



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:42 PM UTC

PDB ID : 1CMK / pdb_00001cmk
Title : CRYSTAL STRUCTURES OF THE MYRISTYLATED CATALYTIC SUB-UNIT OF CAMP-DEPENDENT PROTEIN KINASE REVEAL OPEN AND CLOSED CONFORMATIONS
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Deposited on : 1993-11-18
Resolution : 2.90 Å(reported)

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

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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
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

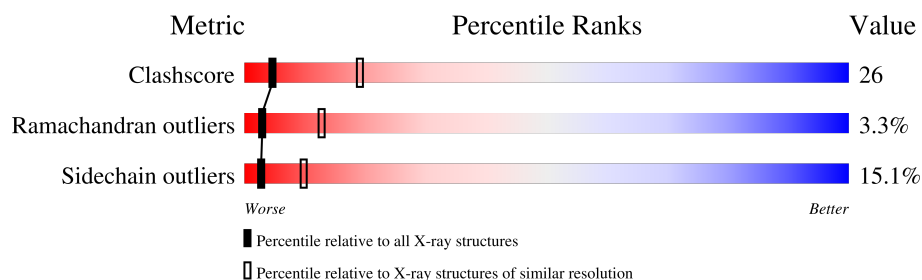
1 Overall quality at a glance

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	E	350	
2	I	22	

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
3	MYR	E	0	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3048 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 cAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	350	Total	C	N	O	P	S	0	0	0
			2874	1857	484	523	2	8			

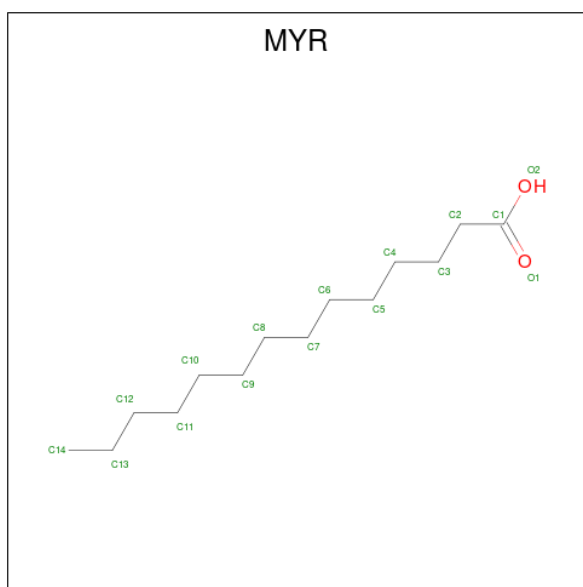
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	63	LYS	MET	conflict	UNP P00517
E	69	PHE	TYR	conflict	UNP P00517
E	108	TYR	PHE	conflict	UNP P00517
E	286	ASP	ASN	conflict	UNP P00517

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor, alpha form.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	1	0
			157	94	33	30			

- Molecule 3 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



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

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

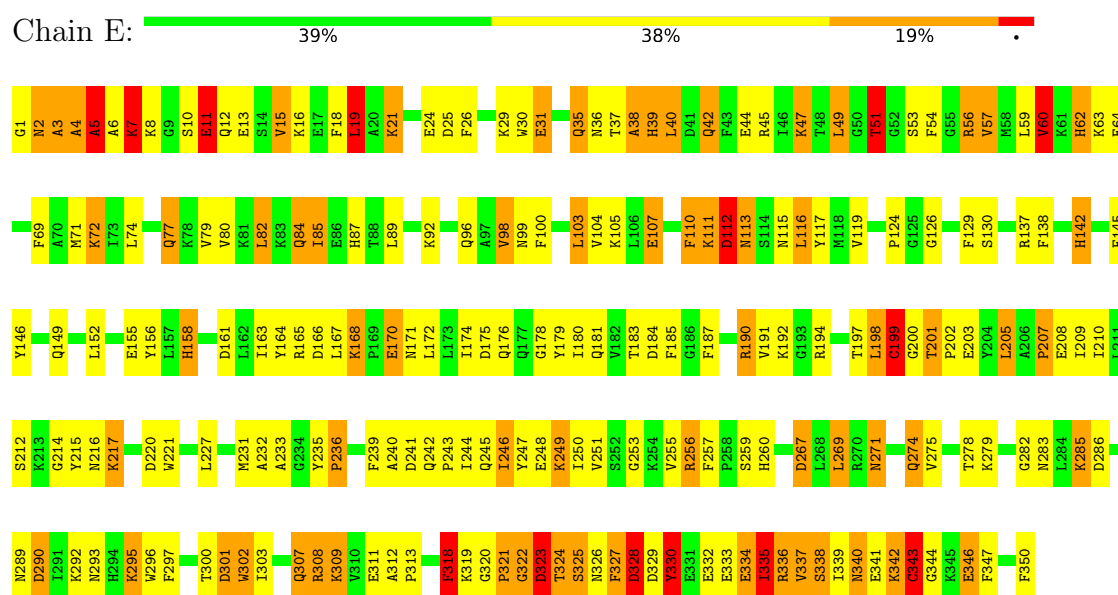
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	2	Total	I	0	0
			2	2		

