



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:13 PM UTC

PDB ID : 1AUG / pdb_00001aug
Title : CRYSTAL STRUCTURE OF THE PYROGLUTAMYL PEPTIDASE I
FROM BACILLUS AMYLOLIQUEFACIENS
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Deposited on : 1997-08-26
Resolution : 2.00 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

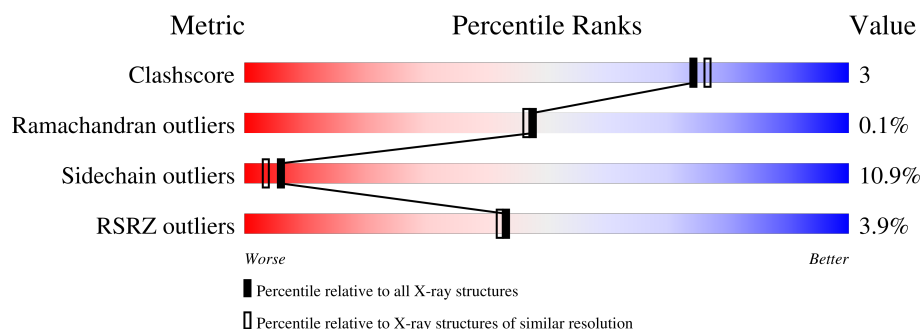
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	
1	B	215	
1	C	215	
1	D	215	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8095 atoms, of which 1388 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 PYROGLUTAMYL PEPTIDASE-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	210	Total	C	H	N	O	S	0	0	0
			1945	1017	347	279	297	5			
1	B	210	Total	C	H	N	O	S	0	0	0
			1945	1017	347	279	297	5			
1	C	210	Total	C	H	N	O	S	0	0	0
			1945	1017	347	279	297	5			
1	D	210	Total	C	H	N	O	S	0	0	0
			1945	1017	347	279	297	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	83	Total	O	0	0
			83	83		
2	C	87	Total	O	0	0
			87	87		
2	D	63	Total	O	0	0
			63	63		

