



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 1CTP / pdb_00001ctp
Title : STRUCTURE OF THE MAMMALIAN CATALYTIC SUBUNIT OF CAMP-DEPENDENT PROTEIN KINASE AND AN INHIBITOR PEPTIDE DISPLAYS AN OPEN CONFORMATION
Authors : Karlsson, R.; Zheng, J.; Xuong, N.H.; Taylor, S.S.; Sowadski, J.M.
Deposited on : 1993-04-08
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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

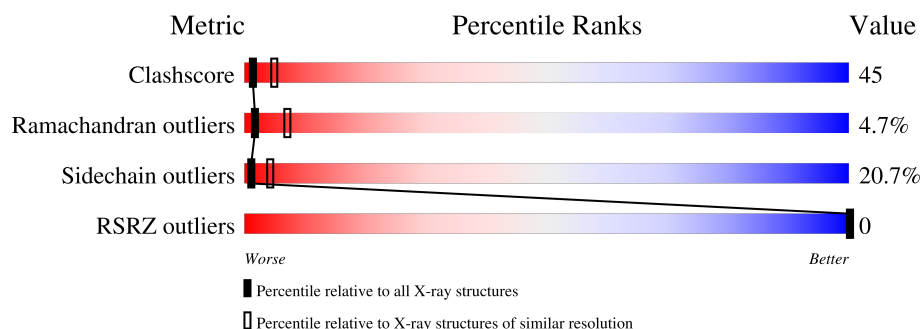
1 Overall quality at a glance

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)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	350	
2	I	20	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2732 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.

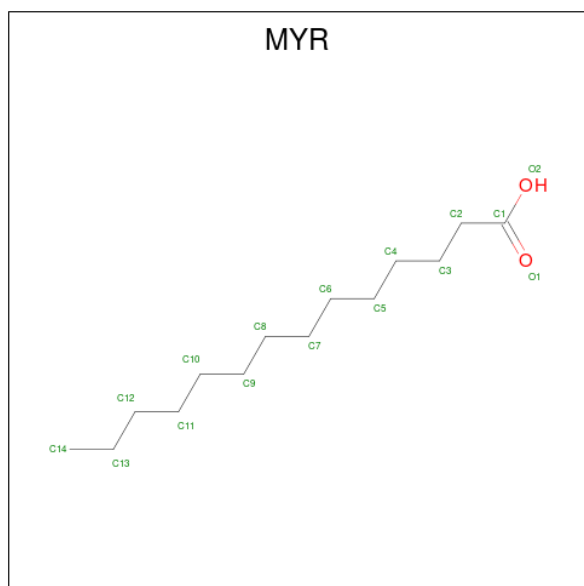
- Molecule 1 is a protein called cAMP-DEPENDENT PROTEIN KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	333	Total	C	N	O	P	S	0	0	0
			2580	1679	431	461	1	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	18	Total	C	I	N	O	0	0	0
			140	84	2	28	26			

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	C	0	0
			10	10		

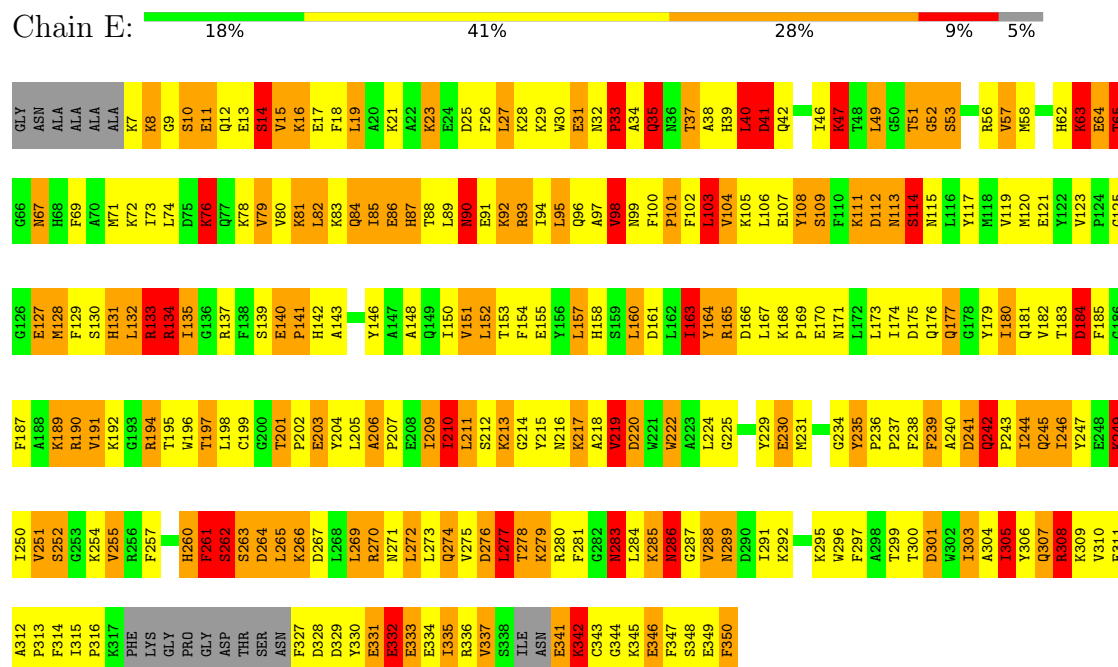
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total	O	0	0
			2	2		

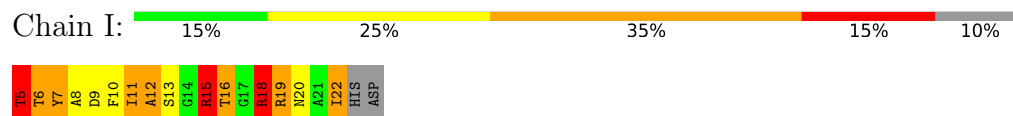
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: cAMP-DEPENDENT PROTEIN KINASE



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	171.50Å 171.50Å 171.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.90 7.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.90) 91.0 (7.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.190 , (Not available) 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 102.1	EDS
L-test for twinning ¹	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2732	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TYI, MYR, TPO