3 Residue-property plots

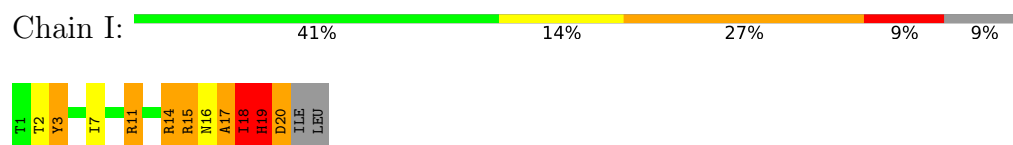
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: cAMP-dependent protein kinase inhibitor, alpha form



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	171.52Å 171.52Å 171.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 2.0	Depositor
R, R_{free}	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3048	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: TPO, IOD, SEP, 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	E	1.41	19/2924 (0.6%)	2.26	164/3936 (4.2%)
2	I	2.65	2/169 (1.2%)	3.43	21/227 (9.3%)
All	All	1.51	21/3093 (0.7%)	2.34	185/4163 (4.4%)

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
1	E	0	9
2	I	0	6
All	All	0	15

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	112	ASP	C-N	-22.49	1.04	1.34
2	I	19[A]	HIS	C-N	20.41	1.61	1.33
2	I	19[B]	HIS	C-N	20.41	1.61	1.33
1	E	292	LYS	C-N	10.36	1.47	1.33
1	E	5	ALA	C-N	9.06	1.46	1.33
1	E	335	ILE	CA-CB	8.57	1.64	1.53
1	E	323	ASP	C-N	8.23	1.45	1.33
1	E	260	HIS	CD2-NE2	-6.75	1.30	1.37
1	E	158	HIS	CD2-NE2	-6.58	1.30	1.37
1	E	15	VAL	C-N	-6.32	1.26	1.33
1	E	85	ILE	CA-CB	6.29	1.61	1.54
1	E	18	PHE	C-N	-5.87	1.25	1.33
1	E	39	HIS	C-N	5.81	1.41	1.33
1	E	297	PHE	C-N	-5.72	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	142	HIS	CD2-NE2	-5.60	1.31	1.37
1	E	174	ILE	CA-CB	5.54	1.60	1.54
1	E	87	HIS	CG-CD2	5.42	1.41	1.35
1	E	30	TRP	NE1-CE2	-5.36	1.31	1.37
1	E	274	GLN	CA-CB	-5.20	1.45	1.53
1	E	62	HIS	CD2-NE2	-5.10	1.32	1.37
1	E	178	GLY	C-N	5.05	1.40	1.33

