



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:58 PM UTC

PDB ID : 1D7K / pdb_00001d7k
Title : CRYSTAL STRUCTURE OF HUMAN ORNITHINE DECARBOXYLASE
AT 2.1 ANGSTROMS RESOLUTION
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Deposited on : 1999-10-18
Resolution : 2.10 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
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

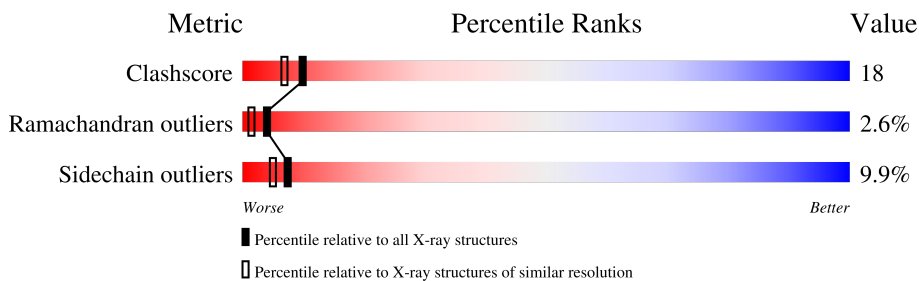
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	A	421	 52% 30% 11% . .
1	B	421	 48% 34% 11% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6824 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 HUMAN ORNITHINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	P	S	0	0	0
			3242	2073	537	610	1	21			
1	B	407	Total	C	N	O	P	S	0	0	0
			3181	2037	531	591	1	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	ARG	LYS	conflict	UNP P11926
A	415	GLN	GLU	conflict	UNP P11926
B	349	ARG	LYS	conflict	UNP P11926
B	415	GLN	GLU	conflict	UNP P11926

- Molecule 2 is water.

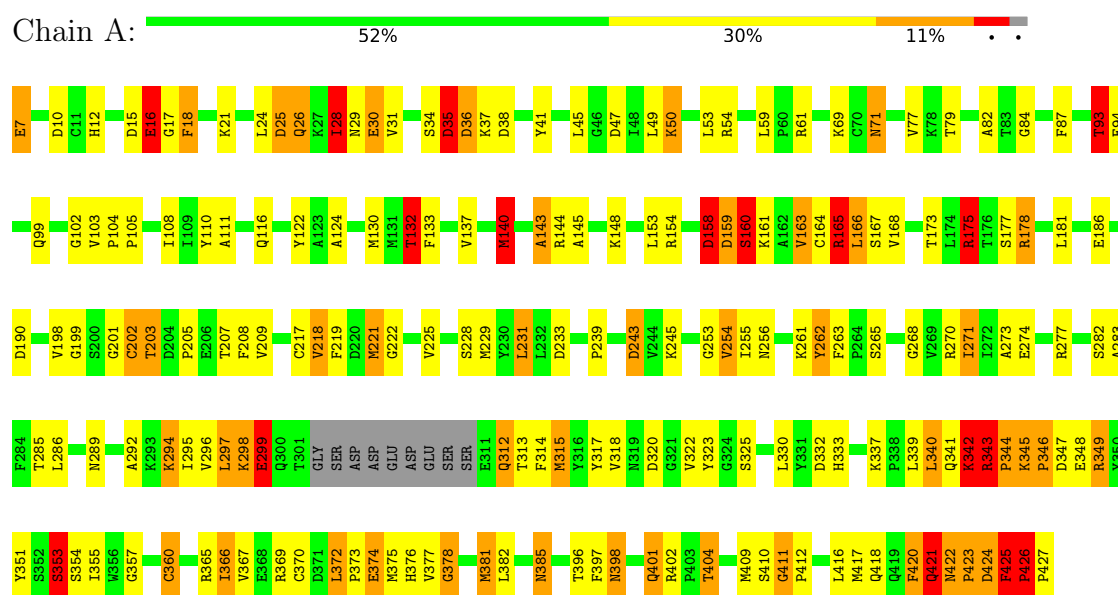
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	219	Total	O	0	0
			219	219		
2	B	182	Total	O	0	0
			182	182		

3 Residue-property plots [i](#)

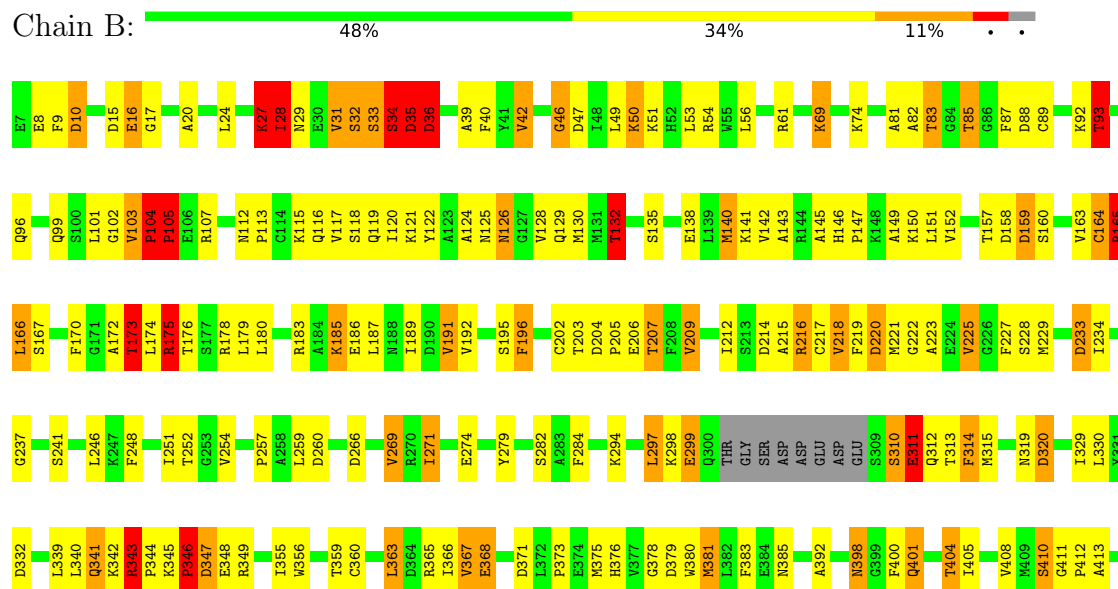
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: HUMAN ORNITHINE DECARBOXYLASE



• Molecule 1: HUMAN ORNITHINE DECARBOXYLASE



L416	M417	Q418	Q419	F420	Q421	ASN	PRO	ASP	PHE	PRO	PRO
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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 21	Depositor
Cell constants a, b, c, α , β , γ	61.68Å 107.45Å 139.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.50 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (30.50-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6824	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: LLP

