



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:02 PM UTC

PDB ID : 1PKN / pdb_00001pkn
Title : STRUCTURE OF RABBIT MUSCLE PYRUVATE KINASE COMPLEXED
WITH MN²⁺, K⁺, AND PYRUVATE
Authors : Larsen, T.M.; Laughlin, L.T.; Holden, H.M.; Rayment, I.; Reed, G.H.
Deposited on : 1994-03-25
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

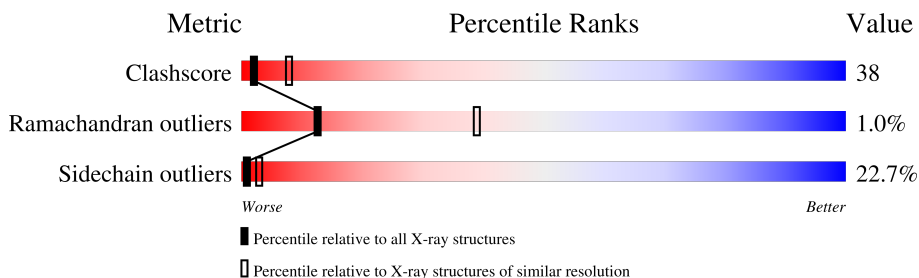
1 Overall quality at a glance

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	A	530	31% 40% 23% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3937 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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3929	2469	698	734	28			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	ALA	GLU	conflict	UNP P11974
A	150	ALA	LYS	conflict	UNP P11974
A	168	GLU	ASP	conflict	UNP P11974
A	233	ASP	GLU	conflict	UNP P11974
A	234	GLU	GLN	conflict	UNP P11974
A	499	ALA	ARG	conflict	UNP P11974

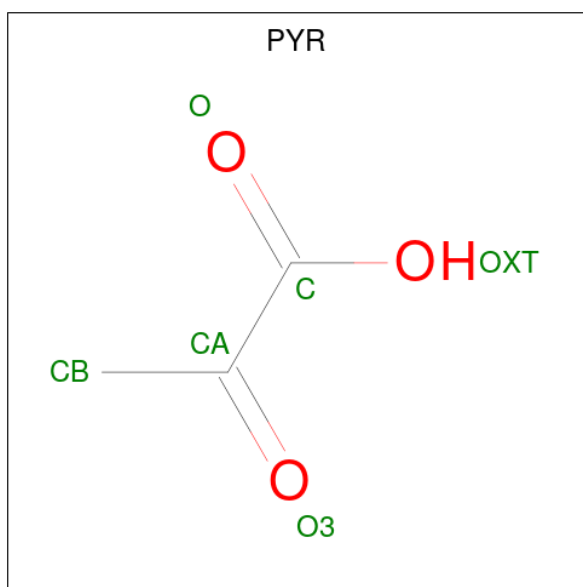
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



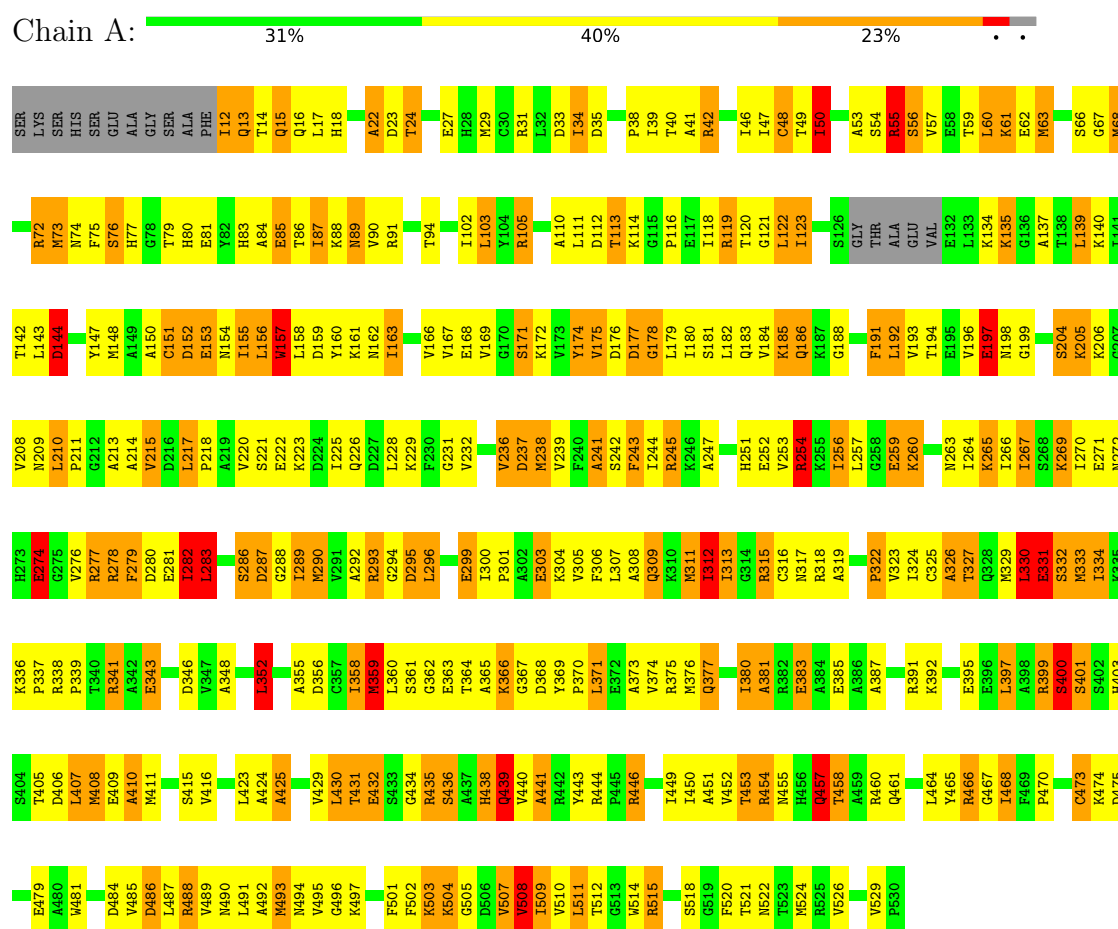
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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: PYRUVATE KINASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.60Å 109.90Å 146.80Å 94.90° 93.60° 112.30°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3937	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: MN, K, PYR

