



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:39 PM UTC

PDB ID : 1GLN / pdb_00001gln
Title : ARCHITECTURES OF CLASS-DEFINING AND SPECIFIC DOMAINS OF GLUTAMYL-TRNA SYNTHETASE
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Deposited on : 1994-07-20
Resolution : 2.50 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
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

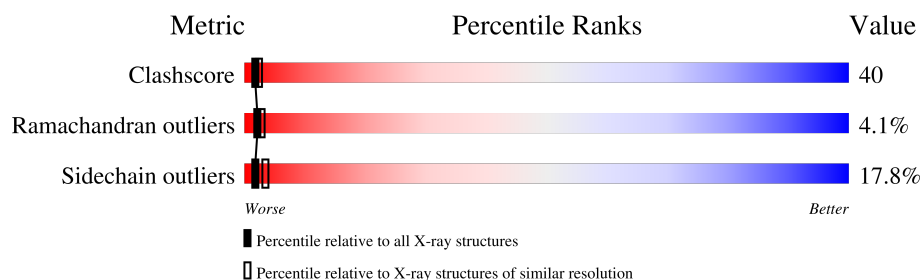
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	468	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3973 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 GLUTAMYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3813	2443	674	688	8			

- Molecule 2 is water.

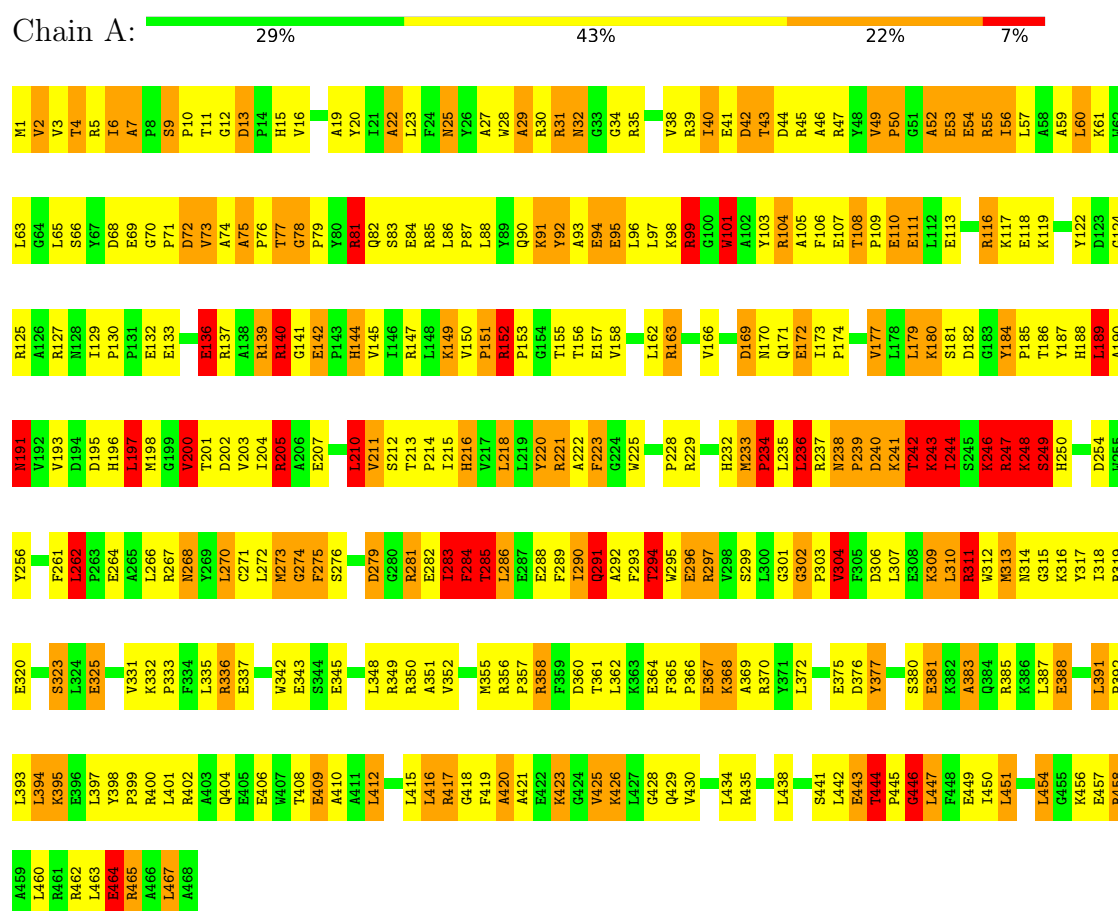
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		

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: GLUTAMYL-TRNA SYNTHETASE



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	75.75Å 110.09Å 67.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3973	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.22	3/3908 (0.1%)	2.39	225/5292 (4.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	PHE	N-CA	-6.54	1.37	1.46
1	A	84	GLU	CA-CB	-6.04	1.45	1.54
1	A	6	ILE	CA-C	5.07	1.58	1.52

