



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:22 PM UTC

PDB ID : 1PNK / pdb_00001pnk
Title : PENICILLIN ACYLASE HAS A SINGLE-AMINO-ACID CATALYTIC CENTRE
Authors : Duggleby, H.J.; Moody, P.C.E.
Deposited on : 1995-03-16
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
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

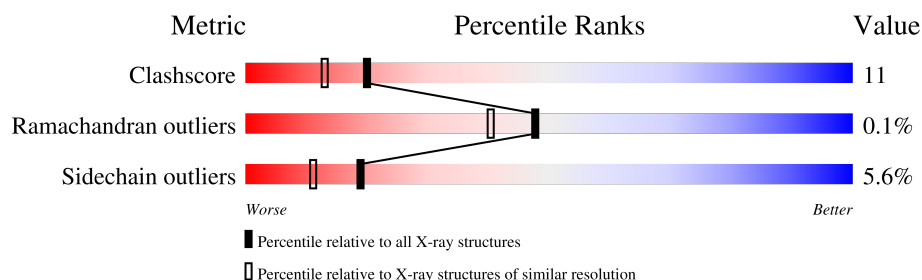
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	209	
2	B	557	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6432 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 PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1545	989	258	290	8			

- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4415	2805	766	834	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		
4	B	350	Total	O	0	0
			350	350		

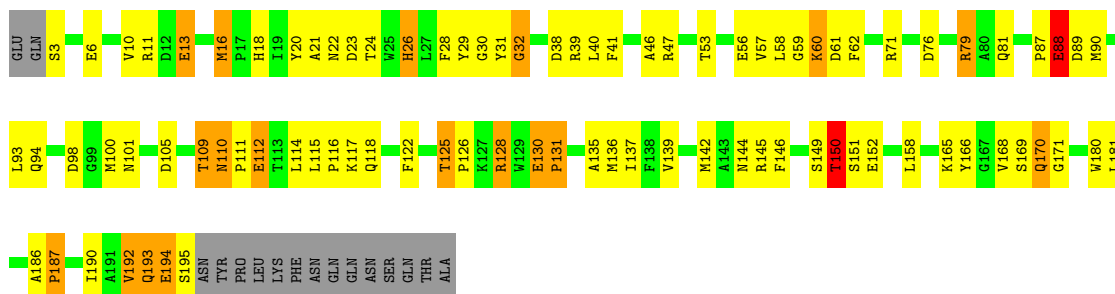
3 Residue-property plots [i](#)

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.

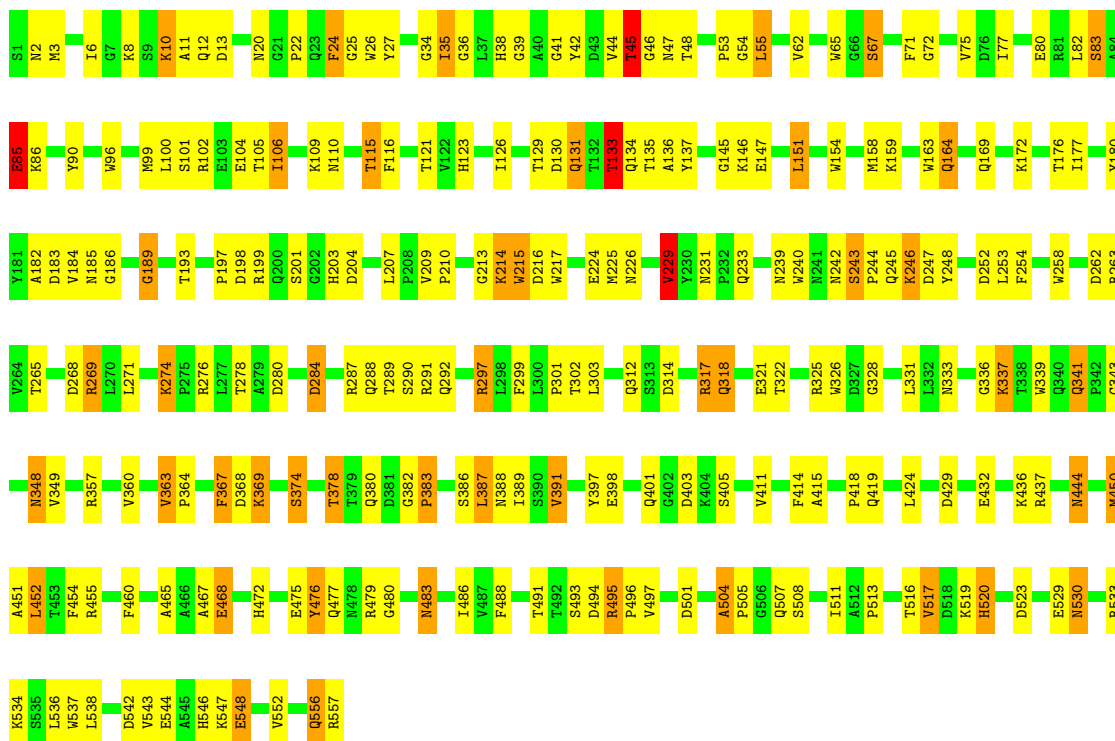
• Molecule 1: PENICILLIN AMIDOHYDROLASE

Chain A: 