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	1.14	7/3991 (0.2%)	2.15	188/5384 (3.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	VAL	CA-CB	-6.70	1.46	1.54
1	A	416	VAL	CA-CB	-6.61	1.46	1.54
1	A	313	ILE	CA-CB	-5.92	1.47	1.54
1	A	507	VAL	CA-CB	-5.56	1.47	1.54
1	A	432	GLU	CD-OE1	5.21	1.35	1.25
1	A	50	ILE	CA-CB	-5.15	1.48	1.54
1	A	259	GLU	CD-OE1	5.06	1.34	1.25

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	HIS	CA-CB-CG	-13.33	100.47	113.80
1	A	77	HIS	CB-CA-C	-10.89	94.72	110.62
1	A	81	GLU	N-CA-CB	10.58	125.35	110.01
1	A	282	ILE	N-CA-CB	10.14	122.42	110.55
1	A	408	MET	CA-CB-CG	-9.68	94.74	114.10
1	A	80	HIS	N-CA-CB	9.59	124.99	110.22
1	A	305	VAL	N-CA-CB	9.54	121.71	110.55
1	A	399	ARG	N-CA-CB	9.54	124.14	110.12
1	A	267	ILE	N-CA-CB	-9.00	100.16	111.41
1	A	330	LEU	N-CA-CB	-8.98	95.31	110.49
1	A	358	ILE	CB-CA-C	8.97	124.02	111.19
1	A	215	VAL	N-CA-CB	8.96	120.76	110.82
1	A	286	SER	N-CA-CB	8.89	123.15	110.44
1	A	12	ILE	O-C-N	8.63	136.80	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LEU	N-CA-CB	-8.51	97.61	110.12
1	A	12	ILE	N-CA-CB	8.50	125.95	111.50
1	A	113	THR	N-CA-CB	-8.40	98.43	110.44
1	A	280	ASP	CA-CB-CG	-8.22	104.38	112.60
1	A	494	ASN	CA-CB-CG	-8.19	104.41	112.60
1	A	66	SER	CB-CA-C	8.03	123.49	110.88
1	A	236	VAL	CA-CB-CG1	-8.00	96.80	110.40
1	A	359	MET	O-C-N	7.94	132.53	123.48
1	A	497	LYS	CB-CA-C	-7.86	97.74	110.79
1	A	238	MET	N-CA-CB	-7.80	97.74	111.39
1	A	55	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	A	29	MET	CB-CA-C	-7.76	98.64	110.90
1	A	504	LYS	N-CA-C	7.67	119.43	111.14
1	A	226	GLN	CB-CA-C	-7.66	98.80	110.90
1	A	265	LYS	CB-CA-C	7.65	122.15	109.53
1	A	410	ALA	CB-CA-C	-7.65	98.57	110.81
1	A	177	ASP	CA-CB-CG	7.58	120.19	112.60
1	A	94	THR	N-CA-CB	7.53	120.92	110.01
1	A	35	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	50	ILE	N-CA-C	7.41	119.14	109.58
1	A	399	ARG	CD-NE-CZ	-7.39	114.05	124.40
1	A	312	ILE	CA-CB-CG2	-7.38	97.96	110.50
1	A	40	THR	CA-CB-OG1	-7.36	98.56	109.60
1	A	119	ARG	CD-NE-CZ	7.32	134.64	124.40
1	A	218	PRO	N-CA-CB	7.29	109.69	103.35
1	A	452	VAL	CB-CA-C	-7.22	102.58	111.32
1	A	24	THR	N-CA-CB	-7.17	98.83	111.08
1	A	197	GLU	O-C-N	7.16	129.76	122.03
1	A	222	GLU	N-CA-CB	7.15	120.78	110.06
1	A	61	LYS	CB-CA-C	-7.10	99.44	110.81
1	A	400	SER	CB-CA-C	-7.10	98.78	110.85
1	A	214	ALA	N-CA-C	7.06	120.41	107.99
1	A	508	VAL	N-CA-CB	-7.05	99.79	111.36
1	A	490	ASN	CA-CB-CG	-7.04	105.56	112.60
1	A	369	TYR	CB-CG-CD1	-6.96	110.37	120.80
1	A	303	GLU	N-CA-CB	-6.94	98.87	110.39
1	A	343	GLU	CB-CG-CD	-6.91	100.86	112.60
1	A	33	ASP	CB-CA-C	-6.90	99.09	110.14
1	A	318	ARG	N-CA-CB	-6.83	99.70	110.22
1	A	89	ASN	CA-CB-CG	6.82	119.42	112.60
1	A	226	GLN	N-CA-CB	6.80	119.93	110.07
1	A	526	VAL	N-CA-CB	6.72	120.26	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	LEU	CB-CA-C	-6.71	99.74	110.81
1	A	119	ARG	NE-CZ-NH1	6.71	128.21	121.50
1	A	510	VAL	CA-CB-CG2	6.71	121.80	110.40
1	A	429	VAL	CB-CA-C	-6.69	102.29	110.99
1	A	443	TYR	N-CA-CB	6.68	119.78	110.56
1	A	279	PHE	N-CA-C	6.67	118.21	111.07
1	A	371	LEU	N-CA-CB	6.66	119.73	110.07
1	A	239	VAL	CA-CB-CG2	-6.64	99.11	110.40
1	A	451	ALA	N-CA-CB	6.64	121.11	110.16
1	A	305	VAL	N-CA-C	6.63	116.78	110.42
1	A	454	ARG	N-CA-C	-6.61	105.13	113.72
1	A	369	TYR	CB-CG-CD2	6.60	130.69	120.80
1	A	34	ILE	N-CA-CB	6.55	121.86	110.65
1	A	370	PRO	N-CA-CB	6.55	110.12	103.25
1	A	368	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	191	PHE	O-C-N	6.49	129.94	122.99
1	A	279	PHE	CB-CA-C	-6.43	100.78	110.88
1	A	380	ILE	CA-CB-CG2	-6.42	99.58	110.50
1	A	94	THR	O-C-N	6.41	128.67	122.07
1	A	373	ALA	N-CA-CB	6.37	119.31	110.07
1	A	157	TRP	CA-CB-CG	6.36	125.69	113.60
1	A	387	ALA	CB-CA-C	6.34	122.57	109.95
1	A	40	THR	CB-CA-C	6.30	121.56	110.85
1	A	316	CYS	CB-CA-C	-6.30	97.53	110.38
1	A	87	ILE	N-CA-C	6.27	116.38	110.30
1	A	259	GLU	CB-CA-C	-6.22	98.03	110.42
1	A	286	SER	N-CA-C	6.22	118.56	110.53
1	A	241	ALA	N-CA-CB	-6.21	99.91	110.16
1	A	374	VAL	N-CA-CB	-6.18	102.14	110.54
1	A	501	PHE	N-CA-CB	-6.18	100.71	110.28
1	A	87	ILE	CA-C-O	-6.17	114.69	121.29
1	A	22	ALA	N-CA-C	6.17	118.26	110.24
1	A	503	LYS	CA-C-N	6.14	128.79	120.44
1	A	503	LYS	C-N-CA	6.14	128.79	120.44
1	A	276	VAL	N-CA-CB	-6.13	101.38	110.58