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	1.63	24/2635 (0.9%)	2.77	248/3578 (6.9%)
2	I	1.62	2/125 (1.6%)	3.35	20/165 (12.1%)
All	All	1.63	26/2760 (0.9%)	2.80	268/3743 (7.2%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	86	GLU	CD-OE2	8.05	1.40	1.25
1	E	349	GLU	CD-OE2	7.42	1.39	1.25
1	E	33	PRO	C-O	7.05	1.33	1.24
1	E	263	SER	CA-C	-6.08	1.47	1.53
1	E	112	ASP	CG-OD1	6.05	1.36	1.25
1	E	230	GLU	C-O	-5.99	1.16	1.24
2	I	9	ASP	CG-OD1	5.90	1.36	1.25
1	E	127	GLU	CD-OE2	5.89	1.36	1.25
1	E	263	SER	N-CA	-5.86	1.40	1.47
1	E	121	GLU	CD-OE1	5.79	1.36	1.25
1	E	263	SER	CA-CB	-5.71	1.46	1.53
1	E	19	LEU	N-CA	-5.59	1.39	1.46
1	E	103	LEU	CA-C	5.51	1.59	1.52
1	E	209	ILE	C-N	-5.45	1.27	1.33
1	E	311	GLU	CD-OE1	5.44	1.35	1.25
1	E	276	ASP	CG-OD1	5.43	1.35	1.25
1	E	341	GLU	N-CA	5.37	1.56	1.46
1	E	177	GLN	N-CA	-5.25	1.39	1.46
2	I	18	ARG	CA-C	-5.24	1.45	1.52
1	E	137	ARG	NE-CZ	5.23	1.38	1.33
1	E	301	ASP	C-O	-5.23	1.17	1.23
1	E	87	HIS	CE1-NE2	5.10	1.37	1.32
1	E	305	ILE	C-O	-5.09	1.18	1.24
1	E	261	PHE	C-O	-5.08	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	PHE	C-N	-5.02	1.27	1.34
1	E	123	VAL	CA-C	-5.00	1.47	1.52

