



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:50 PM UTC

PDB ID : 8R6Z / pdb_00008r6z
Title : Polysaccharide lyase BtPL33HA (BT4410) Apo form 2
Authors : Cartmell, A.
Deposited on : 2023-11-23
Resolution : 2.03 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)	:	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

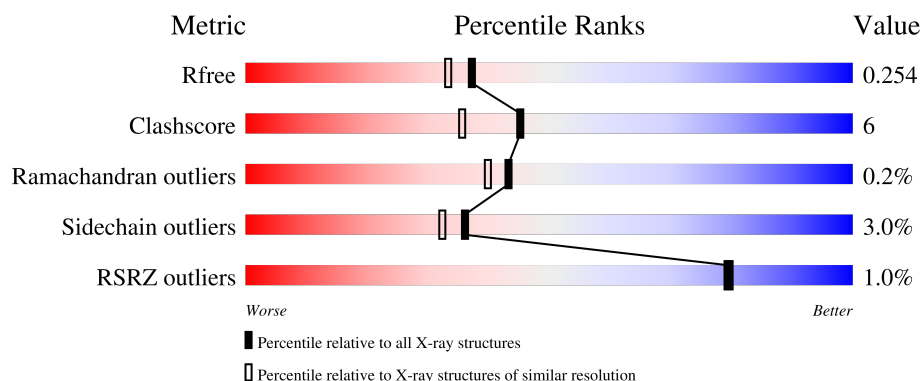
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	644	2% 73% 17% • • 6%
1	B	644	77% 15% • • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10158 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 Heparinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	616	Total	C	N	O	S	0	0	0
			4961	3159	845	923	34			
1	A	604	Total	C	N	O	S	0	1	0
			4862	3095	828	905	34			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q89ZG7
B	2	GLY	-	expression tag	UNP Q89ZG7
B	3	SER	-	expression tag	UNP Q89ZG7
B	4	SER	-	expression tag	UNP Q89ZG7
B	5	HIS	-	expression tag	UNP Q89ZG7
B	6	HIS	-	expression tag	UNP Q89ZG7
B	7	HIS	-	expression tag	UNP Q89ZG7
B	8	HIS	-	expression tag	UNP Q89ZG7
B	9	HIS	-	expression tag	UNP Q89ZG7
B	10	HIS	-	expression tag	UNP Q89ZG7
B	11	SER	-	expression tag	UNP Q89ZG7
B	12	SER	-	expression tag	UNP Q89ZG7
B	13	GLY	-	expression tag	UNP Q89ZG7
B	14	LEU	-	expression tag	UNP Q89ZG7
B	15	VAL	-	expression tag	UNP Q89ZG7
B	16	PRO	-	expression tag	UNP Q89ZG7
B	17	ARG	-	expression tag	UNP Q89ZG7
B	18	GLY	-	expression tag	UNP Q89ZG7
B	19	SER	-	expression tag	UNP Q89ZG7
B	20	HIS	-	expression tag	UNP Q89ZG7
B	21	MET	-	expression tag	UNP Q89ZG7
B	22	ALA	-	expression tag	UNP Q89ZG7
B	23	SER	-	expression tag	UNP Q89ZG7
A	1	MET	-	initiating methionine	UNP Q89ZG7
A	2	GLY	-	expression tag	UNP Q89ZG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	-	expression tag	UNP Q89ZG7
A	4	SER	-	expression tag	UNP Q89ZG7
A	5	HIS	-	expression tag	UNP Q89ZG7
A	6	HIS	-	expression tag	UNP Q89ZG7
A	7	HIS	-	expression tag	UNP Q89ZG7
A	8	HIS	-	expression tag	UNP Q89ZG7
A	9	HIS	-	expression tag	UNP Q89ZG7
A	10	HIS	-	expression tag	UNP Q89ZG7
A	11	SER	-	expression tag	UNP Q89ZG7
A	12	SER	-	expression tag	UNP Q89ZG7
A	13	GLY	-	expression tag	UNP Q89ZG7
A	14	LEU	-	expression tag	UNP Q89ZG7
A	15	VAL	-	expression tag	UNP Q89ZG7
A	16	PRO	-	expression tag	UNP Q89ZG7
A	17	ARG	-	expression tag	UNP Q89ZG7
A	18	GLY	-	expression tag	UNP Q89ZG7
A	19	SER	-	expression tag	UNP Q89ZG7
A	20	HIS	-	expression tag	UNP Q89ZG7
A	21	MET	-	expression tag	UNP Q89ZG7
A	22	ALA	-	expression tag	UNP Q89ZG7
A	23	SER	-	expression tag	UNP Q89ZG7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