• Molecule 2: PENICILLIN AMIDOHYDROLASE

Chain B: 



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	52.12Å 65.08Å 76.30Å 100.20° 111.44° 105.81°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	88.6 (10.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.190 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6432	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.31	3/1584 (0.2%)	2.33	93/2150 (4.3%)
2	B	1.31	16/4541 (0.4%)	2.27	225/6192 (3.6%)
All	All	1.31	19/6125 (0.3%)	2.29	318/8342 (3.8%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	378	THR	C-N	-8.54	1.25	1.33
2	B	231	ASN	C-O	7.19	1.27	1.23
2	B	25	GLY	N-CA	7.12	1.53	1.45
2	B	391	VAL	CA-C	6.82	1.61	1.52
2	B	36	GLY	CA-C	6.76	1.57	1.52
2	B	176	THR	CA-CB	6.30	1.61	1.52
2	B	45	THR	CA-C	6.07	1.59	1.52
2	B	34	GLY	CA-C	6.02	1.60	1.52
2	B	177	ILE	CA-CB	5.89	1.63	1.54
2	B	46	GLY	N-CA	5.83	1.52	1.45
2	B	265	THR	CA-CB	5.63	1.62	1.53
1	A	53	THR	CA-CB	5.48	1.60	1.53
2	B	483	ASN	CA-C	5.46	1.59	1.52
2	B	254	PHE	N-CA	5.43	1.52	1.46
1	A	109	THR	CA-CB	5.38	1.61	1.53
2	B	193	THR	CA-CB	5.21	1.61	1.53
2	B	54	GLY	CA-C	5.07	1.55	1.52
2	B	388	ASN	CA-C	5.06	1.59	1.52
1	A	30	GLY	CA-C	5.04	1.57	1.52

