



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:55 PM UTC

PDB ID : 3RO8 / pdb_00003ro8
Title : Crystal structure of the catalytic domain of XynA1 from Paenibacillus sp. JDR-2
Authors : Pozharski, E.; St John, F.J.
Deposited on : 2011-04-25
Resolution : 1.34 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

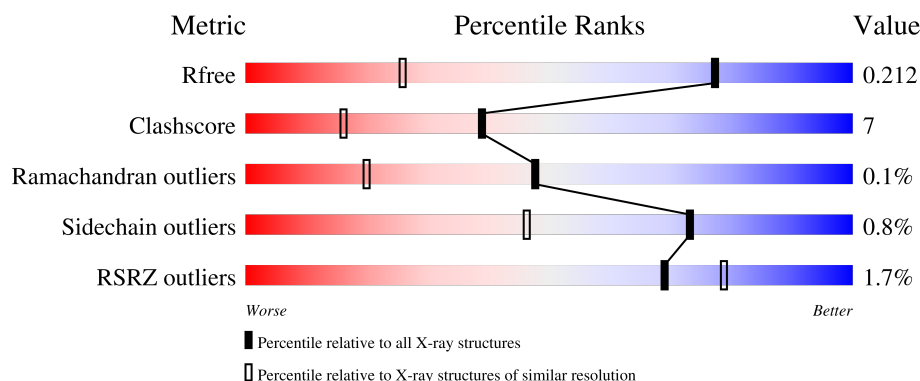
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.34 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	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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	341	2% 73% 15% • 11%
1	B	341	% 78% 11% 11%
1	C	341	% 78% 9% • 11%
1	D	341	% 78% 10% 12%
1	E	341	% 77% 11% 12%

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Mol	Chain	Length	Quality of chain
1	F	341	% 78% 11% 11%
1	G	341	2% 76% 13% 11%
1	H	341	2% 79% 10% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23733 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	19	0
			2575	1626	442	496	11			
1	B	304	Total	C	N	O	S	0	17	0
			2571	1625	444	489	13			
1	C	302	Total	C	N	O	S	0	14	0
			2507	1582	432	481	12			
1	D	301	Total	C	N	O	S	0	17	0
			2530	1594	438	486	12			
1	E	301	Total	C	N	O	S	0	16	0
			2530	1594	439	486	11			
1	F	304	Total	C	N	O	S	0	18	0
			2575	1622	447	494	12			
1	G	304	Total	C	N	O	S	0	13	0
			2527	1592	438	486	11			
1	H	304	Total	C	N	O	S	0	20	0
			2585	1629	446	498	12			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP C6CRV0
A	2	SER	-	expression tag	UNP C6CRV0
A	3	HIS	-	expression tag	UNP C6CRV0
A	4	MET	-	expression tag	UNP C6CRV0
A	339	ALA	-	expression tag	UNP C6CRV0
A	340	GLU	-	expression tag	UNP C6CRV0
A	341	GLN	-	expression tag	UNP C6CRV0
B	1	GLY	-	expression tag	UNP C6CRV0
B	2	SER	-	expression tag	UNP C6CRV0
B	3	HIS	-	expression tag	UNP C6CRV0
B	4	MET	-	expression tag	UNP C6CRV0
B	339	ALA	-	expression tag	UNP C6CRV0
B	340	GLU	-	expression tag	UNP C6CRV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	341	GLN	-	expression tag	UNP C6CRV0
C	1	GLY	-	expression tag	UNP C6CRV0
C	2	SER	-	expression tag	UNP C6CRV0
C	3	HIS	-	expression tag	UNP C6CRV0
C	4	MET	-	expression tag	UNP C6CRV0
C	339	ALA	-	expression tag	UNP C6CRV0
C	340	GLU	-	expression tag	UNP C6CRV0
C	341	GLN	-	expression tag	UNP C6CRV0
D	1	GLY	-	expression tag	UNP C6CRV0
D	2	SER	-	expression tag	UNP C6CRV0
D	3	HIS	-	expression tag	UNP C6CRV0
D	4	MET	-	expression tag	UNP C6CRV0
D	339	ALA	-	expression tag	UNP C6CRV0
D	340	GLU	-	expression tag	UNP C6CRV0
D	341	GLN	-	expression tag	UNP C6CRV0
E	1	GLY	-	expression tag	UNP C6CRV0
E	2	SER	-	expression tag	UNP C6CRV0
E	3	HIS	-	expression tag	UNP C6CRV0
E	4	MET	-	expression tag	UNP C6CRV0
E	339	ALA	-	expression tag	UNP C6CRV0
E	340	GLU	-	expression tag	UNP C6CRV0
E	341	GLN	-	expression tag	UNP C6CRV0
F	1	GLY	-	expression tag	UNP C6CRV0
F	2	SER	-	expression tag	UNP C6CRV0
F	3	HIS	-	expression tag	UNP C6CRV0
F	4	MET	-	expression tag	UNP C6CRV0
F	339	ALA	-	expression tag	UNP C6CRV0
F	340	GLU	-	expression tag	UNP C6CRV0
F	341	GLN	-	expression tag	UNP C6CRV0
G	1	GLY	-	expression tag	UNP C6CRV0
G	2	SER	-	expression tag	UNP C6CRV0
G	3	HIS	-	expression tag	UNP C6CRV0
G	4	MET	-	expression tag	UNP C6CRV0
G	339	ALA	-	expression tag	UNP C6CRV0
G	340	GLU	-	expression tag	UNP C6CRV0
G	341	GLN	-	expression tag	UNP C6CRV0
H	1	GLY	-	expression tag	UNP C6CRV0
H	2	SER	-	expression tag	UNP C6CRV0
H	3	HIS	-	expression tag	UNP C6CRV0
H	4	MET	-	expression tag	UNP C6CRV0
H	339	ALA	-	expression tag	UNP C6CRV0
H	340	GLU	-	expression tag	UNP C6CRV0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	341	GLN	-	expression tag	UNP C6CRV0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	1	Total Mg 2 2	0	1
2	D	1	Total Mg 1 1	0	0
2	E	2	Total Mg 2 2	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	1
3	B	1	Total Cl 1 1	0	1
3	C	1	Total Cl 1 1	0	1
3	D	1	Total Cl 1 1	0	1
3	E	2	Total Cl 2 2	0	1
3	F	1	Total Cl 1 1	0	1
3	G	1	Total Cl 1 1	0	1
3	H	1	Total Cl 1 1	0	1