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	18	ILE	O-C-N	-21.57	95.61	122.57
1	E	216	ASN	OD1-CG-ND2	-12.06	110.54	122.60
2	I	19[A]	HIS	O-C-N	11.94	138.48	122.59
2	I	19[B]	HIS	O-C-N	11.94	138.48	122.59
1	E	7	LYS	N-CA-C	-11.83	99.53	114.56
1	E	5	ALA	O-C-N	-10.83	108.18	122.59
1	E	112	ASP	O-C-N	-10.82	108.78	122.73
1	E	168	LYS	CA-CB-CG	9.62	133.35	114.10
1	E	15	VAL	CA-C-N	9.44	133.11	120.65
1	E	15	VAL	C-N-CA	9.44	133.11	120.65
1	E	62	HIS	CB-CG-CD2	-9.27	119.15	131.20
2	I	19[A]	HIS	CA-C-N	8.82	137.57	121.70
2	I	19[A]	HIS	C-N-CA	8.82	137.57	121.70
2	I	19[B]	HIS	CA-C-N	8.82	137.57	121.70
2	I	19[B]	HIS	C-N-CA	8.82	137.57	121.70
1	E	289	ASN	OD1-CG-ND2	-8.80	113.80	122.60
1	E	267	ASP	CA-CB-CG	8.63	121.23	112.60
2	I	16	ASN	CB-CG-ND2	8.55	129.22	116.40
2	I	17	ALA	N-CA-CB	-8.52	96.33	110.47
1	E	110	PHE	O-C-N	-8.49	114.33	123.42
1	E	51	THR	CA-CB-OG1	-8.31	97.14	109.60
2	I	16	ASN	CA-CB-CG	8.18	120.78	112.60
1	E	295	LYS	O-C-N	-8.14	111.80	122.39
1	E	271	ASN	CA-CB-CG	8.13	120.73	112.60
1	E	216	ASN	CB-CG-ND2	8.09	128.53	116.40
1	E	6	ALA	CA-C-N	8.07	134.43	122.08
1	E	6	ALA	C-N-CA	8.07	134.43	122.08
1	E	220	ASP	CA-CB-CG	8.06	120.66	112.60
1	E	246	ILE	N-CA-C	-7.96	103.04	110.53
1	E	24	GLU	O-C-N	7.94	130.35	122.09
1	E	175	ASP	CA-CB-CG	7.88	120.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	325	SER	CB-CA-C	-7.88	94.73	110.42
1	E	292	LYS	CA-C-N	-7.84	110.20	122.67
1	E	292	LYS	C-N-CA	-7.84	110.20	122.67
1	E	138	PHE	CA-CB-CG	7.83	121.64	113.80
2	I	19[A]	HIS	CB-CA-C	7.79	125.93	110.42
2	I	19[B]	HIS	CB-CA-C	7.79	125.93	110.42
1	E	6	ALA	CA-C-O	7.71	131.54	120.51
1	E	168	LYS	CA-C-N	7.70	127.75	119.28
1	E	168	LYS	C-N-CA	7.70	127.75	119.28
1	E	99	ASN	N-CA-C	7.69	120.74	107.28
1	E	203	GLU	N-CA-C	7.69	121.59	111.75
2	I	15	ARG	CB-CG-CD	-7.62	93.76	111.30
1	E	171	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	E	283	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	E	113	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	E	192	LYS	N-CA-C	-7.44	97.47	109.96
1	E	113	ASN	CB-CG-ND2	7.43	127.55	116.40
1	E	233	ALA	N-CA-C	7.43	122.47	113.41
1	E	37	THR	N-CA-C	7.41	121.73	113.21
1	E	301	ASP	CA-CB-CG	7.38	119.98	112.60
1	E	62	HIS	CB-CG-ND1	7.33	133.70	122.70
1	E	340	ASN	O-C-N	7.32	131.77	123.27
1	E	137	ARG	NE-CZ-NH2	-7.26	112.66	119.20
1	E	142	HIS	CB-CG-CD2	-7.26	121.76	131.20
1	E	313	PRO	CA-C-N	7.13	134.29	121.89
1	E	313	PRO	C-N-CA	7.13	134.29	121.89
1	E	60	VAL	N-CA-CB	-7.06	99.30	112.36
2	I	2	THR	CA-C-O	-7.01	111.52	119.79
1	E	96	GLN	CA-CB-CG	7.00	128.11	114.10
1	E	185	PHE	CA-C-O	7.00	129.18	120.15
1	E	334	GLU	CA-C-N	-7.00	113.76	122.93
1	E	334	GLU	C-N-CA	-7.00	113.76	122.93
1	E	42	GLN	OE1-CD-NE2	-6.96	115.64	122.60
2	I	20	ASP	CA-CB-CG	-6.94	105.66	112.60
1	E	324	THR	CB-CA-C	6.90	124.16	110.42
1	E	60	VAL	CB-CA-C	6.87	121.90	110.30
1	E	158	HIS	CB-CG-CD2	-6.81	122.34	131.20
1	E	335	ILE	N-CA-C	-6.80	97.38	107.51
1	E	249	LYS	O-C-N	-6.78	114.77	122.09
1	E	149	GLN	OE1-CD-NE2	-6.77	115.83	122.60
1	E	166	ASP	N-CA-C	6.69	118.97	110.61
1	E	312	ALA	CA-C-N	6.65	126.90	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	312	ALA	C-N-CA	6.65	126.90	119.32
1	E	124	PRO	O-C-N	-6.63	113.32	122.27
1	E	343	CYS	N-CA-C	6.59	124.84	110.80
1	E	296	TRP	CG-CD2-CE3	6.55	140.45	133.90
1	E	332	GLU	CA-C-O	6.55	128.34	120.81
1	E	207	PRO	CA-C-N	6.50	128.99	120.28
1	E	207	PRO	C-N-CA	6.50	128.99	120.28
1	E	7	LYS	CA-CB-CG	-6.45	101.21	114.10
1	E	332	GLU	N-CA-C	6.40	119.56	109.96
1	E	57	VAL	CB-CA-C	-6.37	101.34	110.83
1	E	175	ASP	CA-C-N	6.35	129.65	120.38
1	E	175	ASP	C-N-CA	6.35	129.65	120.38
1	E	307	GLN	CG-CD-NE2	6.35	125.92	116.40
1	E	31	GLU	O-C-N	-6.30	113.76	122.46
1	E	232	ALA	O-C-N	-6.23	114.29	122.39
1	E	309	LYS	N-CA-C	6.21	121.70	112.94
1	E	26	PHE	CA-CB-CG	6.21	120.01	113.80
1	E	57	VAL	N-CA-CB	6.15	119.61	111.25
1	E	253	GLY	O-C-N	-6.14	116.98	122.57
1	E	164	TYR	N-CA-C	6.11	117.94	111.28
1	E	289	ASN	CB-CG-ND2	6.07	125.50	116.40
1	E	149	GLN	CG-CD-NE2	6.01	125.41	116.40
1	E	321	PRO	CB-CA-C	6.00	119.20	111.64