1	A	313	ILE	CB-CG1-CD1	-6.10	100.99	113.80
1	A	381	ALA	N-CA-CB	6.08	119.05	110.12
1	A	432	GLU	CA-CB-CG	-6.07	101.97	114.10
1	A	33	ASP	CA-CB-CG	-6.06	106.54	112.60
1	A	278	ARG	N-CA-CB	-6.05	102.48	111.43
1	A	48	CYS	CB-CA-C	-6.03	98.53	109.38
1	A	359	MET	N-CA-C	6.02	118.30	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	GLU	N-CA-CB	5.97	118.67	110.01
1	A	440	VAL	CB-CA-C	-5.97	103.24	111.65
1	A	452	VAL	N-CA-C	5.96	116.20	106.72
1	A	492	ALA	O-C-N	5.92	128.24	122.09
1	A	35	ASP	N-CA-CB	5.91	118.71	110.56
1	A	481	TRP	CB-CA-C	-5.90	101.38	110.81
1	A	439	GLN	CB-CG-CD	-5.88	102.60	112.60
1	A	247	ALA	N-CA-C	-5.86	106.30	113.50
1	A	186	GLN	N-CA-C	5.85	118.07	109.24
1	A	303	GLU	CA-CB-CG	-5.83	102.43	114.10
1	A	371	LEU	CB-CA-C	-5.83	101.68	110.90
1	A	259	GLU	CB-CG-CD	-5.82	102.71	112.60
1	A	333	MET	CA-CB-CG	-5.73	102.64	114.10
1	A	85	GLU	N-CA-C	-5.71	105.14	111.36
1	A	466	ARG	CB-CG-CD	-5.70	98.20	111.30
1	A	397	LEU	CB-CA-C	-5.69	98.23	109.67
1	A	185	LYS	CB-CA-C	5.69	121.74	110.42
1	A	438	HIS	CB-CA-C	-5.69	101.35	110.79
1	A	196	VAL	N-CA-CB	-5.69	104.50	111.67
1	A	495	VAL	CA-CB-CG2	-5.69	100.73	110.40
1	A	110	ALA	N-CA-C	5.67	118.64	109.40
1	A	319	ALA	CA-C-N	-5.66	112.97	122.25
1	A	319	ALA	C-N-CA	-5.66	112.97	122.25
1	A	287	ASP	N-CA-CB	-5.64	103.09	110.88
1	A	370	PRO	CB-CA-C	-5.62	102.29	111.56
1	A	457	GLN	CA-CB-CG	-5.61	102.89	114.10
1	A	277	ARG	N-CA-C	5.60	118.15	111.71
1	A	243	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	400	SER	N-CA-C	5.60	117.46	111.36
1	A	429	VAL	CA-CB-CG1	5.60	119.92	110.40
1	A	239	VAL	N-CA-C	5.59	115.93	108.11
1	A	260	LYS	N-CA-CB	5.58	118.10	110.01
1	A	411	MET	CB-CA-C	-5.57	100.32	110.63
1	A	403	HIS	CA-CB-CG	5.56	119.36	113.80
1	A	220	VAL	CB-CA-C	5.52	118.17	110.99
1	A	470	PRO	O-C-N	5.52	129.71	123.03
1	A	174	TYR	N-CA-C	5.50	118.44	109.59
1	A	186	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	A	366	LYS	N-CA-C	-5.50	105.20	111.14
1	A	468	ILE	N-CA-C	5.49	116.78	109.37
1	A	399	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	423	LEU	CB-CA-C	-5.46	103.49	112.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	A	356	ASP	CB-CA-C	-5.42	98.65	109.99
1	A	41	ALA	N-CA-C	5.42	117.86	110.55
1	A	375	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	A	446	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	A	486	ASP	N-CA-CB	-5.38	101.47	110.39
1	A	72	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	84	ALA	N-CA-CB	5.34	118.45	110.22
1	A	488	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	515	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	254	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	217	LEU	CB-CA-C	-5.32	101.07	109.42
1	A	444	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	A	429	VAL	N-CA-CB	5.31	118.59	111.90
1	A	338	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	A	441	ALA	CB-CA-C	5.29	120.83	110.67
1	A	287	ASP	N-CA-C	-5.29	106.77	114.12
1	A	438	HIS	CA-C-O	5.28	126.15	120.55
1	A	274	GLU	N-CA-CB	-5.28	102.15	110.06
1	A	144	ASP	N-CA-CB	5.26	117.69	109.85
1	A	331	GLU	N-CA-CB	5.26	119.37	110.49
1	A	352	LEU	CB-CA-C	-5.25	101.93	110.85
1	A	55	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	A	279	PHE	CA-CB-CG	-5.24	108.56	113.80
1	A	283	LEU	CB-CA-C	-5.24	102.42	110.81
1	A	453	THR	N-CA-CB	-5.24	102.78	110.85
1	A	474	LYS	CB-CA-C	5.24	120.18	109.55
1	A	175	VAL	O-C-N	5.21	128.50	122.82
1	A	244	ILE	CA-C-O	-5.17	114.97	120.39
1	A	473	CYS	N-CA-CB	5.16	118.42	110.21
1	A	322	PRO	N-CA-CB	5.15	107.89	103.31
1	A	155	ILE	N-CA-C	5.13	115.12	108.35
1	A	309	GLN	N-CA-CB	5.12	117.71	110.13
1	A	326	ALA	O-C-N	5.12	129.59	122.78
1	A	491	LEU	O-C-N	5.12	127.35	122.07
1	A	293	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	457	GLN	CB-CG-CD	-5.10	103.94	112.60
1	A	493	MET	CB-CA-C	5.09	118.95	110.81
1	A	425	ALA	N-CA-C	-5.08	106.24	112.90
1	A	290	MET	CA-C-N	-5.06	116.05	122.43
1	A	290	MET	C-N-CA	-5.06	116.05	122.43
1	A	435	ARG	CG-CD-NE	5.04	123.08	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	PRO	CB-CA-C	-5.03	104.97	111.46
1	A	87	ILE	CA-CB-CG1	-5.03	101.85	110.40
1	A	343	GLU	N-CA-CB	5.03	117.61	110.16
1	A	239	VAL	CA-C-N	-5.03	115.86	122.85
1	A	239	VAL	C-N-CA	-5.03	115.86	122.85
1	A	341	ARG	CB-CA-C	5.01	119.90	110.63