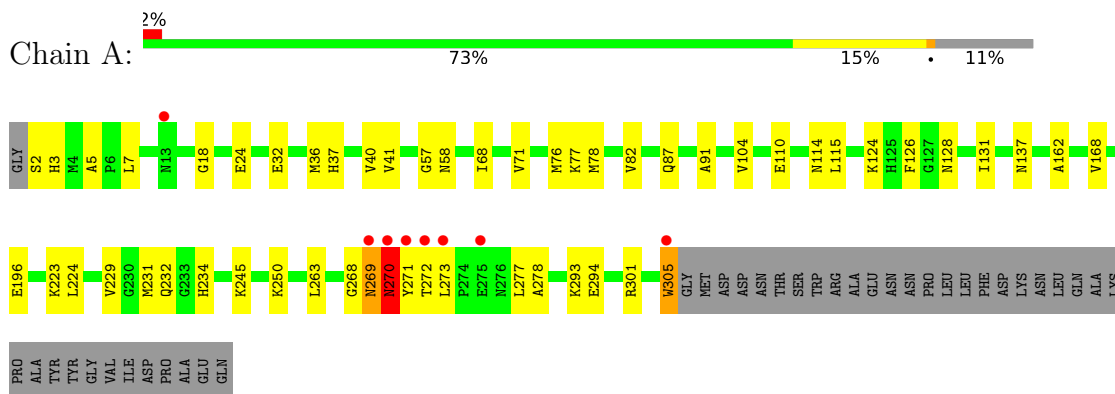
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	431	Total 431	O 431	0	0
4	B	447	Total 447	O 447	0	0
4	C	453	Total 453	O 453	0	0
4	D	400	Total 400	O 400	0	0
4	E	407	Total 407	O 407	0	0
4	F	429	Total 429	O 429	0	0
4	G	392	Total 392	O 392	0	0
4	H	353	Total 353	O 353	0	0