1	E	19	LEU	N-CA-CB	-5.98	100.46	110.39
1	E	175	ASP	N-CA-C	5.98	119.12	109.79
1	E	51	THR	CA-CB-CG2	5.97	120.65	110.50
1	E	297	PHE	CA-C-N	5.96	128.87	120.28
1	E	297	PHE	C-N-CA	5.96	128.87	120.28
1	E	201	THR	N-CA-C	-5.96	102.08	110.31
1	E	194	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	E	235	TYR	CA-C-N	5.95	124.00	119.66
1	E	235	TYR	C-N-CA	5.95	124.00	119.66
1	E	242	GLN	CA-C-N	5.94	126.10	119.32
1	E	242	GLN	C-N-CA	5.94	126.10	119.32
1	E	236	PRO	N-CA-C	5.91	116.15	110.47
1	E	98	VAL	N-CA-CB	-5.91	100.78	112.24
1	E	194	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	E	208	GLU	CB-CA-C	-5.88	101.02	110.79
1	E	190	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	E	307	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	E	105	LYS	N-CA-C	5.85	118.26	108.96
1	E	24	GLU	CA-C-O	5.85	127.16	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	64	GLU	CB-CG-CD	5.80	122.46	112.60
1	E	24	GLU	CA-C-N	5.78	128.30	120.44
1	E	24	GLU	C-N-CA	5.78	128.30	120.44
1	E	242	GLN	CB-CG-CD	5.74	122.36	112.60
2	I	19[A]	HIS	CA-CB-CG	-5.73	108.07	113.80
2	I	19[B]	HIS	CA-CB-CG	-5.73	108.07	113.80
1	E	84	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	E	293	ASN	CB-CA-C	-5.68	101.88	111.02
1	E	158	HIS	CB-CG-ND1	5.66	131.18	122.70
1	E	184	ASP	N-CA-CB	-5.66	100.93	110.49
1	E	142	HIS	CB-CG-ND1	5.65	131.18	122.70
1	E	199	CYS	CA-C-N	5.63	130.07	121.12
1	E	199	CYS	C-N-CA	5.63	130.07	121.12
1	E	107	GLU	N-CA-CB	-5.62	101.82	110.13
1	E	256	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	E	255	VAL	CB-CA-C	-5.61	103.07	110.98
1	E	87	HIS	CA-C-N	5.58	127.70	120.44
1	E	87	HIS	C-N-CA	5.58	127.70	120.44
1	E	212	SER	CA-C-O	5.57	127.72	120.81
1	E	21	LYS	CA-CB-CG	-5.57	102.96	114.10
1	E	16	LYS	CB-CA-C	5.55	119.51	110.96
1	E	98	VAL	CB-CA-C	5.53	119.12	111.38
1	E	318	PHE	N-CA-C	-5.52	102.71	110.50
1	E	35	GLN	N-CA-CB	-5.50	101.58	110.71
1	E	155	GLU	CA-C-O	5.49	126.56	120.63
1	E	214	GLY	CA-C-O	-5.49	118.44	122.23
1	E	174	ILE	CB-CG1-CD1	-5.46	102.33	113.80
2	I	17	ALA	CB-CA-C	5.46	119.69	110.79
1	E	242	GLN	CB-CA-C	5.44	116.00	109.31
1	E	221	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	E	126	GLY	O-C-N	5.43	127.93	122.77
1	E	176	GLN	N-CA-C	5.43	118.70	111.75
1	E	137	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	E	40	LEU	N-CA-C	5.42	117.88	111.33
1	E	21	LYS	O-C-N	5.40	128.54	122.22
1	E	11	GLU	CB-CG-CD	5.37	121.73	112.60
1	E	51	THR	N-CA-CB	-5.36	101.81	110.81
1	E	236	PRO	CA-C-N	5.36	125.00	119.05
1	E	236	PRO	C-N-CA	5.36	125.00	119.05
1	E	85	ILE	CB-CA-C	-5.32	105.07	111.88
1	E	329	ASP	CA-C-N	5.30	131.66	121.54
1	E	329	ASP	C-N-CA	5.30	131.66	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	GLU	CB-CG-CD	5.28	121.58	112.60
1	E	129	PHE	N-CA-C	5.28	117.44	111.11
1	E	283	ASN	CB-CG-ND2	5.26	124.29	116.40
2	I	2	THR	CA-CB-OG1	-5.25	101.72	109.60
1	E	308	ARG	CB-CG-CD	-5.24	99.25	111.30
1	E	241	ASP	CA-C-O	5.23	126.04	120.24
1	E	163	ILE	N-CA-CB	5.23	117.32	111.21
1	E	11	GLU	CA-CB-CG	5.21	124.52	114.10
1	E	215	TYR	CA-CB-CG	5.19	123.24	113.90
1	E	221	TRP	CE2-CD2-CG	-5.17	100.99	107.20
1	E	42	GLN	CG-CD-NE2	5.17	124.16	116.40
1	E	63	LYS	CA-C-O	-5.15	115.09	120.55
1	E	26	PHE	N-CA-C	-5.15	105.56	111.07
1	E	330	TYR	O-C-N	-5.13	115.77	122.59
1	E	311	GLU	CA-C-O	5.12	125.84	120.36
1	E	241	ASP	N-CA-CB	-5.11	102.59	110.20
1	E	145	PHE	O-C-N	5.11	127.53	122.12
1	E	344	GLY	N-CA-C	5.10	118.41	112.50
1	E	116	LEU	N-CA-C	-5.09	101.40	109.59
1	E	290	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	307	GLN	CA-CB-CG	-5.06	103.97	114.10
1	E	302	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	E	221	TRP	CB-CG-CD1	-5.05	119.33	126.90
2	I	11	ARG	CA-CB-CG	-5.04	104.01	114.10
2	I	18	ILE	N-CA-C	5.04	119.82	109.34
1	E	296	TRP	CB-CG-CD1	-5.03	119.35	126.90
1	E	282	GLY	N-CA-C	-5.03	107.58	114.67
1	E	297	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	110	PHE	Mainchain
1	E	112	ASP	Mainchain
1	E	199	CYS	Mainchain
1	E	249	LYS	Mainchain
1	E	31	GLU	Mainchain
1	E	318	PHE	Sidechain
1	E	327	PHE	Peptide
1	E	39	HIS	Mainchain
1	E	5	ALA	Mainchain