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	A	1.06	2/3291 (0.1%)	2.20	142/4458 (3.2%)
1	B	0.99	0/3226	2.26	164/4367 (3.8%)
All	All	1.03	2/6517 (0.0%)	2.23	306/8825 (3.5%)

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	A	0	24
1	B	0	15
All	All	0	39

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	GLY	N-CA	6.81	1.51	1.45
1	A	411	GLY	N-CA	5.09	1.49	1.44

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	CD-NE-CZ	33.54	171.35	124.40
1	B	10	ASP	CA-CB-CG	17.97	130.57	112.60
1	A	426	PRO	N-CA-C	16.25	130.52	110.70
1	B	31	VAL	CA-C-O	14.00	132.71	119.97
1	B	35	ASP	CA-CB-CG	13.45	126.05	112.60
1	A	17	GLY	CA-C-N	12.87	140.76	123.00
1	A	17	GLY	C-N-CA	12.87	140.76	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	PHE	CA-C-N	11.63	132.36	120.38
1	A	425	PHE	C-N-CA	11.63	132.36	120.38
1	B	104	PRO	N-CA-C	11.52	122.91	110.58
1	A	365	ARG	CD-NE-CZ	11.46	140.44	124.40
1	A	144	ARG	CD-NE-CZ	10.59	139.22	124.40
1	A	132	THR	N-CA-CB	-10.42	94.31	110.46
1	B	28	ILE	CA-CB-CG2	10.24	127.91	110.50
1	B	347	ASP	CA-C-O	10.18	132.11	120.60
1	A	61	ARG	CD-NE-CZ	9.83	138.16	124.40
1	B	16	GLU	O-C-N	-9.80	111.83	122.03
1	A	38	ASP	CA-C-O	-9.70	111.27	121.55
1	B	347	ASP	CA-CB-CG	-9.57	103.03	112.60
1	A	143	ALA	O-C-N	-9.50	111.37	122.20
1	B	310	SER	O-C-N	-9.36	114.07	123.62
1	B	165	ARG	CD-NE-CZ	9.28	137.39	124.40
1	A	299	GLU	CA-CB-CG	9.01	132.12	114.10
1	A	320	ASP	CA-C-O	-8.87	111.75	121.33
1	B	15	ASP	CA-CB-CG	8.86	121.46	112.60
1	B	36	ASP	CA-CB-CG	-8.84	103.76	112.60
1	B	398	ASN	CA-CB-CG	8.73	121.33	112.60
1	B	376	HIS	CA-CB-CG	-8.64	105.16	113.80
1	A	243	ASP	CA-CB-CG	-8.63	103.97	112.60
1	B	126	ASN	CA-CB-CG	-8.63	103.97	112.60
1	A	421	GLN	N-CA-CB	8.61	122.52	109.34
1	A	199	GLY	CA-C-O	-8.48	115.82	122.52
1	A	318	VAL	O-C-N	-8.43	113.99	122.76
1	B	87	PHE	CA-CB-CG	-8.42	105.38	113.80
1	A	421	GLN	CA-C-O	8.40	129.35	120.95
1	A	219	PHE	CA-CB-CG	8.38	122.18	113.80
1	A	313	THR	CA-C-O	8.34	130.54	121.11
1	A	132	THR	OG1-CB-CG2	8.30	125.91	109.30
1	B	34	SER	N-CA-C	8.20	128.26	110.80
1	A	255	ILE	O-C-N	8.15	130.33	121.94
1	A	18	PHE	CA-CB-CG	-8.13	105.67	113.80
1	A	209	VAL	N-CA-C	-8.12	102.95	110.82
1	B	401	GLN	O-C-N	-8.05	113.92	122.94
1	B	284	PHE	CA-CB-CG	8.04	121.84	113.80
1	B	175	ARG	CD-NE-CZ	8.03	135.64	124.40
1	A	233	ASP	CA-CB-CG	8.03	120.62	112.60
1	B	378	GLY	N-CA-C	8.01	125.97	115.47
1	A	140	MET	CA-CB-CG	7.98	130.06	114.10
1	A	378	GLY	N-CA-C	-7.96	104.57	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	VAL	CA-C-O	-7.92	112.81	121.05
1	B	346	PRO	O-C-N	-7.90	113.10	123.06
1	B	36	ASP	CA-C-O	7.84	131.72	120.51
1	B	233	ASP	CA-C-O	-7.75	112.26	120.40
1	A	94	GLU	CA-C-O	-7.75	112.20	120.42
1	A	271	ILE	O-C-N	-7.72	115.02	123.20
1	A	202	CYS	CA-CB-SG	7.71	132.14	114.40
1	B	212	ILE	N-CA-C	7.66	117.78	110.42
1	B	10	ASP	N-CA-CB	7.64	122.17	109.56
1	A	299	GLU	CB-CG-CD	7.63	125.57	112.60
1	A	159	ASP	CA-C-O	7.60	129.36	120.69
1	B	347	ASP	CB-CA-C	7.58	123.43	110.77
1	B	363	LEU	N-CA-CB	-7.58	99.50	110.56
1	B	400	PHE	CA-CB-CG	-7.55	106.25	113.80
1	B	215	ALA	CA-C-N	-7.54	110.64	120.44
1	B	215	ALA	C-N-CA	-7.54	110.64	120.44
1	B	220	ASP	CA-CB-CG	7.52	120.12	112.60
1	B	35	ASP	N-CA-CB	7.46	123.10	110.49
1	A	116	GLN	OE1-CD-NE2	-7.41	115.19	122.60
1	B	31	VAL	N-CA-CB	-7.39	102.55	112.16
1	B	310	SER	N-CA-C	7.38	119.75	107.20
1	B	371	ASP	CA-CB-CG	-7.36	105.24	112.60
1	B	340	LEU	CA-C-N	-7.35	110.80	122.79
1	B	340	LEU	C-N-CA	-7.35	110.80	122.79
1	A	404	THR	O-C-N	-7.29	114.00	122.89
1	A	263	PHE	O-C-N	-7.28	115.33	121.23
1	B	27	LYS	CG-CD-CE	7.26	128.01	111.30
1	A	110	TYR	CA-CB-CG	7.25	126.96	113.90
1	B	219	PHE	CA-CB-CG	7.25	121.05	113.80
1	A	61	ARG	NE-CZ-NH1	7.25	128.75	121.50
1	B	165	ARG	CA-C-O	7.24	128.85	120.89
1	B	165	ARG	O-C-N	-7.22	115.39	123.48
1	B	135	SER	CA-C-O	7.15	129.05	121.33
1	B	33	SER	CA-C-O	-7.14	112.32	121.17
1	A	420	PHE	CA-C-O	-7.13	112.86	120.42
1	A	133	PHE	O-C-N	7.09	131.01	123.42
1	B	398	ASN	OD1-CG-ND2	-7.05	115.55	122.60
1	B	349	ARG	N-CA-CB	-7.02	99.65	109.97
1	B	93	THR	O-C-N	-7.00	113.05	122.43
1	A	104	PRO	CA-C-N	6.98	127.27	119.32
1	A	104	PRO	C-N-CA	6.98	127.27	119.32
1	A	145	ALA	CA-C-O	-6.96	111.21	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	CYS	CA-C-N	6.94	132.79	123.00
1	B	360	CYS	C-N-CA	6.94	132.79	123.00
1	B	159	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	420	PHE	O-C-N	6.92	130.04	122.15
1	B	102	GLY	N-CA-C	-6.87	105.57	114.85
1	B	170	PHE	CA-CB-CG	6.80	120.61	113.80