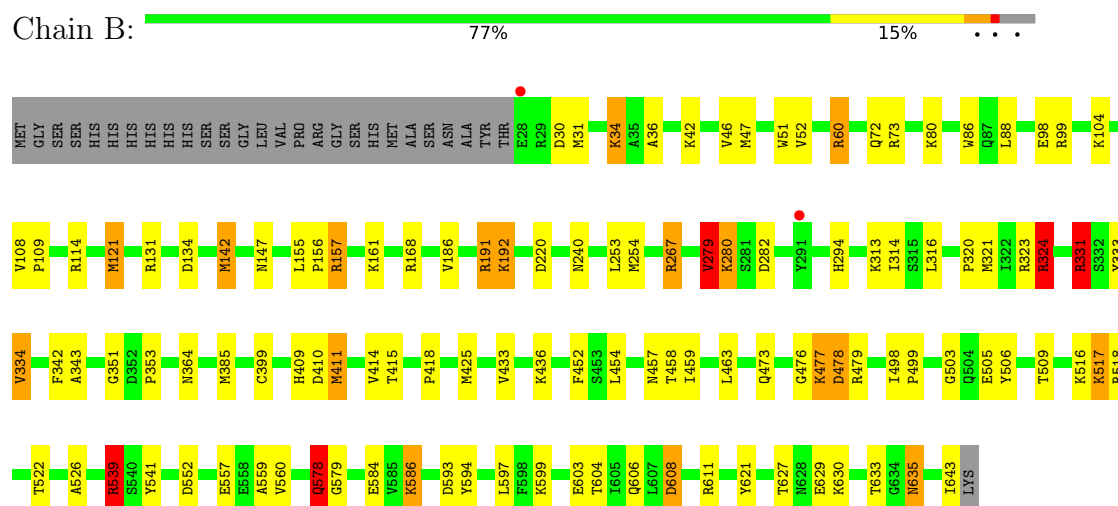
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	215	Total O 215 215	0	0
3	A	118	Total O 118 118	0	0