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	CD-NE-CZ	27.89	163.44	124.40
1	A	283	ILE	CA-C-N	14.72	149.66	121.54
1	A	283	ILE	C-N-CA	14.72	149.66	121.54
1	A	254	ASP	CA-CB-CG	13.98	126.58	112.60
1	A	55	ARG	CD-NE-CZ	11.97	141.16	124.40
1	A	225	TRP	CA-CB-CG	11.35	135.16	113.60
1	A	13	ASP	O-C-N	10.46	129.96	121.38
1	A	430	VAL	N-CA-C	-10.28	103.57	111.90
1	A	6	ILE	N-CA-CB	10.11	130.64	111.93
1	A	49	VAL	CB-CA-C	10.07	120.33	110.16
1	A	279	ASP	CA-CB-CG	-9.95	102.65	112.60
1	A	284	PHE	N-CA-CB	9.88	127.18	110.49
1	A	177	VAL	CB-CA-C	9.52	124.41	111.28
1	A	268	ASN	CA-CB-CG	9.35	121.94	112.60
1	A	191	ASN	CA-CB-CG	9.18	121.78	112.60
1	A	136	GLU	CB-CG-CD	8.58	127.19	112.60
1	A	151	PRO	CA-C-N	8.57	130.81	120.09
1	A	151	PRO	C-N-CA	8.57	130.81	120.09
1	A	32	ASN	CA-CB-CG	8.49	121.09	112.60
1	A	291	GLN	OE1-CD-NE2	8.47	131.07	122.60
1	A	104	ARG	CD-NE-CZ	8.45	136.23	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ILE	N-CA-C	-8.37	95.22	108.86
1	A	73	VAL	N-CA-CB	-8.35	97.46	111.23
1	A	12	GLY	CA-C-N	8.26	132.65	120.83
1	A	12	GLY	C-N-CA	8.26	132.65	120.83
1	A	205	ARG	CB-CG-CD	8.19	130.14	111.30
1	A	84	GLU	CA-CB-CG	8.19	130.48	114.10
1	A	236	LEU	CA-C-O	8.19	130.33	120.92
1	A	169	ASP	CA-CB-CG	8.17	120.77	112.60
1	A	441	SER	N-CA-C	8.00	123.44	111.04
1	A	104	ARG	CA-C-N	7.85	134.01	122.39
1	A	104	ARG	C-N-CA	7.85	134.01	122.39
1	A	358	ARG	N-CA-C	7.82	122.54	112.92
1	A	430	VAL	CB-CA-C	7.77	118.76	111.30
1	A	136	GLU	O-C-N	7.64	129.94	122.07
1	A	285	THR	CA-C-N	7.59	136.03	121.54
1	A	285	THR	C-N-CA	7.59	136.03	121.54
1	A	186	THR	N-CA-C	-7.52	99.69	110.59
1	A	7	ALA	CB-CA-C	7.46	121.24	110.87
1	A	90	GLN	OE1-CD-NE2	-7.40	115.20	122.60
1	A	28	TRP	CB-CA-C	7.40	122.65	110.81
1	A	240	ASP	N-CA-C	-7.40	101.29	111.28
1	A	110	GLU	CB-CG-CD	7.36	125.11	112.60
1	A	319	ARG	NE-CZ-NH2	-7.34	112.60	119.20
1	A	99	ARG	CA-CB-CG	7.25	128.60	114.10
1	A	225	TRP	CB-CA-C	7.21	124.46	109.38
1	A	294	THR	CA-CB-OG1	-7.17	98.84	109.60
1	A	197	LEU	CB-CA-C	7.12	122.07	110.88
1	A	6	ILE	O-C-N	7.12	130.62	123.00
1	A	239	PRO	N-CA-C	-7.12	100.03	111.14
1	A	264	GLU	CB-CG-CD	7.07	124.62	112.60
1	A	25	ASN	O-C-N	7.01	131.34	122.23
1	A	376	ASP	CA-CB-CG	6.97	119.57	112.60
1	A	239	PRO	CA-C-O	-6.96	113.41	121.34
1	A	449	GLU	CB-CG-CD	6.87	124.28	112.60
1	A	2	VAL	CA-C-O	-6.85	112.22	120.78
1	A	271	CYS	N-CA-CB	6.83	119.92	110.01
1	A	49	VAL	CA-C-N	6.80	128.34	119.84
1	A	49	VAL	C-N-CA	6.80	128.34	119.84
1	A	42	ASP	CA-CB-CG	-6.79	105.81	112.60
1	A	336	ARG	CA-C-O	6.76	128.93	121.02
1	A	388	GLU	CB-CG-CD	6.76	124.09	112.60
1	A	240	ASP	CA-C-N	6.73	134.40	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ASP	C-N-CA	6.73	134.40	121.54
1	A	297	ARG	CD-NE-CZ	-6.70	115.03	124.40
1	A	50	PRO	N-CA-C	6.69	126.25	112.47
1	A	189	LEU	CA-C-N	6.68	131.82	121.19
1	A	189	LEU	C-N-CA	6.68	131.82	121.19
1	A	169	ASP	N-CA-C	-6.67	99.16	109.76
1	A	210	LEU	CA-C-N	6.62	129.53	120.46
1	A	210	LEU	C-N-CA	6.62	129.53	120.46
1	A	94	GLU	CB-CG-CD	6.61	123.83	112.60
1	A	40	ILE	CA-C-O	6.59	128.16	120.71
1	A	54	GLU	CB-CG-CD	6.57	123.77	112.60
1	A	92	TYR	N-CA-C	-6.53	103.37	112.45
1	A	52	ALA	O-C-N	6.53	129.04	122.12
1	A	95	GLU	CA-CB-CG	6.52	127.14	114.10
1	A	410	ALA	O-C-N	6.48	129.01	122.08
1	A	416	LEU	O-C-N	6.48	129.54	122.15
1	A	184	TYR	O-C-N	6.46	127.58	121.38
1	A	410	ALA	CA-C-O	-6.44	113.99	121.07
1	A	90	GLN	CB-CG-CD	6.40	123.48	112.60
1	A	250	HIS	N-CA-CB	6.39	120.70	110.16
1	A	234	PRO	CA-C-O	-6.36	109.02	120.60
1	A	294	THR	CB-CA-C	6.36	120.64	109.89
1	A	281	ARG	CD-NE-CZ	-6.29	115.59	124.40
1	A	6	ILE	CA-C-O	-6.25	114.03	121.28
1	A	90	GLN	O-C-N	6.22	129.24	122.15
1	A	53	GLU	O-C-N	6.21	128.48	122.03
1	A	293	PHE	N-CA-CB	6.20	118.73	109.19
1	A	49	VAL	CA-C-O	6.16	123.14	119.94
1	A	211	VAL	N-CA-C	6.14	116.88	110.62
1	A	306	ASP	CA-C-N	6.13	129.63	120.31
1	A	306	ASP	C-N-CA	6.13	129.63	120.31
1	A	345	GLU	CA-C-O	6.13	126.92	119.38
1	A	319	ARG	CD-NE-CZ	6.13	132.98	124.40
1	A	223	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	302	GLY	CA-C-N	6.10	126.04	119.76
1	A	302	GLY	C-N-CA	6.10	126.04	119.76
1	A	216	HIS	O-C-N	6.07	128.56	122.12
1	A	225	TRP	CA-C-O	-6.06	114.02	121.11
1	A	304	VAL	CA-C-N	6.04	132.01	122.34
1	A	304	VAL	C-N-CA	6.04	132.01	122.34
1	A	444	THR	CA-CB-CG2	6.04	120.77	110.50
1	A	465	ARG	CA-C-O	-6.04	114.16	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	GLU	CA-C-O	-6.04	114.46	120.80
1	A	239	PRO	CA-C-N	-6.02	113.96	122.63
1	A	239	PRO	C-N-CA	-6.02	113.96	122.63
1	A	268	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	292	ALA	N-CA-C	-5.98	104.69	112.23
1	A	147	ARG	CD-NE-CZ	-5.98	116.03	124.40
1	A	152	ARG	O-C-N	5.95	126.31	120.71
1	A	296	GLU	CB-CG-CD	5.93	122.69	112.60