1	A	54	ARG	NE-CZ-NH1	-6.76	114.74	121.50
1	B	410	SER	CA-C-O	-6.74	114.31	121.99
1	B	381	MET	CA-CB-CG	6.73	127.57	114.10
1	B	35	ASP	CB-CG-OD1	6.69	133.79	118.40
1	B	47	ASP	CA-C-O	6.69	127.69	119.79
1	B	379	ASP	CA-C-N	6.69	132.23	123.00
1	B	379	ASP	C-N-CA	6.69	132.23	123.00
1	A	108	ILE	O-C-N	-6.65	116.36	123.14
1	A	77	VAL	N-CA-C	6.62	117.41	110.72
1	A	159	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	374	GLU	CB-CG-CD	6.61	123.84	112.60
1	A	110	TYR	O-C-N	-6.60	114.61	122.46
1	A	254	VAL	CA-C-N	6.59	128.94	120.70
1	A	254	VAL	C-N-CA	6.59	128.94	120.70
1	B	81	ALA	CA-C-O	-6.58	113.57	120.55
1	B	320	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	283	ALA	CA-C-O	-6.58	112.67	120.10
1	B	311	GLU	CB-CG-CD	6.57	123.77	112.60
1	A	30	GLU	N-CA-C	-6.56	103.33	112.12
1	A	25	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	178	ARG	CA-C-N	6.56	129.07	120.28
1	A	178	ARG	C-N-CA	6.56	129.07	120.28
1	A	245	LYS	CA-C-N	-6.54	114.34	122.84
1	A	245	LYS	C-N-CA	-6.54	114.34	122.84
1	B	34	SER	CA-C-O	6.52	129.84	120.51
1	B	365	ARG	CD-NE-CZ	6.51	133.52	124.40
1	A	313	THR	N-CA-C	6.51	120.14	109.72
1	A	105	PRO	O-C-N	-6.50	114.76	122.24
1	A	45	LEU	N-CA-C	6.46	120.27	112.38
1	A	239	PRO	O-C-N	-6.46	115.34	123.10
1	B	104	PRO	O-C-N	-6.41	118.14	121.15
1	B	311	GLU	CB-CA-C	-6.38	99.34	109.80
1	B	269	VAL	CA-C-O	6.33	128.69	120.78
1	B	314	PHE	CA-C-N	6.30	131.88	123.05
1	B	314	PHE	C-N-CA	6.30	131.88	123.05
1	A	218	VAL	O-C-N	-6.26	113.57	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	VAL	CA-C-O	6.26	128.24	121.67
1	B	279	TYR	CA-C-N	-6.23	115.23	122.14
1	B	279	TYR	C-N-CA	-6.23	115.23	122.14
1	B	378	GLY	CA-C-O	-6.20	112.05	119.00
1	B	103	VAL	CA-C-N	6.20	124.12	119.66
1	B	103	VAL	C-N-CA	6.20	124.12	119.66
1	B	50	LYS	CA-CB-CG	6.18	126.45	114.10
1	A	10	ASP	CA-C-O	-6.14	115.31	122.37
1	B	365	ARG	NH1-CZ-NH2	6.13	127.27	119.30
1	A	104	PRO	O-C-N	-6.13	118.27	121.15
1	B	104	PRO	CB-CA-C	-6.12	105.41	111.17
1	B	189	ILE	CA-C-O	-6.12	113.99	120.48
1	B	310	SER	CA-C-N	6.09	130.77	122.19
1	B	310	SER	C-N-CA	6.09	130.77	122.19
1	B	28	ILE	CA-C-O	6.08	127.21	120.71
1	B	31	VAL	N-CA-C	-6.06	106.85	112.43
1	A	103	VAL	CA-C-N	6.06	124.02	119.66
1	A	103	VAL	C-N-CA	6.06	124.02	119.66
1	A	277	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	A	165	ARG	CG-CD-NE	6.04	125.29	112.00
1	A	28	ILE	CA-CB-CG2	6.03	120.75	110.50
1	B	165	ARG	N-CA-C	6.03	118.28	108.76
1	A	315	MET	CA-C-O	-6.02	113.86	120.24
1	A	198	VAL	CA-C-O	-5.99	114.41	121.05
1	B	311	GLU	N-CA-C	5.99	119.39	109.46
1	A	360	CYS	N-CA-C	5.98	123.54	110.80
1	A	38	ASP	CA-CB-CG	-5.98	106.62	112.60
1	A	47	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	158	ASP	O-C-N	-5.96	115.19	122.11
1	A	93	THR	N-CA-C	5.95	118.55	111.71
1	B	112	ASN	N-CA-CB	-5.94	101.33	110.07
1	B	151	LEU	CA-C-O	5.93	126.90	120.32
1	A	228	SER	N-CA-C	5.91	118.85	108.56
1	A	87	PHE	CA-CB-CG	-5.89	107.91	113.80
1	A	140	MET	CB-CA-C	-5.89	101.55	110.92
1	B	119	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	B	116	GLN	CA-CB-CG	5.89	125.88	114.10
1	B	132	THR	N-CA-CB	-5.86	101.97	110.70
1	A	398	ASN	CA-CB-CG	5.86	118.46	112.60
1	B	365	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	A	203	THR	CA-CB-CG2	5.84	120.44	110.50
1	A	12	HIS	CA-CB-CG	-5.84	107.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	ASP	O-C-N	-5.84	115.31	122.25
1	A	401	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	372	LEU	O-C-N	-5.81	117.02	121.55
1	B	340	LEU	O-C-N	-5.81	116.56	123.06
1	B	237	GLY	N-CA-C	-5.81	106.98	115.63
1	A	253	GLY	CA-C-O	-5.80	112.60	119.45
1	A	175	ARG	CA-C-O	5.80	126.57	120.42
1	B	126	ASN	OD1-CG-ND2	5.76	128.36	122.60
1	B	61	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	B	54	ARG	NE-CZ-NH2	5.73	124.35	119.20
1	A	221	MET	N-CA-CB	5.71	118.29	110.01
1	B	31	VAL	O-C-N	-5.70	115.88	122.09
1	B	107	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	B	367	VAL	CA-C-O	5.64	125.24	120.22
1	B	408	VAL	N-CA-C	5.63	117.02	108.80
1	B	381	MET	N-CA-CB	-5.63	101.84	110.85
1	A	140	MET	N-CA-CB	5.62	118.37	109.82
1	A	273	ALA	O-C-N	-5.61	116.65	123.10
1	B	360	CYS	CA-CB-SG	-5.60	101.52	114.40
1	A	354	SER	CA-C-O	-5.58	114.81	121.11
1	A	353	SER	CA-C-O	-5.57	113.69	120.54
1	A	103	VAL	CA-C-O	-5.56	114.61	119.62
1	B	417	MET	N-CA-CB	5.56	118.30	110.12
1	B	373	PRO	CA-C-O	-5.55	115.01	121.95
1	A	54	ARG	N-CA-CB	-5.55	101.95	110.16
1	A	372	LEU	CA-C-O	5.55	126.13	120.64
1	A	154	ARG	NH1-CZ-NH2	5.54	126.50	119.30
