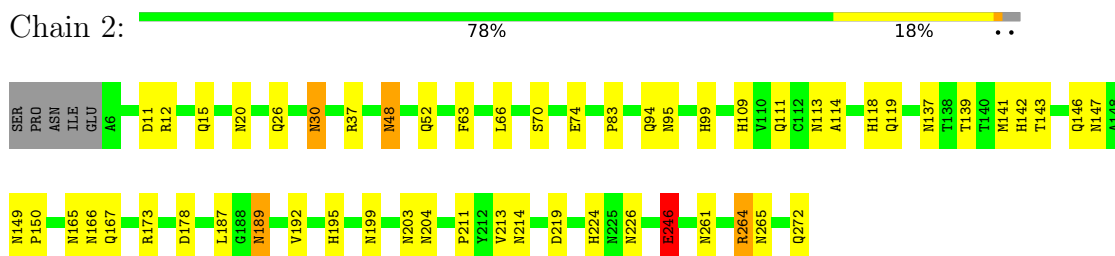
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

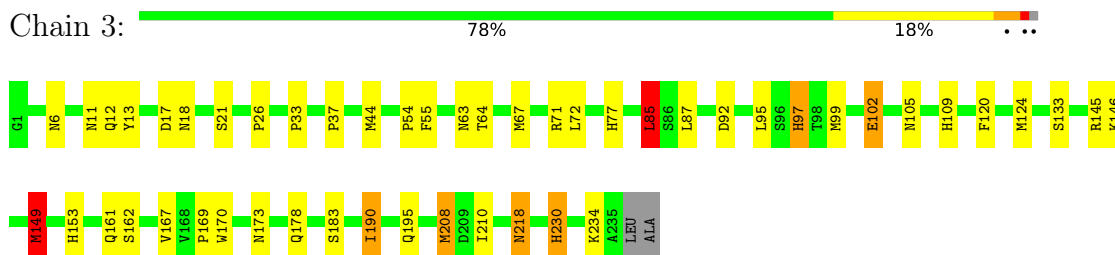
- Molecule 1: GENOME POLYPROTEIN, COAT PROTEIN VP1



- Molecule 2: GENOME POLYPROTEIN, COAT PROTEIN VP2



- Molecule 3: GENOME POLYPROTEIN, COAT PROTEIN VP3



- Molecule 4: GENOME POLYPROTEIN, COAT PROTEIN VP4





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	320.50Å 355.25Å 377.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.268 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: PLM, 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	1	0.97	7/2312 (0.3%)	1.74	51/3160 (1.6%)
2	2	0.95	7/2132 (0.3%)	1.76	51/2916 (1.7%)
3	3	0.99	8/1881 (0.4%)	1.61	36/2562 (1.4%)
4	4	1.12	1/528 (0.2%)	2.08	21/714 (2.9%)
All	All	0.98	23/6853 (0.3%)	1.74	159/9352 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	230	HIS	CD2-NE2	-7.01	1.30	1.37
3	3	109	HIS	CD2-NE2	-6.98	1.30	1.37
3	3	153	HIS	CD2-NE2	-6.80	1.30	1.37
2	2	118	HIS	CD2-NE2	-6.78	1.30	1.37
3	3	97	HIS	CD2-NE2	-6.76	1.30	1.37
2	2	109	HIS	CD2-NE2	-6.54	1.30	1.37
1	1	69	HIS	CD2-NE2	-6.51	1.30	1.37
1	1	65	HIS	CD2-NE2	-6.51	1.30	1.37
3	3	77	HIS	CD2-NE2	-6.47	1.30	1.37
2	2	224	HIS	CD2-NE2	-6.42	1.30	1.37
2	2	195	HIS	CD2-NE2	-6.16	1.31	1.37
1	1	207	HIS	CD2-NE2	-6.11	1.31	1.37
1	1	37	HIS	CD2-NE2	-6.08	1.31	1.37
1	1	265	HIS	CD2-NE2	-6.07	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	153	HIS	CG-ND1	-5.95	1.31	1.38
2	2	99	HIS	CD2-NE2	-5.76	1.31	1.37
1	1	248	HIS	CD2-NE2	-5.48	1.31	1.37
2	2	142	HIS	CD2-NE2	-5.42	1.31	1.37
3	3	71	ARG	NE-CZ	5.38	1.39	1.33
2	2	118	HIS	CG-ND1	-5.30	1.32	1.38
1	1	248	HIS	CG-ND1	-5.29	1.32	1.38
3	3	102	GLU	CB-CG	5.15	1.67	1.52
4	4	20	TYR	CA-CB	5.04	1.61	1.53