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	284	ASP	CA-CB-CG	-14.70	97.90	112.60
2	B	391	VAL	CB-CA-C	-12.77	95.62	111.97
2	B	269	ARG	CD-NE-CZ	12.06	141.28	124.40
1	A	150	THR	N-CA-CB	11.67	133.22	111.52
2	B	269	ARG	CA-CB-CG	11.31	136.72	114.10
2	B	45	THR	OG1-CB-CG2	11.07	131.43	109.30
2	B	472	HIS	CA-CB-CG	-11.01	102.79	113.80
2	B	363	VAL	CA-C-O	10.63	126.10	119.19
2	B	47	ASN	OD1-CG-ND2	10.42	133.02	122.60
2	B	24	PHE	CA-CB-CG	10.37	124.17	113.80
1	A	13	GLU	CB-CG-CD	10.27	130.06	112.60
1	A	28	PHE	CA-CB-CG	-10.12	103.68	113.80
2	B	233	GLN	CB-CG-CD	10.08	129.73	112.60
2	B	391	VAL	N-CA-CB	10.06	122.32	110.55
2	B	229	VAL	N-CA-CB	9.94	127.75	111.45
2	B	437	ARG	NE-CZ-NH1	9.90	131.40	121.50
1	A	110	ASN	N-CA-CB	-9.88	96.90	110.74
1	A	22	ASN	CA-CB-CG	-9.71	102.89	112.60
2	B	269	ARG	NH1-CZ-NH2	-9.64	106.76	119.30
1	A	105	ASP	CA-C-O	-9.38	110.97	120.82
1	A	118	GLN	OE1-CD-NE2	-9.30	113.30	122.60
2	B	62	VAL	O-C-N	9.11	129.00	121.98
2	B	419	GLN	OE1-CD-NE2	8.75	131.35	122.60
2	B	301	PRO	CA-C-N	8.73	131.98	120.28
2	B	301	PRO	C-N-CA	8.73	131.98	120.28
2	B	533	ARG	CD-NE-CZ	8.71	136.59	124.40
2	B	224	GLU	CB-CG-CD	8.69	127.37	112.60
2	B	495	ARG	CG-CD-NE	8.65	131.03	112.00
2	B	552	VAL	CA-C-O	8.60	129.42	120.39
2	B	403	ASP	CA-CB-CG	-8.47	104.13	112.60
2	B	429	ASP	O-C-N	8.47	130.80	122.07
2	B	164	GLN	CB-CG-CD	8.39	126.86	112.60
1	A	62	PHE	CA-CB-CG	-8.38	105.42	113.80
2	B	133	THR	N-CA-CB	8.30	122.59	110.47
1	A	150	THR	CB-CA-C	-8.17	92.55	109.94
1	A	88	GLU	CB-CG-CD	8.14	126.44	112.60
2	B	398	GLU	CA-C-O	-7.96	112.50	120.70
2	B	328	GLY	CA-C-O	-7.95	110.16	119.06
2	B	491	THR	CA-C-N	7.89	134.95	121.14
2	B	491	THR	C-N-CA	7.89	134.95	121.14
1	A	94	GLN	CB-CG-CD	7.85	125.94	112.60
2	B	85	GLU	CA-C-O	-7.82	111.73	121.50
2	B	530	ASN	OD1-CG-ND2	7.82	130.41	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	333	ASN	OD1-CG-ND2	7.81	130.41	122.60
2	B	389	ILE	CA-C-O	-7.80	111.95	120.85
2	B	204	ASP	O-C-N	7.78	128.50	121.19
2	B	374	SER	CA-C-N	7.70	132.20	121.26
2	B	374	SER	C-N-CA	7.70	132.20	121.26
2	B	239	ASN	OD1-CG-ND2	-7.70	114.90	122.60
2	B	325	ARG	CD-NE-CZ	-7.68	113.64	124.40
2	B	75	VAL	CA-C-O	-7.68	112.22	120.36
1	A	168	VAL	N-CA-C	7.65	118.19	110.23
2	B	248	TYR	CA-C-O	7.61	125.90	119.66
2	B	133	THR	N-CA-C	-7.61	104.13	113.41
1	A	38	ASP	N-CA-C	7.53	120.95	111.69
1	A	76	ASP	CA-C-O	-7.51	112.59	120.55
2	B	269	ARG	N-CA-CB	7.50	121.11	109.94
2	B	415	ALA	N-CA-CB	-7.44	100.97	111.62
1	A	125	THR	O-C-N	7.43	126.47	121.71
1	A	71	ARG	CD-NE-CZ	7.42	134.79	124.40
1	A	122	PHE	CA-CB-CG	-7.42	106.38	113.80
1	A	16	MET	O-C-N	7.38	128.04	121.18
2	B	349	VAL	O-C-N	7.34	129.39	121.83
2	B	83	SER	CA-CB-OG	7.30	125.71	111.10
1	A	39	ARG	N-CA-C	7.26	120.17	110.88
2	B	45	THR	N-CA-CB	7.24	125.00	111.53
1	A	192	VAL	CA-C-O	-7.24	112.83	120.57
2	B	493	SER	CA-C-O	7.16	129.53	121.51
2	B	13	ASP	CA-CB-CG	7.13	119.73	112.60
2	B	479	ARG	NE-CZ-NH1	7.13	128.63	121.50
2	B	380	GLN	CB-CG-CD	7.12	124.71	112.60
2	B	391	VAL	O-C-N	7.12	128.89	121.91
1	A	29	TYR	CA-C-N	7.07	127.79	119.94
1	A	29	TYR	C-N-CA	7.07	127.79	119.94
2	B	493	SER	CA-CB-OG	7.06	125.22	111.10
2	B	437	ARG	CD-NE-CZ	7.03	134.25	124.40
2	B	290	SER	CB-CA-C	-7.03	99.13	110.79
2	B	101	SER	CA-C-O	-7.02	113.75	121.33
2	B	314	ASP	O-C-N	6.99	127.25	121.31