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Mol	Chain	Res	Type	Group
2	I	18	ILE	Peptide,Mainchain
2	I	19[A]	HIS	Peptide,Mainchain
2	I	19[B]	HIS	Peptide,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	E	2874	0	2851	153	0
2	I	157	0	146	12	0
3	E	15	0	27	15	0
4	I	2	0	0	0	0
All	All	3048	0	3024	158	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 26.

All (158) 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:E:2:ASN:HB3	1:E:301:ASP:HA	1.10	1.09
1:E:303:ILE:HD12	3:E:0:MYR:C5	1.80	1.09
1:E:318:PHE:CD2	1:E:324:THR:CG2	2.39	1.05
1:E:303:ILE:CG2	3:E:0:MYR:H52	1.86	1.03
1:E:318:PHE:CD2	1:E:324:THR:HG23	1.93	1.03
1:E:303:ILE:HG23	3:E:0:MYR:H52	1.41	1.02
1:E:2:ASN:CB	1:E:301:ASP:HA	1.90	1.01
1:E:1:GLY:O	1:E:11:GLU:OE1	1.81	0.99
1:E:303:ILE:HD12	3:E:0:MYR:H51	1.42	0.98
1:E:318:PHE:CE2	1:E:324:THR:HG23	2.00	0.96
1:E:285:LYS:HD2	1:E:286:ASP:CG	1.91	0.95
1:E:318:PHE:HD2	1:E:324:THR:CG2	1.80	0.94
1:E:327:PHE:O	1:E:328:ASP:HB2	1.66	0.93
1:E:2:ASN:HB3	1:E:301:ASP:CA	1.99	0.92
1:E:318:PHE:CE2	1:E:324:THR:CG2	2.53	0.91
1:E:318:PHE:CD2	1:E:324:THR:HG21	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:PHE:HE2	1:E:324:THR:OG1	1.54	0.90
1:E:303:ILE:HD12	3:E:0:MYR:H52	1.55	0.86
1:E:318:PHE:HD2	1:E:324:THR:HG21	1.38	0.85
1:E:45:ARG:HH22	1:E:56:ARG:HH21	1.22	0.84
1:E:285:LYS:HD3	1:E:286:ASP:N	1.91	0.84
1:E:285:LYS:HD3	1:E:285:LYS:C	2.03	0.83
1:E:303:ILE:CD1	3:E:0:MYR:H51	2.07	0.83
1:E:2:ASN:HD22	1:E:2:ASN:H	1.28	0.80
1:E:285:LYS:HD3	1:E:286:ASP:CA	2.10	0.80
1:E:319:LYS:O	1:E:324:THR:HG23	1.82	0.80
1:E:286:ASP:HB2	1:E:290:ASP:OD1	1.85	0.77
1:E:303:ILE:CD1	3:E:0:MYR:C5	2.59	0.77
1:E:45:ARG:HH22	1:E:56:ARG:NH2	1.83	0.76
1:E:152:LEU:HD22	3:E:0:MYR:H132	1.67	0.76
1:E:322:GLY:O	1:E:323:ASP:HB2	1.84	0.76
1:E:318:PHE:HE2	1:E:324:THR:HG1	0.78	0.76
1:E:285:LYS:CD	1:E:286:ASP:CG	2.60	0.74
1:E:54:PHE:CZ	1:E:84:GLN:HG3	2.21	0.74
1:E:1:GLY:O	1:E:11:GLU:HB2	1.88	0.73
1:E:56:ARG:NH2	1:E:333:GLU:HB2	2.02	0.73
1:E:4:ALA:HB3	1:E:7:LYS:HB2	1.71	0.72
1:E:303:ILE:HG21	3:E:0:MYR:H52	1.73	0.70
1:E:1:GLY:N	1:E:11:GLU:HB2	2.10	0.67
1:E:202:PRO:HA	1:E:205:LEU:HD22	1.75	0.67
1:E:4:ALA:HB3	1:E:7:LYS:CB	2.24	0.67
1:E:172:LEU:HB3	1:E:180:ILE:HD12	1.75	0.67
1:E:243:PRO:HA	1:E:246:ILE:HD12	1.78	0.66
1:E:256:ARG:NE	1:E:256:ARG:HA	2.11	0.66
1:E:340:ASN:HB2	1:E:342:LYS:NZ	2.11	0.65
1:E:340:ASN:HB2	1:E:342:LYS:HZ3	1.61	0.65