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	A	3929	0	4001	301	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	0	3	0
All	All	3937	0	4001	301	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 38.

All (301) 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:279:PHE:CE2	1:A:283:LEU:HD12	1.65	1.29
1:A:122:LEU:O	1:A:151:CYS:HB2	1.29	1.26
1:A:134:LYS:NZ	1:A:139:LEU:HD13	1.56	1.20
1:A:139:LEU:HD12	1:A:153:GLU:O	1.44	1.16
1:A:134:LYS:CE	1:A:139:LEU:HD13	1.84	1.07
1:A:134:LYS:NZ	1:A:139:LEU:CD1	2.17	1.06
1:A:72:ARG:HD2	1:A:359:MET:CE	1.87	1.05
1:A:511:LEU:HB3	1:A:521:THR:HG21	1.09	1.04
1:A:431:THR:HG21	1:A:434:GLY:HA2	1.40	1.03
1:A:511:LEU:HB3	1:A:521:THR:CG2	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:MET:HE2	1:A:86:THR:HG21	1.41	1.00
1:A:49:THR:OG1	1:A:72:ARG:HD3	1.63	0.98
1:A:134:LYS:HZ3	1:A:139:LEU:HD13	1.16	0.96
1:A:294:GLY:CA	1:A:327:THR:HG21	1.96	0.95
1:A:72:ARG:HD2	1:A:359:MET:HE3	1.51	0.92
1:A:279:PHE:CE2	1:A:283:LEU:CD1	2.53	0.91
1:A:15:GLN:HG3	1:A:39:ILE:HG23	1.50	0.90
1:A:333:MET:HE3	1:A:339:PRO:HD3	1.51	0.90
1:A:122:LEU:O	1:A:151:CYS:CB	2.21	0.89
1:A:454:ARG:HG2	1:A:473:CYS:HB3	1.54	0.89
1:A:49:THR:HA	1:A:72:ARG:HB3	1.54	0.87
1:A:294:GLY:HA3	1:A:327:THR:HG21	1.54	0.87
1:A:139:LEU:HG	1:A:140:LYS:H	1.39	0.87
1:A:24:THR:CG2	1:A:27:GLU:HB2	2.05	0.87
1:A:24:THR:HG23	1:A:27:GLU:HB2	1.57	0.86
1:A:425:ALA:HB1	1:A:502:PHE:HB3	1.58	0.86
1:A:139:LEU:CD1	1:A:153:GLU:O	2.24	0.85
1:A:406:ASP:HB3	1:A:409:GLU:HB2	1.58	0.85
1:A:186:GLN:HB3	1:A:193:VAL:HB	1.56	0.85
1:A:134:LYS:HZ3	1:A:139:LEU:CD1	1.82	0.84
1:A:431:THR:CG2	1:A:434:GLY:HA2	2.08	0.82
1:A:511:LEU:CB	1:A:521:THR:HG21	2.03	0.81
1:A:162:ASN:O	1:A:166:VAL:HG23	1.79	0.81
1:A:134:LYS:HE2	1:A:139:LEU:HD13	1.62	0.81
1:A:54:SER:HA	1:A:59:THR:HG21	1.63	0.80
1:A:225:ILE:HG22	1:A:229:LYS:HE2	1.64	0.80
1:A:293:ARG:HD3	1:A:326:ALA:O	1.82	0.80
1:A:504:LYS:O	1:A:529:VAL:O	1.98	0.80
1:A:405:THR:HG22	1:A:405:THR:O	1.82	0.80
1:A:73:MET:HE2	1:A:86:THR:CG2	2.12	0.79
1:A:181:SER:OG	1:A:197:GLU:OE1	1.98	0.79
1:A:75:PHE:HB2	1:A:112:ASP:O	1.84	0.78
1:A:279:PHE:HE2	1:A:283:LEU:HD12	1.45	0.78
1:A:134:LYS:CE	1:A:139:LEU:CD1	2.60	0.77
1:A:15:GLN:HG3	1:A:39:ILE:CG2	2.14	0.77
1:A:182:LEU:HB3	1:A:194:THR:HG21	1.66	0.77
1:A:485:VAL:O	1:A:489:VAL:HG23	1.84	0.77
1:A:237:ASP:OD1	1:A:460:ARG:NH1	2.18	0.76
1:A:122:LEU:C	1:A:151:CYS:HB2	2.10	0.76
1:A:57:VAL:O	1:A:61:LYS:HG3	1.86	0.75
1:A:72:ARG:HD2	1:A:359:MET:HE1	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:PRO:HB3	1:A:464:LEU:O	1.88	0.74
1:A:332:SER:HB3	1:A:343:GLU:OE2	1.87	0.74
1:A:331:GLU:HG2	1:A:334:ILE:HD12	1.68	0.74
1:A:15:GLN:CG	1:A:39:ILE:HG23	2.17	0.73
1:A:139:LEU:HG	1:A:140:LYS:N	2.00	0.73
1:A:512:THR:N	1:A:521:THR:HG23	2.03	0.73
1:A:134:LYS:HE2	1:A:139:LEU:CD1	2.17	0.73
1:A:215:VAL:HG12	1:A:217:LEU:H	1.52	0.73
1:A:308:ALA:O	1:A:312:ILE:HG13	1.88	0.72
1:A:176:ASP:O	1:A:179:LEU:HB2	1.89	0.72
1:A:511:LEU:C	1:A:521:THR:CG2	2.63	0.72
1:A:139:LEU:HD21	1:A:156:LEU:HD12	1.72	0.72
1:A:116:PRO:HB3	1:A:217:LEU:HB2	1.71	0.71
1:A:167:VAL:CG1	1:A:171:SER:HB3	2.21	0.71
1:A:134:LYS:HE2	1:A:153:GLU:O	1.90	0.71
1:A:134:LYS:HZ1	1:A:139:LEU:CD1	2.04	0.71
1:A:134:LYS:HZ1	1:A:139:LEU:HD11	1.53	0.70
1:A:225:ILE:O	1:A:229:LYS:HG3	1.90	0.70
1:A:333:MET:HA	1:A:336:LYS:O	1.91	0.70
1:A:47:ILE:HD13	1:A:324:ILE:HD13	1.73	0.70
1:A:72:ARG:CD	1:A:359:MET:HE3	2.22	0.70