1	A	168	VAL	CA-C-O	-6.94	114.19	121.41
1	A	94	GLN	OE1-CD-NE2	-6.91	115.69	122.60
2	B	25	GLY	N-CA-C	-6.90	102.87	111.70
2	B	530	ASN	CA-CB-CG	6.86	119.46	112.60
2	B	480	GLY	CA-C-N	6.84	129.75	120.38
2	B	480	GLY	C-N-CA	6.84	129.75	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	331	LEU	CA-C-O	-6.83	112.81	120.66
2	B	146	LYS	O-C-N	6.82	130.79	122.20
2	B	83	SER	N-CA-CB	6.80	121.73	110.85
2	B	240	TRP	N-CA-C	-6.80	102.39	110.41
2	B	102	ARG	CA-C-O	-6.78	112.20	120.54
2	B	341	GLN	OE1-CD-NE2	6.77	129.37	122.60
1	A	137	ILE	N-CA-CB	6.76	118.45	110.55
1	A	81	GLN	OE1-CD-NE2	6.75	129.35	122.60
1	A	149	SER	N-CA-C	6.74	119.67	108.96
2	B	233	GLN	OE1-CD-NE2	-6.72	115.88	122.60
2	B	321	GLU	CG-CD-OE2	-6.71	102.97	118.40
1	A	41	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	128	ARG	NE-CZ-NH2	6.70	125.23	119.20
2	B	269	ARG	NE-CZ-NH2	6.69	125.22	119.20
1	A	79	ARG	NE-CZ-NH1	6.63	128.13	121.50
2	B	55	LEU	O-C-N	6.60	131.14	123.02
2	B	424	LEU	CA-C-O	-6.59	113.56	120.55
2	B	317	ARG	NE-CZ-NH1	6.58	128.08	121.50
2	B	185	ASN	CA-C-O	-6.58	111.32	119.28
2	B	215	TRP	CA-CB-CG	-6.55	101.15	113.60
2	B	398	GLU	O-C-N	6.55	129.16	122.09
2	B	183	ASP	CA-CB-CG	6.55	119.15	112.60
2	B	225	MET	CA-C-O	-6.55	111.19	119.31
2	B	444	ASN	CA-CB-CG	6.54	119.14	112.60
2	B	176	THR	CA-CB-OG1	-6.51	99.83	109.60
2	B	269	ARG	NE-CZ-NH1	6.50	128.00	121.50
2	B	303	LEU	CA-C-N	6.46	129.22	120.44
2	B	303	LEU	C-N-CA	6.46	129.22	120.44
2	B	248	TYR	CB-CA-C	6.45	118.68	109.08
2	B	268	ASP	CA-C-O	-6.43	114.02	120.90
2	B	243	SER	CA-C-O	6.42	125.78	119.75
2	B	268	ASP	O-C-N	6.40	128.75	122.09
2	B	363	VAL	N-CA-C	6.40	115.60	108.05
1	A	112	GLU	CB-CG-CD	6.40	123.47	112.60
2	B	299	PHE	CA-C-O	-6.39	111.72	119.32
1	A	13	GLU	CA-CB-CG	6.37	126.85	114.10
2	B	391	VAL	CA-C-O	-6.37	114.41	121.17
2	B	333	ASN	N-CA-C	-6.35	102.34	110.53
2	B	460	PHE	CA-CB-CG	6.33	120.13	113.80
1	A	59	GLY	CA-C-N	6.32	133.62	121.54
1	A	59	GLY	C-N-CA	6.32	133.62	121.54
1	A	94	GLN	O-C-N	6.32	128.91	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	233	GLN	CA-C-O	-6.28	113.00	120.10
2	B	71	PHE	CA-CB-CG	-6.27	107.53	113.80
2	B	508	SER	CA-C-O	-6.26	114.07	120.71
1	A	40	LEU	CA-C-O	-6.26	113.92	120.55
1	A	194	GLU	CA-C-O	-6.26	114.23	120.80
2	B	199	ARG	O-C-N	6.26	130.07	123.06
2	B	45	THR	CA-C-O	-6.23	113.83	121.06
2	B	367	PHE	CA-CB-CG	-6.23	107.57	113.80
2	B	245	GLN	N-CA-CB	-6.22	101.92	111.56
2	B	229	VAL	CB-CA-C	-6.22	99.95	110.71
2	B	100	LEU	N-CA-C	-6.21	100.40	110.20
2	B	137	TYR	CA-C-O	-6.16	113.71	120.43
2	B	520	HIS	CA-CB-CG	-6.11	107.69	113.80
2	B	271	LEU	CA-C-O	-6.10	112.95	119.97
2	B	548	GLU	CA-CB-CG	6.09	126.29	114.10
2	B	496	PRO	CA-C-N	6.07	131.45	122.71
2	B	496	PRO	C-N-CA	6.07	131.45	122.71
1	A	89	ASP	CA-CB-CG	-6.07	106.53	112.60
1	A	130	GLU	CA-CB-CG	6.07	126.24	114.10
2	B	411	VAL	N-CA-CB	6.06	121.94	111.39
2	B	546	HIS	CA-CB-CG	-6.06	107.74	113.80
2	B	67	SER	N-CA-C	6.03	118.35	109.24
2	B	110	ASN	OD1-CG-ND2	-5.99	116.61	122.60
2	B	465	ALA	O-C-N	5.99	129.28	123.29
2	B	231	ASN	CB-CA-C	5.97	116.20	111.00
2	B	292	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	79	ARG	NE-CZ-NH2	-5.96	113.84	119.20
1	A	109	THR	CA-CB-CG2	5.96	120.62	110.50
2	B	204	ASP	CA-CB-CG	5.94	118.54	112.60
2	B	529	GLU	CA-C-O	-5.94	114.22	120.63
1	A	31	TYR	CA-C-N	5.92	126.66	120.03