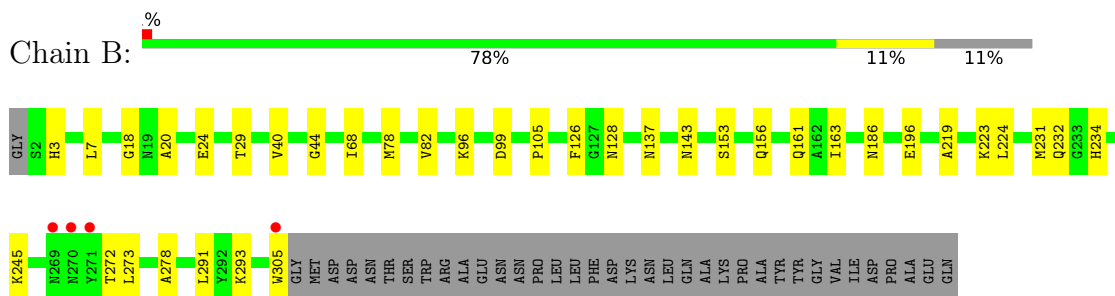
3 Residue-property plots [i](#)

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 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.

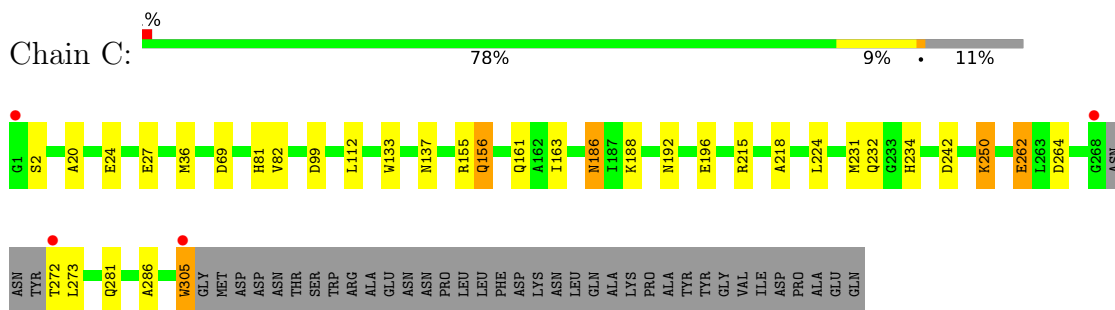
- Molecule 1: Endo-1,4-beta-xylanase



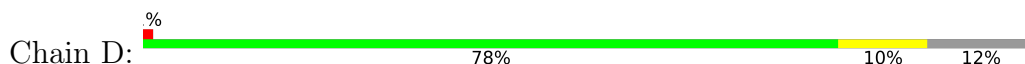
- Molecule 1: Endo-1,4-beta-xylanase

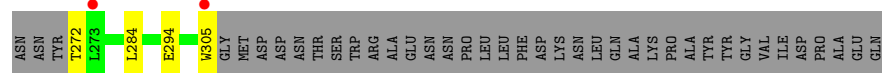


- Molecule 1: Endo-1,4-beta-xylanase

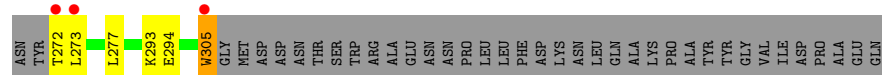
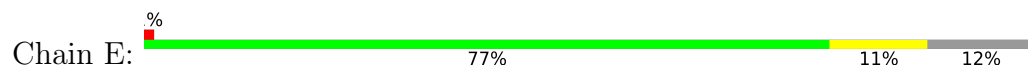


- Molecule 1: Endo-1,4-beta-xylanase

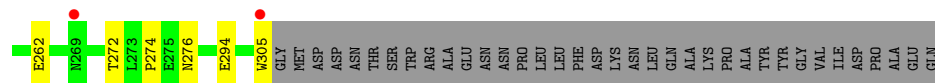
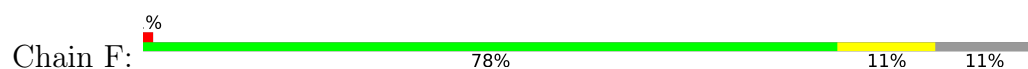