1:E:179:TYR:HB2	1:E:308:ARG:HH21	1.62	0.65
1:E:240:ALA:O	2:I:11:ARG:HD3	1.95	0.65
1:E:244:ILE:HD12	1:E:247:TYR:HD2	1.60	0.65
1:E:62:HIS:HB2	1:E:69:PHE:HE2	1.63	0.64
1:E:303:ILE:CD1	3:E:0:MYR:H52	2.24	0.64
1:E:45:ARG:NH2	1:E:56:ARG:HH21	1.95	0.63
1:E:104:VAL:HG11	1:E:183:THR:HG22	1.81	0.63
1:E:200:GLY:N	2:I:19[A]:HIS:NE2	2.47	0.63
1:E:285:LYS:HD3	1:E:286:ASP:HA	1.79	0.63
1:E:285:LYS:HD2	1:E:286:ASP:OD1	1.99	0.62
1:E:246:ILE:O	1:E:250:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LEU:HD22	3:E:0:MYR:C13	2.30	0.62
1:E:2:ASN:CB	1:E:300:THR:O	2.47	0.61
1:E:327:PHE:O	1:E:328:ASP:CB	2.47	0.60
1:E:5:ALA:H	1:E:7:LYS:HB2	1.67	0.59
1:E:2:ASN:HB2	1:E:300:THR:O	2.01	0.59
1:E:54:PHE:HZ	1:E:84:GLN:HG3	1.66	0.59
1:E:100:PHE:HB3	1:E:103:LEU:HD22	1.83	0.59
1:E:1:GLY:O	1:E:11:GLU:CD	2.45	0.59
1:E:322:GLY:O	1:E:323:ASP:CB	2.51	0.59
1:E:3:ALA:O	1:E:4:ALA:C	2.44	0.59
1:E:111:LYS:HB3	1:E:116:LEU:HD23	1.83	0.59
1:E:324:THR:HG21	1:E:327:PHE:HD2	1.70	0.56
1:E:319:LYS:O	1:E:324:THR:CG2	2.54	0.56
1:E:256:ARG:HA	1:E:256:ARG:HE	1.70	0.56
1:E:2:ASN:CG	1:E:301:ASP:HA	2.31	0.56
1:E:200:GLY:N	2:I:19[B]:HIS:NE2	2.54	0.56
1:E:56:ARG:CZ	1:E:333:GLU:HB2	2.36	0.56
1:E:303:ILE:CG1	3:E:0:MYR:H52	2.36	0.56
1:E:236:PRO:HG2	1:E:239:PHE:HB3	1.89	0.55
1:E:54:PHE:HE1	1:E:82:LEU:HD12	1.72	0.55
1:E:285:LYS:CD	1:E:286:ASP:N	2.68	0.55
1:E:69:PHE:CE1	1:E:107:GLU:HG2	2.42	0.55
1:E:2:ASN:H	1:E:2:ASN:ND2	1.96	0.54
1:E:45:ARG:NH2	1:E:56:ARG:NH2	2.55	0.54
1:E:285:LYS:C	1:E:285:LYS:CD	2.71	0.54
1:E:245:GLN:HA	1:E:248:GLU:HB3	1.89	0.54
1:E:187:PHE:HE1	2:I:20:ASP:HA	1.73	0.54
1:E:85:ILE:H	1:E:85:ILE:HD12	1.73	0.53
1:E:62:HIS:HB2	1:E:69:PHE:CE2	2.44	0.53
1:E:318:PHE:HE2	1:E:324:THR:CB	2.20	0.53
1:E:77:GLN:OE1	1:E:342:LYS:HD3	2.08	0.53
1:E:11:GLU:O	1:E:15:VAL:HG23	2.08	0.53
1:E:318:PHE:HE2	1:E:324:THR:CG2	2.10	0.53
1:E:201:THR:HG21	2:I:15:ARG:HD3	1.90	0.53
1:E:285:LYS:HD2	1:E:286:ASP:OD2	2.09	0.53
1:E:198:LEU:HD13	1:E:209:ILE:HG22	1.91	0.53
1:E:307:GLN:HB3	1:E:309:LYS:HE3	1.91	0.52
1:E:320:GLY:HA3	1:E:324:THR:HA	1.90	0.52
1:E:334:GLU:CD	1:E:336:ARG:HB3	2.36	0.51
1:E:318:PHE:CE2	1:E:324:THR:OG1	2.40	0.51
1:E:2:ASN:HA	1:E:302:TRP:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:ILE:HG13	3:E:0:MYR:C1	2.41	0.50
1:E:244:ILE:HD12	1:E:247:TYR:CD2	2.45	0.50
1:E:71:MET:HG3	1:E:119:VAL:HG22	1.94	0.50
1:E:338:SEP:HB2	1:E:340:ASN:O	2.11	0.49