1	B	152	VAL	N-CA-CB	-5.53	104.49	111.46
1	A	357	GLY	CA-C-O	-5.52	116.69	122.38
1	B	56	LEU	CA-C-O	-5.52	115.02	120.82
1	A	173	THR	O-C-N	-5.51	115.87	122.65
1	B	311	GLU	CA-CB-CG	5.51	125.12	114.10
1	A	143	ALA	CA-C-N	5.50	133.69	121.80
1	A	143	ALA	C-N-CA	5.50	133.69	121.80
1	A	186	GLU	CB-CG-CD	-5.50	103.25	112.60
1	B	413	ALA	O-C-N	-5.46	115.92	122.15
1	B	179	LEU	N-CA-C	5.46	120.37	111.37
1	B	35	ASP	OD1-CG-OD2	-5.46	109.81	122.90
1	A	218	VAL	CA-C-O	5.44	126.53	120.71
1	A	425	PHE	CB-CG-CD1	5.44	129.95	120.70
1	B	28	ILE	O-C-N	-5.43	114.67	121.84
1	B	112	ASN	CA-C-O	5.42	123.92	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	VAL	N-CA-C	5.42	114.26	108.95
1	A	277	ARG	CA-C-N	5.40	127.83	120.54
1	A	277	ARG	C-N-CA	5.40	127.83	120.54
1	B	368	GLU	N-CA-CB	-5.38	101.94	110.28
1	B	35	ASP	CB-CA-C	5.37	121.11	110.42
1	A	175	ARG	CD-NE-CZ	5.37	131.92	124.40
1	A	318	VAL	CA-C-O	5.37	128.20	121.92
1	B	209	VAL	N-CA-CB	-5.36	104.99	110.62
1	B	129	GLN	CA-C-N	-5.35	114.65	122.19
1	B	129	GLN	C-N-CA	-5.35	114.65	122.19
1	A	332	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	144	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	B	61	ARG	CA-C-N	-5.33	116.20	123.12
1	B	61	ARG	C-N-CA	-5.33	116.20	123.12
1	A	294	LYS	CA-C-O	-5.31	115.04	120.99
1	A	82	ALA	N-CA-C	-5.30	105.67	111.82
1	B	116	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	B	196	PHE	CA-CB-CG	-5.29	108.51	113.80
1	B	271	ILE	N-CA-CB	5.29	118.51	111.64
1	B	380	TRP	N-CA-CB	5.28	118.85	110.57
1	B	420	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	20	ALA	CA-C-N	5.26	127.77	120.29
1	B	20	ALA	C-N-CA	5.26	127.77	120.29
1	B	392	ALA	CA-C-O	-5.26	114.98	120.55
1	A	323	TYR	CA-C-O	-5.25	113.59	119.79
1	A	273	ALA	CA-C-N	5.25	129.46	123.21
1	A	273	ALA	C-N-CA	5.25	129.46	123.21
1	A	225	VAL	CA-C-O	-5.24	114.17	119.89
1	A	268	GLY	O-C-N	-5.23	116.38	122.60
1	B	20	ALA	O-C-N	-5.23	115.84	122.27
1	B	314	PHE	O-C-N	-5.22	116.44	123.23
1	B	312	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	366	ILE	N-CA-C	5.20	116.28	111.81
1	A	381	MET	CA-CB-CG	5.20	124.51	114.10
1	B	112	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	B	46	GLY	O-C-N	-5.19	116.74	122.24
1	B	8	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	71	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	B	356	TRP	CA-C-O	5.16	126.28	120.70
1	A	102	GLY	CA-C-O	-5.16	113.12	119.06
1	A	243	ASP	N-CA-CB	-5.16	103.36	110.42
1	B	355	ILE	CA-C-N	5.16	130.68	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ILE	C-N-CA	5.16	130.68	122.94
1	B	319	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	B	405	ILE	N-CA-CB	-5.15	104.81	110.99
1	A	93	THR	CA-CB-OG1	5.15	117.32	109.60
1	B	311	GLU	CA-C-O	-5.15	114.72	120.54
1	A	159	ASP	N-CA-C	5.14	117.93	109.76
1	B	89	CYS	CA-C-O	-5.14	114.81	120.36
1	B	228	SER	N-CA-C	5.13	117.52	107.57
1	B	47	ASP	N-CA-C	-5.12	105.78	112.23
1	A	231	LEU	O-C-N	-5.11	116.97	123.05
1	B	212	ILE	CA-C-N	5.11	127.09	120.44
1	B	212	ILE	C-N-CA	5.11	127.09	120.44
1	A	190	ASP	CA-C-O	-5.11	114.83	120.60
1	B	85	THR	N-CA-CB	5.11	117.66	110.36
1	A	262	TYR	CB-CA-C	5.09	118.15	109.24
1	B	359	THR	N-CA-CB	5.08	118.18	110.45
1	B	31	VAL	CB-CA-C	5.08	117.85	111.65
1	A	256	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	B	39	ALA	N-CA-C	5.08	116.85	110.24
1	B	115	LYS	N-CA-C	5.08	117.77	109.59
1	B	346	PRO	CA-C-N	-5.08	114.42	121.99
1	B	346	PRO	C-N-CA	-5.08	114.42	121.99
1	B	16	GLU	CA-C-O	-5.08	115.67	121.00
1	A	402	ARG	CA-C-O	-5.07	115.06	120.23
1	B	212	ILE	N-CA-CB	-5.07	104.62	110.55
1	B	216	ARG	N-CA-CB	5.06	117.35	110.01
1	B	312	GLN	CA-C-O	-5.06	113.27	120.51
1	A	16	GLU	CA-CB-CG	5.06	124.22	114.10
1	A	178	ARG	O-C-N	-5.06	116.76	122.12
1	B	9	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	59	LEU	CA-C-O	5.05	126.44	121.29
1	A	325	SER	N-CA-C	5.05	117.52	111.71
1	A	16	GLU	O-C-N	-5.05	115.87	122.59
1	A	285	THR	CA-C-N	-5.05	115.61	122.93
1	A	285	THR	C-N-CA	-5.05	115.61	122.93
1	B	17	GLY	N-CA-C	5.05	125.14	113.18
1	A	122	TYR	O-C-N	-5.04	116.77	122.12
1	B	51	LYS	O-C-N	-5.04	116.77	122.12
1	B	173	THR	CA-CB-OG1	-5.04	102.03	109.60
1	A	122	TYR	CA-C-O	5.04	125.89	120.55
1	A	418	GLN	N-CA-C	5.04	116.77	111.28
1	A	385	ASN	N-CA-CB	-5.02	104.28	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	VAL	N-CA-C	5.01	116.97	109.20
1	A	333	HIS	CA-CB-CG	-5.01	108.79	113.80
1	B	42	VAL	CA-C-N	-5.01	115.93	123.00
1	B	42	VAL	C-N-CA	-5.01	115.93	123.00
1	B	191	VAL	N-CA-C	5.00	115.30	107.99