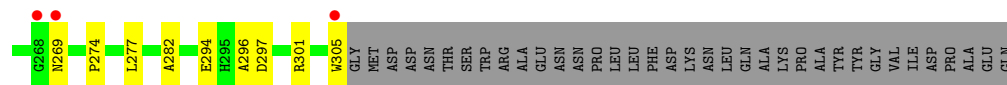
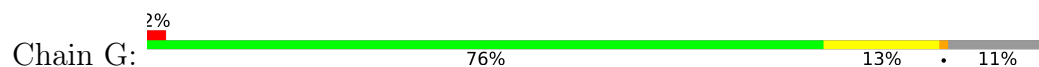
• Molecule 1: Endo-1,4-beta-xylanase



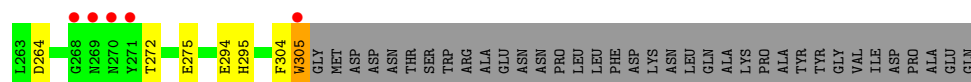
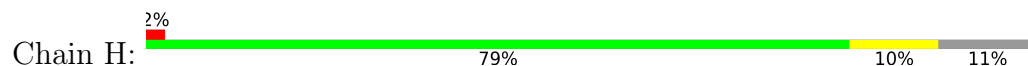
• Molecule 1: Endo-1,4-beta-xylanase



• Molecule 1: Endo-1,4-beta-xylanase



• Molecule 1: Endo-1,4-beta-xylanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.07Å 93.17Å 182.95Å 90.00° 99.96° 90.00°	Depositor
Resolution (Å)	42.61 – 1.34 42.61 – 1.34	Depositor EDS
% Data completeness (in resolution range)	86.7 (42.61-1.34) 86.7 (42.61-1.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.34Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.142 , 0.185 (Not available) , 0.212	Depositor DCC
R_{free} test set	26358 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	23733	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1846e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.55	15/2633 (0.6%)	1.30	6/3580 (0.2%)
1	B	1.49	7/2635 (0.3%)	1.20	2/3578 (0.1%)
1	C	1.52	6/2566 (0.2%)	1.24	7/3485 (0.2%)
1	D	1.51	5/2586 (0.2%)	1.21	0/3512
1	E	1.49	4/2588 (0.2%)	1.22	3/3512 (0.1%)
1	F	1.56	11/2633 (0.4%)	1.27	5/3574 (0.1%)
1	G	1.56	12/2584 (0.5%)	1.28	3/3512 (0.1%)
1	H	1.50	9/2642 (0.3%)	1.21	1/3591 (0.0%)
All	All	1.52	69/20867 (0.3%)	1.24	27/28344 (0.1%)