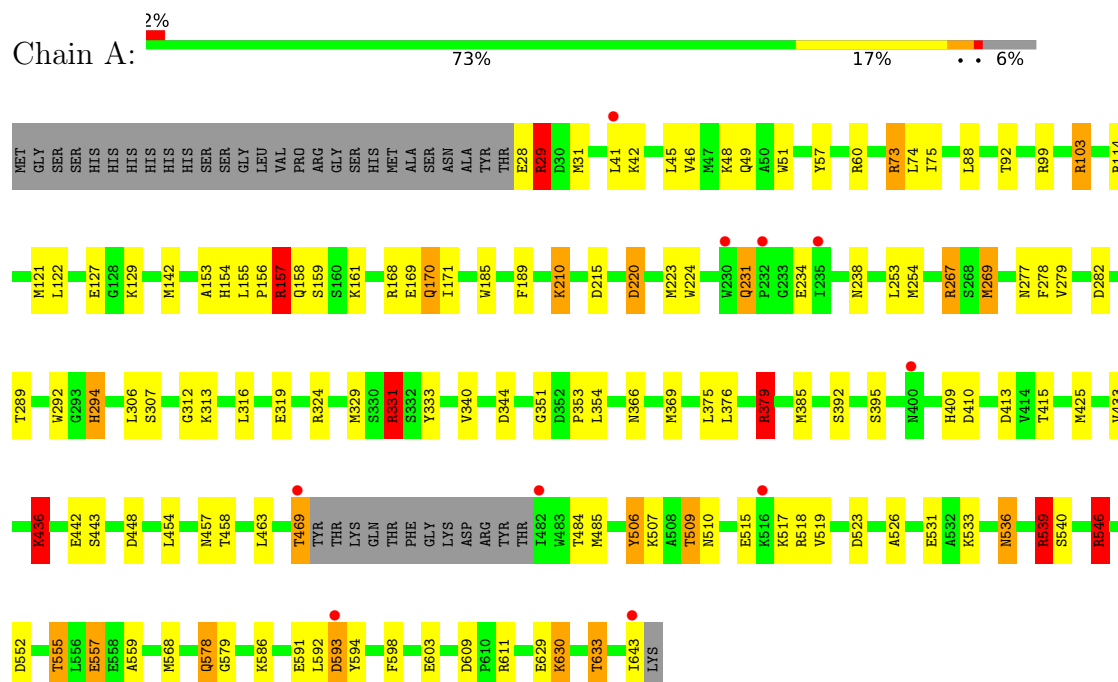
3 Residue-property plots

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: Heparinase



• Molecule 1: Heparinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.53Å 137.67Å 202.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.85 – 2.03 113.85 – 2.03	Depositor EDS
% Data completeness (in resolution range)	75.0 (113.85-2.03) 75.1 (113.85-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.191 , 0.251 0.198 , 0.254	Depositor DCC
R_{free} test set	3607 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10158	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

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

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	1.00	1/4980 (0.0%)	1.53	51/6741 (0.8%)
1	B	1.07	7/5083 (0.1%)	1.57	62/6880 (0.9%)
All	All	1.03	8/10063 (0.1%)	1.55	113/13621 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	12
All	All	0	23

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	611	ARG	NE-CZ	7.79	1.41	1.33
1	B	240	ASN	C-O	-6.64	1.18	1.24
1	A	643	ILE	CB-CG1	5.99	1.65	1.53
1	B	418	PRO	C-O	-5.52	1.17	1.24
1	B	334	VAL	C-O	-5.39	1.18	1.24
1	B	593	ASP	CG-OD1	5.31	1.35	1.25
1	B	80	LYS	C-O	-5.21	1.17	1.24
1	B	147	ASN	C-O	-5.09	1.17	1.24