All (268) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	ASN	CA-CB-CG	-15.85	96.75	112.60
1	E	103	LEU	O-C-N	-15.16	105.94	123.22
1	E	32	ASN	CB-CA-C	14.88	126.12	110.65
1	E	164	TYR	CA-C-N	-13.11	102.80	122.86
1	E	164	TYR	C-N-CA	-13.11	102.80	122.86
1	E	289	ASN	CA-CB-CG	-13.03	99.57	112.60
1	E	252	SER	CB-CA-C	-11.99	87.64	110.67
1	E	262	SER	CA-C-O	-11.27	107.35	121.55
2	I	20	ASN	CA-CB-CG	-10.68	101.92	112.60
1	E	241	ASP	CA-C-O	-10.57	109.55	120.54
1	E	15	VAL	CA-CB-CG2	-10.43	92.68	110.40
1	E	262	SER	N-CA-C	-10.42	93.58	109.94
1	E	63	LYS	CA-C-N	-10.32	107.28	122.65
1	E	63	LYS	C-N-CA	-10.32	107.28	122.65
1	E	184	ASP	N-CA-CB	-10.28	93.12	110.49
1	E	115	ASN	CA-CB-CG	10.19	122.78	112.60
1	E	261	PHE	O-C-N	-10.07	109.20	122.59
1	E	209	ILE	O-C-N	-10.02	112.07	121.89
1	E	177	GLN	N-CA-CB	-9.90	95.39	110.73
1	E	209	ILE	CA-C-O	9.64	131.07	121.05
1	E	161	ASP	CA-CB-CG	-9.61	102.99	112.60
2	I	16	THR	CA-CB-OG1	-9.58	95.23	109.60
1	E	184	ASP	CA-CB-CG	-9.55	103.05	112.60
1	E	213	LYS	N-CA-CB	-9.22	96.69	110.61
1	E	164	TYR	O-C-N	-9.19	111.62	122.93
1	E	342	LYS	CA-C-O	-8.97	107.68	120.51
1	E	275	VAL	CA-C-N	-8.89	108.11	122.34
1	E	275	VAL	C-N-CA	-8.89	108.11	122.34
1	E	263	SER	N-CA-C	-8.88	93.33	110.56
1	E	262	SER	CB-CA-C	-8.81	93.59	112.63
1	E	14	SER	CA-C-N	-8.80	109.47	120.56
1	E	14	SER	C-N-CA	-8.80	109.47	120.56
1	E	342	LYS	N-CA-CB	8.79	125.35	110.49
1	E	286	ASN	CB-CG-ND2	-8.67	103.39	116.40
1	E	32	ASN	CA-C-O	8.66	129.30	120.38
1	E	34	ALA	CB-CA-C	8.64	122.85	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	212	SER	N-CA-C	8.59	123.25	111.39
1	E	194	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	E	37	THR	CA-CB-CG2	-8.45	96.13	110.50
2	I	6	THR	CB-CA-C	-8.45	90.51	109.10
1	E	41	ASP	CA-C-N	-8.40	108.70	122.65
1	E	41	ASP	C-N-CA	-8.40	108.70	122.65
1	E	330	TYR	CA-C-N	-8.18	111.48	122.85
1	E	330	TYR	C-N-CA	-8.18	111.48	122.85
2	I	13	SER	CA-C-N	-8.15	103.08	121.82
2	I	13	SER	C-N-CA	-8.15	103.08	121.82
1	E	333	GLU	CA-C-N	-8.14	108.39	121.58
1	E	333	GLU	C-N-CA	-8.14	108.39	121.58
1	E	98	VAL	CA-CB-CG2	-8.09	96.66	110.40
1	E	345	LYS	N-CA-CB	8.02	121.70	110.07
1	E	348	SER	CA-CB-OG	-8.00	95.10	111.10
1	E	137	ARG	NE-CZ-NH2	7.87	126.28	119.20
1	E	98	VAL	N-CA-CB	-7.83	98.39	111.38
1	E	163	ILE	CA-CB-CG1	7.77	123.61	110.40
1	E	267	ASP	CA-CB-CG	-7.75	104.85	112.60
1	E	114	SER	N-CA-C	7.69	123.24	113.55
2	I	5	THR	CA-C-N	-7.69	107.86	121.70
2	I	5	THR	C-N-CA	-7.69	107.86	121.70
1	E	180	ILE	CB-CG1-CD1	-7.62	97.80	113.80
1	E	16	LYS	CA-C-O	7.61	131.40	120.51
1	E	237	PRO	O-C-N	-7.52	112.12	122.27
1	E	225	GLY	O-C-N	-7.45	115.04	122.19
1	E	277	LEU	CB-CA-C	-7.44	95.62	110.42
1	E	210	ILE	CB-CG1-CD1	-7.42	98.22	113.80
1	E	286	ASN	CB-CA-C	-7.38	95.73	110.42
1	E	220	ASP	CA-CB-CG	7.32	119.92	112.60
1	E	262	SER	CA-CB-OG	-7.28	96.54	111.10
1	E	81	LYS	N-CA-CB	7.27	120.78	109.94
1	E	63	LYS	O-C-N	-7.24	112.97	122.59
2	I	9	ASP	CB-CA-C	-7.23	95.62	110.38
1	E	280	ARG	NE-CZ-NH1	7.21	128.71	121.50
1	E	18	PHE	CA-C-O	7.17	128.09	120.70
1	E	330	TYR	CA-C-O	7.08	130.18	121.89
1	E	163	ILE	CB-CA-C	7.08	120.83	110.77
1	E	133	ARG	CG-CD-NE	-7.08	96.43	112.00
2	I	18	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	E	206	ALA	CA-C-O	7.00	126.80	119.80
1	E	194	ARG	CA-C-N	-6.96	110.24	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	194	ARG	C-N-CA	-6.96	110.24	123.32
2	I	6	THR	N-CA-CB	-6.95	99.68	111.50
2	I	22	ILE	CA-CB-CG2	-6.94	98.70	110.50
1	E	330	TYR	O-C-N	-6.93	114.57	122.68
1	E	262	SER	O-C-N	6.93	131.01	122.14
1	E	38	ALA	CB-CA-C	-6.92	102.23	113.37
1	E	109	SER	N-CA-CB	-6.91	98.63	111.13
1	E	143	ALA	CA-C-N	6.89	129.51	120.28
1	E	143	ALA	C-N-CA	6.89	129.51	120.28
1	E	41	ASP	N-CA-CB	-6.87	98.88	110.49
1	E	57	VAL	CB-CA-C	6.81	120.90	110.96
1	E	175	ASP	N-CA-C	6.80	120.91	110.36
1	E	93	ARG	N-CA-C	6.72	118.39	111.14
1	E	99	ASN	O-C-N	-6.69	117.34	123.50
1	E	35	GLN	N-CA-C	6.63	119.42	108.48
1	E	103	LEU	CA-C-O	6.61	127.43	120.36
1	E	344	GLY	CA-C-O	-6.60	113.72	120.45
1	E	102	PHE	N-CA-C	6.53	120.56	112.59
1	E	11	GLU	CA-C-O	6.53	127.68	120.82
1	E	276	ASP	CA-C-O	-6.51	114.29	121.58
2	I	15	ARG	N-CA-C	6.51	122.05	113.20
1	E	288	VAL	CA-CB-CG2	-6.50	99.34	110.40
1	E	199	CYS	N-CA-C	6.49	118.07	108.60
1	E	274	GLN	CA-C-O	6.47	128.08	120.58
1	E	104	VAL	CA-CB-CG1	-6.45	99.43	110.40
1	E	297	PHE	CA-CB-CG	6.45	120.25	113.80
1	E	263	SER	CA-CB-OG	-6.44	98.22	111.10
2	I	22	ILE	CA-C-O	-6.42	109.89	120.80
1	E	47	LYS	O-C-N	-6.36	116.82	123.56
1	E	312	ALA	CA-C-O	-6.36	114.09	120.64
1	E	121	GLU	CA-C-O	-6.34	113.52	120.81
1	E	255	VAL	CB-CA-C	-6.33	102.75	111.49
1	E	250	ILE	CA-C-O	6.33	127.53	120.95
1	E	21	LYS	CB-CA-C	-6.31	100.32	110.79
1	E	307	GLN	CA-C-N	-6.30	112.82	122.08
1	E	307	GLN	C-N-CA	-6.30	112.82	122.08
1	E	131	HIS	O-C-N	6.30	129.33	122.15
1	E	313	PRO	N-CA-CB	6.28	110.47	103.44
1	E	97	ALA	CA-C-O	6.27	126.49	119.41
1	E	239	PHE	O-C-N	-6.26	116.72	123.42
1	E	278	THR	CA-C-O	6.23	127.14	120.10
1	E	329	ASP	O-C-N	-6.23	114.31	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	279	LYS	CA-C-O	-6.22	112.21	119.05
1	E	266	LYS	CA-C-O	6.21	127.34	120.63
1	E	331	GLU	N-CA-CB	-6.18	100.18	110.39
1	E	163	ILE	CB-CG1-CD1	-6.18	100.82	113.80
1	E	330	TYR	N-CA-C	6.18	119.55	110.59
1	E	127	GLU	CA-C-O	-6.17	114.52	121.81
1	E	29	LYS	N-CA-CB	-6.15	100.75	110.28
1	E	270	ARG	N-CA-CB	6.14	120.58	110.39
1	E	238	PHE	CA-C-O	-6.14	113.60	120.66
1	E	201	THR	CA-C-O	6.11	125.87	120.19
1	E	337	VAL	CA-C-N	-6.10	110.72	121.70
1	E	337	VAL	C-N-CA	-6.10	110.72	121.70
1	E	76	LYS	CG-CD-CE	6.08	125.28	111.30