1:A:279:PHE:CZ	1:A:283:LEU:HD12	2.26	0.70
1:A:333:MET:CE	1:A:339:PRO:HD3	2.22	0.70
1:A:120:THR:HG23	1:A:156:LEU:HD23	1.73	0.70
1:A:174:TYR:HB3	1:A:178:GLY:HA2	1.74	0.69
1:A:72:ARG:CD	1:A:359:MET:CE	2.70	0.68
1:A:371:LEU:N	1:A:371:LEU:HD12	2.09	0.68
1:A:120:THR:HG22	1:A:121:GLY:H	1.57	0.68
1:A:188:GLY:HA3	1:A:191:PHE:CE1	2.28	0.68
1:A:102:ILE:HG22	1:A:103:LEU:HD12	1.75	0.67
1:A:167:VAL:HG13	1:A:171:SER:HB3	1.75	0.67
1:A:182:LEU:HB3	1:A:194:THR:CG2	2.24	0.67
1:A:391:ARG:HG2	1:A:391:ARG:HH11	1.61	0.66
1:A:22:ALA:O	1:A:391:ARG:NH2	2.29	0.66
1:A:120:THR:HG23	1:A:156:LEU:CD2	2.26	0.66
1:A:74:ASN:OD1	1:A:76:SER:OG	2.14	0.66
1:A:270:ILE:HD13	1:A:312:ILE:HD13	1.79	0.65
1:A:265:LYS:HA	1:A:287:ASP:OD2	1.97	0.64
1:A:355:ALA:O	1:A:466:ARG:NH1	2.30	0.64
1:A:135:LYS:C	1:A:137:ALA:H	2.05	0.64
1:A:279:PHE:HE2	1:A:283:LEU:CD1	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:CE1	1:A:162:ASN:HB2	2.32	0.63
1:A:120:THR:HG22	1:A:121:GLY:N	2.14	0.63
1:A:228:LEU:CD1	1:A:256:ILE:HG21	2.28	0.62
1:A:466:ARG:HG3	1:A:467:GLY:N	2.14	0.62
1:A:143:LEU:N	1:A:143:LEU:HD12	2.14	0.62
1:A:408:MET:SD	1:A:436:SER:HA	2.39	0.62
1:A:511:LEU:C	1:A:521:THR:HG23	2.21	0.62
1:A:435:ARG:O	1:A:438:HIS:HB2	1.99	0.62
1:A:457:GLN:O	1:A:461:GLN:HG3	2.00	0.62
1:A:334:ILE:HD11	1:A:362:GLY:HA3	1.80	0.62
1:A:119:ARG:H	1:A:159:ASP:HB2	1.64	0.61
1:A:269:LYS:HD2	1:A:290:MET:HE2	1.82	0.61
1:A:358:ILE:HG13	1:A:377:GLN:NE2	2.16	0.61
1:A:511:LEU:CB	1:A:521:THR:CG2	2.74	0.60
1:A:139:LEU:HD12	1:A:153:GLU:C	2.25	0.60
1:A:504:LYS:HG3	1:A:505:GLY:N	2.16	0.60
1:A:134:LYS:HE3	1:A:153:GLU:HA	1.83	0.60
1:A:209:ASN:C	1:A:211:PRO:HD3	2.26	0.60
1:A:188:GLY:HA3	1:A:191:PHE:CD1	2.36	0.60
1:A:360:LEU:HB3	1:A:364:THR:HG23	1.83	0.60
1:A:225:ILE:CG2	1:A:229:LYS:HE2	2.31	0.60
1:A:24:THR:HG23	1:A:27:GLU:H	1.67	0.59
1:A:50:ILE:HD11	1:A:68:MET:CE	2.31	0.59
1:A:177:ASP:O	1:A:179:LEU:N	2.35	0.59
1:A:72:ARG:O	1:A:73:MET:HE3	2.02	0.59
1:A:134:LYS:CE	1:A:153:GLU:HA	2.31	0.59
1:A:181:SER:HB3	1:A:198:ASN:HB2	1.83	0.59
1:A:446:ARG:O	1:A:446:ARG:HG3	2.02	0.59
1:A:118:ILE:HG12	1:A:160:TYR:HB2	1.84	0.59
1:A:47:ILE:CD1	1:A:324:ILE:HD13	2.33	0.59
1:A:18:HIS:CE1	1:A:31:ARG:NH1	2.71	0.58
1:A:503:LYS:O	1:A:529:VAL:HG11	2.03	0.58
1:A:177:ASP:C	1:A:179:LEU:H	2.11	0.58
1:A:264:ILE:HG22	1:A:265:LYS:N	2.17	0.58
1:A:333:MET:HE3	1:A:337:PRO:O	2.03	0.58
1:A:182:LEU:CB	1:A:194:THR:HG21	2.32	0.58
1:A:270:ILE:HD13	1:A:312:ILE:CD1	2.33	0.58
1:A:484:ASP:O	1:A:487:LEU:HB3	2.04	0.58
1:A:333:MET:CE	1:A:337:PRO:O	2.52	0.58
1:A:430:LEU:N	1:A:430:LEU:HD12	2.18	0.57
1:A:47:ILE:O	1:A:359:MET:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD12	1:A:256:ILE:HG21	1.87	0.57
1:A:14:THR:O	1:A:17:LEU:HG	2.04	0.57
1:A:15:GLN:CG	1:A:39:ILE:CG2	2.80	0.57
1:A:277:ARG:O	1:A:277:ARG:HG2	2.03	0.56
1:A:142:THR:HG22	1:A:144:ASP:N	2.20	0.56
1:A:271:GLU:HG3	1:A:292:ALA:HB3	1.87	0.56
1:A:381:ALA:O	1:A:385:GLU:HG3	2.05	0.56
1:A:182:LEU:CG	1:A:194:THR:HG21	2.34	0.56
1:A:12:ILE:HG22	1:A:13:GLN:O	2.05	0.56
1:A:431:THR:O	1:A:432:GLU:HG2	2.05	0.56
1:A:186:GLN:HB3	1:A:193:VAL:CB	2.31	0.56
1:A:512:THR:CA	1:A:521:THR:HG23	2.36	0.56
1:A:142:THR:HG22	1:A:144:ASP:H	1.72	0.55
1:A:48:CYS:SG	1:A:68:MET:HG3	2.46	0.55
1:A:50:ILE:HD11	1:A:68:MET:HE1	1.89	0.55
1:A:293:ARG:CD	1:A:326:ALA:O	2.54	0.55
1:A:142:THR:O	1:A:157:TRP:HA	2.07	0.54
1:A:38:PRO:HG3	1:A:383:GLU:OE1	2.08	0.54