1	A	31	TYR	C-N-CA	5.92	126.66	120.03
2	B	72	GLY	N-CA-C	-5.92	103.33	112.85
2	B	556	GLN	N-CA-CB	5.89	121.66	111.00
2	B	20	ASN	CA-CB-CG	5.88	118.48	112.60
2	B	357	ARG	NE-CZ-NH1	5.87	127.37	121.50
2	B	504	ALA	CA-C-O	-5.87	114.59	120.63
2	B	207	LEU	O-C-N	5.84	126.03	121.88
2	B	169	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	114	LEU	O-C-N	5.83	129.53	122.48
1	A	11	ARG	CD-NE-CZ	5.83	132.56	124.40
1	A	61	ASP	O-C-N	5.83	129.04	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	321	GLU	CA-CB-CG	-5.80	102.50	114.10
1	A	60	LYS	CA-CB-CG	5.78	125.66	114.10
2	B	35	ILE	O-C-N	-5.77	117.65	123.19
1	A	88	GLU	N-CA-CB	5.77	118.70	110.16
1	A	193	GLN	N-CA-CB	5.77	119.10	110.22
2	B	258	TRP	O-C-N	5.77	130.40	123.13
2	B	284	ASP	OD1-CG-OD2	5.75	136.71	122.90
2	B	27	TYR	O-C-N	5.75	129.94	123.27
2	B	54	GLY	CA-C-N	5.74	130.04	121.72
2	B	54	GLY	C-N-CA	5.74	130.04	121.72
1	A	170	GLN	O-C-N	5.74	128.69	122.15
2	B	229	VAL	O-C-N	5.72	129.41	123.05
2	B	45	THR	O-C-N	5.72	129.90	123.27
2	B	444	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	22	ASN	O-C-N	5.70	130.13	122.49
2	B	336	GLY	CA-C-O	-5.70	112.46	119.69
2	B	242	ASN	OD1-CG-ND2	5.66	128.26	122.60
2	B	556	GLN	OE1-CD-NE2	-5.66	116.94	122.60
2	B	450	MET	O-C-N	5.66	129.35	122.96
1	A	151	SER	N-CA-C	-5.65	104.00	112.54
2	B	321	GLU	CB-CG-CD	-5.65	102.99	112.60
2	B	45	THR	CB-CA-C	-5.64	97.04	109.56
1	A	23	ASP	O-C-N	5.64	130.07	122.96
2	B	341	GLN	O-C-N	5.63	127.04	121.57
2	B	83	SER	N-CA-C	-5.62	101.01	109.95
1	A	24	THR	CA-C-O	-5.61	114.93	120.82
2	B	468	GLU	CG-CD-OE2	-5.59	105.54	118.40
2	B	419	GLN	CG-CD-NE2	-5.59	108.02	116.40
1	A	149	SER	CA-C-O	-5.58	114.18	120.43
1	A	193	GLN	CB-CA-C	-5.58	100.31	110.63
1	A	90	MET	CA-C-N	5.58	127.75	120.28
1	A	90	MET	C-N-CA	5.58	127.75	120.28
2	B	213	GLY	N-CA-C	5.57	126.38	113.18
1	A	131	PRO	CA-C-N	5.57	127.74	120.28
1	A	131	PRO	C-N-CA	5.57	127.74	120.28
2	B	380	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	58	LEU	CA-C-O	-5.56	112.81	119.15
2	B	538	LEU	O-C-N	5.55	128.44	121.95
2	B	106	ILE	CA-C-O	-5.54	114.56	120.59
2	B	383	PRO	CA-C-O	5.53	127.98	121.56
2	B	454	PHE	N-CA-CB	5.53	118.67	110.49
2	B	542	ASP	CA-CB-CG	-5.53	107.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	322	THR	CA-CB-OG1	-5.52	101.32	109.60
2	B	189	GLY	O-C-N	-5.52	118.46	123.54
1	A	180	TRP	CA-CB-CG	5.51	124.07	113.60
2	B	477	GLN	OE1-CD-NE2	-5.51	117.09	122.60
2	B	203	HIS	CA-C-O	-5.51	114.10	120.49
2	B	297	ARG	CA-C-N	5.51	128.11	120.29
2	B	297	ARG	C-N-CA	5.51	128.11	120.29
1	A	135	ALA	CA-C-O	-5.50	114.71	120.55
2	B	145	GLY	CA-C-N	5.50	130.83	122.08
2	B	145	GLY	C-N-CA	5.50	130.83	122.08
2	B	475	GLU	N-CA-C	5.49	117.69	108.73
2	B	533	ARG	CA-C-O	5.48	126.92	120.89
2	B	414	PHE	CA-C-N	5.47	130.17	122.46
2	B	414	PHE	C-N-CA	5.47	130.17	122.46
2	B	544	GLU	O-C-N	5.47	127.70	122.07
2	B	54	GLY	CA-C-O	5.46	125.89	120.92
1	A	112	GLU	CG-CD-OE1	5.46	130.96	118.40
2	B	54	GLY	O-C-N	-5.45	117.81	123.48
2	B	386	SER	CA-C-O	5.45	127.50	121.56
2	B	35	ILE	CA-C-N	5.45	126.31	122.33
2	B	35	ILE	C-N-CA	5.45	126.31	122.33
2	B	106	ILE	N-CA-CB	5.45	117.58	111.21
2	B	137	TYR	O-C-N	5.42	129.40	123.27
2	B	476	TYR	N-CA-CB	5.42	117.93	109.85
1	A	6	GLU	CG-CD-OE1	-5.42	105.93	118.40
2	B	429	ASP	CA-C-O	-5.42	115.13	120.82