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	539	ARG	CD-NE-CZ	12.23	141.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	MET	CG-SD-CE	-11.89	74.74	100.90
1	A	539	ARG	CD-NE-CZ	11.54	140.56	124.40
1	B	539	ARG	NE-CZ-NH2	-11.32	109.01	119.20
1	B	324	ARG	NE-CZ-NH2	-10.64	109.62	119.20
1	A	282	ASP	CA-CB-CG	8.68	121.28	112.60
1	A	269	MET	CG-SD-CE	-8.56	82.07	100.90
1	A	267	ARG	NE-CZ-NH2	-8.38	111.66	119.20
1	A	294	HIS	CA-CB-CG	-8.36	105.44	113.80
1	A	539	ARG	NE-CZ-NH2	-8.28	111.75	119.20
1	A	42	LYS	N-CA-CB	-8.03	97.86	110.22
1	A	92	THR	CA-CB-OG1	-8.02	97.58	109.60
1	B	282	ASP	CA-CB-CG	7.77	120.37	112.60
1	B	324	ARG	CD-NE-CZ	7.71	135.20	124.40
1	B	633	THR	CA-CB-OG1	-7.71	98.03	109.60
1	A	568	MET	CG-SD-CE	-7.58	84.22	100.90
1	B	539	ARG	NE-CZ-NH1	7.56	129.06	121.50
1	A	598	PHE	CB-CA-C	-7.33	95.97	109.37
1	A	633	THR	CA-CB-OG1	-7.31	98.64	109.60
1	B	121	MET	CG-SD-CE	-7.24	84.97	100.90
1	A	515	GLU	CB-CG-CD	7.22	124.88	112.60
1	B	60	ARG	CD-NE-CZ	7.09	134.32	124.40
1	B	629	GLU	CB-CA-C	-7.08	96.52	109.54
1	B	34	LYS	N-CA-CB	7.07	120.62	110.16
1	B	578	GLN	CB-CA-C	-7.01	97.08	109.62
1	A	603	GLU	CB-CA-C	6.91	121.67	109.72
1	B	324	ARG	NE-CZ-NH1	6.86	128.36	121.50
1	B	604	THR	CA-CB-OG1	-6.85	99.32	109.60
1	B	134	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	46	VAL	N-CA-CB	-6.71	103.36	111.21
1	A	598	PHE	N-CA-CB	6.70	121.56	110.85
1	B	294	HIS	CA-CB-CG	-6.66	107.14	113.80
1	B	364	ASN	CB-CA-C	-6.54	102.60	111.89
1	A	231	GLN	CB-CA-C	-6.52	99.10	108.88
1	A	157	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	A	170	GLN	N-CA-CB	-6.45	99.64	110.80
1	B	267	ARG	NE-CZ-NH2	-6.43	113.42	119.20
1	A	340	VAL	CA-C-O	-6.39	113.75	121.04
1	B	192	LYS	CD-CE-NZ	6.36	132.25	111.90
1	A	586	LYS	CB-CA-C	6.36	123.07	110.42
1	A	630	LYS	N-CA-CB	-6.33	100.21	110.71
1	B	73	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	A	73	ARG	N-CA-CB	-6.22	101.05	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	LEU	N-CA-CB	-6.19	100.86	109.97
1	A	410	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	506	TYR	CB-CA-C	6.13	121.40	111.05
1	B	578	GLN	CA-C-O	-6.12	115.06	121.55
1	A	510	ASN	CB-CA-C	-6.10	103.07	111.73
1	B	42	LYS	CB-CA-C	-6.02	99.50	110.63
1	B	603	GLU	CB-CA-C	5.98	120.06	109.72
1	B	331	ARG	CG-CD-NE	5.97	125.14	112.00
1	A	319	GLU	CG-CD-OE1	-5.96	104.69	118.40
1	B	584	GLU	CB-CG-CD	-5.94	102.50	112.60
1	B	578	GLN	CA-C-N	5.93	132.37	121.70
1	B	578	GLN	C-N-CA	5.93	132.37	121.70
1	A	484	THR	CA-CB-OG1	-5.91	100.74	109.60
1	A	279	VAL	N-CA-CB	5.88	121.14	111.38