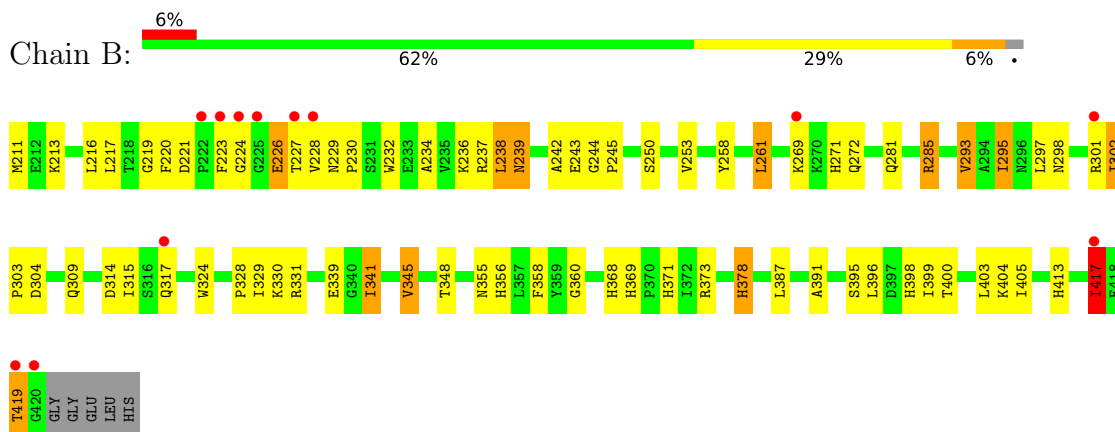
3 Residue-property plots

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

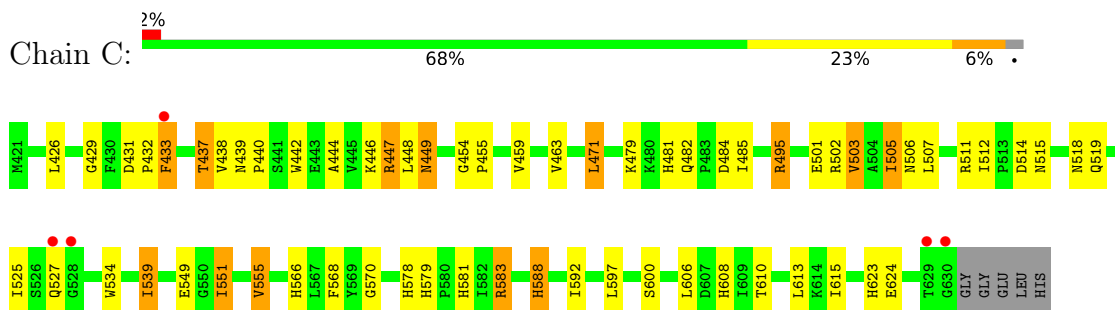
• Molecule 1: PYROGLUTAMYL PEPTIDASE-1



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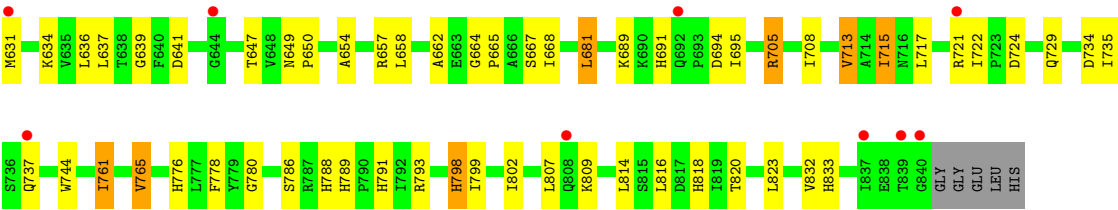


• Molecule 1: PYROGLUTAMYL PEPTIDASE-1



• Molecule 1: PYROGLUTAMYL PEPTIDASE-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.71Å 80.80Å 69.16Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 83.6 (30.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.95Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.197 , 0.259 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.001 for -k,-h,-l 0.004 for k,h,-l 0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.27	13/1635 (0.8%)	1.87	47/2222 (2.1%)
1	B	1.28	13/1635 (0.8%)	1.87	52/2222 (2.3%)
1	C	1.29	12/1635 (0.7%)	1.85	51/2222 (2.3%)
1	D	1.23	13/1635 (0.8%)	1.78	42/2222 (1.9%)
All	All	1.27	51/6540 (0.8%)	1.84	192/8888 (2.2%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	VAL	CA-CB	8.90	1.66	1.54
1	C	551	ILE	CA-CB	7.98	1.64	1.54
1	B	345	VAL	CA-CB	7.96	1.64	1.54
1	C	555	VAL	CA-CB	7.89	1.64	1.54
1	A	131	ILE	CA-CB	7.81	1.64	1.54
1	C	588	HIS	CD2-NE2	-7.75	1.29	1.37
1	D	765	VAL	CA-CB	7.73	1.64	1.54
1	C	566	HIS	CG-ND1	-7.70	1.29	1.38
1	B	368	HIS	CD2-NE2	-7.65	1.29	1.37
1	C	579	HIS	CD2-NE2	-7.32	1.29	1.37
1	A	188	HIS	CD2-NE2	-7.25	1.29	1.37
1	C	623	HIS	CD2-NE2	-7.14	1.29	1.37
1	B	271	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	158	HIS	CD2-NE2	-6.80	1.30	1.37
1	B	398	HIS	CD2-NE2	-6.76	1.30	1.37
1	D	788	HIS	CD2-NE2	-6.66	1.30	1.37
1	D	691	HIS	CD2-NE2	-6.42	1.30	1.37
1	C	578	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	341	ILE	CA-CB	6.39	1.62	1.54
1	B	378	HIS	CD2-NE2	-6.39	1.30	1.37
1	D	761	ILE	CA-CB	6.34	1.62	1.54
1	C	566	HIS	CD2-NE2	-6.23	1.30	1.37
1	C	581	HIS	CD2-NE2	-6.17	1.31	1.37
1	C	608	HIS	CD2-NE2	-6.08	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	413	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	203	HIS	CD2-NE2	-6.05	1.31	1.37
1	D	789	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	146	HIS	CG-ND1	-5.94	1.31	1.38
1	D	798	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	356	HIS	CG-ND1	-5.82	1.31	1.38
1	D	818	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	161	HIS	CD2-NE2	-5.71	1.31	1.37
1	A	209	THR	CA-C	5.71	1.56	1.52
1	D	833	HIS	CD2-NE2	-5.66	1.31	1.37
1	D	791	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	61	HIS	CD2-NE2	-5.61	1.31	1.37
1	D	799	ILE	CA-CB	5.58	1.59	1.55
1	A	159	HIS	CD2-NE2	-5.55	1.31	1.37
1	C	438	VAL	CA-CB	5.51	1.62	1.54
1	B	369	HIS	CG-ND1	-5.34	1.32	1.38
1	C	481	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	163	ARG	CA-CB	-5.26	1.46	1.53
1	D	833	HIS	CG-ND1	-5.25	1.32	1.38
1	D	818	HIS	CG-ND1	-5.23	1.32	1.38
1	B	371	HIS	CD2-NE2	-5.19	1.32	1.37
1	B	369	HIS	CD2-NE2	-5.18	1.32	1.37
1	B	356	HIS	CD2-NE2	-5.15	1.32	1.37
1	D	776	HIS	CG-ND1	-5.14	1.32	1.38
1	B	398	HIS	CG-ND1	-5.12	1.32	1.38
1	A	209	THR	CA-CB	5.12	1.60	1.53