1	E	348	SER	CA-C-O	6.07	126.96	120.10
1	E	168	LYS	CA-C-O	-6.06	111.85	120.16
1	E	252	SER	CA-CB-OG	-6.04	99.02	111.10
1	E	113	ASN	N-CA-CB	6.03	119.11	110.06
1	E	141	PRO	N-CA-CB	6.01	109.56	103.25
1	E	35	GLN	CA-C-N	-6.00	113.94	122.41
1	E	35	GLN	C-N-CA	-6.00	113.94	122.41
1	E	234	GLY	CA-C-N	6.00	134.93	123.65
1	E	234	GLY	C-N-CA	6.00	134.93	123.65
1	E	187	PHE	N-CA-CB	6.00	118.98	111.00
1	E	291	ILE	N-CA-C	-6.00	105.87	111.45
1	E	14	SER	N-CA-C	5.97	118.28	111.11
1	E	176	GLN	N-CA-C	5.97	119.66	112.38
1	E	58	MET	CA-CB-CG	-5.92	102.26	114.10
1	E	28	LYS	N-CA-CB	5.92	118.82	110.12
1	E	128	MET	CG-SD-CE	-5.91	87.91	100.90
1	E	51	THR	CB-CA-C	-5.90	98.68	110.42
1	E	130	SER	CB-CA-C	-5.85	99.43	110.67
1	E	49	LEU	CA-C-O	5.84	126.44	119.60
1	E	137	ARG	NH1-CZ-NH2	-5.84	111.71	119.30
1	E	332	GLU	N-CA-C	5.84	123.24	110.80
1	E	108	TYR	CB-CG-CD1	-5.84	112.04	120.80
1	E	190	ARG	N-CA-CB	5.83	119.37	109.87
1	E	277	LEU	CB-CG-CD2	-5.81	93.26	110.70
1	E	276	ASP	N-CA-C	5.81	118.90	107.98
2	I	11	ILE	O-C-N	5.80	129.82	122.57
1	E	266	LYS	O-C-N	-5.78	115.99	122.12
1	E	280	ARG	NE-CZ-NH2	-5.78	114.00	119.20
2	I	15	ARG	CD-NE-CZ	-5.77	116.33	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	88	THR	CA-CB-OG1	-5.76	100.95	109.60
1	E	245	GLN	O-C-N	5.76	128.23	122.12
1	E	164	TYR	N-CA-CB	-5.76	101.27	109.85
1	E	130	SER	CA-CB-OG	-5.75	99.59	111.10
1	E	217	LYS	O-C-N	-5.74	114.95	122.59
1	E	283	ASN	CB-CA-C	-5.74	98.67	110.38
1	E	280	ARG	O-C-N	-5.74	115.87	122.93
1	E	303	ILE	CA-CB-CG1	-5.72	100.67	110.40
2	I	13	SER	O-C-N	-5.72	114.62	122.23
1	E	251	VAL	CB-CA-C	5.71	119.85	112.14
1	E	95	LEU	N-CA-CB	5.70	118.28	110.01
1	E	241	ASP	N-CA-C	-5.68	98.49	108.20
1	E	93	ARG	CA-C-N	5.67	127.71	120.56
1	E	93	ARG	C-N-CA	5.67	127.71	120.56
1	E	152	LEU	O-C-N	5.66	127.91	122.03
1	E	101	PRO	N-CA-CB	5.65	109.19	103.25
1	E	283	ASN	CA-CB-CG	-5.65	106.95	112.60
1	E	272	LEU	N-CA-C	-5.65	106.44	113.55
1	E	283	ASN	N-CA-C	5.64	119.34	112.23
1	E	343	CYS	CA-CB-SG	-5.64	101.44	114.40
1	E	254	LYS	CB-CA-C	5.63	120.33	111.77
1	E	219	VAL	CA-CB-CG2	5.63	119.97	110.40
1	E	341	GLU	CG-CD-OE2	5.63	131.35	118.40
1	E	33	PRO	N-CA-CB	5.62	109.15	103.25
1	E	76	LYS	N-CA-CB	5.62	118.94	109.78
1	E	47	LYS	CB-CG-CD	-5.59	98.45	111.30
2	I	11	ILE	CB-CA-C	-5.58	102.14	111.29
1	E	90	ASN	CA-CB-CG	-5.58	107.02	112.60
1	E	182	VAL	CA-C-N	-5.58	113.05	123.03
1	E	182	VAL	C-N-CA	-5.58	113.05	123.03
1	E	273	LEU	CA-C-N	5.57	129.25	121.24
1	E	273	LEU	C-N-CA	5.57	129.25	121.24
1	E	291	ILE	CB-CA-C	5.56	119.21	111.92
1	E	345	LYS	O-C-N	5.55	128.09	122.09
1	E	31	GLU	CA-C-N	-5.54	113.56	123.08
1	E	31	GLU	C-N-CA	-5.54	113.56	123.08
1	E	10	SER	N-CA-CB	-5.53	101.76	110.06
1	E	58	MET	N-CA-C	5.53	119.07	110.17
1	E	192	LYS	CA-C-O	-5.51	115.91	122.13
1	E	245	GLN	N-CA-C	5.51	117.99	111.33
1	E	235	TYR	CA-C-O	5.50	126.09	120.64
1	E	292	LYS	CA-C-N	-5.50	110.94	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	292	LYS	C-N-CA	-5.50	110.94	121.94
1	E	262	SER	N-CA-CB	-5.49	100.13	110.07
1	E	310	VAL	N-CA-CB	-5.49	101.05	111.21
1	E	115	ASN	N-CA-CB	-5.47	102.72	111.43
1	E	33	PRO	N-CA-C	5.47	123.74	112.47
1	E	189	LYS	CA-C-N	-5.46	113.80	121.72
1	E	189	LYS	C-N-CA	-5.46	113.80	121.72
1	E	300	THR	N-CA-C	5.43	118.47	109.46
1	E	260	HIS	N-CA-C	-5.41	106.65	113.20
1	E	288	VAL	O-C-N	5.40	127.34	121.94
1	E	64	GLU	O-C-N	5.39	129.50	123.19
1	E	135	ILE	CA-C-O	-5.38	114.66	120.47
1	E	35	GLN	CG-CD-NE2	-5.38	108.34	116.40
1	E	151	VAL	CA-C-N	5.37	127.74	120.65
1	E	151	VAL	C-N-CA	5.37	127.74	120.65
1	E	134	ARG	CD-NE-CZ	5.36	131.91	124.40
1	E	108	TYR	CB-CG-CD2	5.36	128.84	120.80
1	E	307	GLN	N-CA-CB	5.34	118.66	110.70
1	E	72	LYS	O-C-N	-5.34	116.99	123.13
1	E	152	LEU	CA-C-O	-5.34	115.40	121.00
1	E	308	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	E	239	PHE	CA-C-O	5.33	126.93	121.23
1	E	166	ASP	N-CA-CB	-5.33	101.49	110.49
1	E	335	ILE	N-CA-C	-5.33	98.26	109.34
2	I	12	ALA	CA-C-O	5.31	124.89	119.05
1	E	343	CYS	CB-CA-C	-5.30	102.58	111.23
1	E	67	ASN	CB-CA-C	5.29	118.56	109.51
1	E	51	THR	CA-C-N	-5.29	111.05	121.41
1	E	51	THR	C-N-CA	-5.29	111.05	121.41
1	E	52	GLY	O-C-N	-5.28	115.84	122.70
1	E	265	LEU	CD1-CG-CD2	-5.25	99.25	110.80
1	E	187	PHE	CA-CB-CG	-5.25	108.55	113.80
1	E	51	THR	CA-C-O	5.25	128.01	120.51
1	E	212	SER	CA-C-O	5.23	127.91	121.84
1	E	344	GLY	N-CA-C	5.23	120.23	113.27
1	E	237	PRO	N-CA-CB	5.23	109.06	103.52
2	I	11	ILE	CA-CB-CG1	-5.22	101.52	110.40
1	E	242	GLN	N-CA-CB	5.20	119.62	110.37
1	E	85	ILE	O-C-N	5.17	127.27	121.94
1	E	272	LEU	N-CA-CB	5.17	117.89	110.40
1	E	79	VAL	O-C-N	5.16	126.88	121.87
1	E	249	LYS	CB-CA-C	-5.15	102.09	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	121	GLU	CG-CD-OE1	-5.15	106.56	118.40
2	I	5	THR	CB-CA-C	-5.13	97.80	109.10
1	E	350	PHE	CA-C-O	-5.13	112.08	120.80
1	E	25	ASP	N-CA-CB	5.11	117.64	110.12
1	E	131	HIS	CA-CB-CG	-5.11	108.69	113.80
1	E	278	THR	CA-CB-OG1	-5.10	101.95	109.60
1	E	106	LEU	CB-CA-C	-5.08	103.19	111.68
1	E	236	PRO	N-CA-C	5.08	116.90	110.70
1	E	79	VAL	N-CA-CB	5.06	117.42	110.54
1	E	123	VAL	O-C-N	5.05	126.86	121.10
1	E	171	ASN	CB-CA-C	-5.05	102.84	111.02
1	E	194	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	E	152	LEU	N-CA-CB	5.04	117.26	109.91
1	E	216	ASN	CA-CB-CG	-5.03	107.57	112.60
1	E	285	LYS	N-CA-CB	-5.02	101.94	109.88
1	E	231	MET	N-CA-C	-5.02	105.52	111.69
1	E	264	ASP	CA-CB-CG	5.02	117.62	112.60
1	E	132	LEU	CA-C-N	-5.01	112.34	120.72
1	E	132	LEU	C-N-CA	-5.01	112.34	120.72
1	E	131	HIS	CA-C-N	5.01	127.75	120.79
1	E	131	HIS	C-N-CA	5.01	127.75	120.79
1	E	113	ASN	CA-CB-CG	-5.01	107.59	112.60