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	218	ASN	OD1-CG-ND2	-11.68	110.92	122.60
1	1	83	ARG	NE-CZ-NH2	-10.32	109.92	119.20
2	2	26	GLN	OE1-CD-NE2	-9.96	112.64	122.60
4	4	44	GLN	OE1-CD-NE2	-9.13	113.47	122.60
2	2	165	ASN	CA-CB-CG	-8.89	103.71	112.60
4	4	46	PHE	CA-CB-CG	-8.51	105.29	113.80
1	1	117	GLN	OE1-CD-NE2	-8.24	114.36	122.60
2	2	137	ASN	OD1-CG-ND2	-8.23	114.37	122.60
4	4	31	ASN	OD1-CG-ND2	-8.14	114.46	122.60
3	3	97	HIS	CB-CG-CD2	-8.13	120.63	131.20
4	4	48	GLN	OE1-CD-NE2	-8.09	114.51	122.60
4	4	8	GLN	OE1-CD-NE2	-7.96	114.64	122.60
1	1	266	ILE	N-CA-C	7.90	120.48	108.71
1	1	83	ARG	NE-CZ-NH1	7.89	129.39	121.50
3	3	149	MET	CA-CB-CG	7.88	129.87	114.10
1	1	232	ALA	O-C-N	-7.83	114.71	123.48
4	4	4	GLN	OE1-CD-NE2	-7.82	114.78	122.60
2	2	261	ASN	OD1-CG-ND2	-7.67	114.93	122.60
1	1	235	ASN	OD1-CG-ND2	-7.66	114.94	122.60
3	3	105	ASN	OD1-CG-ND2	-7.63	114.97	122.60
3	3	173	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	1	215	VAL	CB-CA-C	-7.44	102.75	110.71
2	2	48	ASN	OD1-CG-ND2	-7.44	115.16	122.60
4	4	51	SER	N-CA-C	7.37	121.19	111.75
1	1	235	ASN	CA-CB-CG	-7.29	105.31	112.60
1	1	53	ASN	OD1-CG-ND2	-7.29	115.31	122.60
2	2	219	ASP	CA-CB-CG	7.26	119.86	112.60
1	1	263	PRO	N-CA-CB	7.24	106.97	102.92
2	2	95	ASN	OD1-CG-ND2	-7.21	115.39	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	220	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	1	147	ASN	OD1-CG-ND2	-7.12	115.48	122.60
2	2	20	ASN	OD1-CG-ND2	-7.07	115.53	122.60
2	2	165	ASN	OD1-CG-ND2	-7.02	115.58	122.60
4	4	39	ASN	OD1-CG-ND2	-6.99	115.61	122.60
4	4	49	ASP	CA-CB-CG	6.91	119.51	112.60
3	3	162	SER	N-CA-C	6.87	120.76	112.38
2	2	214	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	1	100	ASN	OD1-CG-ND2	-6.75	115.85	122.60
2	2	204	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	1	149	HIS	CB-CG-CD2	-6.74	122.44	131.20
2	2	147	ASN	OD1-CG-ND2	-6.72	115.88	122.60
3	3	161	GLN	OE1-CD-NE2	-6.67	115.93	122.60
4	4	18	ARG	N-CA-C	-6.65	103.32	112.03
3	3	17	ASP	CA-CB-CG	6.65	119.25	112.60
2	2	264	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	1	116	VAL	N-CA-C	6.63	119.59	112.96
2	2	167	GLN	CA-CB-CG	-6.63	100.83	114.10
2	2	178	ASP	N-CA-C	6.63	119.06	111.11
2	2	226	ASN	OD1-CG-ND2	-6.61	115.99	122.60
2	2	113	ASN	OD1-CG-ND2	-6.60	116.00	122.60
2	2	146	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	1	69	HIS	CB-CG-CD2	-6.58	122.64	131.20