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	ILE	N-CA-CB	-12.84	100.75	111.67
1	A	75	ARG	NE-CZ-NH1	11.89	133.39	121.50
1	A	75	ARG	NE-CZ-NH2	-10.39	109.84	119.20
1	C	514	ASP	CA-CB-CG	9.86	122.46	112.60
1	A	105	ILE	N-CA-C	-9.42	102.69	111.45
1	B	221	ASP	CA-CB-CG	9.09	121.69	112.60
1	C	431	ASP	CA-CB-CG	8.85	121.45	112.60
1	A	209	THR	N-CA-C	8.68	124.22	111.02
1	D	705	ARG	NE-CZ-NH1	8.30	129.80	121.50
1	C	525	ILE	N-CA-C	-8.20	102.87	110.82
1	A	75	ARG	CB-CG-CD	8.19	130.14	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	649	ASN	OD1-CG-ND2	-8.06	114.53	122.60
1	B	272	GLN	O-C-N	-8.05	117.83	121.53
1	B	285	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	A	92	ILE	N-CA-CB	-7.85	100.22	111.21
1	A	11	ASP	CA-CB-CG	7.81	120.41	112.60
1	B	391	ALA	N-CA-C	-7.80	101.20	108.22
1	B	304	ASP	CA-CB-CG	7.74	120.34	112.60
1	B	314	ASP	CA-CB-CG	7.69	120.29	112.60
1	C	579	HIS	CB-CG-CD2	-7.62	121.30	131.20
1	D	724	ASP	CA-CB-CG	7.57	120.17	112.60
1	D	735	ILE	N-CA-C	-7.50	103.54	110.82
1	C	568	PHE	CA-CB-CG	7.46	121.27	113.80
1	C	512	ILE	N-CA-CB	-7.41	100.84	111.21
1	D	649	ASN	N-CA-C	-7.38	93.39	109.11
1	C	495	ARG	NE-CZ-NH2	-7.28	112.65	119.20
1	B	315	ILE	N-CA-C	-7.24	103.79	110.82
1	A	159	HIS	CB-CG-CD2	-7.14	121.92	131.20
1	D	722	ILE	N-CA-CB	-7.06	101.33	111.21
1	D	705	ARG	CB-CG-CD	6.96	127.31	111.30
1	A	85	ILE	CA-CB-CG2	6.95	122.32	110.50
1	B	317	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	D	789	HIS	CB-CG-CD2	-6.89	122.24	131.20
1	A	27	ARG	CA-CB-CG	6.85	127.81	114.10
1	B	223	PHE	O-C-N	6.81	131.30	123.27
1	C	495	ARG	NE-CZ-NH1	6.81	128.31	121.50
1	B	285	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	B	358	PHE	CA-CB-CG	6.64	120.44	113.80
1	B	295	ILE	CB-CA-C	6.61	120.47	110.62
1	C	454	GLY	CA-C-N	6.55	126.68	119.87
1	C	454	GLY	C-N-CA	6.55	126.68	119.87
1	B	293	VAL	CB-CA-C	-6.53	99.97	110.28
1	A	7	LEU	O-C-N	-6.48	114.98	123.21
1	C	608	HIS	CB-CG-CD2	-6.46	122.81	131.20
1	C	623	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	C	482	GLN	O-C-N	-6.42	118.58	121.53
1	B	417	ILE	CB-CA-C	6.42	118.65	111.59
1	B	229	ASN	CA-C-N	6.41	126.91	119.47
1	B	229	ASN	C-N-CA	6.41	126.91	119.47
1	A	94	ASP	CA-CB-CG	6.41	119.00	112.60
1	B	419	THR	O-C-N	-6.35	115.62	123.44
1	B	417	ILE	N-CA-CB	-6.34	100.85	111.38
1	B	295	ILE	CA-CB-CG2	6.33	121.26	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	C	623	HIS	CA-CB-CG	-6.32	107.48	113.80
1	A	83	VAL	CB-CA-C	-6.29	99.83	110.71
1	C	583	ARG	CA-CB-CG	-6.26	101.58	114.10
1	C	439	ASN	CA-C-N	6.24	126.71	119.47
1	C	439	ASN	C-N-CA	6.24	126.71	119.47
1	D	649	ASN	CA-C-O	6.23	125.48	119.62
1	C	503	VAL	CB-CA-C	-6.22	100.46	110.28
1	B	239	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	B	295	ILE	N-CA-CB	-6.16	100.68	111.39
1	C	505	ILE	CA-CB-CG2	6.15	120.96	110.50
1	B	373	ARG	CA-CB-CG	-6.13	101.83	114.10
1	B	237	ARG	CA-CB-CG	6.13	126.36	114.10