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	E	2580	0	2409	223	1
2	I	140	0	132	22	0
3	E	10	0	19	0	0
4	E	2	0	0	0	0
All	All	2732	0	2560	238	1

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 45.

All (238) 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:15:VAL:HG23	1:E:16:LYS:N	1.61	1.10
1:E:65:THR:HG22	1:E:67:ASN:H	1.14	1.10
2:I:11:ILE:HD12	2:I:11:ILE:C	1.78	1.09
1:E:23:LYS:HD2	1:E:27:LEU:HD22	1.36	1.03
1:E:284:LEU:N	1:E:284:LEU:HD12	1.75	0.99
1:E:15:VAL:CG2	1:E:16:LYS:N	2.30	0.95
1:E:23:LYS:HD2	1:E:27:LEU:CD2	1.98	0.94
1:E:140:GLU:HB3	1:E:141:PRO:HD3	1.50	0.94
1:E:346:GLU:N	1:E:346:GLU:OE1	2.03	0.91
1:E:128:MET:HE2	1:E:169:PRO:HB3	1.50	0.91
1:E:284:LEU:CD1	1:E:284:LEU:H	1.84	0.90
1:E:301:ASP:HB3	1:E:304:ALA:HB3	1.54	0.90
1:E:31:GLU:O	1:E:33:PRO:HD3	1.73	0.89
1:E:100:PHE:CG	1:E:101:PRO:HD2	2.08	0.88
1:E:64:GLU:O	1:E:65:THR:HB	1.74	0.88
1:E:39:HIS:O	1:E:42:GLN:HG2	1.74	0.87
1:E:189:LYS:HD3	1:E:191:VAL:HG11	1.55	0.87
1:E:284:LEU:N	1:E:284:LEU:CD1	2.37	0.87
1:E:140:GLU:OE2	1:E:262:SER:OG	1.95	0.84
1:E:31:GLU:C	1:E:33:PRO:HD3	2.03	0.84
1:E:184:ASP:OD1	1:E:184:ASP:C	2.19	0.84
1:E:65:THR:CG2	1:E:67:ASN:HB2	2.10	0.82
2:I:11:ILE:C	2:I:11:ILE:CD1	2.53	0.81
1:E:158:HIS:HE1	1:E:220:ASP:OD2	1.63	0.81
1:E:198:LEU:HD12	1:E:209:ILE:HG22	1.62	0.80
1:E:37:THR:HG21	1:E:108:TYR:HD1	1.43	0.80
2:I:11:ILE:HD12	2:I:11:ILE:O	1.81	0.79
1:E:194:ARG:NH2	1:E:213:LYS:O	2.16	0.78
1:E:205:LEU:HD12	1:E:247:TYR:HE1	1.47	0.78
1:E:153:THR:HG22	1:E:157:LEU:HD22	1.66	0.77
1:E:7:LYS:O	1:E:8:LYS:C	2.27	0.77
1:E:15:VAL:CG2	1:E:16:LYS:H	1.96	0.76
1:E:84:GLN:NE2	1:E:87:HIS:HD2	1.84	0.76
1:E:205:LEU:HD12	1:E:247:TYR:CE1	2.21	0.76
2:I:6:THR:HG22	2:I:7:TYI:N	1.99	0.75
1:E:65:THR:CG2	1:E:67:ASN:H	1.98	0.75
1:E:65:THR:HG22	1:E:67:ASN:N	1.99	0.74
1:E:15:VAL:HG23	1:E:16:LYS:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:GLU:OE2	2:I:19:ARG:HD2	1.86	0.74
1:E:303:ILE:O	1:E:307:GLN:HG3	1.87	0.74
1:E:69:PHE:CE2	1:E:107:GLU:HG2	2.23	0.73
1:E:203:GLU:OE2	2:I:15:ARG:NH2	2.20	0.71
1:E:7:LYS:N	1:E:10:SER:HB3	2.06	0.70
1:E:245:GLN:O	1:E:249:LYS:HD2	1.92	0.70
1:E:197:TPO:HG23	1:E:198:LEU:N	2.06	0.70
1:E:230:GLU:CD	2:I:19:ARG:HH22	2.00	0.69
2:I:11:ILE:CD1	2:I:11:ILE:O	2.39	0.69
1:E:7:LYS:O	1:E:10:SER:HB3	1.93	0.69
1:E:37:THR:HG21	1:E:108:TYR:CD1	2.26	0.68
1:E:131:HIS:O	1:E:135:ILE:HG13	1.93	0.68
1:E:286:ASN:O	1:E:287:GLY:C	2.35	0.68
1:E:27:LEU:HD11	1:E:190:ARG:NH2	2.09	0.67
1:E:262:SER:HB2	1:E:265:LEU:HB3	1.76	0.67
1:E:65:THR:HG23	1:E:67:ASN:HB2	1.76	0.67
1:E:76:LYS:HB3	1:E:347:PHE:CE2	2.29	0.67
1:E:189:LYS:HG2	1:E:191:VAL:HG12	1.77	0.66
1:E:40:LEU:O	1:E:42:GLN:N	2.28	0.66
1:E:112:ASP:OD1	1:E:112:ASP:C	2.36	0.66
1:E:243:PRO:O	1:E:244:ILE:C	2.37	0.66
1:E:104:VAL:HG13	1:E:104:VAL:O	1.96	0.65
1:E:211:LEU:HD22	1:E:251:VAL:HG22	1.79	0.64
1:E:307:GLN:O	1:E:308:ARG:C	2.35	0.64
1:E:180:ILE:HD12	1:E:180:ILE:C	2.23	0.63
1:E:103:LEU:O	1:E:104:VAL:C	2.30	0.63
1:E:152:LEU:O	1:E:155:GLU:HB3	1.98	0.63
1:E:284:LEU:H	1:E:284:LEU:HD13	1.64	0.63
1:E:51:THR:HA	1:E:56:ARG:HA	1.82	0.62
1:E:23:LYS:HG3	1:E:23:LYS:O	1.80	0.62
1:E:100:PHE:CD1	1:E:101:PRO:HD2	2.34	0.61
1:E:84:GLN:HE22	1:E:87:HIS:HD2	1.48	0.61
1:E:100:PHE:CD2	1:E:101:PRO:HD2	2.36	0.61
1:E:194:ARG:HH21	1:E:214:GLY:HA3	1.66	0.61
1:E:197:TPO:CG2	1:E:198:LEU:N	2.63	0.61
1:E:78:LYS:O	1:E:82:LEU:HD12	2.01	0.60
1:E:83:LYS:C	1:E:84:GLN:HG2	2.26	0.60
1:E:183:THR:O	1:E:184:ASP:HB3	2.00	0.60