1	A	420	ALA	N-CA-C	-5.93	104.51	110.97
1	A	101	TRP	N-CA-C	-5.93	105.88	114.12
1	A	248	LYS	CA-CB-CG	5.90	125.90	114.10
1	A	52	ALA	CA-C-O	-5.89	114.31	120.55
1	A	16	VAL	CB-CA-C	5.87	121.26	112.16
1	A	238	ASN	O-C-N	5.86	128.05	121.32
1	A	93	ALA	N-CA-C	-5.80	104.31	111.33
1	A	289	PHE	O-C-N	5.80	128.84	122.11
1	A	383	ALA	CA-C-N	5.80	128.30	120.65
1	A	383	ALA	C-N-CA	5.80	128.30	120.65
1	A	220	TYR	O-C-N	5.78	128.24	122.12
1	A	152	ARG	NH1-CZ-NH2	5.74	126.76	119.30
1	A	319	ARG	N-CA-C	5.74	120.44	113.38
1	A	381	GLU	CB-CG-CD	5.74	122.35	112.60
1	A	95	GLU	N-CA-C	-5.72	104.24	111.11
1	A	293	PHE	CA-CB-CG	-5.72	108.08	113.80
1	A	400	ARG	CD-NE-CZ	5.72	132.41	124.40
1	A	409	GLU	CA-C-N	5.70	128.71	120.79
1	A	409	GLU	C-N-CA	5.70	128.71	120.79
1	A	20	TYR	CA-C-O	-5.69	115.02	121.00
1	A	136	GLU	N-CA-CB	5.69	118.26	110.01
1	A	458	ARG	N-CA-C	-5.69	104.69	111.69
1	A	72	ASP	CA-CB-CG	-5.68	106.92	112.60
1	A	417	ARG	CD-NE-CZ	-5.67	116.47	124.40
1	A	90	GLN	N-CA-C	-5.66	105.19	111.36
1	A	108	THR	N-CA-C	-5.65	102.06	110.20
1	A	351	ALA	CA-C-N	5.63	128.18	120.46
1	A	351	ALA	C-N-CA	5.63	128.18	120.46
1	A	273	MET	N-CA-C	-5.62	101.06	109.15
1	A	185	PRO	CB-CA-C	-5.61	104.05	111.23
1	A	147	ARG	O-C-N	5.60	130.75	122.97
1	A	446	GLY	CA-C-N	5.60	128.34	120.28
1	A	446	GLY	C-N-CA	5.60	128.34	120.28
1	A	140	ARG	NE-CZ-NH1	5.59	127.09	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	SER	CA-C-O	-5.59	115.02	120.89
1	A	247	ARG	N-CA-C	-5.59	100.01	108.67
1	A	19	ALA	CA-C-N	5.58	128.02	120.65
1	A	19	ALA	C-N-CA	5.58	128.02	120.65
1	A	311	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	2	VAL	N-CA-CB	-5.55	102.07	111.23
1	A	81	ARG	CA-C-N	5.55	127.98	120.38
1	A	81	ARG	C-N-CA	5.55	127.98	120.38
1	A	242	THR	N-CA-CB	5.54	119.85	110.49
1	A	284	PHE	CB-CA-C	-5.52	99.43	110.42
1	A	311	ARG	N-CA-CB	5.52	118.84	110.28
1	A	370	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	443	GLU	N-CA-C	-5.49	99.14	108.26
1	A	16	VAL	CA-CB-CG1	5.49	119.73	110.40
1	A	335	LEU	N-CA-C	-5.49	104.99	110.97
1	A	136	GLU	CG-CD-OE2	5.45	130.92	118.40
1	A	136	GLU	CB-CA-C	-5.43	102.35	110.88
1	A	133	GLU	N-CA-C	-5.42	105.06	110.97
1	A	246	LYS	N-CA-C	-5.42	104.40	111.02
1	A	16	VAL	CA-C-N	5.42	126.00	119.98
1	A	16	VAL	C-N-CA	5.42	126.00	119.98
1	A	233	MET	CA-C-O	5.42	124.58	119.76
1	A	205	ARG	CA-CB-CG	5.39	124.89	114.10
1	A	316	LYS	N-CA-CB	5.38	118.13	110.16
1	A	313	MET	CA-C-N	5.36	127.47	120.28
1	A	313	MET	C-N-CA	5.36	127.47	120.28
1	A	394	LEU	CA-C-O	5.36	125.97	119.38
1	A	400	ARG	CA-C-N	5.35	127.40	120.44
1	A	400	ARG	C-N-CA	5.35	127.40	120.44
1	A	368	LYS	N-CA-C	5.35	117.19	111.36
1	A	284	PHE	CA-C-O	-5.33	112.88	120.51
1	A	349	ARG	CD-NE-CZ	5.33	131.86	124.40
1	A	54	GLU	CA-C-N	5.30	129.58	120.72
1	A	54	GLU	C-N-CA	5.30	129.58	120.72
1	A	132	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	457	GLU	CB-CG-CD	5.28	121.58	112.60
1	A	200	VAL	N-CA-CB	5.28	119.00	110.13
1	A	444	THR	N-CA-CB	-5.27	100.98	110.37
1	A	22	ALA	N-CA-C	5.26	117.01	111.28
1	A	191	ASN	CA-C-O	-5.26	114.95	120.63
1	A	454	LEU	N-CA-CB	-5.23	102.22	110.06
1	A	77	THR	CA-C-O	5.22	127.97	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	TYR	O-C-N	5.21	125.78	121.35
1	A	416	LEU	CA-C-O	-5.20	114.91	120.42
1	A	270	LEU	N-CA-C	-5.20	105.61	111.28
1	A	149	LYS	CA-C-O	5.20	130.36	122.20
1	A	249	SER	CA-C-O	-5.20	113.08	120.51
1	A	464	GLU	N-CA-CB	5.19	117.60	110.07
1	A	315	GLY	N-CA-C	-5.18	106.42	113.37
1	A	186	THR	N-CA-CB	5.18	118.29	110.42
1	A	449	GLU	N-CA-C	-5.18	105.72	111.36
1	A	101	TRP	N-CA-CB	5.17	118.02	110.88
1	A	312	TRP	N-CA-CB	5.17	117.72	110.12
1	A	380	SER	N-CA-C	-5.17	103.66	110.33
1	A	417	ARG	N-CA-CB	5.12	118.11	110.22
1	A	323	SER	O-C-N	5.12	128.80	123.06
1	A	293	PHE	CB-CA-C	-5.12	103.51	109.80
1	A	31	ARG	N-CA-C	-5.11	106.87	113.01
1	A	465	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	A	172	GLU	CG-CD-OE1	-5.10	106.68	118.40
1	A	216	HIS	N-CA-C	-5.09	105.74	111.28
1	A	205	ARG	CD-NE-CZ	5.08	131.52	124.40
1	A	243	LYS	CA-C-O	-5.07	116.12	120.88
1	A	395	LYS	N-CA-C	-5.07	105.65	111.07
1	A	325	GLU	N-CA-C	-5.07	106.26	112.90
1	A	144	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	195	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	319	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	A	457	GLU	CG-CD-OE1	5.04	129.99	118.40
1	A	204	ILE	CB-CA-C	5.03	117.53	110.99
1	A	262	LEU	CA-CB-CG	5.03	133.90	116.30
1	A	320	GLU	O-C-N	5.02	128.97	122.15
1	A	291	GLN	CB-CG-CD	-5.02	104.07	112.60
1	A	4	THR	CA-CB-OG1	-5.01	102.08	109.60
1	A	284	PHE	CA-CB-CG	-5.01	108.78	113.80
1	A	447	LEU	N-CA-CB	-5.01	102.50	110.22
1	A	22	ALA	CA-C-O	-5.01	115.24	120.55
1	A	325	GLU	CG-CD-OE2	5.00	129.91	118.40