1	B	378	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	B	226	GLU	CA-C-O	-6.12	114.90	121.45
1	B	242	ALA	N-CA-C	-6.11	98.44	108.76
1	A	188	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	D	657	ARG	CA-CB-CG	6.08	126.27	114.10
1	A	181	ALA	O-C-N	-6.01	117.26	121.65
1	B	244	GLY	CA-C-N	5.99	126.10	119.87
1	B	244	GLY	C-N-CA	5.99	126.10	119.87
1	A	29	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	D	793	ARG	CA-CB-CG	-5.93	102.25	114.10
1	C	581	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	D	715	ILE	N-CA-CB	-5.92	101.73	111.44
1	D	664	GLY	CA-C-N	5.91	125.53	119.56
1	D	664	GLY	C-N-CA	5.91	125.53	119.56
1	C	527	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	C	592	ILE	CA-C-N	5.85	125.99	119.32
1	C	592	ILE	C-N-CA	5.85	125.99	119.32
1	B	220	PHE	O-C-N	5.84	129.56	122.96
1	A	168	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	D	791	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	D	662	ALA	N-CA-C	-5.78	98.99	108.76
1	A	168	HIS	CB-CG-ND1	5.77	131.36	122.70
1	B	302	ILE	CB-CA-C	5.77	119.17	110.97
1	C	481	HIS	CB-CG-CD2	-5.77	123.69	131.20
1	A	209	THR	CA-C-O	-5.77	113.00	119.98
1	A	85	ILE	N-CA-CB	-5.76	99.98	111.91
1	C	588	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	D	734	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	505	ILE	CB-CA-C	5.76	119.20	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	298	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	B	398	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	C	505	ILE	N-CA-CB	-5.66	101.54	111.39
1	A	178	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	B	368	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	C	484	ASP	CA-CB-CG	-5.63	106.97	112.60
1	A	85	ILE	CB-CA-C	5.62	119.48	110.82
1	B	295	ILE	CA-CB-CG1	-5.61	100.86	110.40
1	A	85	ILE	CA-CB-CG1	-5.60	100.88	110.40
1	B	324	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	D	809	LYS	CA-C-O	-5.59	114.31	120.24
1	C	506	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	78	ILE	N-CA-C	-5.56	101.55	108.89
1	C	515	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	C	623	HIS	CA-C-O	5.53	126.41	120.32
1	C	539	ILE	CB-CG1-CD1	-5.53	102.20	113.80
1	C	449	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	D	639	GLY	N-CA-C	-5.51	102.75	110.96
1	D	713	VAL	CB-CA-C	-5.49	101.22	110.71
1	B	219	GLY	N-CA-C	-5.47	102.53	110.90
1	A	22	TRP	CE2-CD2-CG	-5.46	100.64	107.20
1	D	802	ILE	CA-C-N	5.45	125.54	119.32
1	D	802	ILE	C-N-CA	5.45	125.54	119.32
1	D	789	HIS	CB-CG-ND1	5.44	130.86	122.70
1	A	61	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	B	285	ARG	CB-CG-CD	5.43	123.80	111.30
1	D	715	ILE	CA-CB-CG2	5.42	119.72	110.50
1	A	114	TRP	CG-CD2-CE3	5.42	139.32	133.90
1	B	329	ILE	N-CA-C	5.41	117.85	111.09
1	A	104	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	159	HIS	CB-CG-ND1	5.40	130.80	122.70