3	3	183	SER	N-CA-C	6.50	118.36	111.28
1	1	83	ARG	CG-CD-NE	-6.48	97.75	112.00
2	2	224	HIS	CA-CB-CG	6.45	120.25	113.80
2	2	15	GLN	OE1-CD-NE2	-6.42	116.18	122.60
3	3	218	ASN	CB-CG-ND2	6.38	125.97	116.40
1	1	141	ASN	OD1-CG-ND2	-6.38	116.22	122.60
2	2	142	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	1	149	HIS	CA-CB-CG	-6.37	107.43	113.80
2	2	94	GLN	OE1-CD-NE2	-6.32	116.28	122.60
3	3	54	PRO	N-CA-CB	6.25	106.79	102.35
3	3	11	ASN	OD1-CG-ND2	-6.25	116.35	122.60
4	4	10	VAL	N-CA-C	6.24	117.77	108.54
3	3	6	ASN	OD1-CG-ND2	-6.23	116.37	122.60
4	4	69	ASN	OD1-CG-ND2	-6.17	116.42	122.60
4	4	24	THR	CA-C-N	-6.17	115.00	122.90
4	4	24	THR	C-N-CA	-6.17	115.00	122.90
1	1	68	GLN	OE1-CD-NE2	-6.16	116.44	122.60
4	4	17	ASN	CA-C-O	6.14	126.55	121.02
4	4	13	HIS	CB-CG-CD2	-6.12	123.24	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	263	PRO	O-C-N	-6.08	118.42	122.73
1	1	172	ASP	CA-CB-CG	6.06	118.66	112.60
2	2	178	ASP	CA-CB-CG	6.00	118.60	112.60
2	2	63	PHE	N-CA-C	5.99	118.40	109.59
2	2	52	GLN	OE1-CD-NE2	-5.99	116.61	122.60
2	2	199	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	1	246	ASN	OD1-CG-ND2	-5.98	116.62	122.60
3	3	149	MET	N-CA-CB	-5.97	100.48	110.39
1	1	94	ASN	OD1-CG-ND2	-5.97	116.63	122.60
2	2	99	HIS	CB-CG-CD2	-5.95	123.47	131.20
3	3	63	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	1	93	ASP	CA-CB-CG	5.89	118.49	112.60
1	1	237	PHE	CA-CB-CG	-5.88	107.92	113.80
1	1	256	LYS	CA-CB-CG	-5.86	102.37	114.10
2	2	119	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	1	153	GLN	OE1-CD-NE2	-5.86	116.74	122.60
3	3	85	LEU	CD1-CG-CD2	-5.86	97.91	110.80
1	1	9	SER	N-CA-C	5.82	117.89	108.41
3	3	97	HIS	CB-CG-ND1	5.81	131.42	122.70
2	2	246	GLU	CA-CB-CG	5.78	125.65	114.10
2	2	137	ASN	CA-CB-CG	-5.74	106.86	112.60
2	2	272	GLN	OE1-CD-NE2	-5.73	116.87	122.60
2	2	265	ASN	OD1-CG-ND2	-5.72	116.88	122.60
4	4	67	MET	CG-SD-CE	-5.72	88.32	100.90
3	3	102	GLU	CG-CD-OE1	-5.68	105.33	118.40
2	2	111	GLN	OE1-CD-NE2	-5.68	116.92	122.60
2	2	203	ASN	OD1-CG-ND2	-5.68	116.92	122.60
3	3	18	ASN	OD1-CG-ND2	-5.68	116.92	122.60
4	4	18	ARG	CA-CB-CG	5.63	125.37	114.10
2	2	137	ASN	CB-CG-ND2	5.62	124.83	116.40
3	3	170	TRP	CG-CD2-CE3	5.62	139.52	133.90
1	1	177	THR	CB-CA-C	-5.61	99.25	110.42
2	2	141	MET	CG-SD-CE	-5.61	88.56	100.90
3	3	26	PRO	N-CA-CB	5.61	108.23	103.35
3	3	21	SER	O-C-N	-5.60	117.93	121.85
3	3	133	SER	N-CA-C	5.60	118.59	109.24