1:E:101:PRO:HG3	1:E:306:TYR:CE1	2.36	0.60
1:E:257:PHE:HE1	1:E:269:LEU:HD23	1.67	0.59
1:E:285:LYS:O	1:E:286:ASN:CG	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:LYS:O	1:E:10:SER:N	2.36	0.59
1:E:16:LYS:O	1:E:17:GLU:C	2.43	0.59
1:E:301:ASP:HB3	1:E:304:ALA:CB	2.31	0.59
2:I:6:THR:CG2	2:I:7:TYI:N	2.62	0.58
1:E:189:LYS:CD	1:E:191:VAL:HG11	2.30	0.58
1:E:52:GLY:C	1:E:53:SER:O	2.45	0.58
1:E:112:ASP:OD1	1:E:114:SER:N	2.34	0.58
1:E:341:GLU:HG3	1:E:342:LYS:H	1.68	0.58
1:E:179:TYR:CZ	1:E:308:ARG:HA	2.39	0.57
1:E:131:HIS:HA	1:E:134:ARG:HH11	1.69	0.57
1:E:257:PHE:CE1	1:E:269:LEU:HD23	2.40	0.57
2:I:5:THR:HG23	2:I:5:THR:O	2.05	0.57
1:E:140:GLU:HB3	1:E:141:PRO:CD	2.32	0.56
1:E:206:ALA:O	1:E:207:PRO:C	2.48	0.56
1:E:334:GLU:O	1:E:335:ILE:C	2.48	0.56
2:I:18:ARG:CB	2:I:18:ARG:HH11	2.18	0.56
1:E:163:ILE:HG12	1:E:165:ARG:HD3	1.87	0.55
1:E:133:ARG:HD2	2:I:16:THR:O	2.05	0.55
1:E:189:LYS:HE2	1:E:195:THR:OG1	2.06	0.55
1:E:112:ASP:O	1:E:113:ASN:C	2.47	0.55
1:E:98:VAL:HG13	1:E:103:LEU:HD23	1.88	0.54
1:E:262:SER:CB	1:E:265:LEU:H	2.20	0.54
1:E:98:VAL:CG1	1:E:103:LEU:HD23	2.37	0.54
1:E:239:PHE:CZ	2:I:10:PHE:HB2	2.42	0.54
1:E:30:TRP:O	1:E:93:ARG:NH2	2.41	0.54
1:E:15:VAL:HG22	1:E:16:LYS:H	1.70	0.54
1:E:164:TYR:O	1:E:220:ASP:OD1	2.27	0.53
1:E:78:LYS:O	1:E:82:LEU:CD1	2.57	0.53
1:E:12:GLN:O	1:E:15:VAL:HG22	2.09	0.52
1:E:346:GLU:H	1:E:346:GLU:CD	2.16	0.52
1:E:93:ARG:O	1:E:96:GLN:NE2	2.34	0.52
1:E:217:LYS:O	1:E:218:ALA:C	2.49	0.52
1:E:84:GLN:HE22	1:E:87:HIS:CD2	2.28	0.52
1:E:230:GLU:OE1	2:I:19:ARG:NH2	2.42	0.52
1:E:276:ASP:O	1:E:278:THR:N	2.43	0.52
1:E:101:PRO:CG	1:E:306:TYR:CE1	2.93	0.52
1:E:154:PHE:CE2	1:E:220:ASP:HB3	2.45	0.52
1:E:14:SER:O	1:E:15:VAL:C	2.52	0.51
1:E:229:TYR:CD1	1:E:229:TYR:C	2.88	0.51
2:I:6:THR:HG22	2:I:8:ALA:H	1.75	0.51
1:E:128:MET:CE	1:E:169:PRO:HB3	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:VAL:O	1:E:16:LYS:C	2.53	0.51
1:E:241:ASP:O	1:E:242:GLN:CB	2.58	0.51
1:E:23:LYS:CD	1:E:27:LEU:HD22	2.24	0.51
1:E:62:HIS:CD2	1:E:65:THR:HB	2.47	0.50
1:E:210:ILE:HD12	1:E:247:TYR:HB3	1.92	0.50
1:E:76:LYS:HE3	1:E:113:ASN:O	2.11	0.50
2:I:5:THR:C	2:I:6:THR:OG1	2.54	0.50
1:E:263:SER:O	1:E:266:LYS:N	2.45	0.50
1:E:8:LYS:O	1:E:11:GLU:N	2.44	0.50
1:E:142:HIS:NE2	1:E:146:TYR:CE2	2.80	0.50
1:E:206:ALA:HB1	1:E:207:PRO:HD2	1.92	0.50
1:E:276:ASP:O	1:E:279:LYS:N	2.30	0.50
1:E:85:ILE:HG22	1:E:89:LEU:HD11	1.93	0.49
1:E:239:PHE:CD1	1:E:239:PHE:C	2.90	0.49
1:E:195:THR:N	1:E:215:TYR:O	2.45	0.49
1:E:307:GLN:HB2	1:E:309:LYS:HD2	1.94	0.49
2:I:18:ARG:CB	2:I:18:ARG:NH1	2.75	0.49
2:I:5:THR:O	2:I:6:THR:OG1	2.26	0.49
1:E:91:GLU:HG3	1:E:185:PHE:HB2	1.94	0.48
1:E:180:ILE:HD12	1:E:181:GLN:N	2.28	0.48
1:E:262:SER:HB2	1:E:265:LEU:H	1.77	0.48
1:E:307:GLN:C	1:E:309:LYS:N	2.70	0.48
1:E:209:ILE:HD11	1:E:219:VAL:HG11	1.96	0.48
1:E:314:PHE:O	1:E:315:ILE:HG12	2.14	0.48
1:E:46:ILE:O	1:E:47:LYS:CB	2.59	0.48
1:E:206:ALA:HB3	1:E:219:VAL:HG12	1.95	0.48
1:E:260:HIS:O	1:E:261:PHE:O	2.32	0.48
1:E:271:ASN:HB3	1:E:281:PHE:CD1	2.49	0.48
1:E:37:THR:CG2	1:E:108:TYR:HD1	2.20	0.48
2:I:18:ARG:NH1	2:I:18:ARG:HB3	2.29	0.48
1:E:139:SER:O	1:E:140:GLU:C	2.57	0.47
1:E:169:PRO:HD3	1:E:204:TYR:OH	2.14	0.47
1:E:150:ILE:O	1:E:151:VAL:C	2.55	0.47
1:E:9:GLY:O	1:E:10:SER:C	2.56	0.47
1:E:82:LEU:O	1:E:84:GLN:HG2	2.14	0.47
1:E:160:LEU:O	1:E:190:ARG:HD2	2.14	0.47
1:E:83:LYS:O	1:E:84:GLN:HG2	2.13	0.47
1:E:205:LEU:CD1	1:E:247:TYR:CE1	2.95	0.47