1	A	158	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	D	818	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	C	437	THR	CA-C-O	5.37	124.96	119.05
1	A	119	ILE	CB-CG1-CD1	-5.37	102.52	113.80
1	C	429	GLY	N-CA-C	-5.37	102.97	110.96
1	A	43	VAL	CA-C-N	5.36	125.27	119.85
1	A	43	VAL	C-N-CA	5.36	125.27	119.85
1	D	667	SER	N-CA-C	-5.36	99.56	108.34
1	D	737	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	D	814	LEU	O-C-N	-5.35	116.75	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	ILE	CA-C-O	-5.34	115.12	121.05
1	C	433	PHE	N-CA-CB	-5.32	102.77	111.66
1	C	455	PRO	N-CA-CB	5.30	108.39	103.41
1	B	355	ASN	CA-CB-CG	5.30	117.90	112.60
1	C	505	ILE	CA-CB-CG1	-5.29	101.41	110.40
1	A	43	VAL	N-CA-CB	-5.27	103.83	111.21
1	A	163	ARG	CA-CB-CG	-5.26	103.57	114.10
1	B	238	LEU	N-CA-C	-5.26	106.54	113.17
1	A	107	GLN	CG-CD-NE2	5.26	124.29	116.40
1	B	232	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	C	495	ARG	CB-CG-CD	5.25	123.37	111.30
1	D	729	GLN	CA-C-N	5.24	125.16	119.76
1	D	729	GLN	C-N-CA	5.24	125.16	119.76
1	D	778	PHE	CA-CB-CG	5.24	119.04	113.80
1	D	641	ASP	O-C-N	-5.22	115.31	121.32
1	D	788	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	B	253	VAL	N-CA-CB	-5.21	103.92	111.21
1	A	3	LYS	N-CA-C	-5.21	100.41	108.90
1	B	309	GLN	CA-C-N	5.21	125.12	119.76
1	B	309	GLN	C-N-CA	5.21	125.12	119.76
1	C	534	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	B	271	HIS	CB-CG-CD2	-5.19	124.46	131.20
1	C	518	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	D	715	ILE	CA-CB-CG1	-5.18	101.60	110.40
1	A	164	GLY	O-C-N	-5.17	118.72	123.42
1	A	109	GLY	CA-C-O	-5.16	117.45	122.46
1	C	579	HIS	CB-CG-ND1	5.15	130.43	122.70
1	C	608	HIS	CB-CG-ND1	5.15	130.43	122.70
1	D	789	HIS	CA-C-N	5.14	124.86	119.82
1	D	789	HIS	C-N-CA	5.14	124.86	119.82
1	D	715	ILE	CB-CA-C	5.14	118.42	110.50
1	A	37	SER	N-CA-C	-5.14	100.03	108.41
1	D	798	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	A	22	TRP	CB-CG-CD1	-5.13	119.20	126.90
1	D	668	ILE	O-C-N	-5.13	117.91	123.14
1	B	378	HIS	CB-CG-ND1	5.12	130.39	122.70
1	D	649	ASN	CB-CG-ND2	5.12	124.08	116.40
1	D	744	TRP	CG-CD2-CE3	5.12	139.02	133.90
1	B	328	PRO	CB-CA-C	5.11	120.05	113.09
1	C	519	GLN	O-C-N	-5.11	116.79	121.34
1	C	624	GLU	CA-C-O	5.11	125.96	120.70
1	A	204	GLU	N-CA-C	-5.10	106.22	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	188	HIS	CB-CG-ND1	5.08	130.31	122.70
1	D	708	ILE	N-CA-C	-5.07	102.96	109.30
1	C	442	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	C	463	VAL	N-CA-CB	-5.06	104.13	111.21
1	C	446	LYS	CB-CG-CD	-5.05	99.67	111.30
1	B	236	LYS	CB-CG-CD	-5.03	99.72	111.30
1	C	501	GLU	CA-C-O	-5.03	114.86	120.54
1	C	447	ARG	CA-CB-CG	5.03	124.16	114.10
1	C	481	HIS	CB-CG-ND1	5.02	130.23	122.70
1	A	85	ILE	O-C-N	-5.02	117.76	123.03
1	A	92	ILE	CB-CA-C	5.02	120.49	111.36
1	B	398	HIS	CB-CG-ND1	5.01	130.22	122.70