1:A:241:ALA:O	1:A:269:LYS:HG3	2.07	0.54
1:A:408:MET:SD	1:A:436:SER:HB3	2.47	0.54
1:A:143:LEU:HD23	1:A:161:LYS:HA	1.89	0.54
1:A:53:ALA:HB3	1:A:365:ALA:O	2.07	0.54
1:A:512:THR:N	1:A:521:THR:CG2	2.71	0.54
1:A:295:ASP:HB2	4:A:533:PYR:OXT	2.08	0.53
1:A:441:ALA:HB1	1:A:466:ARG:O	2.07	0.53
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.43	0.53
1:A:209:ASN:ND2	1:A:299:GLU:OE1	2.41	0.53
1:A:454:ARG:CG	1:A:473:CYS:HB3	2.34	0.53
1:A:391:ARG:HG2	1:A:391:ARG:NH1	2.23	0.53
1:A:221:SER:C	1:A:225:ILE:HD12	2.33	0.53
1:A:162:ASN:O	1:A:166:VAL:CG2	2.54	0.52
1:A:72:ARG:HH11	1:A:359:MET:HE2	1.74	0.52
1:A:38:PRO:HG3	1:A:383:GLU:CD	2.35	0.52
1:A:325:CYS:SG	1:A:329:MET:HE3	2.50	0.52
1:A:400:SER:OG	1:A:401:SER:N	2.39	0.52
1:A:24:THR:HG22	1:A:27:GLU:HB2	1.90	0.51
1:A:182:LEU:HD23	1:A:194:THR:HG21	1.92	0.51
1:A:441:ALA:HB2	1:A:449:ILE:HD12	1.92	0.51
1:A:507:VAL:HG12	1:A:508:VAL:N	2.26	0.51
1:A:322:PRO:HD3	1:A:465:TYR:CE1	2.45	0.51
1:A:208:VAL:HG12	1:A:209:ASN:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:HB3	1:A:274:GLU:HB3	1.91	0.51
1:A:301:PRO:O	1:A:304:LYS:HB2	2.10	0.51
1:A:160:TYR:CE2	1:A:166:VAL:HG21	2.46	0.51
1:A:278:ARG:O	1:A:282:ILE:HD12	2.11	0.51
1:A:243:PHE:N	1:A:271:GLU:OE1	2.37	0.50
1:A:166:VAL:HG12	1:A:213:ALA:HB1	1.94	0.50
1:A:294:GLY:N	1:A:327:THR:HG21	2.26	0.50
1:A:274:GLU:O	1:A:278:ARG:HB2	2.12	0.50
1:A:168:GLU:O	1:A:171:SER:HB2	2.11	0.50
1:A:54:SER:HA	1:A:59:THR:CG2	2.38	0.49
1:A:228:LEU:HD22	1:A:257:LEU:HD11	1.95	0.49
1:A:228:LEU:O	1:A:231:GLY:N	2.42	0.49
1:A:514:TRP:C	1:A:515:ARG:HG2	2.37	0.49
1:A:120:THR:CG2	1:A:121:GLY:H	2.24	0.49
1:A:72:ARG:NH1	1:A:359:MET:HE2	2.27	0.49
1:A:140:LYS:HG2	1:A:193:VAL:HG13	1.94	0.49
1:A:431:THR:C	1:A:432:GLU:HG2	2.38	0.49
1:A:76:SER:HA	1:A:114:LYS:HB2	1.93	0.48
1:A:434:GLY:O	1:A:438:HIS:ND1	2.46	0.48
1:A:512:THR:O	1:A:521:THR:HA	2.13	0.48
1:A:116:PRO:HD2	1:A:243:PHE:HB2	1.95	0.48
1:A:453:THR:HG21	1:A:458:THR:HG22	1.96	0.48
1:A:446:ARG:O	1:A:446:ARG:CG	2.61	0.48
1:A:309:GLN:O	1:A:313:ILE:HG13	2.13	0.48
1:A:330:LEU:O	1:A:363:GLU:HG2	2.13	0.48
1:A:473:CYS:SG	1:A:475:ASP:HB2	2.54	0.47
1:A:245:ARG:HD2	1:A:274:GLU:OE1	2.13	0.47
1:A:55:ARG:NH2	1:A:85:GLU:HB3	2.29	0.47
1:A:329:MET:O	1:A:330:LEU:HD13	2.14	0.47
1:A:266:ILE:O	1:A:287:ASP:HB2	2.15	0.47
1:A:237:ASP:O	1:A:264:ILE:HG23	2.15	0.47
1:A:371:LEU:HD12	1:A:371:LEU:H	1.79	0.47
1:A:54:SER:O	1:A:60:LEU:HD13	2.15	0.46
1:A:134:LYS:HE2	1:A:153:GLU:C	2.41	0.46
1:A:313:ILE:HG23	1:A:323:VAL:HG11	1.98	0.46
1:A:142:THR:CG2	1:A:144:ASP:H	2.28	0.46
1:A:182:LEU:CB	1:A:194:THR:CG2	2.91	0.46
1:A:348:ALA:O	1:A:352:LEU:HD22	2.15	0.46
1:A:15:GLN:CD	1:A:39:ILE:CG2	2.89	0.46
1:A:300:ILE:HB	1:A:301:PRO:HD2	1.98	0.46
1:A:23:ASP:OD1	1:A:23:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:O	1:A:91:ARG:HG3	2.16	0.46
1:A:102:ILE:O	1:A:102:ILE:CG2	2.64	0.46
1:A:143:LEU:CD2	1:A:161:LYS:HA	2.45	0.46
1:A:147:TYR:O	1:A:150:ALA:O	2.34	0.46
1:A:186:GLN:O	1:A:192:LEU:HA	2.16	0.46
1:A:152:ASP:C	1:A:154:ASN:H	2.25	0.45
1:A:430:LEU:N	1:A:430:LEU:CD1	2.80	0.45
1:A:439:GLN:HE21	1:A:439:GLN:HB2	1.43	0.45
1:A:229:LYS:O	1:A:232:VAL:HB	2.17	0.45
1:A:294:GLY:HA3	4:A:533:PYR:O	2.16	0.45
1:A:120:THR:CG2	1:A:121:GLY:N	2.80	0.45
1:A:158:LEU:HD22	1:A:163:ILE:HD12	1.98	0.45
1:A:18:His:O	1:A:31:ARG:HD3	2.17	0.45
1:A:252:GLU:O	1:A:256:ILE:CD1	2.65	0.45
1:A:358:ILE:HG13	1:A:377:GLN:HE22	1.81	0.45