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ALA	Mainchain
1	A	143	ALA	Mainchain
1	A	158	ASP	Peptide
1	A	16	GLU	Peptide
1	A	160	SER	Peptide
1	A	161	LYS	Peptide
1	A	165	ARG	Peptide
1	A	201	GLY	Peptide
1	A	208	PHE	Mainchain
1	A	26	GLN	Peptide
1	A	271	ILE	Mainchain
1	A	274	GLU	Mainchain
1	A	29	ASN	Mainchain
1	A	297	LEU	Peptide
1	A	342	LYS	Peptide
1	A	343	ARG	Peptide
1	A	35	ASP	Peptide
1	A	421	GLN	Peptide
1	A	422	ASN	Peptide
1	A	424	ASP	Peptide
1	A	425	PHE	Peptide
1	A	50	LYS	Mainchain
1	A	7	GLU	Peptide
1	A	99	GLN	Mainchain
1	B	101	LEU	Peptide
1	B	104	PRO	Mainchain
1	B	160	SER	Peptide
1	B	164	CYS	Peptide
1	B	165	ARG	Peptide
1	B	172	ALA	Peptide
1	B	241	SER	Mainchain
1	B	297	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	320	ASP	Mainchain
1	B	34	SER	Peptide
1	B	341	GLN	Peptide
1	B	342	LYS	Peptide
1	B	346	PRO	Peptide
1	B	347	ASP	Peptide
1	B	417	MET	Peptide