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	1598	347	1605	10	0
1	B	1598	347	1602	14	0
1	C	1598	347	1602	11	0
1	D	1598	347	1602	5	0
2	A	82	0	0	1	0
2	B	83	0	0	2	0
2	C	87	0	0	2	0
2	D	63	0	0	0	0
All	All	6707	1388	6411	40	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 3.

All (40) 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:186:LEU:O	1:A:190:THR:HG23	1.98	0.64
1:B:396:LEU:O	1:B:400:THR:HG23	2.01	0.60
1:C:606:LEU:O	1:C:610:THR:HG23	2.04	0.57
1:C:502:ARG:HD3	1:C:539:ILE:HD11	1.87	0.56
1:D:816:LEU:O	1:D:820:THR:HG23	2.04	0.56
1:B:331:ARG:CZ	1:B:417:ILE:HD13	2.38	0.54
1:B:261:LEU:HD11	1:B:360:GLY:HA3	1.93	0.51
1:B:234:ALA:HA	1:B:400:THR:HG22	1.94	0.49
1:C:444:ALA:HA	1:C:610:THR:HG22	1.93	0.49
1:B:302:ILE:HG13	1:B:303:PRO:HD2	1.94	0.49
1:B:395:SER:HB2	2:B:998:HOH:O	2.11	0.49
1:D:681:LEU:HD11	1:D:780:GLY:HA3	1.95	0.49
1:B:339:GLU:HG3	1:B:405:ILE:HD11	1.96	0.48
1:B:230:PRO:HG2	1:B:281:GLN:HE22	1.78	0.47
1:A:179:LYS:HG2	2:A:952:HOH:O	2.15	0.47
1:C:549:GLU:HG3	1:C:615:ILE:HD11	1.97	0.46
1:C:471:LEU:HD11	1:C:570:GLY:HA3	1.97	0.46
1:D:654:ALA:HA	1:D:820:THR:HG22	1.97	0.46
1:A:24:ALA:HA	1:A:190:THR:HG22	1.98	0.45
1:D:665:PRO:HG2	1:D:832:VAL:HG22	1.99	0.45
1:C:432:PRO:HA	2:C:912:HOH:O	2.16	0.45
1:A:207:ILE:HD12	1:A:207:ILE:HA	1.84	0.44
1:A:13:PHE:HD1	1:A:95:ASN:OD1	2.01	0.44
1:A:33:GLU:HG3	1:A:194:LYS:HD2	2.00	0.44
1:B:211:MET:HE3	1:B:213:LYS:HE3	2.00	0.43
1:B:330:LYS:HD3	1:B:419:THR:H	1.84	0.43
1:B:211:MET:O	1:B:245:PRO:HB3	2.18	0.43
1:C:600:SER:HA	2:C:897:HOH:O	2.19	0.43
1:C:447:ARG:HD2	1:C:610:THR:HG21	2.01	0.42
1:A:77:GLN:HG2	1:A:132:PRO:HB2	2.00	0.42
1:B:258:TYR:HD1	2:B:1079:HOH:O	2.02	0.42
1:D:694:ASP:C	1:D:695:ILE:HG13	2.45	0.42
1:A:119:ILE:HG21	1:A:119:ILE:HD13	1.88	0.42
1:C:449:ASN:HD22	1:C:459:VAL:HA	1.83	0.41
1:C:502:ARG:CD	1:C:539:ILE:HD11	2.49	0.41
1:C:485:ILE:HA	1:C:583:ARG:O	2.21	0.41
1:A:7:LEU:HA	1:A:67:ILE:O	2.21	0.41
1:B:243:GLU:HG3	1:B:404:LYS:HD2	2.02	0.41
1:A:92:ILE:HG13	1:A:93:PRO:HD2	2.03	0.41
1:B:239:ASN:ND2	1:B:250:SER:H	2.19	0.41