1:A:60:LEU:O	1:A:63:MET:HB2	2.16	0.45
1:A:74:ASN:HA	1:A:112:ASP:HB3	1.98	0.45
1:A:180:ILE:HG23	1:A:199:GLY:HA2	1.99	0.44
1:A:182:LEU:HG	1:A:194:THR:CG2	2.47	0.44
1:A:264:ILE:CG2	1:A:265:LYS:N	2.80	0.44
1:A:406:ASP:HB3	1:A:409:GLU:CB	2.37	0.44
1:A:294:GLY:CA	4:A:533:PYR:O	2.65	0.44
1:A:430:LEU:HD21	1:A:488:ARG:HB2	1.99	0.44
1:A:228:LEU:HD13	1:A:256:ILE:HG21	1.97	0.44
1:A:267:ILE:HG22	1:A:267:ILE:O	2.17	0.44
1:A:311:MET:O	1:A:311:MET:HG2	2.13	0.44
1:A:424:ALA:HB2	1:A:509:ILE:HD12	1.99	0.44
1:A:134:LYS:HZ3	1:A:139:LEU:CD2	2.30	0.44
1:A:134:LYS:HZ3	1:A:139:LEU:HD22	1.83	0.44
1:A:238:MET:HA	1:A:264:ILE:CG2	2.47	0.44
1:A:288:GLY:O	1:A:289:ILE:HG13	2.16	0.44
1:A:380:ILE:O	1:A:380:ILE:HG22	2.10	0.44
1:A:135:LYS:C	1:A:137:ALA:N	2.74	0.44
1:A:236:VAL:H	1:A:236:VAL:HG13	1.61	0.44
1:A:306:PHE:CE2	1:A:307:LEU:HD23	2.53	0.44
1:A:85:GLU:O	1:A:89:ASN:ND2	2.38	0.44
1:A:407:LEU:O	1:A:410:ALA:HB3	2.18	0.44
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.54	0.44
1:A:42:ARG:NH2	1:A:46:ILE:HD12	2.32	0.43
1:A:56:SER:O	1:A:56:SER:OG	2.33	0.43
1:A:453:THR:HG23	1:A:455:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:PHE:CE2	1:A:522:ASN:HB3	2.53	0.43
1:A:123:ILE:HG23	1:A:204:SER:OG	2.18	0.43
1:A:172:LYS:NZ	1:A:197:GLU:OE2	2.49	0.43
1:A:174:TYR:O	1:A:208:VAL:HA	2.17	0.43
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.47	0.43
1:A:360:LEU:CB	1:A:364:THR:HG23	2.46	0.43
1:A:63:MET:CE	1:A:364:THR:HB	2.48	0.43
1:A:152:ASP:C	1:A:154:ASN:N	2.75	0.43
1:A:134:LYS:NZ	1:A:156:LEU:HD12	2.32	0.43
1:A:408:MET:O	1:A:408:MET:HG2	2.18	0.43
1:A:134:LYS:HE2	1:A:153:GLU:HA	1.98	0.43
1:A:253:VAL:O	1:A:257:LEU:HD13	2.19	0.43
1:A:49:THR:HB	1:A:361:SER:HA	2.01	0.42
1:A:50:ILE:HD11	1:A:68:MET:HE2	2.01	0.42
1:A:169:VAL:HG13	1:A:185:LYS:O	2.19	0.42
1:A:251:HIS:O	1:A:254:ARG:N	2.52	0.42
1:A:289:ILE:CG2	1:A:290:MET:N	2.82	0.42
1:A:267:ILE:HD11	1:A:464:LEU:HD21	2.00	0.42
1:A:139:LEU:HD21	1:A:156:LEU:CD1	2.47	0.42
1:A:139:LEU:CD2	1:A:156:LEU:HD12	2.44	0.42
1:A:210:LEU:HB3	1:A:213:ALA:HB3	2.01	0.42
1:A:311:MET:HE3	1:A:311:MET:HB3	1.81	0.42
1:A:143:LEU:N	1:A:143:LEU:CD1	2.83	0.42
1:A:171:SER:O	1:A:184:VAL:HB	2.19	0.42
1:A:313:ILE:HD13	1:A:313:ILE:HG21	1.54	0.42
1:A:405:THR:O	1:A:405:THR:CG2	2.54	0.42
1:A:311:MET:O	1:A:315:ARG:HB2	2.20	0.42
1:A:53:ALA:CB	1:A:365:ALA:O	2.68	0.42
1:A:263:ASN:CB	1:A:457:GLN:HE22	2.33	0.41
1:A:119:ARG:HB2	1:A:159:ASP:OD2	2.20	0.41
1:A:331:GLU:O	1:A:334:ILE:N	2.35	0.41
1:A:507:VAL:CG1	1:A:508:VAL:N	2.82	0.41
1:A:391:ARG:O	1:A:395:GLU:HG3	2.20	0.41
1:A:167:VAL:HG13	1:A:171:SER:CB	2.45	0.41
1:A:432:GLU:O	1:A:458:THR:HG21	2.20	0.41
1:A:252:GLU:O	1:A:256:ILE:HD12	2.21	0.41
1:A:175:VAL:HG22	1:A:208:VAL:HG22	2.03	0.41
1:A:177:ASP:C	1:A:179:LEU:N	2.72	0.41
1:A:228:LEU:HD13	1:A:256:ILE:CG2	2.51	0.41
1:A:139:LEU:CG	1:A:140:LYS:N	2.76	0.41
1:A:293:ARG:HH22	1:A:346:ASP:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:O	1:A:90:VAL:HG23	2.21	0.40
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.91	0.40
1:A:333:MET:HE2	1:A:337:PRO:O	2.20	0.40
1:A:204:SER:O	1:A:205:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/530 (96%)	460 (90%)	45 (9%)	5 (1%)	12	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	GLY
1	A	178	GLY
1	A	259	GLU
1	A	327	THR
1	A	67	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	419/431 (97%)	324 (77%)	95 (23%)	1 3