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	3813	0	3821	307	0
2	A	160	0	0	15	0
All	All	3973	0	3821	307	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 40.

All (307) 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:127:ARG:HH21	1:A:149:LYS:HG3	1.24	1.02
1:A:77:THR:HG21	1:A:198:MET:HA	1.40	1.01
1:A:75:ALA:HB1	1:A:76:PRO:HD2	1.47	0.96
1:A:262:LEU:H	1:A:314:ASN:HD21	1.15	0.94
1:A:268:ASN:HA	1:A:285:THR:HG23	1.55	0.89
1:A:284:PHE:HD2	1:A:288:GLU:HB2	1.40	0.86
1:A:136:GLU:HG3	1:A:137:ARG:N	1.90	0.85
1:A:75:ALA:HB1	1:A:76:PRO:CD	2.06	0.85
1:A:127:ARG:HH21	1:A:149:LYS:CG	1.90	0.84
1:A:444:THR:HG23	1:A:445:PRO:HD2	1.59	0.84
1:A:152:ARG:HG3	1:A:171:GLN:HE22	1.41	0.83
1:A:279:ASP:OD1	1:A:281:ARG:HB2	1.80	0.82
1:A:4:THR:HB	1:A:25:ASN:HD22	1.44	0.81
1:A:311:ARG:NH2	1:A:364:GLU:OE2	2.13	0.81
1:A:127:ARG:NH2	1:A:149:LYS:HG3	1.95	0.81
1:A:262:LEU:H	1:A:314:ASN:ND2	1.81	0.79
1:A:332:LYS:HD3	1:A:342:TRP:CZ2	2.18	0.78
1:A:385:ARG:O	1:A:388:GLU:HG2	1.85	0.76
1:A:291:GLN:HG2	2:A:804:HOH:O	1.85	0.76
1:A:237:ARG:CZ	1:A:302:GLY:HA3	2.17	0.74
1:A:267:ARG:HG2	1:A:285:THR:HG21	1.69	0.74
1:A:74:ALA:O	1:A:75:ALA:HB2	1.86	0.73
1:A:213:THR:N	1:A:214:PRO:HD2	2.03	0.73
1:A:272:LEU:HD21	1:A:282:GLU:HB3	1.68	0.73
1:A:435:ARG:HD2	1:A:444:THR:HB	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:HH12	1:A:171:GLN:HA	1.53	0.72
1:A:77:THR:HG21	1:A:198:MET:CA	2.19	0.72
1:A:267:ARG:HE	1:A:285:THR:HB	1.55	0.72
1:A:404:GLN:NE2	1:A:415:LEU:HD12	2.05	0.72
1:A:268:ASN:CA	1:A:285:THR:HG23	2.22	0.70
1:A:234:PRO:O	1:A:235:LEU:HB3	1.91	0.70
1:A:55:ARG:HD2	2:A:555:HOH:O	1.93	0.69
1:A:273:MET:HE2	1:A:273:MET:HA	1.75	0.69
1:A:152:ARG:HG3	1:A:171:GLN:NE2	2.08	0.68
1:A:57:LEU:O	1:A:61:LYS:HD2	1.92	0.68
1:A:92:TYR:HB3	1:A:223:PHE:CE1	2.29	0.68
1:A:202:ASP:OD2	1:A:229:ARG:NH1	2.27	0.68
1:A:77:THR:CG2	1:A:198:MET:HG2	2.24	0.67
1:A:11:THR:CG2	1:A:47:ARG:HB3	2.25	0.67
1:A:5:ARG:HG2	1:A:200:VAL:HG11	1.77	0.67
1:A:406:GLU:HG2	1:A:408:THR:HG23	1.76	0.67
1:A:205:ARG:HH22	1:A:216:HIS:CD2	2.13	0.67
1:A:221:ARG:HH11	1:A:221:ARG:HB3	1.60	0.67
1:A:247:ARG:O	1:A:248:LYS:HB2	1.95	0.67
1:A:137:ARG:HD2	1:A:142:GLU:OE2	1.95	0.66
1:A:307:LEU:O	1:A:311:ARG:HG3	1.96	0.66
1:A:294:THR:HG22	1:A:296:GLU:HB3	1.78	0.65
1:A:284:PHE:HA	2:A:631:HOH:O	1.96	0.65
1:A:239:PRO:O	1:A:240:ASP:HB2	1.97	0.64
1:A:332:LYS:HE3	1:A:348:LEU:CD2	2.27	0.64
1:A:15:HIS:HE1	1:A:244:ILE:HD12	1.62	0.64
1:A:10:PRO:HD3	1:A:40:ILE:HG23	1.79	0.64
1:A:39:ARG:HG3	1:A:198:MET:HE1	1.81	0.63
1:A:79:PRO:HB2	1:A:85:ARG:HG2	1.80	0.63
1:A:11:THR:HG21	1:A:47:ARG:HB3	1.81	0.63
1:A:408:THR:O	1:A:412:LEU:HB2	1.98	0.63
1:A:332:LYS:HB2	1:A:333:PRO:HD3	1.80	0.63
1:A:170:ASN:HA	1:A:173:ILE:HD12	1.80	0.62
1:A:96:LEU:HD13	1:A:223:PHE:CZ	2.34	0.62
1:A:262:LEU:N	1:A:314:ASN:HD21	1.93	0.62
1:A:74:ALA:O	1:A:75:ALA:CB	2.47	0.62
1:A:29:ALA:O	1:A:32:ASN:N	2.27	0.62
1:A:5:ARG:CG	1:A:200:VAL:HG11	2.30	0.62
1:A:169:ASP:O	1:A:172:GLU:HG3	2.01	0.61
1:A:284:PHE:HD2	1:A:288:GLU:CB	2.13	0.61
1:A:365:PHE:HB3	1:A:366:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HD11	1:A:243:LYS:HG2	1.83	0.61
1:A:77:THR:O	1:A:77:THR:HG22	2.01	0.60
1:A:119:LYS:NZ	1:A:125:ARG:HH22	1.99	0.60
1:A:221:ARG:HH11	1:A:221:ARG:CB	2.14	0.60
1:A:325:GLU:OE1	1:A:325:GLU:N	2.34	0.60
1:A:77:THR:HG21	1:A:198:MET:HG2	1.83	0.60
1:A:238:ASN:O	1:A:241:LYS:HA	2.01	0.60
1:A:113:GLU:OE2	1:A:116:ARG:NH1	2.35	0.59