1	A	220	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	240	ASN	O-C-N	-5.77	116.29	120.27
1	A	586	LYS	N-CA-CB	-5.77	100.74	110.49
1	B	168	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	A	46	VAL	N-CA-CB	-5.76	104.47	111.21
1	A	99	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	B	99	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	B	635	ASN	CA-CB-CG	-5.72	106.88	112.60
1	B	313	LYS	CA-CB-CG	-5.67	102.76	114.10
1	B	643	ILE	CA-C-O	-5.66	111.18	120.80
1	A	42	LYS	CB-CA-C	5.66	121.10	110.63
1	B	34	LYS	CB-CG-CD	5.64	124.26	111.30
1	B	411	MET	CG-SD-CE	-5.63	88.51	100.90
1	B	606	GLN	CB-CA-C	5.59	118.21	110.16
1	B	220	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	103	ARG	CA-CB-CG	5.58	125.25	114.10
1	B	509	THR	OG1-CB-CG2	-5.56	98.17	109.30
1	B	399	CYS	N-CA-CB	5.55	118.06	110.01
1	A	540	SER	CA-CB-OG	-5.55	100.00	111.10
1	A	142	MET	CG-SD-CE	-5.54	88.71	100.90
1	B	73	ARG	N-CA-CB	-5.54	101.98	110.12
1	A	168	ARG	CD-NE-CZ	5.52	132.13	124.40
1	B	52	VAL	N-CA-CB	5.52	115.22	110.08
1	A	442	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	88	LEU	N-CA-CB	-5.48	101.35	110.23
1	B	608	ASP	CB-CA-C	-5.46	99.23	110.38
1	A	436	LYS	CG-CD-CE	5.44	123.82	111.30
1	A	557	GLU	CB-CA-C	-5.41	102.35	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	GLU	N-CA-CB	5.41	118.45	110.56
1	B	611	ARG	CG-CD-NE	5.40	123.87	112.00
1	A	57	TYR	N-CA-CB	-5.39	101.97	110.06
1	B	503	GLY	CA-C-N	5.34	128.84	120.82
1	B	503	GLY	C-N-CA	5.34	128.84	120.82
1	B	98	GLU	N-CA-CB	5.32	118.50	110.30
1	A	103	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	531	GLU	N-CA-CB	5.27	119.26	110.41
1	B	478	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	279	VAL	N-CA-CB	-5.21	100.30	110.45
1	B	586	LYS	CB-CG-CD	5.18	123.23	111.30
1	A	278	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	523	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	280	LYS	N-CA-CB	5.17	118.15	110.29
1	B	476	GLY	CA-C-O	-5.14	117.17	122.26
1	A	586	LYS	CB-CG-CD	5.13	123.10	111.30
1	B	191	ARG	CG-CD-NE	-5.12	100.74	112.00
1	B	557	GLU	CB-CG-CD	5.11	121.28	112.60
1	A	267	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	B	516	LYS	N-CA-CB	5.08	117.68	110.16
1	A	289	THR	OG1-CB-CG2	5.08	119.46	109.30
1	A	331	ARG	CG-CD-NE	5.07	123.15	112.00
1	A	220	ASP	CB-CA-C	5.06	118.89	110.74
1	B	522	THR	CA-CB-OG1	-5.05	102.02	109.60
1	B	627	THR	CA-CB-OG1	-5.05	102.02	109.60
1	A	593	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	267	ARG	NE-CZ-NH1	5.01	126.51	121.50
1	B	557	GLU	N-CA-CB	5.01	117.55	110.13