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	1
1	H	0	1
All	All	0	2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	ASN	C-O	8.83	1.28	1.23
1	A	115	LEU	N-CA	7.17	1.54	1.46
1	H	143	ASN	C-O	6.99	1.27	1.23
1	H	191	TYR	N-CA	6.79	1.54	1.46
1	B	105	PRO	N-CA	6.76	1.55	1.47
1	F	104	VAL	C-O	-6.60	1.19	1.24
1	F	66	ALA	CA-CB	6.51	1.63	1.53
1	G	32	GLU	N-CA	6.41	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	143	ASN	C-O	6.29	1.27	1.23
1	H	66	ALA	N-CA	6.19	1.53	1.46
1	A	87	GLN	C-O	6.01	1.31	1.23
1	H	255	GLY	C-N	6.01	1.38	1.33
1	G	138	GLU	C-O	5.99	1.31	1.23
1	G	282	ALA	C-O	5.97	1.31	1.24
1	F	143	ASN	CA-CB	5.94	1.57	1.52
1	F	103	THR	C-O	5.86	1.31	1.24
1	A	229	VAL	C-N	5.86	1.37	1.33
1	F	43	ALA	N-CA	5.78	1.53	1.46
1	D	124	LYS	C-O	5.78	1.31	1.24
1	F	38	HIS	N-CA	5.72	1.53	1.46
1	G	258	VAL	C-O	5.70	1.29	1.24
1	A	5	ALA	CA-C	5.67	1.58	1.52
1	G	41	VAL	C-O	5.66	1.29	1.23
1	B	293	LYS	C-O	5.62	1.30	1.24
1	F	97	LYS	C-O	5.58	1.30	1.24
1	F	124	LYS	N-CA	5.53	1.53	1.46
1	D	284	LEU	N-CA	5.52	1.53	1.46
1	C	192	ASN	CG-OD1	5.51	1.34	1.23
1	D	55	THR	C-O	5.46	1.30	1.23
1	G	33	LEU	CA-C	5.45	1.59	1.52
1	H	193	ASP	N-CA	5.44	1.52	1.46
1	G	277	LEU	C-O	5.44	1.30	1.24
1	E	66	ALA	CA-C	5.42	1.59	1.52
1	A	162	ALA	CA-CB	-5.41	1.44	1.53
1	D	155	ARG	CB-CG	-5.37	1.36	1.52
1	H	156	GLN	CA-CB	5.34	1.59	1.52
1	A	278	ALA	CA-CB	5.32	1.61	1.53
1	G	192	ASN	N-CA	5.30	1.52	1.46
1	C	262	GLU	CA-CB	5.26	1.58	1.53
1	A	263	LEU	N-CA	5.26	1.52	1.46
1	B	278	ALA	CA-CB	5.26	1.61	1.53
1	A	104	VAL	CA-C	5.23	1.57	1.52
1	B	163	ILE	CA-C	-5.23	1.47	1.52
1	E	203	THR	C-O	-5.22	1.18	1.24
1	H	272	THR	CA-C	-5.22	1.46	1.52
1	F	47	MET	SD-CE	-5.22	1.66	1.79
1	A	110	GLU	CA-C	5.19	1.59	1.52
1	G	143	ASN	C-O	5.17	1.26	1.23
1	C	218	ALA	N-CA	5.15	1.52	1.46
1	H	47	MET	SD-CE	-5.13	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	SER	CA-C	5.13	1.59	1.52
1	C	242	ASP	CA-C	5.12	1.59	1.52
1	A	131	ILE	CA-CB	5.09	1.60	1.54
1	B	219	ALA	N-CA	5.09	1.52	1.46
1	A	293	LYS	CA-C	5.08	1.59	1.52
1	C	281	GLN	N-CA	5.07	1.52	1.46
1	G	11	TYR	C-O	5.07	1.30	1.24
1	G	133	TRP	N-CA	5.07	1.52	1.46
1	G	296	ALA	C-O	5.04	1.30	1.24
1	A	250	LYS	CE-NZ	5.04	1.64	1.49
1	E	293	LYS	C-O	5.03	1.30	1.24
1	H	56	LYS	C-O	5.03	1.29	1.24
1	E	146	ASN	N-CA	5.03	1.52	1.46
1	A	91	ALA	C-O	-5.03	1.17	1.24
1	F	274	PRO	C-O	5.03	1.30	1.24
1	A	76	MET	N-CA	5.02	1.52	1.45
1	D	168	VAL	N-CA	5.01	1.52	1.46
1	C	250	LYS	CE-NZ	5.01	1.64	1.49
1	A	58	ASN	CA-CB	5.00	1.59	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ASN	O-C-N	7.10	130.24	122.15
1	C	163	ILE	N-CA-C	6.96	117.80	111.81
1	G	24	GLU	CA-CB-CG	6.89	127.88	114.10
1	F	143	ASN	O-C-N	-6.81	118.40	121.53
1	A	91	ALA	N-CA-C	6.57	119.26	111.71
1	A	301	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	E	273	LEU	N-CA-C	6.08	117.55	109.83
1	C	2	SER	N-CA-C	5.95	118.46	107.99
1	E	212	ILE	O-C-N	5.93	127.72	121.91
1	H	66	ALA	N-CA-C	-5.85	104.81	111.07
1	F	135	VAL	N-CA-C	-5.85	105.15	110.82
1	B	161	GLN	CB-CG-CD	5.82	122.50	112.60
1	E	163	ILE	CA-C-O	-5.71	114.04	120.32
1	F	156	GLN	CA-CB-CG	-5.54	103.02	114.10
1	F	168	VAL	O-C-N	5.49	127.61	121.90
1	G	301	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	B	223	LYS	CD-CE-NZ	-5.32	94.89	111.90
1	G	21	ILE	N-CA-C	5.18	117.50	108.95
1	C	133	TRP	CA-C-O	-5.16	114.72	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	226	ILE	N-CA-CB	-5.15	105.18	111.21
1	C	215	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	A	250	LYS	CG-CD-CE	5.13	123.10	111.30
1	C	156	GLN	CB-CG-CD	5.12	121.30	112.60
1	C	24	GLU	CA-CB-CG	5.11	124.32	114.10
1	A	168	VAL	O-C-N	5.02	127.00	121.83
1	A	57	GLY	N-CA-C	5.01	122.52	115.30
1	C	155	ARG	CB-CG-CD	-5.01	99.78	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ASN	Peptide
1	H	304	PHE	Peptide