1	A	110	ASN	CB-CA-C	5.41	118.88	111.41
2	B	337	LYS	O-C-N	5.41	127.67	121.93
2	B	475	GLU	CG-CD-OE1	5.38	130.78	118.40
1	A	117	LYS	CA-C-N	5.38	128.02	120.28
1	A	117	LYS	C-N-CA	5.38	128.02	120.28
2	B	291	ARG	N-CA-C	5.35	119.96	113.38
1	A	142	MET	N-CA-C	-5.34	105.88	112.72
2	B	507	GLN	CA-C-O	5.33	126.20	120.55
1	A	93	LEU	O-C-N	5.32	128.22	122.15
2	B	169	GLN	CG-CD-OE1	5.32	131.44	120.80
2	B	182	ALA	CA-C-O	-5.32	115.03	120.99
2	B	209	VAL	N-CA-CB	5.31	118.64	111.21
1	A	187	PRO	N-CA-CB	5.29	108.03	103.27
1	A	87	PRO	CA-C-O	-5.29	111.61	119.86
1	A	71	ARG	NE-CZ-NH1	5.27	126.77	121.50
2	B	271	LEU	N-CA-CB	5.26	118.44	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	483	ASN	N-CA-CB	5.25	120.51	111.00
2	B	536	LEU	N-CA-CB	5.24	118.97	110.43
2	B	41	GLY	CA-C-N	5.24	130.45	122.65
2	B	41	GLY	C-N-CA	5.24	130.45	122.65
2	B	348	ASN	OD1-CG-ND2	-5.24	117.36	122.60
2	B	101	SER	O-C-N	5.23	129.22	123.25
2	B	322	THR	CA-C-N	5.23	127.28	120.28
2	B	322	THR	C-N-CA	5.23	127.28	120.28
2	B	325	ARG	CA-C-N	5.22	129.82	122.09
2	B	325	ARG	C-N-CA	5.22	129.82	122.09
2	B	289	THR	CA-C-N	5.22	127.27	120.28
2	B	289	THR	C-N-CA	5.22	127.27	120.28
2	B	415	ALA	N-CA-C	5.21	118.39	111.30
2	B	543	VAL	O-C-N	5.21	127.01	121.91
2	B	516	THR	CA-C-N	5.21	129.52	121.71
2	B	516	THR	C-N-CA	5.21	129.52	121.71
2	B	130	ASP	CB-CA-C	5.20	119.97	111.23
2	B	216	ASP	CA-CB-CG	5.20	117.80	112.60
2	B	233	GLN	CA-CB-CG	5.20	124.50	114.10
2	B	231	ASN	N-CA-CB	-5.20	104.08	111.51
1	A	71	ARG	CB-CA-C	-5.19	99.46	110.31
1	A	3	SER	CA-C-N	5.19	130.22	121.14
1	A	3	SER	C-N-CA	5.19	130.22	121.14
2	B	278	THR	N-CA-C	-5.19	103.07	110.59
2	B	318	GLN	CA-C-N	5.19	127.54	120.54
2	B	318	GLN	C-N-CA	5.19	127.54	120.54
1	A	98	ASP	CA-C-N	5.18	125.84	119.99
1	A	98	ASP	C-N-CA	5.18	125.84	119.99
1	A	32	GLY	CA-C-N	5.18	127.17	120.44
1	A	32	GLY	C-N-CA	5.18	127.17	120.44
1	A	26	HIS	CA-CB-CG	-5.17	108.63	113.80
2	B	198	ASP	CB-CG-OD2	-5.16	106.54	118.40
1	A	61	ASP	CA-C-O	-5.15	114.28	120.10
2	B	253	LEU	CA-C-O	-5.13	115.36	120.96
2	B	538	LEU	CA-C-O	-5.11	113.27	119.61
2	B	263	ARG	CA-C-O	-5.10	113.11	119.38
1	A	101	ASN	CA-C-N	5.09	127.41	120.54
1	A	101	ASN	C-N-CA	5.09	127.41	120.54
1	A	76	ASP	O-C-N	5.09	127.51	122.12
2	B	204	ASP	CA-C-O	-5.09	115.09	119.36
2	B	333	ASN	CA-CB-CG	5.08	117.68	112.60
2	B	246	LYS	CA-CB-CG	-5.08	103.94	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	MET	O-C-N	5.07	128.69	122.96
2	B	543	VAL	CA-C-O	-5.06	115.80	121.17
2	B	467	ALA	CA-C-N	5.06	128.69	120.60
2	B	467	ALA	C-N-CA	5.06	128.69	120.60
2	B	172	LYS	O-C-N	5.05	128.57	122.35
2	B	302	THR	N-CA-CB	5.05	117.55	110.12
1	A	169	SER	CA-C-N	5.05	127.45	120.29
1	A	169	SER	C-N-CA	5.05	127.45	120.29
2	B	269	ARG	CB-CA-C	-5.05	102.74	110.81
2	B	455	ARG	NE-CZ-NH2	-5.05	114.66	119.20
2	B	486	ILE	CB-CG1-CD1	5.04	124.39	113.80
2	B	226	ASN	O-C-N	5.04	125.87	121.18
2	B	378	THR	CA-CB-CG2	5.04	119.07	110.50
2	B	552	VAL	O-C-N	-5.04	117.82	123.26
1	A	136	MET	CA-C-N	5.03	126.90	120.56
1	A	136	MET	C-N-CA	5.03	126.90	120.56
2	B	444	ASN	CB-CA-C	5.02	119.10	111.02
1	A	193	GLN	OE1-CD-NE2	5.01	127.61	122.60
2	B	548	GLU	O-C-N	5.01	127.85	122.34
1	A	46	ALA	CA-C-O	-5.01	115.11	120.42
2	B	418	PRO	CB-CA-C	5.00	117.87	111.21
1	A	171	GLY	CA-C-N	5.00	127.40	120.29
1	A	171	GLY	C-N-CA	5.00	127.40	120.29