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	267	ARG	Sidechain
1	A	29	ARG	Sidechain
1	A	324	ARG	Sidechain
1	A	331	ARG	Sidechain
1	A	379	ARG	Sidechain
1	A	539	ARG	Sidechain
1	A	546	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	578	GLN	Peptide
1	A	60	ARG	Sidechain
1	B	114	ARG	Sidechain
1	B	131	ARG	Sidechain
1	B	157	ARG	Sidechain
1	B	191	ARG	Sidechain
1	B	267	ARG	Sidechain
1	B	323	ARG	Sidechain
1	B	324	ARG	Sidechain
1	B	331	ARG	Sidechain
1	B	518	ARG	Sidechain
1	B	539	ARG	Sidechain
1	B	578	GLN	Peptide
1	B	60	ARG	Sidechain

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	4862	0	4754	74	0
1	B	4961	0	4851	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	118	0	0	5	0
3	B	215	0	0	5	0
All	All	10158	0	9605	115	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 6.

All (115) 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:121:MET:HE1	1:A:185:TRP:HB3	1.41	0.98
1:B:31:MET:HE3	1:B:316:LEU:HD13	1.50	0.90
1:B:254:MET:HE1	3:B:889:HOH:O	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HG2	1:A:28:GLU:O	1.77	0.84
1:B:31:MET:CE	1:B:316:LEU:HD13	2.08	0.82
1:A:254:MET:CE	3:A:901:HOH:O	2.32	0.77
1:A:385:MET:HE2	3:A:829:HOH:O	1.85	0.77
1:A:74:LEU:HD23	1:A:385:MET:HE1	1.70	0.73
1:A:28:GLU:O	1:A:28:GLU:CG	2.38	0.72
1:A:436:LYS:HE3	1:A:448:ASP:OD1	1.90	0.71
1:A:121:MET:HE2	1:A:189:PHE:HD2	1.58	0.68
1:A:536:ASN:ND2	1:A:555:THR:OG1	2.26	0.68
1:B:86:TRP:HB3	1:B:142:MET:HE3	1.76	0.68
1:B:539:ARG:HD3	1:B:552:ASP:OD1	1.93	0.68
1:A:121:MET:HE2	1:A:189:PHE:CD2	2.29	0.68
1:A:539:ARG:HD3	1:A:552:ASP:OD1	1.94	0.68
1:A:611:ARG:NH2	1:A:611:ARG:HG2	2.09	0.67
1:A:254:MET:HE1	3:A:901:HOH:O	1.91	0.66
1:B:254:MET:CE	3:B:889:HOH:O	2.36	0.66
1:B:459:ILE:HD13	1:B:586:LYS:HB2	1.79	0.65
1:A:292:TRP:CD2	1:A:329:MET:HG2	2.34	0.62
1:A:31:MET:HE3	1:A:316:LEU:HD13	1.82	0.61
1:A:331:ARG:HG3	1:A:415:THR:HG21	1.83	0.61
1:B:608:ASP:OD1	1:A:517:LYS:NZ	2.35	0.59
1:A:269:MET:HE2	1:A:306:LEU:HD21	1.86	0.57
1:A:559:ALA:HB1	1:A:630:LYS:HG2	1.86	0.57
1:A:333:TYR:O	1:A:409:HIS:HE1	1.89	0.56
1:B:331:ARG:HG3	1:B:415:THR:HG21	1.89	0.55
1:A:313:LYS:HA	1:A:313:LYS:HE2	1.88	0.55
1:B:463:LEU:C	1:B:463:LEU:HD12	2.32	0.54
1:B:517:LYS:N	1:B:517:LYS:HD2	2.23	0.54
1:A:254:MET:HE2	3:A:901:HOH:O	2.01	0.53
1:A:171:ILE:HA	1:A:223:MET:HE2	1.91	0.53
1:B:559:ALA:HB1	1:B:630:LYS:HG2	1.90	0.53
1:B:155:LEU:N	1:B:156:PRO:CD	2.72	0.53
1:B:279:VAL:HG12	1:B:321:MET:HE3	1.91	0.52
1:A:579:GLY:HA2	1:A:594:TYR:CZ	2.45	0.51
1:A:506:TYR:HA	1:A:526:ALA:O	2.09	0.51
1:B:157:ARG:HD2	3:B:1007:HOH:O	2.10	0.51
1:A:74:LEU:CD2	1:A:385:MET:HE1	2.39	0.51
1:B:579:GLY:HA2	1:B:594:TYR:CZ	2.45	0.51
1:A:463:LEU:C	1:A:463:LEU:HD12	2.35	0.51
1:B:333:TYR:O	1:B:409:HIS:HE1	1.94	0.50
1:A:48:LYS:O	1:A:49:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:O	1:A:45:LEU:HG	2.11	0.50
1:A:509:THR:HG23	3:A:844:HOH:O	2.11	0.50
1:A:122:LEU:HD11	1:A:392:SER:HB3	1.94	0.49
1:A:155:LEU:N	1:A:156:PRO:CD	2.74	0.49
1:A:425:MET:HE2	1:A:518:ARG:HA	1.94	0.49
1:A:425:MET:HE1	1:A:519:VAL:N	2.28	0.49