1:E:54:PHE:CE1	1:E:82:LEU:HD12	2.47	0.48
1:E:38:ALA:HB1	1:E:42:GLN:NE2	2.28	0.48
1:E:179:TYR:CB	1:E:308:ARG:HH21	2.27	0.48
1:E:51:THR:OG1	1:E:56:ARG:HG3	2.13	0.48
1:E:227:LEU:HG	1:E:231:MET:HE2	1.96	0.48
1:E:80:VAL:HG23	1:E:347:PHE:CE2	2.49	0.47
1:E:338:SEP:OG	1:E:339:ILE:N	2.46	0.47
1:E:62:HIS:CB	1:E:69:PHE:HE2	2.28	0.47
1:E:25:ASP:O	1:E:29:LYS:HG3	2.15	0.47
1:E:112:ASP:O	1:E:113:ASN:C	2.52	0.47
1:E:21:LYS:O	1:E:25:ASP:HB2	2.16	0.46
1:E:240:ALA:HB3	1:E:246:ILE:HG13	1.96	0.46
2:I:3:TYR:CZ	2:I:7:ILE:HD11	2.51	0.45
1:E:328:ASP:HB3	1:E:330:TYR:CD2	2.51	0.45
1:E:89:LEU:HD23	1:E:350:PHE:HD2	1.80	0.45
1:E:112:ASP:OD1	1:E:112:ASP:C	2.60	0.45
1:E:247:TYR:O	1:E:251:VAL:HG22	2.17	0.44
1:E:72:LYS:HE3	1:E:74:LEU:HD11	1.98	0.44
1:E:15:VAL:O	1:E:19:LEU:HB2	2.17	0.44
1:E:271:ASN:HA	1:E:274:GLN:HG2	1.98	0.44
1:E:4:ALA:HB3	1:E:7:LYS:HB3	1.99	0.44
2:I:3:TYR:O	2:I:7:ILE:HG12	2.18	0.44
1:E:161:ASP:O	1:E:190:ARG:HG3	2.18	0.44
1:E:49:LEU:HD12	1:E:49:LEU:HA	1.88	0.43
1:E:80:VAL:HG23	1:E:347:PHE:CZ	2.53	0.43
1:E:47:LYS:HB2	1:E:47:LYS:HE3	1.58	0.43
1:E:167:LEU:HD21	1:E:227:LEU:HD22	2.00	0.43
1:E:8:LYS:O	1:E:11:GLU:HB3	2.18	0.43
1:E:210:ILE:HD11	1:E:250:ILE:HD12	2.00	0.43
1:E:207:PRO:HG3	1:E:275:VAL:HG13	2.01	0.43
1:E:343:CYS:HB3	1:E:346:GLU:HG2	2.01	0.43
1:E:113:ASN:ND2	1:E:341:GLU:HB2	2.34	0.42
1:E:115:ASN:HB2	1:E:117:TYR:CZ	2.54	0.42
1:E:7:LYS:HA	1:E:7:LYS:HD2	1.78	0.42
1:E:72:LYS:HE3	1:E:72:LYS:HB3	1.83	0.42
1:E:142:HIS:HE1	1:E:146:TYR:OH	2.03	0.42
1:E:158:HIS:CD2	1:E:217:LYS:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:VAL:HA	1:E:85:ILE:HD11	2.02	0.41
1:E:152:LEU:O	3:E:0:MYR:H141	2.20	0.41
1:E:156:TYR:HB2	3:E:0:MYR:H142	2.02	0.41
1:E:7:LYS:HD2	1:E:10:SER:OG	2.19	0.41
1:E:170:GLU:HG2	2:I:14:ARG:HG2	2.02	0.41
1:E:321:PRO:O	1:E:322:GLY:O	2.38	0.41
1:E:3:ALA:O	1:E:5:ALA:N	2.53	0.41
1:E:44:GLU:O	1:E:60:VAL:HA	2.20	0.41
1:E:257:PHE:HE1	1:E:269:LEU:HD23	1.86	0.40
1:E:335:ILE:CD1	1:E:337:VAL:HG12	2.51	0.40
1:E:202:PRO:HD3	2:I:18:ILE:HG23	2.03	0.40
1:E:2:ASN:ND2	1:E:2:ASN:N	2.68	0.40
1:E:11:GLU:HG3	1:E:12:GLN:HG2	2.02	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	E	346/350 (99%)	318 (92%)	19 (6%)	9 (3%)	4	17
2	I	19/22 (86%)	14 (74%)	1 (5%)	4 (21%)	0	0
All	All	365/372 (98%)	332 (91%)	20 (6%)	13 (4%)	3	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	4	ALA
1	E	328	ASP
1	E	330	TYR
1	E	343	CYS
2	I	18	ILE