1:A:205:ARG:HD3	1:A:232:HIS:CE1	2.38	0.59
1:A:438:LEU:HD11	1:A:451:LEU:HG	1.84	0.59
1:A:45:ARG:NH1	1:A:83:SER:HB2	2.17	0.59
1:A:40:ILE:HB	1:A:81:ARG:HG3	1.84	0.58
1:A:242:THR:O	1:A:243:LYS:C	2.46	0.58
1:A:445:PRO:O	1:A:446:GLY:C	2.45	0.58
1:A:276:SER:O	1:A:297:ARG:NH1	2.36	0.58
1:A:3:VAL:HG13	1:A:35:ARG:HB2	1.87	0.57
1:A:205:ARG:HH11	1:A:232:HIS:HE1	1.51	0.57
1:A:86:LEU:HB3	1:A:87:PRO:HD3	1.86	0.57
1:A:275:PHE:HA	1:A:297:ARG:O	2.04	0.57
1:A:45:ARG:NE	2:A:528:HOH:O	2.36	0.57
1:A:267:ARG:HG2	1:A:285:THR:CG2	2.34	0.57
1:A:267:ARG:CG	1:A:285:THR:HG21	2.35	0.56
1:A:136:GLU:CD	1:A:140:ARG:HH11	2.13	0.56
1:A:323:SER:HB2	2:A:511:HOH:O	2.04	0.56
1:A:52:ALA:O	1:A:56:ILE:HG13	2.05	0.56
1:A:444:THR:HG23	1:A:445:PRO:CD	2.34	0.56
1:A:456:LYS:HG2	1:A:460:LEU:HD12	1.87	0.56
1:A:23:LEU:HD13	1:A:65:LEU:HD21	1.87	0.55
1:A:122:TYR:CE2	1:A:124:GLY:HA2	2.41	0.55
1:A:276:SER:CB	1:A:297:ARG:HH12	2.18	0.55
1:A:91:LYS:NZ	1:A:91:LYS:CB	2.70	0.55
1:A:446:GLY:O	1:A:450:ILE:HG12	2.07	0.55
1:A:91:LYS:HZ3	1:A:91:LYS:HB2	1.72	0.55
1:A:106:PHE:CD2	1:A:144:HIS:HB3	2.42	0.54
1:A:276:SER:OG	1:A:297:ARG:NH1	2.35	0.54
1:A:464:GLU:O	1:A:465:ARG:C	2.49	0.54
1:A:196:HIS:HD2	2:A:508:HOH:O	1.91	0.54
1:A:237:ARG:HD3	1:A:241:LYS:HB3	1.90	0.53
1:A:415:LEU:HD23	1:A:415:LEU:C	2.33	0.53
1:A:163:ARG:NH2	1:A:232:HIS:O	2.41	0.53
1:A:94:GLU:CD	1:A:98:LYS:HZ2	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASN:O	1:A:318:ILE:HG13	2.08	0.53
1:A:77:THR:HG22	1:A:198:MET:HG2	1.89	0.53
1:A:393:LEU:HD23	1:A:429:GLN:O	2.09	0.53
1:A:1:MET:O	1:A:3:VAL:HG23	2.09	0.53
1:A:243:LYS:HZ3	1:A:244:ILE:HG13	1.73	0.53
1:A:95:GLU:HG2	1:A:99:ARG:HH21	1.74	0.53
1:A:103:TYR:CE2	1:A:127:ARG:HG2	2.44	0.53
1:A:290:ILE:HG13	1:A:290:ILE:O	2.09	0.53
1:A:82:GLN:OE1	1:A:190:ALA:HB1	2.09	0.52
1:A:86:LEU:HD21	1:A:184:TYR:CE1	2.44	0.52
1:A:398:TYR:N	1:A:399:PRO:HD2	2.23	0.52
1:A:75:ALA:CB	1:A:76:PRO:CD	2.78	0.52
1:A:72:ASP:OD1	1:A:73:VAL:N	2.42	0.52
1:A:40:ILE:HG22	1:A:42:ASP:HB3	1.91	0.52
1:A:332:LYS:HE3	1:A:348:LEU:HD21	1.90	0.52
1:A:267:ARG:NH2	2:A:607:HOH:O	2.42	0.52
1:A:332:LYS:HD3	1:A:342:TRP:CH2	2.45	0.52
1:A:267:ARG:HE	1:A:285:THR:CB	2.22	0.51
1:A:237:ARG:HH11	1:A:241:LYS:CE	2.23	0.51
1:A:119:LYS:HZ1	1:A:125:ARG:HH22	1.57	0.51
1:A:179:LEU:HD23	1:A:189:LEU:HD12	1.93	0.51
1:A:97:LEU:O	1:A:99:ARG:N	2.43	0.51
1:A:282:GLU:OE2	1:A:309:LYS:NZ	2.43	0.51
1:A:27:ALA:CB	1:A:290:ILE:HG22	2.41	0.51
1:A:22:ALA:CB	1:A:60:LEU:HD21	2.41	0.51
1:A:188:HIS:CD2	1:A:216:HIS:HE1	2.29	0.51
1:A:398:TYR:O	1:A:402:ARG:HG3	2.11	0.50
1:A:124:GLY:O	1:A:127:ARG:HG3	2.11	0.50
1:A:188:HIS:CD2	1:A:216:HIS:CE1	2.98	0.50
1:A:136:GLU:CG	1:A:137:ARG:N	2.66	0.50
1:A:71:PRO:C	1:A:73:VAL:H	2.20	0.50
1:A:237:ARG:HH11	1:A:241:LYS:NZ	2.10	0.50
1:A:136:GLU:OE2	1:A:140:ARG:HD2	2.12	0.50
1:A:237:ARG:NH1	1:A:301:GLY:O	2.44	0.50
1:A:361:THR:OG1	1:A:364:GLU:HG3	2.11	0.50
1:A:381:GLU:O	1:A:385:ARG:HG2	2.12	0.50
1:A:237:ARG:NH2	1:A:302:GLY:HA3	2.26	0.49
1:A:92:TYR:O	1:A:96:LEU:HB2	2.11	0.49
1:A:237:ARG:NH1	1:A:241:LYS:NZ	2.61	0.49
1:A:246:LYS:NZ	1:A:247:ARG:HH12	2.10	0.49
1:A:213:THR:N	1:A:214:PRO:CD	2.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:CE2	1:A:423:LYS:NZ	2.80	0.49
1:A:95:GLU:OE2	1:A:99:ARG:NH2	2.44	0.49
1:A:236:LEU:HD12	1:A:303:PRO:HG2	1.95	0.49
1:A:332:LYS:O	1:A:336:ARG:HG2	2.12	0.49
1:A:152:ARG:CG	1:A:171:GLN:HE22	2.21	0.49
1:A:92:TYR:HB3	1:A:223:PHE:CZ	2.47	0.49