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	1545	0	1501	45	0
2	B	4415	0	4242	107	0
3	B	1	0	0	0	0
4	A	121	0	0	9	0
4	B	350	0	0	16	0
All	All	6432	0	5743	133	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 11.

All (133) 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:16:MET:HE1	2:B:45:THR:HG22	1.48	0.93
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.66	0.93
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.37	0.89
2:B:288:GLN:HG2	4:B:756:HOH:O	1.77	0.84
2:B:214:LYS:H	2:B:214:LYS:HD2	1.40	0.84
2:B:164:GLN:HG3	4:B:904:HOH:O	1.77	0.81
2:B:318:GLN:HG2	4:B:906:HOH:O	1.79	0.81
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.45	0.81
1:A:190:ILE:HG12	2:B:229:VAL:HG22	1.60	0.81
1:A:10:VAL:HG13	2:B:547:LYS:HG3	1.64	0.80
1:A:150:THR:HG22	2:B:252:ASP:OD2	1.81	0.80
4:A:235:HOH:O	2:B:534:LYS:HE3	1.82	0.79
2:B:214:LYS:HD2	2:B:214:LYS:N	2.00	0.77
2:B:6:ILE:HG23	2:B:10:LYS:HB3	1.65	0.77
1:A:60:LYS:HG3	4:B:707:HOH:O	1.85	0.76
1:A:16:MET:CE	2:B:45:THR:HG22	2.18	0.74
2:B:501:ASP:OD1	2:B:534:LYS:HE2	1.90	0.71
1:A:166:TYR:O	1:A:170:GLN:HB3	1.91	0.70
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.54	0.70
2:B:12:GLN:HB2	2:B:276:ARG:HB3	1.74	0.70
2:B:288:GLN:CG	4:B:756:HOH:O	2.38	0.68
1:A:56:GLU:O	2:B:109:LYS:HB2	1.93	0.68
2:B:104:GLU:O	2:B:115:THR:HA	1.94	0.68
2:B:387:LEU:HD21	2:B:450:MET:HE1	1.75	0.67
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.06	0.67
1:A:150:THR:HG22	2:B:252:ASP:CG	2.21	0.66
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.32	0.65
2:B:269:ARG:NH2	2:B:297:ARG:HB2	2.14	0.63
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.58	0.61
1:A:145:ARG:HG2	1:A:146:PHE:CD2	2.35	0.61
2:B:397:TYR:O	2:B:401:GLN:HG2	2.00	0.61
1:A:194:GLU:O	1:A:195:SER:HB3	2.02	0.60
1:A:150:THR:CG2	2:B:252:ASP:OD2	2.48	0.60
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.11	0.60
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.84	0.59
2:B:214:LYS:H	2:B:214:LYS:CD	2.13	0.59
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.83	0.59
1:A:166:TYR:HB3	1:A:170:GLN:CG	2.33	0.59
1:A:110:ASN:N	1:A:111:PRO:HD3	2.20	0.56
2:B:80:GLU:OE2	2:B:123:HIS:ND1	2.39	0.56
2:B:129:THR:HA	2:B:136:ALA:HA	1.88	0.56
1:A:166:TYR:HB3	1:A:170:GLN:HG3	1.88	0.56
1:A:57:VAL:HG12	4:A:323:HOH:O	2.06	0.55
1:A:88:GLU:CG	4:A:295:HOH:O	2.54	0.55
2:B:534:LYS:NZ	4:B:640:HOH:O	2.39	0.55
2:B:274:LYS:NZ	4:B:701:HOH:O	2.33	0.55
1:A:187:PRO:HG2	2:B:262:ASP:HB3	1.89	0.55
1:A:21:ALA:O	2:B:39:GLY:HA3	2.07	0.55
2:B:326:TRP:CD1	2:B:341:GLN:HG3	2.42	0.55
2:B:382:GLY:HA3	2:B:451:ALA:O	2.07	0.55
1:A:125:THR:HB	1:A:126:PRO:HD2	1.88	0.54
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.90	0.54
1:A:26:HIS:HE1	2:B:556:GLN:NE2	2.06	0.53
2:B:11:ALA:O	2:B:276:ARG:NH1	2.39	0.53
2:B:42:TYR:CZ	2:B:159:LYS:HE3	2.44	0.53
2:B:129:THR:HG22	2:B:136:ALA:CB	2.38	0.53
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.43	0.52
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.45	0.52
2:B:210:PRO:HD2	2:B:215:TRP:CD1	2.45	0.51
2:B:383:PRO:HD2	2:B:476:TYR:CD1	2.46	0.51
1:A:115:LEU:O	2:B:513:PRO:HG3	2.11	0.50
2:B:106:ILE:HD11	2:B:116:PHE:CE1	2.41	0.50
2:B:8:LYS:HG3	2:B:186:GLY:HA3	1.94	0.50
2:B:318:GLN:HA	4:B:906:HOH:O	2.11	0.50
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.94	0.50
1:A:145:ARG:HG2	1:A:146:PHE:CE2	2.47	0.49
1:A:150:THR:HG22	2:B:252:ASP:OD1	2.10	0.49
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.94	0.49
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.48	0.49
2:B:378:THR:HG22	2:B:383:PRO:HG3	1.95	0.48
1:A:88:GLU:HG3	4:A:295:HOH:O	2.12	0.48
2:B:280:ASP:O	2:B:284:ASP:HB2	2.13	0.48
2:B:65:TRP:HA	2:B:180:TYR:O	2.14	0.47
2:B:488:PHE:CD1	2:B:497:VAL:HG22	2.49	0.47
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.50	0.47
2:B:274:LYS:HE2	4:B:701:HOH:O	2.13	0.47
1:A:60:LYS:CG	4:B:707:HOH:O	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:MET:HE3	2:B:180:TYR:HB2	1.97	0.46
1:A:20:TYR:HA	2:B:38:HIS:O	2.15	0.46
2:B:85:GLU:O	2:B:86:LYS:C	2.58	0.46
1:A:130:GLU:HB2	1:A:131:PRO:CD	2.46	0.46
1:A:144:ASN:C	4:A:327:HOH:O	2.59	0.46
1:A:150:THR:HG22	1:A:152:GLU:HG3	1.96	0.45
2:B:504:ALA:HA	2:B:505:PRO:C	2.40	0.45
2:B:274:LYS:CE	4:B:701:HOH:O	2.64	0.45
2:B:495:ARG:HH12	2:B:537:TRP:HZ3	1.65	0.44
1:A:32:GLY:O	1:A:100:MET:HG2	2.18	0.44
2:B:360:VAL:HG13	2:B:368:ASP:HB2	2.00	0.44
1:A:16:MET:HE1	2:B:45:THR:CG2	2.35	0.44
2:B:287:ARG:NH1	4:B:756:HOH:O	2.51	0.44
2:B:284:ASP:OD2	2:B:287:ARG:NH2	2.51	0.44
2:B:312:GLN:HG3	4:B:888:HOH:O	2.16	0.44
2:B:339:TRP:CH2	2:B:450:MET:HE2	2.37	0.44
2:B:269:ARG:HH21	2:B:297:ARG:HB2	1.82	0.43
2:B:348:ASN:ND2	2:B:374:SER:OG	2.50	0.43
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.92	0.43
2:B:483:ASN:O	2:B:501:ASP:HA	2.19	0.43
1:A:79:ARG:NE	4:A:307:HOH:O	2.46	0.43
1:A:165:LYS:HG2	1:A:166:TYR:CE2	2.54	0.43
2:B:164:GLN:HG3	2:B:164:GLN:H	1.43	0.43
2:B:133:THR:HB	2:B:135:THR:OG1	2.19	0.42
2:B:494:ASP:OD1	2:B:495:ARG:HG3	2.18	0.42
2:B:105:THR:HG23	2:B:115:THR:HG22	2.00	0.42
2:B:48:THR:HB	2:B:55:LEU:HA	2.01	0.42
2:B:164:GLN:CG	4:B:904:HOH:O	2.53	0.42
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.96	0.42
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.85	0.42
1:A:47:ARG:NE	4:A:317:HOH:O	2.52	0.42
2:B:129:THR:HG22	2:B:136:ALA:HB2	2.02	0.42
2:B:488:PHE:CE1	2:B:497:VAL:HG22	2.55	0.42
2:B:164:GLN:CD	4:B:904:HOH:O	2.63	0.41
1:A:139:VAL:HG22	2:B:147:GLU:HB3	2.01	0.41
1:A:130:GLU:HB2	1:A:131:PRO:HD2	2.02	0.41
2:B:556:GLN:OE1	2:B:557:ARG:N	2.48	0.41
2:B:341:GLN:HG2	4:B:659:HOH:O	2.20	0.41
1:A:145:ARG:HA	4:A:327:HOH:O	2.19	0.41
2:B:246:LYS:O	2:B:247:ASP:HB2	2.20	0.41
2:B:53:PRO:HD2	2:B:151:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLN:H	2:B:131:GLN:HG3	1.52	0.41
2:B:35:ILE:HG23	2:B:55:LEU:HD11	2.03	0.41
2:B:90:TYR:CZ	2:B:121:THR:HB	2.55	0.41
2:B:363:VAL:HA	2:B:364:PRO:HD3	1.87	0.41
2:B:378:THR:HG21	2:B:450:MET:HG2	2.01	0.41
1:A:158:LEU:HD13	2:B:367:PHE:HB3	2.02	0.41
2:B:83:SER:HB3	2:B:96:TRP:CH2	2.56	0.41
2:B:369:LYS:HA	2:B:369:LYS:HD2	1.87	0.41
2:B:210:PRO:O	2:B:215:TRP:HB2	2.21	0.40
2:B:45:THR:HG21	2:B:537:TRP:O	2.21	0.40
2:B:243:SER:HA	2:B:244:PRO:HD3	1.91	0.40
1:A:88:GLU:HG2	4:A:295:HOH:O	2.20	0.40
2:B:401:GLN:HB2	2:B:405:SER:HB2	2.03	0.40
2:B:432:GLU:O	2:B:436: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	191/209 (91%)	189 (99%)	2 (1%)	0	100	100
2	B	555/557 (100%)	538 (97%)	16 (3%)	1 (0%)	43	36
All	All	746/766 (97%)	727 (98%)	18 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	GLN