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Mol	Chain	Res	Type
2	I	19[A]	HIS
2	I	19[B]	HIS
1	E	3	ALA
1	E	38	ALA
1	E	322	GLY
1	E	323	ASP
1	E	325	SER
2	I	3	TYR

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	E	303/303 (100%)	257 (85%)	46 (15%)	3	9
2	I	16/17 (94%)	14 (88%)	2 (12%)	4	15
All	All	319/320 (100%)	271 (85%)	48 (15%)	3	10

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	ASN
1	E	7	LYS
1	E	11	GLU
1	E	13	GLU
1	E	19	LEU
1	E	35	GLN
1	E	36	ASN
1	E	40	LEU
1	E	47	LYS
1	E	49	LEU
1	E	51	THR
1	E	53	SER
1	E	56	ARG
1	E	57	VAL
1	E	59	LEU

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Mol	Chain	Res	Type
1	E	60	VAL
1	E	72	LYS
1	E	77	GLN
1	E	79	VAL
1	E	82	LEU
1	E	92	LYS
1	E	98	VAL
1	E	103	LEU
1	E	111	LYS
1	E	130	SER
1	E	165	ARG
1	E	168	LYS
1	E	181	GLN
1	E	191	VAL
1	E	198	LEU
1	E	205	LEU
1	E	217	LYS
1	E	259	SER
1	E	267	ASP
1	E	269	LEU
1	E	278	THR
1	E	279	LYS
1	E	285	LYS
1	E	295	LYS
1	E	326	ASN
1	E	328	ASP
1	E	335	ILE
1	E	336	ARG
1	E	337	VAL
1	E	342	LYS
1	E	346	GLU
2	I	14	ARG
2	I	18	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	2	ASN
1	E	32	ASN
1	E	62	HIS
1	E	113	ASN
1	E	115	ASN

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Mol	Chain	Res	Type
1	E	142	HIS
1	E	158	HIS
1	E	181	GLN
1	E	260	HIS
1	E	274	GLN
1	E	283	ASN
1	E	293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	TPO	E	197	1	8,10,11	1.13	1 (12%)	10,14,16	1.36	1 (10%)
1	SEP	E	338	1	8,9,10	1.34	1 (12%)	7,12,14	1.81	2 (28%)

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
1	TPO	E	197	1	-	1/9/11/13	-
1	SEP	E	338	1	-	4/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	338	SEP	P-O3P	3.27	1.67	1.54
1	E	197	TPO	P-O2P	-2.58	1.45	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	197	TPO	O2P-P-O1P	3.06	122.76	110.83
1	E	338	SEP	O2P-P-O1P	2.91	122.16	110.83
1	E	338	SEP	OG-CB-CA	-2.75	105.47	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	338	SEP	CB-OG-P-O2P
1	E	338	SEP	CB-OG-P-O3P
1	E	338	SEP	N-CA-CB-OG
1	E	338	SEP	CB-OG-P-O1P
1	E	197	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	338	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
3	MYR	E	0	1	13,14,15	0.87	1 (7%)	12,13,15	1.54	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
3	MYR	E	0	1	-	8/12/12/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	0	MYR	O1-C1	-2.70	1.04	1.20

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	0	MYR	O1-C1-C2	-3.73	95.13	126.30
3	E	0	MYR	C5-C4-C3	-2.13	103.62	114.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	0	MYR	C1-C2-C3-C4
3	E	0	MYR	C5-C6-C7-C8
3	E	0	MYR	C2-C3-C4-C5
3	E	0	MYR	C4-C5-C6-C7
3	E	0	MYR	C11-C10-C9-C8
3	E	0	MYR	C3-C4-C5-C6
3	E	0	MYR	C11-C12-C13-C14
3	E	0	MYR	C6-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	0	MYR	15	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	19:HIS	C	20:ASP	N	1.61
1	E	112:ASP	C	113:ASN	N	1.04

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.