1:A:103:ARG:HG2	1:A:153:ALA:HB2	1.94	0.49
1:B:72:GLN:HG3	3:B:825:HOH:O	2.13	0.48
1:A:121:MET:HE1	1:A:185:TRP:CB	2.30	0.48
1:B:36:ALA:CB	1:B:314:ILE:HD13	2.44	0.48
1:B:253:LEU:O	1:B:254:MET:HE2	2.14	0.47
1:A:159:SER:HB2	1:A:169:GLU:OE1	2.15	0.47
1:A:171:ILE:HA	1:A:223:MET:CE	2.45	0.47
1:A:536:ASN:HD22	1:A:555:THR:HG1	1.61	0.47
1:B:506:TYR:HA	1:B:526:ALA:O	2.15	0.47
1:A:517:LYS:HB2	1:A:519:VAL:HG23	1.97	0.47
1:A:292:TRP:CD2	1:A:329:MET:CG	2.97	0.47
1:A:611:ARG:HG2	1:A:611:ARG:HH21	1.79	0.47
1:A:533:LYS:HB3	1:A:557:GLU:HB2	1.97	0.46
1:B:433:VAL:HG22	1:B:454:LEU:HD13	1.95	0.46
1:B:253:LEU:C	1:B:254:MET:HE2	2.41	0.46
1:A:127:GLU:HG2	1:A:129:LYS:HG3	1.98	0.46
1:A:253:LEU:O	1:A:254:MET:HE2	2.16	0.46
1:B:473:GLN:O	1:B:479:ARG:HA	2.16	0.46
1:B:121:MET:HE3	1:B:186:VAL:HG22	1.99	0.45
1:B:414:VAL:HG22	1:B:425:MET:HG2	1.98	0.45
1:A:436:LYS:HE3	1:A:448:ASP:CG	2.42	0.45
1:B:498:ILE:HG23	1:B:499:PRO:HD2	1.98	0.45
1:B:30:ASP:O	1:B:34:LYS:HG2	2.18	0.44
1:A:29:ARG:HD3	1:A:277:ASN:HA	1.99	0.44
1:A:155:LEU:O	1:A:158:GLN:HG2	2.17	0.44
1:A:354:LEU:HD23	1:A:395:SER:HB2	1.98	0.44
1:A:469:THR:HG23	1:A:611:ARG:HH21	1.82	0.44
1:B:351:GLY:O	1:B:353:PRO:HD3	2.18	0.44
1:B:108:VAL:N	1:B:109:PRO:HD2	2.32	0.44
1:B:342:PHE:O	1:B:343:ALA:HB3	2.17	0.44
1:A:376:LEU:O	1:A:379:ARG:HD2	2.18	0.44
1:B:47:MET:HE3	3:B:824:HOH:O	2.17	0.44
1:B:156:PRO:O	1:B:161:LYS:HA	2.17	0.44
1:A:413:ASP:O	1:A:425:MET:HA	2.18	0.44
1:A:220:ASP:OD2	1:A:223:MET:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLN:HB3	1:A:234:GLU:HG3	1.99	0.43
1:A:292:TRP:CE3	1:A:329:MET:HG3	2.53	0.43
1:B:457:ASN:C	1:B:458:THR:HG23	2.44	0.43
1:B:51:TRP:H	1:B:51:TRP:CD1	2.36	0.43
1:A:433:VAL:HG22	1:A:454:LEU:HD13	2.00	0.43
1:A:154:HIS:C	1:A:156:PRO:HD2	2.44	0.43
1:A:351:GLY:O	1:A:353:PRO:HD3	2.18	0.43
1:A:307:SER:OG	1:A:312:GLY:HA2	2.18	0.43
1:A:210:LYS:HD2	1:A:215:ASP:CG	2.44	0.42
1:A:507:LYS:O	1:A:526:ALA:HB3	2.20	0.42
1:B:452:PHE:CD1	1:B:541:TYR:CE1	3.08	0.42
1:B:477:LYS:O	1:B:478:ASP:HB2	2.18	0.42
1:A:157:ARG:HH11	1:A:224:TRP:HE1	1.67	0.42
1:A:292:TRP:CG	1:A:329:MET:HG2	2.54	0.42
1:A:75:ILE:HG12	1:A:127:GLU:HB2	2.01	0.42
1:B:334:VAL:HG12	1:B:458:THR:HA	2.02	0.42
1:B:320:PRO:HB2	1:B:324:ARG:HH22	1.85	0.41
1:B:477:LYS:O	1:B:478:ASP:CB	2.67	0.41
1:A:469:THR:N	1:A:609:ASP:OD2	2.53	0.41
1:A:51:TRP:CD1	1:A:51:TRP:H	2.39	0.41
1:A:591:GLU:OE2	1:A:593:ASP:OD1	2.38	0.41
1:A:457:ASN:C	1:A:458:THR:HG23	2.46	0.41
1:A:592:LEU:C	1:A:592:LEU:HD23	2.46	0.41
1:B:410:ASP:O	1:B:411:MET:HB3	2.21	0.41
1:B:621:TYR:OH	1:A:546:ARG:HD2	2.21	0.40
1:A:156:PRO:O	1:A:161:LYS:HA	2.21	0.40
1:A:269:MET:CE	1:A:306:LEU:HD11	2.51	0.40
1:A:238:ASN:HB2	1:A:294:HIS:O	2.20	0.40
1:B:552:ASP:O	1:B:635:ASN:HA	2.21	0.40
1:A:366:ASN:HA	1:A:369:MET:HE3	2.03	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	601/644 (93%)	580 (96%)	21 (4%)	0	100	100
1	B	614/644 (95%)	593 (97%)	19 (3%)	2 (0%)	36	31
All	All	1215/1288 (94%)	1173 (96%)	40 (3%)	2 (0%)	43	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	597	LEU
1	B	385	MET