1:E:239:PHE:O	1:E:240:ALA:HB2	2.15	0.47
1:E:189:LYS:CG	1:E:191:VAL:HG12	2.44	0.47
2:I:11:ILE:H	2:I:11:ILE:HG13	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:GLU:HA	1:E:173:LEU:HA	1.97	0.46
1:E:46:ILE:O	1:E:47:LYS:HB3	2.14	0.46
1:E:40:LEU:HD23	1:E:40:LEU:HA	1.74	0.46
1:E:80:VAL:O	1:E:81:LYS:C	2.59	0.46
1:E:203:GLU:H	1:E:203:GLU:HG2	1.21	0.46
1:E:194:ARG:HA	1:E:215:TYR:O	2.15	0.46
1:E:100:PHE:CG	1:E:101:PRO:CD	2.91	0.46
1:E:125:GLY:HA3	1:E:316:PRO:HG2	1.97	0.46
1:E:26:PHE:O	1:E:27:LEU:C	2.58	0.46
1:E:105:LYS:O	1:E:120:MET:HG3	2.16	0.45
2:I:11:ILE:HD12	2:I:12:ALA:N	2.25	0.45
1:E:84:GLN:HE21	1:E:84:GLN:HA	1.81	0.45
1:E:100:PHE:O	1:E:101:PRO:C	2.58	0.45
1:E:104:VAL:O	1:E:104:VAL:CG1	2.58	0.45
1:E:307:GLN:O	1:E:309:LYS:N	2.49	0.45
1:E:19:LEU:HD23	1:E:19:LEU:HA	1.66	0.45
1:E:286:ASN:O	1:E:289:ASN:HB2	2.17	0.45
1:E:210:ILE:HG21	1:E:210:ILE:HD13	1.24	0.45
1:E:174:ILE:CD1	1:E:180:ILE:HG22	2.47	0.45
1:E:111:LYS:HE2	1:E:350:PHE:O	2.17	0.45
1:E:132:LEU:O	1:E:133:ARG:C	2.59	0.44
1:E:40:LEU:C	1:E:42:GLN:N	2.75	0.44
1:E:109:SER:HA	1:E:117:TYR:O	2.17	0.44
1:E:184:ASP:OD1	1:E:184:ASP:O	2.34	0.44
1:E:189:LYS:CD	1:E:191:VAL:CG1	2.95	0.44
1:E:276:ASP:O	1:E:277:LEU:C	2.60	0.44
1:E:189:LYS:CG	1:E:191:VAL:CG1	2.96	0.44
1:E:69:PHE:HB3	1:E:120:MET:O	2.17	0.44
1:E:91:GLU:HG3	1:E:185:PHE:CB	2.48	0.44
1:E:135:ILE:O	1:E:135:ILE:HG22	2.18	0.44
1:E:243:PRO:O	1:E:246:ILE:N	2.49	0.44
1:E:31:GLU:O	1:E:33:PRO:CD	2.56	0.43
1:E:266:LYS:O	1:E:270:ARG:HG2	2.18	0.43
1:E:277:LEU:HD23	1:E:277:LEU:HA	1.08	0.43
1:E:82:LEU:O	1:E:83:LYS:C	2.61	0.43
1:E:240:ALA:HB2	1:E:249:LYS:HE3	1.99	0.43
1:E:327:PHE:O	1:E:328:ASP:C	2.61	0.43
1:E:26:PHE:CG	1:E:160:LEU:HG	2.53	0.43
1:E:92:LYS:HG3	1:E:350:PHE:CE2	2.53	0.43
1:E:71:MET:HG3	1:E:119:VAL:HG22	2.01	0.43
1:E:84:GLN:NE2	1:E:87:HIS:CD2	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:HIS:C	1:E:261:PHE:O	2.61	0.43
1:E:241:ASP:O	1:E:245:GLN:NE2	2.52	0.43
1:E:63:LYS:H	1:E:63:LYS:HG2	1.68	0.42
1:E:158:HIS:CE1	1:E:220:ASP:OD2	2.55	0.42
1:E:271:ASN:HB3	1:E:281:PHE:CG	2.54	0.42
1:E:222:TRP:CD1	1:E:222:TRP:C	2.98	0.42
1:E:272:LEU:C	1:E:274:GLN:H	2.27	0.42
1:E:295:LYS:O	1:E:296:TRP:C	2.59	0.42
1:E:133:ARG:NH2	1:E:230:GLU:OE2	2.48	0.42
1:E:269:LEU:HD12	1:E:269:LEU:HA	1.89	0.42
1:E:81:LYS:C	1:E:83:LYS:H	2.28	0.42
1:E:190:ARG:C	1:E:191:VAL:HG12	2.45	0.42
1:E:39:HIS:O	1:E:40:LEU:C	2.62	0.42
1:E:165:ARG:NH1	1:E:215:TYR:OH	2.53	0.42
1:E:179:TYR:CE2	1:E:308:ARG:HA	2.55	0.42
1:E:235:TYR:CD1	1:E:235:TYR:N	2.87	0.42
1:E:12:GLN:O	1:E:13:GLU:C	2.62	0.41
1:E:195:THR:O	1:E:214:GLY:HA2	2.19	0.41
1:E:249:LYS:HZ2	1:E:249:LYS:HG2	1.59	0.41
1:E:92:LYS:HD2	1:E:92:LYS:C	2.45	0.41
1:E:201:THR:O	1:E:202:PRO:C	2.61	0.41
1:E:95:LEU:HA	1:E:95:LEU:HD23	1.81	0.41
1:E:283:ASN:HD22	1:E:283:ASN:HA	1.59	0.41
1:E:35:GLN:NE2	1:E:350:PHE:C	2.78	0.41
1:E:49:LEU:HA	1:E:49:LEU:HD23	1.78	0.41
1:E:303:ILE:H	1:E:303:ILE:HG13	1.73	0.41
1:E:262:SER:HB3	1:E:265:LEU:H	1.85	0.41
1:E:288:VAL:H	1:E:288:VAL:HG23	1.71	0.41
1:E:169:PRO:HD2	2:I:19:ARG:HH12	1.86	0.41
1:E:270:ARG:HH11	1:E:270:ARG:HD2	1.77	0.41
1:E:331:GLU:O	1:E:332:GLU:O	2.39	0.41
1:E:334:GLU:O	1:E:336:ARG:N	2.54	0.41
1:E:49:LEU:HB2	1:E:57:VAL:O	2.21	0.40
1:E:40:LEU:O	1:E:41:ASP:C	2.63	0.40
1:E:90:ASN:O	1:E:94:ILE:HG13	2.21	0.40
1:E:148:ALA:HB3	1:E:305:ILE:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:GLU:OE2	1:E:196:TRP:CZ3[24_555]	2.10	0.10