2	2	109	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	1	153	GLN	N-CA-C	5.58	118.73	110.48
3	3	33	PRO	N-CA-CB	5.57	109.23	103.38
1	1	203	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	1	177	THR	OG1-CB-CG2	5.57	120.43	109.30
1	1	144	GLU	CB-CG-CD	5.56	122.06	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	248	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	1	104	LEU	N-CA-C	5.51	117.22	108.67
3	3	195	GLN	OE1-CD-NE2	-5.50	117.10	122.60
3	3	153	HIS	CB-CG-CD2	-5.45	124.12	131.20
2	2	12	ARG	CB-CG-CD	-5.43	98.82	111.30
4	4	66	PRO	N-CA-CB	5.42	108.15	103.27
2	2	118	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	1	29	ASN	OD1-CG-ND2	-5.39	117.21	122.60
2	2	95	ASN	CB-CG-ND2	5.39	124.48	116.40
4	4	18	ARG	CA-C-O	5.39	125.04	119.97
2	2	189	ASN	OD1-CG-ND2	-5.36	117.24	122.60
2	2	246	GLU	CB-CG-CD	5.36	121.71	112.60
2	2	30	ASN	OD1-CG-ND2	-5.33	117.27	122.60
2	2	83	PRO	N-CA-CB	5.33	108.46	102.60
2	2	149	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	1	156	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	1	102	ASP	N-CA-C	5.32	117.74	110.24
1	1	83	ARG	CA-CB-CG	5.31	124.72	114.10
1	1	216	PRO	N-CA-CB	5.30	108.02	103.36
3	3	102	GLU	CB-CG-CD	5.29	121.59	112.60
1	1	152	ASN	OD1-CG-ND2	-5.29	117.31	122.60
2	2	26	GLN	CG-CD-NE2	5.26	124.30	116.40
1	1	146	ASN	N-CA-CB	-5.26	103.09	111.62
1	1	111	THR	O-C-N	-5.25	118.26	123.46
2	2	211	PRO	N-CA-CB	5.25	108.89	103.38
3	3	102	GLU	CG-CD-OE2	5.23	130.44	118.40
2	2	48	ASN	CB-CG-ND2	5.23	124.25	116.40
4	4	69	ASN	CA-CB-CG	-5.23	107.37	112.60
3	3	170	TRP	CB-CG-CD1	-5.22	119.06	126.90
1	1	175	TRP	CG-CD2-CE3	5.20	139.10	133.90
3	3	170	TRP	CE2-CD2-CG	-5.19	100.97	107.20
3	3	55	PHE	N-CA-C	5.18	116.92	111.28
2	2	166	ASN	OD1-CG-ND2	-5.14	117.45	122.60
3	3	12	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	1	37	HIS	CA-CB-CG	5.11	118.91	113.80
3	3	109	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	1	117	GLN	N-CA-C	5.10	116.65	111.14
1	1	73	SER	N-CA-C	5.09	116.83	111.28
2	2	264	ARG	CB-CG-CD	5.08	122.98	111.30
2	2	150	PRO	N-CA-CB	5.07	108.01	103.20
3	3	92	ASP	CA-C-N	5.04	124.82	119.28
3	3	92	ASP	C-N-CA	5.04	124.82	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	105	ASN	CA-CB-CG	-5.02	107.58	112.60
1	1	175	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	1	69	HIS	CB-CG-ND1	5.02	130.22	122.70
1	1	35	PRO	N-CA-CB	5.00	108.09	103.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	11	ASP	Mainchain