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	519/552 (94%)	499 (96%)	20 (4%)	28	22
1	B	529/552 (96%)	518 (98%)	11 (2%)	47	47
All	All	1048/1104 (95%)	1017 (97%)	31 (3%)	36	32

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	LYS
1	B	192	LYS
1	B	279	VAL
1	B	280	LYS
1	B	331	ARG
1	B	436	LYS
1	B	477	LYS
1	B	517	LYS
1	B	560	VAL
1	B	578	GLN
1	B	599	LYS

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Mol	Chain	Res	Type
1	A	29	ARG
1	A	73	ARG
1	A	157	ARG
1	A	170	GLN
1	A	210	LYS
1	A	331	ARG
1	A	344	ASP
1	A	375	LEU
1	A	379	ARG
1	A	436	LYS
1	A	443	SER
1	A	469	THR
1	A	485	MET
1	A	509	THR
1	A	536	ASN
1	A	546	ARG
1	A	555	THR
1	A	578	GLN
1	A	629	GLU
1	A	633	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	GLN
1	B	115	GLN
1	B	204	GLN
1	B	231	GLN
1	B	256	ASN
1	B	294	HIS
1	B	409	HIS
1	B	510	ASN
1	A	348	GLN
1	A	394	GLN
1	A	409	HIS
1	A	486	GLN
1	A	536	ASN
1	A	582	GLN
1	A	641	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](#)

Of 2 ligands modelled in this entry, 2 are 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 [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 [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	604/644 (93%)	0.13	10 (1%) 69 69	15, 35, 57, 74	1 (0%)
1	B	616/644 (95%)	-0.20	2 (0%) 90 90	15, 26, 47, 86	0
All	All	1220/1288 (94%)	-0.04	12 (0%) 79 80	15, 30, 55, 86	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	ILE	4.0
1	A	232	PRO	3.7
1	A	643	ILE	3.7
1	A	235	ILE	3.2
1	A	469	THR	3.1
1	B	28	GLU	2.9
1	B	291	TYR	2.7
1	A	230	TRP	2.6
1	A	400	ASN	2.2
1	A	593	ASP	2.2
1	A	516	LYS	2.1
1	A	41	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	701	1/1	0.99	0.04	32,32,32,32	0
2	ZN	B	701	1/1	1.00	0.01	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.