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	2575	0	2475	49	0
1	B	2571	0	2483	33	0
1	C	2507	0	2412	38	0
1	D	2530	0	2424	31	1
1	E	2530	0	2438	37	1
1	F	2575	0	2467	27	0
1	G	2527	0	2422	34	0
1	H	2585	0	2480	31	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	1	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	431	0	0	12	1
4	B	447	0	0	15	0
4	C	453	0	0	15	0
4	D	400	0	0	15	0
4	E	407	0	0	14	1
4	F	429	0	0	11	0
4	G	392	0	0	11	0
4	H	353	0	0	9	1
All	All	23733	0	19601	272	3

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 7.

All (272) 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:270[B]:ASN:ND2	1:A:271[B]:TYR:H	0.93	1.40
1:A:270[B]:ASN:ND2	1:A:271[B]:TYR:N	1.71	1.35
1:A:224[B]:LEU:HD12	4:A:821:HOH:O	1.28	1.24
1:H:149[A]:ASP:OD1	4:H:852:HOH:O	1.58	1.21
1:B:224[B]:LEU:HD12	4:B:863:HOH:O	0.99	1.14
4:A:851:HOH:O	1:C:36[B]:MET:SD	2.06	1.13
1:B:224[A]:LEU:HA	4:B:752:HOH:O	1.45	1.13
1:A:270[B]:ASN:CG	1:A:271[B]:TYR:H	1.51	1.13
1:A:268:GLY:O	1:A:270[B]:ASN:HB2	1.48	1.12
1:C:27:GLU:HB3	4:C:713:HOH:O	1.50	1.11
1:G:24:GLU:HG3	4:G:657:HOH:O	1.54	1.05
1:D:186[A]:ASN:ND2	4:D:897:HOH:O	1.89	1.04
1:F:305[A]:TRP:CE3	4:F:912:HOH:O	2.09	1.04
1:H:305[C]:TRP:CZ3	4:H:757:HOH:O	2.12	1.02
1:B:186[B]:ASN:O	1:B:186[B]:ASN:ND2	1.93	1.01
1:A:270[B]:ASN:HD22	1:A:271[B]:TYR:N	1.42	1.01
1:F:305[A]:TRP:HE3	4:F:912:HOH:O	1.42	1.00
1:H:305[C]:TRP:HZ3	4:H:757:HOH:O	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:TRP:HE3	1:E:305:TRP:HA	1.28	0.97
1:E:305:TRP:HA	1:E:305:TRP:CE3	2.00	0.96
1:A:305:TRP:HA	1:A:305:TRP:CE3	1.99	0.96
1:A:305:TRP:HA	1:A:305:TRP:HE3	1.27	0.96
1:H:112[B]:LEU:HD21	1:H:116[B]:ARG:NH2	1.81	0.95
1:E:24:GLU:HG3	4:E:784:HOH:O	1.65	0.95
1:A:41[B]:VAL:HG11	1:A:71:VAL:HG11	1.48	0.93
1:E:68[C]:ILE:CD1	1:E:129:LYS:HD3	1.99	0.92
1:G:269:ASN:HB2	4:G:886:HOH:O	1.70	0.92
1:B:128[B]:ASN:OD1	4:B:945:HOH:O	1.87	0.92
1:D:27:GLU:HB3	4:D:778:HOH:O	1.68	0.92
1:H:250:LYS:HE2	4:H:844:HOH:O	1.72	0.90
1:B:186[B]:ASN:C	1:B:186[B]:ASN:HD22	1.79	0.90