1:A:129:ILE:O	1:A:130:PRO:C	2.56	0.49
1:A:243:LYS:NZ	1:A:244:ILE:HG13	2.28	0.48
1:A:267:ARG:NH1	2:A:556:HOH:O	2.43	0.48
1:A:152:ARG:HG3	1:A:152:ARG:NH1	2.28	0.48
1:A:276:SER:O	1:A:297:ARG:HD3	2.12	0.48
1:A:182:ASP:OD1	1:A:182:ASP:C	2.56	0.48
1:A:220:TYR:CZ	1:A:228:PRO:HD3	2.48	0.48
1:A:1:MET:O	1:A:2:VAL:C	2.56	0.48
1:A:356:ARG:N	1:A:357:PRO:CD	2.76	0.48
1:A:96:LEU:HD13	1:A:223:PHE:CE1	2.48	0.48
1:A:152:ARG:NH1	1:A:170:ASN:O	2.46	0.48
1:A:7:ALA:HA	1:A:39:ARG:O	2.12	0.48
1:A:205:ARG:HH11	1:A:232:HIS:CE1	2.32	0.48
1:A:187:TYR:O	1:A:191:ASN:HB3	2.14	0.48
1:A:191:ASN:ND2	2:A:538:HOH:O	2.45	0.48
1:A:247:ARG:O	1:A:248:LYS:CB	2.61	0.48
1:A:137:ARG:CD	1:A:142:GLU:OE2	2.61	0.48
1:A:201:THR:HB	2:A:821:HOH:O	2.13	0.48
1:A:241:LYS:O	1:A:242:THR:HG23	2.13	0.47
1:A:53:GLU:O	1:A:56:ILE:HB	2.14	0.47
1:A:88:LEU:O	1:A:92:TYR:HD2	1.96	0.47
1:A:401:LEU:HD12	1:A:463:LEU:CD1	2.44	0.47
1:A:381:GLU:OE2	1:A:385:ARG:NH2	2.48	0.47
1:A:43:THR:O	1:A:45:ARG:HG2	2.15	0.47
1:A:248:LYS:O	1:A:249:SER:HB2	2.14	0.47
1:A:294:THR:C	1:A:296:GLU:N	2.71	0.47
1:A:355:MET:HG3	1:A:369:ALA:HB2	1.95	0.47
1:A:63:LEU:O	1:A:267:ARG:HD3	2.15	0.47
1:A:163:ARG:NH1	1:A:207:GLU:OE2	2.48	0.47
1:A:404:GLN:O	1:A:456:LYS:NZ	2.40	0.47
1:A:157:GLU:HG3	2:A:560:HOH:O	2.15	0.47
1:A:458:ARG:NE	2:A:635:HOH:O	2.43	0.47
1:A:348:LEU:O	1:A:352:VAL:HG23	2.16	0.46
1:A:401:LEU:HD12	1:A:463:LEU:HD12	1.97	0.46
1:A:72:ASP:C	1:A:73:VAL:HG23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:HB3	1:A:111:GLU:HB3	1.98	0.46
1:A:152:ARG:N	1:A:153:PRO:CD	2.78	0.46
1:A:391:LEU:CD2	1:A:394:LEU:HD12	2.46	0.46
1:A:72:ASP:OD1	1:A:73:VAL:HB	2.15	0.46
1:A:417:ARG:NH1	1:A:417:ARG:CB	2.78	0.46
1:A:59:ALA:O	1:A:63:LEU:HD12	2.15	0.46
1:A:79:PRO:HB2	1:A:85:ARG:CG	2.45	0.46
1:A:274:GLY:O	1:A:275:PHE:CB	2.63	0.46
1:A:166:VAL:HG23	2:A:502:HOH:O	2.15	0.46
1:A:210:LEU:O	1:A:210:LEU:HD12	2.16	0.46
1:A:98:LYS:O	1:A:99:ARG:HG3	2.16	0.46
1:A:101:TRP:C	1:A:149:LYS:HB3	2.40	0.46
1:A:356:ARG:CB	1:A:357:PRO:HD3	2.46	0.46
1:A:139:ARG:C	1:A:141:GLY:N	2.74	0.46
1:A:248:LYS:O	1:A:249:SER:CB	2.63	0.46
1:A:86:LEU:CB	1:A:87:PRO:HD3	2.46	0.45
1:A:418:GLY:O	1:A:421:ALA:HB3	2.16	0.45
1:A:158:VAL:HG21	1:A:214:PRO:HA	1.98	0.45
1:A:284:PHE:CD2	1:A:285:THR:O	2.69	0.45
1:A:218:LEU:O	1:A:222:ALA:N	2.42	0.45
1:A:239:PRO:HA	1:A:304:VAL:HG21	1.98	0.45
1:A:247:ARG:HG2	1:A:247:ARG:HH11	1.82	0.45
1:A:434:LEU:CD2	1:A:451:LEU:HD11	2.47	0.45
1:A:234:PRO:HG3	1:A:299:SER:O	2.17	0.45
1:A:358:ARG:O	1:A:368:LYS:HD2	2.15	0.45
1:A:284:PHE:CD2	1:A:288:GLU:HB2	2.32	0.45
1:A:377:TYR:OH	1:A:462:ARG:HD3	2.17	0.45
1:A:152:ARG:NH2	1:A:173:ILE:O	2.50	0.45
1:A:193:VAL:HG13	1:A:197:LEU:HD22	1.99	0.45
1:A:261:PHE:CE1	1:A:310:LEU:HD13	2.52	0.45
1:A:297:ARG:HB3	1:A:297:ARG:HH11	1.80	0.45
1:A:9:SER:HB3	1:A:41:GLU:O	2.16	0.45
1:A:387:LEU:HD12	1:A:387:LEU:O	2.17	0.45
1:A:355:MET:O	1:A:356:ARG:C	2.60	0.44
1:A:314:ASN:OD1	1:A:360:ASP:O	2.35	0.44
1:A:398:TYR:CE2	1:A:402:ARG:HD2	2.53	0.44
1:A:203:VAL:HG12	1:A:205:ARG:HD2	2.00	0.44
1:A:434:LEU:HD21	1:A:451:LEU:HD11	2.00	0.44
1:A:282:GLU:C	1:A:283:ILE:HG12	2.42	0.44
1:A:297:ARG:NH1	1:A:297:ARG:HB3	2.33	0.44
1:A:91:LYS:CB	1:A:91:LYS:HZ3	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD21	1:A:295:TRP:CE3	2.53	0.43
1:A:274:GLY:HA2	2:A:832:HOH:O	2.18	0.43
1:A:15:HIS:CE1	1:A:244:ILE:HD12	2.48	0.43
1:A:44:ASP:OD1	1:A:46:ALA:HB3	2.18	0.43
1:A:463:LEU:O	1:A:467:LEU:HG	2.19	0.43