5.2 Too-close contacts [i](#)

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	A	3242	0	3185	110	0
1	B	3181	0	3133	121	0
2	A	219	0	0	9	0
2	B	182	0	0	10	0
All	All	6824	0	6318	223	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 18.

All (223) 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:A:426:PRO:CB	1:A:427:PRO:HD3	1.77	1.13
1:A:426:PRO:HB2	1:A:427:PRO:HD3	1.18	1.11
1:A:409:MET:HE1	1:A:417:MET:HE3	1.33	1.09
1:A:15:ASP:O	1:A:16:GLU:O	1.71	1.06
1:B:173:THR:HB	1:B:175:ARG:HD3	1.43	1.01
1:A:218:VAL:HA	1:A:221:MET:HE2	1.45	0.95
1:A:426:PRO:HB2	1:A:427:PRO:CD	1.97	0.95
1:A:217:CYS:HB2	2:A:612:HOH:O	1.72	0.90
1:A:343:ARG:O	1:A:344:PRO:O	1.90	0.89
1:A:84:GLY:HA2	1:A:422:ASN:ND2	1.91	0.85
1:B:410:SER:HB2	1:B:412:PRO:HD2	1.59	0.85
1:B:345:LYS:HB2	1:B:348:GLU:HG3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PRO:CB	1:A:427:PRO:CD	2.54	0.81
1:A:79:THR:HG23	1:A:417:MET:HE2	1.63	0.79
1:A:35:ASP:HB2	1:A:37:LYS:HG3	1.67	0.77
1:A:322:VAL:HB	1:A:330:LEU:HD11	1.67	0.77
1:B:341:GLN:HB3	2:B:506:HOH:O	1.85	0.76
1:A:282:SER:HA	1:A:385:ASN:HD22	1.50	0.76
1:A:79:THR:HG23	1:A:417:MET:CE	2.16	0.75
1:B:159:ASP:HB2	1:B:207:THR:HG21	1.68	0.75
1:B:173:THR:OG1	1:B:176:THR:HB	1.87	0.75
1:A:165:ARG:HD2	1:A:166:LEU:CD1	2.17	0.74
1:A:137:VAL:HA	1:A:140:MET:HG3	1.69	0.74
1:A:222:GLY:HA3	1:A:229:MET:HE3	1.70	0.74
1:B:205:PRO:HB2	1:B:254:VAL:HG21	1.67	0.74
1:B:375:MET:HE1	1:B:381:MET:HE1	1.71	0.72
1:A:165:ARG:HD2	1:A:166:LEU:HD12	1.72	0.71
1:B:404:THR:HG22	2:B:445:HOH:O	1.91	0.71
1:A:202:CYS:HB3	2:A:561:HOH:O	1.90	0.70
1:B:298:LYS:HE2	1:B:313:THR:HG21	1.74	0.70
1:A:348:GLU:O	1:A:349:ARG:HB3	1.91	0.69
1:B:345:LYS:HB3	1:B:346:PRO:HD2	1.74	0.69
1:B:82:ALA:HB1	1:B:421:GLN:HG3	1.75	0.68
1:B:53:LEU:HD11	1:B:416:LEU:HD11	1.75	0.68
1:B:159:ASP:OD2	1:B:202:CYS:HA	1.94	0.67
1:A:165:ARG:HA	1:A:165:ARG:HH11	1.60	0.66
1:B:375:MET:HE1	1:B:381:MET:CE	2.26	0.66
1:A:424:ASP:O	1:A:425:PHE:HB2	1.96	0.65
1:B:183:ARG:O	1:B:187:LEU:HG	1.98	0.64
1:B:24:LEU:HD12	1:B:40:PHE:CE1	2.32	0.64
1:A:163:VAL:HG22	1:A:164:CYS:H	1.62	0.64
1:B:117:VAL:HG22	1:B:141:LYS:HG2	1.78	0.64
1:A:409:MET:HE1	1:A:417:MET:CE	2.21	0.63
1:A:175:ARG:H	1:A:175:ARG:HD2	1.64	0.62
1:A:372:LEU:HD13	1:A:375:MET:CE	2.28	0.62
1:B:298:LYS:HG2	1:B:313:THR:HG23	1.82	0.62
1:B:345:LYS:HB3	1:B:346:PRO:CD	2.29	0.62
1:A:148:LYS:HE2	1:A:148:LYS:HA	1.81	0.62
1:B:24:LEU:HD12	1:B:40:PHE:HE1	1.65	0.62
1:B:218:VAL:HA	1:B:221:MET:HE3	1.80	0.62
1:A:15:ASP:O	1:A:16:GLU:C	2.42	0.61
1:B:257:PRO:HA	1:B:260:ASP:HB2	1.81	0.61
1:A:165:ARG:HG2	1:B:368:GLU:OE2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:HD3	1:A:166:LEU:N	2.15	0.61
1:A:175:ARG:H	1:A:175:ARG:CD	2.13	0.61
1:A:165:ARG:CG	1:A:166:LEU:H	2.14	0.60
1:A:404:THR:HG22	2:A:544:HOH:O	2.01	0.60
1:A:348:GLU:O	1:A:349:ARG:CB	2.48	0.60
1:B:130:MET:HA	1:B:150:LYS:O	2.03	0.59
1:B:185:LYS:HD3	1:B:227:PHE:CE2	2.38	0.58
1:B:82:ALA:O	1:B:421:GLN:HA	2.03	0.58
1:A:270:ARG:NH2	2:A:444:HOH:O	2.37	0.58
1:A:426:PRO:HB3	1:A:427:PRO:HD3	1.81	0.57
2:A:584:HOH:O	1:B:93:THR:HG23	2.05	0.57
1:B:117:VAL:HG23	2:B:534:HOH:O	2.04	0.57
1:A:165:ARG:CD	1:A:166:LEU:H	2.18	0.57
1:A:178:ARG:HH11	1:A:221:MET:HB3	1.70	0.56
1:A:411:GLY:N	1:A:412:PRO:CD	2.69	0.56
1:B:216:ARG:O	1:B:217:CYS:O	2.24	0.56
1:B:174:LEU:H	1:B:174:LEU:HD12	1.71	0.55
1:B:216:ARG:O	1:B:217:CYS:C	2.48	0.55
1:B:159:ASP:CB	1:B:207:THR:HG21	2.35	0.55
1:B:298:LYS:O	1:B:299:GLU:CB	2.53	0.55
1:B:344:PRO:HD3	2:B:442:HOH:O	2.06	0.55
1:B:191:VAL:HG12	1:B:229:MET:HE3	1.88	0.55
1:B:33:SER:O	1:B:34:SER:CB	2.52	0.55
1:B:173:THR:HG1	1:B:176:THR:HB	1.71	0.55
1:B:311:GLU:HG3	1:B:314:PHE:HZ	1.72	0.55
1:A:165:ARG:HG3	1:A:166:LEU:H	1.72	0.54
1:B:117:VAL:HG12	1:B:121:LYS:HE2	1.88	0.54
1:A:37:LYS:NZ	1:A:378:GLY:O	2.41	0.54
1:A:372:LEU:HD13	1:A:375:MET:HE2	1.90	0.53
1:B:27:LYS:NZ	2:B:604:HOH:O	2.40	0.53
1:B:183:ARG:NH2	1:B:186:GLU:OE1	2.41	0.53
1:A:292:ALA:HB3	1:A:317:TYR:HB2	1.91	0.53
1:B:92:LYS:O	1:B:96:GLN:HG3	2.09	0.53
1:B:159:ASP:HB2	1:B:207:THR:CG2	2.38	0.53
1:B:259:LEU:HD22	1:B:271:ILE:HD13	1.90	0.53
1:A:353:SER:HB2	1:A:370:CYS:O	2.08	0.53
1:B:128:VAL:O	1:B:146:HIS:HE1	1.91	0.53
1:B:132:THR:HG21	2:B:542:HOH:O	2.09	0.53
1:B:163:VAL:O	1:B:164:CYS:C	2.52	0.52
1:B:29:ASN:O	1:B:32:SER:HB2	2.09	0.52
1:A:341:GLN:HE21	1:A:342:LYS:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASP:O	1:B:36:ASP:C	2.53	0.52
1:B:147:PRO:HD2	2:B:475:HOH:O	2.10	0.52
1:B:297:LEU:HD21	1:B:310:SER:O	2.10	0.52
1:A:177:SER:HB3	1:A:221:MET:HE1	1.90	0.52
1:A:84:GLY:HA2	1:A:422:ASN:HD22	1.70	0.52
1:B:69:LLP:H6	1:B:274:GLU:O	2.10	0.52
1:A:355:ILE:HD13	1:A:381:MET:SD	2.50	0.51
1:B:298:LYS:HG2	1:B:313:THR:CG2	2.40	0.51
1:A:93:THR:HG23	2:B:502:HOH:O	2.11	0.51
1:A:132:THR:HG21	2:A:447:HOH:O	2.10	0.51
1:A:165:ARG:HD2	1:A:166:LEU:CG	2.41	0.51
1:A:24:LEU:HD21	1:A:382:LEU:HD13	1.92	0.51
1:B:282:SER:HA	1:B:385:ASN:HD22	1.74	0.51
1:A:401:GLN:NE2	1:B:93:THR:HG21	2.25	0.51
1:B:33:SER:O	1:B:34:SER:HB2	2.10	0.51
1:A:421:GLN:O	1:A:423:PRO:HD2	2.11	0.51
1:B:251:ILE:O	1:B:254:VAL:HG22	2.11	0.51
1:A:295:ILE:HG12	1:A:314:PHE:CE1	2.46	0.51