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	208/215 (97%)	203 (98%)	5 (2%)	0	100	100
1	B	208/215 (97%)	202 (97%)	5 (2%)	1 (0%)	24	21
1	C	208/215 (97%)	202 (97%)	6 (3%)	0	100	100
1	D	208/215 (97%)	201 (97%)	7 (3%)	0	100	100
All	All	832/860 (97%)	808 (97%)	23 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	GLY

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	169/174 (97%)	152 (90%)	17 (10%)	7	4
1	B	169/174 (97%)	149 (88%)	20 (12%)	5	3
1	C	169/174 (97%)	152 (90%)	17 (10%)	7	4
1	D	169/174 (97%)	149 (88%)	20 (12%)	5	3
All	All	676/696 (97%)	602 (89%)	74 (11%)	6	3

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	6	LEU
1	A	7	LEU
1	A	28	LEU
1	A	51	LEU
1	A	59	LYS
1	A	75	ARG
1	A	83	VAL
1	A	85	ILE
1	A	87	LEU
1	A	91	ARG
1	A	131	ILE
1	A	135	VAL
1	A	168	HIS
1	A	177	LEU
1	A	193	LEU
1	B	216	LEU
1	B	217	LEU
1	B	226	GLU
1	B	227	THR
1	B	228	VAL
1	B	238	LEU
1	B	261	LEU
1	B	269	LYS
1	B	285	ARG
1	B	293	VAL
1	B	295	ILE
1	B	297	LEU
1	B	301	ARG
1	B	341	ILE
1	B	345	VAL
1	B	348	THR
1	B	378	HIS
1	B	387	LEU
1	B	403	LEU
1	B	417	ILE
1	C	426	LEU
1	C	433	PHE
1	C	437	THR
1	C	440	PRO
1	C	448	LEU
1	C	471	LEU

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Mol	Chain	Res	Type
1	C	479	LYS
1	C	495	ARG
1	C	503	VAL
1	C	505	ILE
1	C	507	LEU
1	C	511	ARG
1	C	551	ILE
1	C	555	VAL
1	C	588	HIS
1	C	597	LEU
1	C	613	LEU
1	D	631	MET
1	D	634	LYS
1	D	636	LEU
1	D	637	LEU
1	D	647	THR
1	D	650	PRO
1	D	658	LEU
1	D	681	LEU
1	D	689	LYS
1	D	705	ARG
1	D	713	VAL
1	D	715	ILE
1	D	717	LEU
1	D	721	ARG
1	D	761	ILE
1	D	765	VAL
1	D	786	SER
1	D	798	HIS
1	D	807	LEU
1	D	823	LEU

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	29	ASN
1	A	42	GLN
1	A	77	GLN
1	A	107	GLN
1	A	159	HIS
1	B	239	ASN
1	B	252	GLN

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Mol	Chain	Res	Type
1	B	272	GLN
1	B	317	GLN
1	C	449	ASN
1	C	462	GLN
1	C	527	GLN
1	D	659	ASN
1	D	737	GLN

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 ⓘ

There are no ligands in this entry.

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	210/215 (97%)	-0.22	7 (3%) 49 48	2, 11, 27, 49	0
1	B	210/215 (97%)	-0.08	12 (5%) 29 28	3, 12, 34, 50	0
1	C	210/215 (97%)	-0.18	5 (2%) 59 59	3, 10, 33, 47	0
1	D	210/215 (97%)	-0.11	9 (4%) 40 39	3, 11, 33, 59	0
All	All	840/860 (97%)	-0.15	33 (3%) 43 42	2, 11, 34, 59	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	840	GLY	6.9
1	D	631	MET	4.7
1	B	224	GLY	4.4
1	B	225	GLY	4.3
1	D	839	THR	3.5
1	D	737	GLN	3.4
1	C	629	THR	3.4
1	B	419	THR	3.3
1	C	630	GLY	3.3
1	C	527	GLN	3.3
1	B	223	PHE	3.3
1	A	1	MET	3.2
1	D	644	GLY	3.1
1	A	209	THR	2.9
1	A	91	ARG	2.9
1	A	107	GLN	2.8
1	D	808	GLN	2.8
1	B	222	PRO	2.8
1	D	837	ILE	2.7
1	B	420	GLY	2.7
1	A	179	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	210	GLY	2.5
1	B	269	LYS	2.5
1	B	227	THR	2.4
1	B	417	ILE	2.4
1	B	317	GLN	2.3
1	B	301	ARG	2.3
1	C	433	PHE	2.2
1	C	528	GLY	2.2
1	A	178	GLN	2.2
1	D	721	ARG	2.2
1	B	228	VAL	2.1
1	D	692	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.