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	15	GLN
1	A	16	GLN
1	A	34	ILE
1	A	42	ARG
1	A	50	ILE
1	A	55	ARG
1	A	56	SER
1	A	60	LEU
1	A	62	GLU
1	A	63	MET
1	A	68	MET
1	A	73	MET
1	A	76	SER
1	A	79	THR
1	A	88	LYS
1	A	103	LEU
1	A	105	ARG
1	A	111	LEU
1	A	113	THR
1	A	122	LEU
1	A	123	ILE
1	A	135	LYS
1	A	139	LEU
1	A	144	ASP
1	A	148	MET
1	A	151	CYS
1	A	152	ASP
1	A	153	GLU
1	A	155	ILE
1	A	156	LEU
1	A	157	TRP
1	A	163	ILE
1	A	171	SER
1	A	183	GLN
1	A	192	LEU
1	A	197	GLU
1	A	204	SER

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Mol	Chain	Res	Type
1	A	205	LYS
1	A	206	LYS
1	A	210	LEU
1	A	223	LYS
1	A	237	ASP
1	A	242	SER
1	A	245	ARG
1	A	254	ARG
1	A	256	ILE
1	A	260	LYS
1	A	269	LYS
1	A	272	ASN
1	A	274	GLU
1	A	282	ILE
1	A	283	LEU
1	A	286	SER
1	A	289	ILE
1	A	295	ASP
1	A	299	GLU
1	A	303	GLU
1	A	311	MET
1	A	312	ILE
1	A	315	ARG
1	A	317	ASN
1	A	330	LEU
1	A	331	GLU
1	A	332	SER
1	A	334	ILE
1	A	341	ARG
1	A	352	LEU
1	A	359	MET
1	A	366	LYS
1	A	376	MET
1	A	377	GLN
1	A	383	GLU
1	A	392	LYS
1	A	397	LEU
1	A	399	ARG
1	A	400	SER
1	A	401	SER
1	A	407	LEU
1	A	415	SER

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Mol	Chain	Res	Type
1	A	431	THR
1	A	436	SER
1	A	439	GLN
1	A	450	ILE
1	A	457	GLN
1	A	458	THR
1	A	468	ILE
1	A	479	GLU
1	A	486	ASP
1	A	493	MET
1	A	508	VAL
1	A	509	ILE
1	A	511	LEU
1	A	518	SER
1	A	524	MET

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

Mol	Chain	Res	Type
1	A	43	ASN
1	A	162	ASN
1	A	183	GLN
1	A	209	ASN
1	A	226	GLN
1	A	349	ASN
1	A	377	GLN
1	A	439	GLN
1	A	457	GLN
1	A	463	HIS
1	A	478	GLN
1	A	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	PYR	A	533	3	5,5,5	2.29	2 (40%)	3,6,6	4.31	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PYR	A	533	3	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	533	PYR	O-C	4.25	1.33	1.22
4	A	533	PYR	OXT-C	-2.18	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	533	PYR	O3-CA-CB	5.61	132.33	119.77
4	A	533	PYR	OXT-C-O	4.77	135.25	123.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	533	PYR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.