1:A:218:VAL:CA	1:A:221:MET:HE2	2.31	0.50
1:B:121:LYS:HG2	1:B:145:ALA:HB1	1.93	0.50
1:B:196:PHE:CZ	1:B:234:ILE:HG22	2.47	0.50
1:B:175:ARG:CD	1:B:175:ARG:H	2.24	0.50
1:A:35:ASP:CB	1:A:37:LYS:HG3	2.40	0.50
1:B:142:VAL:O	1:B:143:ALA:C	2.54	0.50
1:A:205:PRO:HB2	1:A:254:VAL:HG21	1.94	0.50
1:A:376:HIS:O	1:A:377:VAL:C	2.54	0.50
1:A:340:LEU:HD11	1:A:375:MET:SD	2.52	0.50
1:A:425:PHE:C	1:A:425:PHE:CD2	2.91	0.49
1:B:83:THR:HG22	1:B:85:THR:HG23	1.94	0.49
1:B:173:THR:OG1	1:B:176:THR:N	2.44	0.49
1:A:166:LEU:HD11	1:B:368:GLU:HG2	1.94	0.49
1:A:373:PRO:O	1:A:374:GLU:C	2.55	0.49
1:A:28:ILE:HD12	1:A:28:ILE:O	2.12	0.49
1:B:140:MET:HE3	1:B:140:MET:HA	1.94	0.49
1:A:165:ARG:HD2	1:A:166:LEU:HG	1.94	0.48
1:A:366:ILE:HG22	1:A:367:VAL:HG23	1.94	0.48
1:A:298:LYS:HA	1:A:298:LYS:HE2	1.95	0.48
1:A:35:ASP:O	1:A:36:ASP:HB2	2.14	0.48
1:A:165:ARG:CD	1:A:166:LEU:N	2.75	0.48
1:A:243:ASP:OD2	1:A:337:LYS:HE3	2.13	0.48
1:B:246:LEU:HG	1:B:251:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ILE:HD12	1:B:28:ILE:C	2.38	0.48
1:A:111:ALA:HA	1:A:132:THR:HB	1.96	0.48
1:A:294:LYS:HD2	1:A:315:MET:CE	2.43	0.48
1:A:93:THR:HG21	1:B:401:GLN:NE2	2.29	0.47
1:A:342:LYS:HB2	2:A:559:HOH:O	2.14	0.47
1:B:366:ILE:HG22	1:B:367:VAL:HG23	1.96	0.47
1:A:159:ASP:HB3	1:A:207:THR:HG21	1.97	0.47
1:A:21:LYS:HD2	2:A:464:HOH:O	2.14	0.47
1:A:165:ARG:CG	1:A:166:LEU:N	2.78	0.47
1:B:104:PRO:O	1:B:105:PRO:C	2.58	0.47
1:B:158:ASP:O	1:B:159:ASP:HB3	2.15	0.47
1:B:175:ARG:H	1:B:175:ARG:HD2	1.78	0.47
1:B:217:CYS:SG	1:B:221:MET:HE2	2.54	0.47
1:A:297:LEU:O	1:A:312:GLN:HB2	2.15	0.47
1:B:96:GLN:HG2	1:B:122:TYR:OH	2.13	0.47
1:B:165:ARG:HA	1:B:165:ARG:HD3	1.69	0.46
1:B:329:ILE:HG13	1:B:330:LEU:HD12	1.97	0.46
1:B:178:ARG:HA	1:B:178:ARG:HD2	1.73	0.46
1:B:214:ASP:O	1:B:217:CYS:HB3	2.14	0.46
1:A:166:LEU:CD1	1:B:368:GLU:HG2	2.46	0.46
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.77	0.46
1:A:37:LYS:HD3	1:A:289:ASN:ND2	2.30	0.45
1:A:25:ASP:O	1:A:26:GLN:C	2.55	0.45
1:B:138:GLU:O	1:B:142:VAL:HG23	2.17	0.45
1:A:153:LEU:HD23	1:A:153:LEU:C	2.42	0.45
1:A:410:SER:HB2	1:A:412:PRO:HD2	1.99	0.45
1:A:16:GLU:O	1:A:18:PHE:N	2.35	0.45
1:A:41:TYR:CE1	1:A:286:LEU:HB2	2.52	0.45
1:B:248:PHE:O	1:B:252:THR:HG23	2.15	0.45
1:A:417:MET:O	1:A:421:GLN:N	2.49	0.45
1:B:218:VAL:HG22	1:B:221:MET:CE	2.47	0.45
1:A:37:LYS:HD3	1:A:289:ASN:HD21	1.82	0.45
1:A:21:LYS:HG3	2:A:585:HOH:O	2.16	0.44
1:B:294:LYS:HB2	1:B:315:MET:HB2	1.98	0.44
1:B:206:GLU:OE2	1:B:209:VAL:HG21	2.17	0.44
1:A:312:GLN:HA	1:A:312:GLN:OE1	2.16	0.44
1:A:79:THR:HG23	1:A:417:MET:HE1	1.96	0.44
1:A:165:ARG:HA	1:A:165:ARG:NH1	2.29	0.44
1:B:164:CYS:O	1:B:165:ARG:HB2	2.17	0.44
1:A:351:TYR:N	1:A:372:LEU:O	2.47	0.43
1:B:166:LEU:O	1:B:167:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:O	1:A:425:PHE:CB	2.65	0.43
1:B:204:ASP:HA	1:B:205:PRO:HD2	1.90	0.43
1:A:93:THR:HG21	1:B:401:GLN:HE21	1.82	0.43
1:B:343:ARG:HA	1:B:344:PRO:HD3	1.77	0.43
1:B:124:ALA:HB2	1:B:146:HIS:CG	2.54	0.43
1:B:157:THR:CG2	1:B:196:PHE:HB2	2.49	0.43
1:B:83:THR:CG2	1:B:85:THR:HG23	2.49	0.42
1:B:411:GLY:N	1:B:412:PRO:CD	2.82	0.42
1:B:375:MET:HE3	1:B:375:MET:HB2	1.82	0.42
1:B:183:ARG:O	1:B:186:GLU:HB2	2.20	0.42
1:A:421:GLN:HG3	1:A:422:ASN:H	1.84	0.42
1:B:220:ASP:O	1:B:223:ALA:HB3	2.20	0.42
1:A:346:PRO:O	1:A:347:ASP:HB3	2.19	0.42
1:B:122:TYR:O	1:B:126:ASN:ND2	2.37	0.42
1:B:195:SER:HB3	1:B:233:ASP:HB3	2.01	0.42
1:B:381:MET:HE3	1:B:381:MET:HB2	1.81	0.42
1:B:88:ASP:OD1	1:B:88:ASP:C	2.62	0.42
1:B:142:VAL:HG12	1:B:146:HIS:O	2.20	0.42
1:B:185:LYS:HD2	1:B:185:LYS:HA	1.90	0.42
1:B:381:MET:HG2	1:B:383:PHE:CE1	2.55	0.42
1:B:146:HIS:CG	1:B:149:ALA:HB2	2.55	0.41
1:A:36:ASP:HA	1:B:118:SER:HB3	2.02	0.41
1:B:195:SER:CB	1:B:233:ASP:HB3	2.50	0.41
1:B:176:THR:O	1:B:180:LEU:HG	2.21	0.41
1:B:222:GLY:O	1:B:225:VAL:HG22	2.20	0.41
1:B:254:VAL:O	1:B:257:PRO:HD2	2.20	0.41
1:A:148:LYS:HE2	1:A:148:LYS:CA	2.48	0.41
1:A:411:GLY:N	1:A:412:PRO:HD2	2.35	0.41
1:B:103:VAL:HG13	1:B:104:PRO:HD2	2.02	0.41
1:A:165:ARG:CD	1:B:368:GLU:OE2	2.68	0.41
1:A:181:LEU:HD12	1:A:221:MET:HE3	2.02	0.41
1:B:46:GLY:HA3	2:B:435:HOH:O	2.21	0.41
1:A:130:MET:HE3	1:A:130:MET:HB2	1.83	0.41
1:A:165:ARG:CD	1:A:166:LEU:HG	2.50	0.41
1:A:261:LYS:HE2	1:A:262:TYR:CZ	2.55	0.41
1:A:343:ARG:O	1:A:344:PRO:C	2.61	0.41
1:B:24:LEU:HD13	1:B:42:VAL:CG2	2.51	0.41
1:B:53:LEU:CD1	1:B:416:LEU:HD11	2.49	0.41
1:B:120:ILE:O	1:B:121:LYS:C	2.64	0.41
1:B:164:CYS:O	1:B:165:ARG:NH1	2.54	0.41
1:A:420:PHE:O	1:A:421:GLN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:HD3	2:B:542:HOH:O	2.21	0.41
1:A:345:LYS:O	1:A:348:GLU:HB2	2.21	0.40
1:A:396:THR:O	1:A:397:PHE:C	2.63	0.40
1:B:222:GLY:O	1:B:227:PHE:HB2	2.21	0.40
1:B:166:LEU:O	1:B:167:SER:CB	2.70	0.40
1:A:49:LEU:HB3	1:A:416:LEU:HD23	2.03	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	A	407/421 (97%)	371 (91%)	23 (6%)	13 (3%)	3	1
1	B	402/421 (96%)	362 (90%)	32 (8%)	8 (2%)	6	2
All	All	809/842 (96%)	733 (91%)	55 (7%)	21 (3%)	4	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	160	SER
1	A	312	GLN
1	A	344	PRO
1	A	360	CYS
1	A	423	PRO
1	A	425	PHE
1	A	426	PRO
1	B	35	ASP
1	B	173	THR
1	A	299	GLU
1	B	36	ASP