1:G:305[B]:TRP:CZ3	4:G:842:HOH:O	2.26	0.89
1:F:27:GLU:HB3	4:F:795:HOH:O	1.77	0.85
1:G:78[B]:MET:O	1:G:130[B]:VAL:HG23	1.78	0.84
1:E:234[B]:HIS:HD2	4:E:717:HOH:O	1.61	0.83
1:H:305[B]:TRP:HA	4:H:833:HOH:O	1.79	0.82
1:C:232:GLN:OE1	1:C:234[B]:HIS:CE1	2.32	0.81
1:C:188:LYS:HE3	4:C:834:HOH:O	1.79	0.81
1:D:24:GLU:HG3	4:D:734:HOH:O	1.78	0.81
1:C:250:LYS:HD3	4:C:837:HOH:O	1.78	0.80
1:C:305[A]:TRP:CE3	1:C:305[A]:TRP:HA	2.16	0.80
1:C:305[A]:TRP:HA	1:C:305[A]:TRP:HE3	1.43	0.80
1:B:305[A]:TRP:HA	1:B:305[A]:TRP:CE3	2.17	0.80
1:A:41[B]:VAL:CG1	1:A:71:VAL:HG11	2.12	0.80
1:D:224:LEU:HA	4:D:748:HOH:O	1.80	0.80
1:D:32:GLU:OE2	4:D:771:HOH:O	1.99	0.80
1:C:305[B]:TRP:CZ2	4:C:806:HOH:O	2.34	0.79
1:G:128[B]:ASN:OD1	4:G:891:HOH:O	2.00	0.78
1:A:232:GLN:OE1	1:A:234[B]:HIS:CE1	2.37	0.78
1:F:224[B]:LEU:HA	4:F:671:HOH:O	1.82	0.78
1:A:245[B]:LYS:NZ	4:A:616:HOH:O	2.17	0.78
1:B:232:GLN:OE1	1:B:234[B]:HIS:CE1	2.37	0.77
1:G:297[B]:ASP:OD1	4:G:884:HOH:O	2.02	0.77
1:B:305[A]:TRP:HA	1:B:305[A]:TRP:HE3	1.49	0.77
1:E:112[B]:LEU:HD21	1:E:116[B]:ARG:NH2	1.99	0.77
1:C:224:LEU:HA	4:C:852:HOH:O	1.84	0.77
1:H:27:GLU:HB2	4:H:742:HOH:O	1.84	0.76
1:A:41[B]:VAL:HG12	1:A:77:LYS:O	1.86	0.76
1:A:32[B]:GLU:OE2	4:A:931:HOH:O	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:VAL:HG21	1:E:137:ASN:HB2	1.68	0.76
1:A:68[B]:ILE:HG12	1:A:78[B]:MET:HE3	1.66	0.75
1:A:223[B]:LYS:HG2	1:A:224[B]:LEU:H	1.52	0.75
1:C:250:LYS:CD	4:C:837:HOH:O	2.34	0.74
1:E:68[C]:ILE:HD11	1:E:129:LYS:HD3	1.67	0.74
1:H:294[B]:GLU:HG2	1:H:295:HIS:CE1	2.22	0.74
1:C:156:GLN:HB3	1:C:161[B]:GLN:NE2	2.02	0.73
1:G:305[B]:TRP:HZ3	4:G:842:HOH:O	1.66	0.73
1:B:24:GLU:HG3	4:B:740:HOH:O	1.87	0.73
1:F:67[B]:MET:HG3	4:F:532:HOH:O	1.89	0.72
1:A:41[B]:VAL:HG11	1:A:71:VAL:CG1	2.19	0.72
1:D:29[A]:THR:HG21	4:D:805:HOH:O	1.88	0.72
1:F:232:GLN:OE1	1:F:234[B]:HIS:CE1	2.42	0.72
1:F:58:ASN:HB2	4:F:727:HOH:O	1.89	0.71
1:D:69:ASP:OD1	4:D:760:HOH:O	2.09	0.71
1:D:112[A]:LEU:HD21	4:D:824:HOH:O	1.91	0.71