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	E	326/350 (93%)	272 (83%)	38 (12%)	16 (5%)	1	6
2	I	15/20 (75%)	12 (80%)	3 (20%)	0	100	100
All	All	341/370 (92%)	284 (83%)	41 (12%)	16 (5%)	2	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	33	PRO
1	E	41	ASP
1	E	242	GLN
1	E	332	GLU
1	E	337	VAL
1	E	342	LYS
1	E	8	LYS
1	E	40	LEU
1	E	65	THR
1	E	277	LEU
1	E	286	ASN
1	E	184	ASP
1	E	261	PHE
1	E	264	ASP
1	E	244	ILE
1	E	333	GLU

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	249/304 (82%)	200 (80%)	49 (20%)	1	5
2	I	12/14 (86%)	7 (58%)	5 (42%)	0	0
All	All	261/318 (82%)	207 (79%)	54 (21%)	1	4

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	14	SER
1	E	23	LYS
1	E	27	LEU
1	E	35	GLN
1	E	40	LEU
1	E	47	LYS
1	E	53	SER
1	E	63	LYS
1	E	65	THR
1	E	73	ILE
1	E	74	LEU
1	E	76	LYS
1	E	79	VAL
1	E	82	LEU
1	E	84	GLN
1	E	90	ASN
1	E	92	LYS
1	E	98	VAL
1	E	103	LEU
1	E	111	LYS
1	E	114	SER
1	E	133	ARG
1	E	134	ARG
1	E	140	GLU
1	E	157	LEU
1	E	160	LEU
1	E	163	ILE

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Mol	Chain	Res	Type
1	E	165	ARG
1	E	167	LEU
1	E	177	GLN
1	E	191	VAL
1	E	203	GLU
1	E	210	ILE
1	E	211	LEU
1	E	219	VAL
1	E	222	TRP
1	E	224	LEU
1	E	246	ILE
1	E	249	LYS
1	E	252	SER
1	E	255	VAL
1	E	262	SER
1	E	269	LEU
1	E	277	LEU
1	E	283	ASN
1	E	299	THR
1	E	305	ILE
1	E	308	ARG
1	E	346	GLU
2	I	5	THR
2	I	15	ARG
2	I	18	ARG
2	I	19	ARG
2	I	22	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	35	GLN
1	E	62	HIS
1	E	84	GLN
1	E	87	HIS
1	E	158	HIS
1	E	245	GLN
1	E	283	ASN
1	E	289	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$
2	TYI	I	7	2	13,14,15	2.29	1 (7%)	14,19,21	3.25	7 (50%)
1	TPO	E	197	1	8,10,11	1.58	1 (12%)	10,14,16	2.03	2 (20%)

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
2	TYI	I	7	2	-	0/5/6/8	0/1/1/1
1	TPO	E	197	1	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	7	TYI	CE1-I1	-7.59	1.93	2.10
1	E	197	TPO	P-OG1	-3.58	1.53	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	7	TYI	CD1-CE1-I1	-7.12	105.10	118.46
2	I	7	TYI	CB-CG-CD1	5.19	129.33	120.43
2	I	7	TYI	CB-CG-CD2	-4.98	111.88	120.43
1	E	197	TPO	CG2-CB-CA	-4.92	103.68	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	197	TPO	P-OG1-CB	-3.62	113.49	123.33
2	I	7	TYI	CD2-CE2-CZ	3.12	127.21	121.33
2	I	7	TYI	CD2-CE2-I2	-3.11	112.62	118.46
2	I	7	TYI	CG-CD2-CE2	-2.66	115.60	120.45
2	I	7	TYI	CD1-CE1-CZ	-2.64	116.36	121.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	197	TPO	CB-OG1-P-O1P
1	E	197	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	7	TYI	2	0
1	E	197	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	MYR	E	0	-	9,9,15	0.56	0	8,8,15	0.72	0

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	-	-	2/7/7/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	0	MYR	C6-C7-C8-C9
3	E	0	MYR	C11-C12-C13-C14

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	332/350 (94%)	-1.00	0 100 100	16, 20, 30, 40	0
2	I	17/20 (85%)	-0.93	0 100 100	16, 22, 30, 31	0
All	All	349/370 (94%)	-1.00	0 100 100	16, 20, 30, 40	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	E	197	11/12	0.99	0.06	16,18,25,28	0
2	TYI	I	7	14/15	1.00	0.05	16,25,33,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MYR	E	0	10/16	0.98	0.04	16,16,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.