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Mol	Chain	Res	Type
1	B	269	VAL
1	B	299	GLU
1	B	419	GLN
1	A	34	SER
1	A	346	PRO
1	B	105	PRO
1	B	343	ARG
1	A	71	ASN
1	A	35	ASP

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	A	348/358 (97%)	314 (90%)	34 (10%)	7	5
1	B	337/358 (94%)	303 (90%)	34 (10%)	7	5
All	All	685/716 (96%)	617 (90%)	68 (10%)	7	5

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	16	GLU
1	A	28	ILE
1	A	30	GLU
1	A	31	VAL
1	A	36	ASP
1	A	50	LYS
1	A	53	LEU
1	A	93	THR
1	A	132	THR
1	A	140	MET
1	A	158	ASP
1	A	160	SER
1	A	165	ARG

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Mol	Chain	Res	Type
1	A	166	LEU
1	A	167	SER
1	A	168	VAL
1	A	175	ARG
1	A	203	THR
1	A	231	LEU
1	A	265	SER
1	A	296	VAL
1	A	298	LYS
1	A	299	GLU
1	A	339	LEU
1	A	340	LEU
1	A	342	LYS
1	A	343	ARG
1	A	345	LYS
1	A	349	ARG
1	A	353	SER
1	A	369	ARG
1	A	398	ASN
1	A	426	PRO
1	B	10	ASP
1	B	16	GLU
1	B	27	LYS
1	B	28	ILE
1	B	31	VAL
1	B	32	SER
1	B	34	SER
1	B	49	LEU
1	B	50	LYS
1	B	74	LYS
1	B	83	THR
1	B	93	THR
1	B	99	GLN
1	B	105	PRO
1	B	125	ASN
1	B	132	THR
1	B	140	MET
1	B	165	ARG
1	B	166	LEU
1	B	175	ARG
1	B	185	LYS
1	B	192	VAL

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Mol	Chain	Res	Type
1	B	203	THR
1	B	207	THR
1	B	225	VAL
1	B	266	ASP
1	B	311	GLU
1	B	339	LEU
1	B	343	ARG
1	B	363	LEU
1	B	398	ASN
1	B	404	THR
1	B	420	PHE
1	B	421	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	341	GLN
1	A	385	ASN
1	B	125	ASN
1	B	146	HIS
1	B	188	ASN
1	B	312	GLN
1	B	333	HIS
1	B	385	ASN
1	B	401	GLN
1	B	419	GLN

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	LLP	A	69	1	23,24,25	1.20	2 (8%)	25,32,34	2.24	8 (32%)
1	LLP	B	69	1	23,24,25	1.12	2 (8%)	25,32,34	2.30	12 (48%)

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	LLP	A	69	1	-	3/16/17/19	0/1/1/1
1	LLP	B	69	1	-	6/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	LLP	C2'-C2	2.61	1.54	1.50
1	A	69	LLP	P-OP3	-2.50	1.45	1.54
1	B	69	LLP	P-OP3	-2.39	1.45	1.54
1	B	69	LLP	C5'-C5	2.16	1.56	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	LLP	CE-NZ-C4'	7.01	141.17	118.72
1	B	69	LLP	C3-C2-N1	-4.33	115.49	120.96
1	B	69	LLP	C4-C3-C2	3.75	122.25	120.14
1	B	69	LLP	CE-NZ-C4'	3.68	130.50	118.72
1	B	69	LLP	C6-N1-C2	3.63	125.79	119.20
1	A	69	LLP	OP3-P-OP4	-3.39	97.84	106.67
1	A	69	LLP	C5-C6-N1	-3.33	118.42	123.83
1	B	69	LLP	CD-CE-NZ	3.31	119.59	110.83
1	B	69	LLP	C5-C6-N1	-3.22	118.59	123.83
1	A	69	LLP	C6-N1-C2	3.15	124.90	119.20
1	B	69	LLP	C2'-C2-C3	2.99	124.30	120.80
1	A	69	LLP	C5'-C5-C6	2.83	123.97	119.36
1	B	69	LLP	CG-CD-CE	2.79	123.09	113.38
1	B	69	LLP	OP3-P-OP1	2.53	120.69	110.83
1	A	69	LLP	CD-CE-NZ	2.51	117.47	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	LLP	C5'-C5-C6	2.46	123.37	119.36
1	B	69	LLP	C3-C4-C5	-2.39	116.36	118.28
1	A	69	LLP	C3-C2-N1	-2.22	118.16	120.96
1	A	69	LLP	O3-C3-C4	2.22	125.41	119.44
1	B	69	LLP	OP4-C5'-C5	-2.11	105.39	109.36

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	69	LLP	C5-C4-C4'-NZ
1	A	69	LLP	C3-C4-C4'-NZ
1	B	69	LLP	CE-CD-CG-CB
1	B	69	LLP	CG-CD-CE-NZ
1	A	69	LLP	CD-CE-NZ-C4'
1	B	69	LLP	C3-C4-C4'-NZ
1	B	69	LLP	C4-C4'-NZ-CE
1	B	69	LLP	C5-C4-C4'-NZ
1	B	69	LLP	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	69	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.