1:A:91:LYS:NZ	1:A:91:LYS:C	2.77	0.43
1:A:9:SER:C	1:A:11:THR:H	2.26	0.43
1:A:240:ASP:O	1:A:241:LYS:O	2.37	0.43
1:A:435:ARG:NH1	1:A:447:LEU:HB2	2.34	0.43
1:A:71:PRO:C	1:A:73:VAL:N	2.75	0.43
1:A:284:PHE:CD2	1:A:288:GLU:HG3	2.53	0.43
1:A:391:LEU:HD23	1:A:394:LEU:HD12	2.00	0.43
1:A:77:THR:O	1:A:78:GLY:C	2.61	0.43
1:A:94:GLU:HG3	1:A:98:LYS:CD	2.48	0.43
1:A:281:ARG:NH1	1:A:288:GLU:OE1	2.50	0.43
1:A:417:ARG:HH11	1:A:417:ARG:HB3	1.84	0.43
1:A:279:ASP:OD1	1:A:279:ASP:C	2.62	0.42
1:A:372:LEU:CD2	1:A:454:LEU:HD21	2.49	0.42
1:A:152:ARG:HG3	1:A:152:ARG:HH11	1.83	0.42
1:A:237:ARG:O	1:A:244:ILE:HG23	2.19	0.42
1:A:109:PRO:HD2	1:A:110:GLU:OE1	2.19	0.42
1:A:69:GLU:HG2	1:A:75:ALA:CB	2.50	0.42
1:A:77:THR:HG21	1:A:198:MET:CG	2.49	0.42
1:A:137:ARG:O	1:A:142:GLU:HB2	2.19	0.42
1:A:425:VAL:HG13	1:A:429:GLN:HB2	2.00	0.42
1:A:4:THR:HB	1:A:25:ASN:ND2	2.24	0.42
1:A:127:ARG:HH12	1:A:152:ARG:HD3	1.84	0.42
1:A:150:VAL:HA	1:A:151:PRO:HD3	1.78	0.42
1:A:180:LYS:HG3	1:A:184:TYR:O	2.19	0.42
1:A:262:LEU:HD23	1:A:317:TYR:HB3	2.01	0.42
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.93	0.42
1:A:31:ARG:HD2	1:A:31:ARG:O	2.19	0.42
1:A:45:ARG:HH12	1:A:83:SER:HB2	1.84	0.42
1:A:38:VAL:O	1:A:70:GLY:HA2	2.20	0.42
1:A:221:ARG:CB	1:A:221:ARG:NH1	2.82	0.42
1:A:256:TYR:O	1:A:261:PHE:HB2	2.19	0.42
1:A:284:PHE:CD2	1:A:288:GLU:CG	3.03	0.42
1:A:13:ASP:HB3	2:A:613:HOH:O	2.20	0.42
1:A:398:TYR:CD2	1:A:402:ARG:HD2	2.54	0.42
1:A:104:ARG:HA	1:A:145:VAL:O	2.20	0.42
1:A:94:GLU:CD	1:A:98:LYS:NZ	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ARG:CG	1:A:152:ARG:HH11	2.33	0.41
1:A:207:GLU:HB2	1:A:233:MET:O	2.19	0.41
1:A:391:LEU:N	1:A:392:PRO:CD	2.83	0.41
1:A:454:LEU:N	1:A:454:LEU:HD23	2.35	0.41
1:A:30:ARG:HB2	1:A:290:ILE:HD12	2.03	0.41
1:A:188:HIS:HD2	1:A:216:HIS:CE1	2.37	0.41
1:A:212:SER:HA	1:A:215:ILE:HD12	2.02	0.41
1:A:284:PHE:HD2	1:A:288:GLU:CG	2.34	0.41
1:A:47:ARG:HH11	1:A:47:ARG:HD2	1.73	0.41
1:A:92:TYR:HB3	1:A:223:PHE:HE1	1.79	0.41
1:A:104:ARG:HG2	1:A:144:HIS:CD2	2.55	0.41
1:A:108:THR:OG1	1:A:111:GLU:HB2	2.19	0.41
1:A:156:THR:OG1	1:A:170:ASN:ND2	2.52	0.41
1:A:116:ARG:C	1:A:118:GLU:H	2.29	0.41
1:A:158:VAL:HG11	1:A:213:THR:HB	2.03	0.41
1:A:397:LEU:C	1:A:399:PRO:HD2	2.46	0.41
1:A:95:GLU:HG2	1:A:99:ARG:NH2	2.34	0.41
1:A:152:ARG:HD2	1:A:152:ARG:HA	1.75	0.41
1:A:212:SER:C	1:A:214:PRO:HD2	2.45	0.41
1:A:274:GLY:O	1:A:275:PHE:HB2	2.20	0.41
1:A:398:TYR:N	1:A:399:PRO:CD	2.82	0.41
1:A:383:ALA:HA	1:A:442:LEU:HD22	2.02	0.41
1:A:442:LEU:HD12	1:A:442:LEU:HA	1.89	0.41
1:A:1:MET:SD	1:A:34:GLY:HA2	2.61	0.41
1:A:30:ARG:C	1:A:32:ASN:N	2.78	0.41
1:A:72:ASP:OD1	1:A:73:VAL:HG23	2.21	0.41
1:A:105:ALA:HB1	1:A:107:GLU:OE1	2.21	0.41
1:A:406:GLU:HG2	1:A:408:THR:CG2	2.48	0.41
1:A:420:ALA:HB1	1:A:425:VAL:O	2.20	0.41
1:A:262:LEU:CD1	1:A:362:LEU:HD11	2.51	0.40
1:A:286:LEU:HA	1:A:286:LEU:HD23	1.56	0.40
1:A:15:HIS:HE1	1:A:244:ILE:CD1	2.31	0.40
1:A:173:ILE:HA	1:A:174:PRO:HD3	1.88	0.40
1:A:426:LYS:HD2	1:A:428:GLY:H	1.86	0.40
1:A:152:ARG:N	1:A:153:PRO:HD2	2.37	0.40
1:A:417:ARG:CB	1:A:417:ARG:HH11	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	466/468 (100%)	394 (84%)	53 (11%)	19 (4%)	2 3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ALA
1	A	99	ARG
1	A	241	LYS
1	A	242	THR
1	A	248	LYS
1	A	249	SER
1	A	275	PHE
1	A	284	PHE
1	A	286	LEU
1	A	29	ALA
1	A	274	GLY
1	A	285	THR
1	A	446	GLY
1	A	117	LYS
1	A	244	ILE
1	A	290	ILE
1	A	78	GLY
1	A	291	GLN
1	A	234	PRO