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	165/180 (92%)	157 (95%)	8 (5%)	23	15
2	B	460/460 (100%)	433 (94%)	27 (6%)	18	10
All	All	625/640 (98%)	590 (94%)	35 (6%)	19	11

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	88	GLU
1	A	109	THR
1	A	112	GLU
1	A	150	THR
1	A	181	LEU
1	A	192	VAL
1	A	193	GLN
2	B	2	ASN
2	B	10	LYS
2	B	45	THR
2	B	67	SER
2	B	77	ILE
2	B	85	GLU
2	B	115	THR
2	B	131	GLN
2	B	133	THR
2	B	151	LEU
2	B	154	TRP
2	B	184	VAL
2	B	201	SER
2	B	214	LYS
2	B	229	VAL
2	B	274	LYS
2	B	317	ARG
2	B	337	LYS
2	B	369	LYS

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Mol	Chain	Res	Type
2	B	387	LEU
2	B	391	VAL
2	B	444	ASN
2	B	452	LEU
2	B	468	GLU
2	B	517	VAL
2	B	519	LYS
2	B	530	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	110	ASN
2	B	2	ASN
2	B	93	ASN
2	B	134	GLN
2	B	245	GLN
2	B	288	GLN
2	B	292	GLN
2	B	295	ASN
2	B	348	ASN
2	B	440	ASN
2	B	441	ASN
2	B	444	ASN
2	B	520	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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.