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	1	2250	0	2197	17	0
2	2	2075	0	1994	8	0
3	3	1834	0	1816	19	0
4	4	519	0	497	6	0
5	1	18	0	31	6	0
6	4	15	0	27	0	0
7	1	213	0	0	2	0
7	2	136	0	0	1	0
7	3	144	0	0	1	0
7	4	52	0	0	0	0
All	All	7256	0	6562	43	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 3.

All (43) 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)
1:1:158:MET:SD	1:1:177:THR:HG23	2.23	0.79
1:1:132:MET:HE1	5:1:2000:PLM:H82	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:159:TYR:HB2	5:1:2000:PLM:HE2	1.72	0.71
1:1:237:PHE:CE2	5:1:2000:PLM:H21	2.32	0.64
1:1:177:THR:HG22	1:1:180:ASN:HB2	1.79	0.63
1:1:107:VAL:HG13	1:1:239:ILE:HD13	1.80	0.63
4:4:14:GLU:HB3	4:4:20:TYR:CD2	2.33	0.62
1:1:144:GLU:HG2	7:1:2107:HOH:O	1.99	0.62
3:3:72:LEU:HB2	3:3:208:MET:CE	2.30	0.61
1:1:177:THR:HG21	1:1:182:SER:OG	2.01	0.60
3:3:97:HIS:HA	3:3:102:GLU:HG2	1.85	0.58
1:1:235:ASN:HA	1:1:237:PHE:CZ	2.39	0.58
3:3:72:LEU:HB2	3:3:208:MET:HE2	1.85	0.57
7:2:1049:HOH:O	3:3:124:MET:HG2	2.06	0.55
1:1:191:PRO:HG2	3:3:13:TYR:HB2	1.88	0.54
1:1:273:PRO:HB3	2:2:189:ASN:HB2	1.91	0.52
2:2:213:VAL:HG22	3:3:37:PRO:HG2	1.90	0.52
2:2:192:VAL:HG11	3:3:99:MET:HE2	1.92	0.50
3:3:85:LEU:HD21	3:3:95:LEU:HD11	1.94	0.50
1:1:237:PHE:HE2	5:1:2000:PLM:H21	1.76	0.50
1:1:132:MET:SD	5:1:2000:PLM:H62	2.52	0.49
3:3:167:VAL:O	3:3:169:PRO:HD3	2.12	0.49
2:2:37:ARG:HG3	3:3:37:PRO:HB3	1.94	0.49
3:3:87:LEU:HD13	3:3:190:ILE:HD11	1.94	0.49
4:4:22:GLY:O	4:4:24:THR:N	2.47	0.48
3:3:97:HIS:ND1	3:3:102:GLU:OE2	2.43	0.48
1:1:237:PHE:CE2	5:1:2000:PLM:H52	2.48	0.48
3:3:44:MET:HE2	3:3:44:MET:HA	1.96	0.47
2:2:30:ASN:HD21	4:4:59:ASP:HB2	1.80	0.46
3:3:102:GLU:OE2	3:3:230:HIS:ND1	2.46	0.46
1:1:96:ALA:HA	1:1:249:ASN:O	2.16	0.46
3:3:146:LYS:HB2	7:3:1072:HOH:O	2.15	0.45
1:1:149:HIS:HB3	7:1:2174:HOH:O	2.18	0.44
3:3:145:ARG:O	3:3:149:MET:HB3	2.18	0.43
4:4:6:SER:HB2	4:4:27:TYR:CE1	2.54	0.43
2:2:187:LEU:O	2:2:187:LEU:HG	2.17	0.43
3:3:120:PHE:HA	3:3:210:ILE:HG22	2.01	0.43
3:3:64:THR:O	3:3:67:MET:HG2	2.20	0.41
2:2:143:THR:HG23	2:2:173:ARG:HA	2.02	0.41
3:3:234:LYS:HA	3:3:234:LYS:HD3	1.66	0.40
4:4:20:TYR:CD2	4:4:21:GLY:N	2.90	0.40
1:1:42:PRO:HA	4:4:63:LYS:O	2.22	0.40
2:2:70:SER:OG	2:2:246:GLU:HG2	2.21	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	1	284/302 (94%)	275 (97%)	8 (3%)	1 (0%)	30	34
2	2	265/272 (97%)	252 (95%)	11 (4%)	2 (1%)	16	16
3	3	233/237 (98%)	224 (96%)	9 (4%)	0	100	100
4	4	66/68 (97%)	54 (82%)	6 (9%)	6 (9%)	0	0
All	All	848/879 (96%)	805 (95%)	34 (4%)	9 (1%)	11	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	15	ASN
4	4	23	SER
4	4	24	THR
4	4	19	ALA
4	4	21	GLY
2	2	48	ASN
1	1	145	THR
2	2	114	ALA
4	4	60	VAL