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	393/393 (100%)	323 (82%)	70 (18%)	2 3

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	9	SER
1	A	43	THR
1	A	49	VAL
1	A	50	PRO
1	A	54	GLU
1	A	56	ILE
1	A	60	LEU
1	A	66	SER
1	A	68	ASP
1	A	81	ARG
1	A	91	LYS
1	A	101	TRP
1	A	111	GLU
1	A	116	ARG
1	A	136	GLU
1	A	139	ARG
1	A	140	ARG
1	A	142	GLU
1	A	152	ARG
1	A	155	THR
1	A	163	ARG
1	A	177	VAL
1	A	179	LEU
1	A	180	LYS
1	A	181	SER
1	A	189	LEU
1	A	191	ASN
1	A	197	LEU
1	A	200	VAL
1	A	205	ARG
1	A	210	LEU
1	A	211	VAL
1	A	218	LEU
1	A	221	ARG
1	A	236	LEU
1	A	243	LYS
1	A	244	ILE

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Mol	Chain	Res	Type
1	A	246	LYS
1	A	247	ARG
1	A	262	LEU
1	A	266	LEU
1	A	270	LEU
1	A	283	ILE
1	A	285	THR
1	A	294	THR
1	A	304	VAL
1	A	309	LYS
1	A	310	LEU
1	A	311	ARG
1	A	313	MET
1	A	331	VAL
1	A	337	GLU
1	A	343	GLU
1	A	350	ARG
1	A	367	GLU
1	A	375	GLU
1	A	391	LEU
1	A	395	LYS
1	A	409	GLU
1	A	412	LEU
1	A	416	LEU
1	A	423	LYS
1	A	425	VAL
1	A	426	LYS
1	A	443	GLU
1	A	444	THR
1	A	451	LEU
1	A	464	GLU
1	A	467	LEU

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	25	ASN
1	A	32	ASN
1	A	82	GLN
1	A	170	ASN
1	A	171	GLN
1	A	188	HIS

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Mol	Chain	Res	Type
1	A	191	ASN
1	A	196	HIS
1	A	216	HIS
1	A	232	HIS
1	A	314	ASN
1	A	404	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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.