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	1	249/260 (96%)	244 (98%)	5 (2%)	48	64
2	2	227/232 (98%)	222 (98%)	5 (2%)	45	61
3	3	210/211 (100%)	204 (97%)	6 (3%)	37	51
4	4	57/57 (100%)	55 (96%)	2 (4%)	32	43
All	All	743/760 (98%)	725 (98%)	18 (2%)	43	58

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	83	ARG
1	1	147	ASN
1	1	177	THR
1	1	196	VAL
1	1	224	LEU
2	2	66	LEU
2	2	74	GLU
2	2	139	THR
2	2	246	GLU
2	2	264	ARG
3	3	85	LEU
3	3	149	MET
3	3	178	GLN
3	3	190	ILE
3	3	208	MET
3	3	218	ASN
4	4	18	ARG
4	4	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	94	GLN
2	2	183	ASN
2	2	238	ASN
2	2	261	ASN
2	2	272	GLN
3	3	6	ASN
3	3	218	ASN
4	4	8	GLN
4	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$
5	PLM	1	2000	-	17,17,17	0.90	1 (5%)	17,17,17	1.01	1 (5%)
6	MYR	4	1	4	13,14,15	0.65	0	12,13,15	1.11	2 (16%)

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
5	PLM	1	2000	-	-	2/15/15/15	-
6	MYR	4	1	4	-	5/12/12/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	2000	PLM	C2-C1	2.11	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	4	1	MYR	C4-C3-C2	-2.37	102.45	113.86
6	4	1	MYR	C5-C4-C3	-2.11	103.70	114.37
5	1	2000	PLM	O1-C1-C2	2.08	120.57	114.00

There are no chirality outliers.

All (7) torsion outliers are listed below:

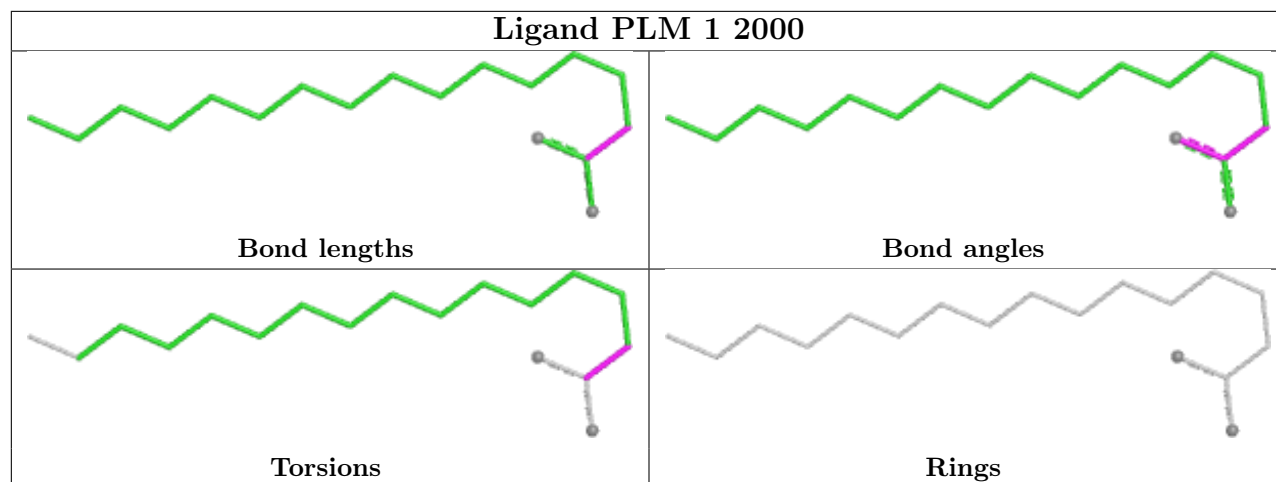
Mol	Chain	Res	Type	Atoms
6	4	1	MYR	C6-C7-C8-C9
6	4	1	MYR	C5-C6-C7-C8
6	4	1	MYR	C1-C2-C3-C4
5	1	2000	PLM	O2-C1-C2-C3
5	1	2000	PLM	O1-C1-C2-C3
6	4	1	MYR	C11-C12-C13-C14
6	4	1	MYR	C10-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	2000	PLM	6	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.