1:B:68[B]:ILE:HG12	1:B:78[B]:MET:HE3	1.74	0.70
4:F:647:HOH:O	1:G:29:THR:HG21	1.93	0.69
1:C:156:GLN:HB3	1:C:161[B]:GLN:HE21	1.55	0.68
1:B:305[B]:TRP:CZ2	4:B:753:HOH:O	2.46	0.68
1:C:69:ASP:OD1	4:C:879:HOH:O	2.10	0.68
1:B:224[B]:LEU:CD1	4:B:863:HOH:O	1.81	0.68
1:D:32:GLU:OE1	4:D:742:HOH:O	2.11	0.68
1:E:3:HIS:CE1	1:E:7[A]:LEU:HD11	2.29	0.67
1:F:305[A]:TRP:HB2	4:F:912:HOH:O	1.95	0.67
1:D:32:GLU:O	1:D:36[B]:MET:HG2	1.94	0.67
1:F:112:LEU:HD21	1:F:116[B]:ARG:NH2	2.10	0.66
1:F:272:THR:HG22	4:F:793:HOH:O	1.94	0.66
1:G:269:ASN:CB	4:G:886:HOH:O	2.36	0.66
1:C:82:VAL:HG21	1:C:137[B]:ASN:HB2	1.78	0.66
1:D:3:HIS:CE1	1:D:7[A]:LEU:HD11	2.31	0.65
1:A:305:TRP:CE3	1:A:305:TRP:CA	2.77	0.65
1:A:223[B]:LYS:HG2	1:A:224[B]:LEU:N	2.10	0.65
1:A:234[B]:HIS:CE1	4:A:824:HOH:O	2.49	0.65
1:C:36[B]:MET:O	1:C:36[B]:MET:HG3	1.94	0.65
1:C:186:ASN:CG	4:C:735:HOH:O	2.39	0.65
1:D:272:THR:N	4:D:834:HOH:O	2.29	0.65
1:F:82:VAL:HG21	1:F:137:ASN:HB2	1.79	0.64
1:G:130[B]:VAL:HG22	1:G:131:ILE:N	2.12	0.64
1:H:82:VAL:HG21	1:H:137:ASN:HB2	1.79	0.64
1:A:268:GLY:O	1:A:270[B]:ASN:CB	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:VAL:HG21	1:B:137:ASN:HB2	1.80	0.64
1:A:270[B]:ASN:CG	1:A:271[B]:TYR:N	2.26	0.63
1:G:82:VAL:HG21	1:G:137:ASN:HB2	1.81	0.63
1:A:272[A]:THR:O	1:A:273[A]:LEU:CB	2.46	0.63
1:D:234[B]:HIS:HD2	4:D:801:HOH:O	1.80	0.62
1:C:112[A]:LEU:HD21	4:C:826:HOH:O	2.00	0.62
1:D:82:VAL:HG21	1:D:137:ASN:HB2	1.82	0.62
1:A:270[B]:ASN:ND2	1:A:271[B]:TYR:CA	2.63	0.62
1:H:112[B]:LEU:HD21	1:H:116[B]:ARG:CZ	2.28	0.62
1:A:68[B]:ILE:HD12	1:A:126:PHE:CE1	2.35	0.61
1:D:234[B]:HIS:HE1	1:D:262:GLU:OE1	1.83	0.61
1:H:3:HIS:CE1	1:H:7[A]:LEU:HD11	2.35	0.61
1:A:305:TRP:C	4:A:833:HOH:O	2.44	0.60
1:C:250:LYS:CE	4:C:837:HOH:O	2.50	0.60
1:B:156:GLN:NE2	4:B:862:HOH:O	2.31	0.60
1:G:130[B]:VAL:HG22	1:G:132:SER:H	1.67	0.59
1:H:224:LEU:HA	4:H:732:HOH:O	2.00	0.59
1:E:2:SER:N	4:E:677:HOH:O	2.34	0.59
1:A:128:ASN:HB2	4:A:899:HOH:O	2.02	0.59
1:A:272[B]:THR:CG2	1:A:277:LEU:HB2	2.32	0.59
1:B:29[B]:THR:HG22	4:B:916:HOH:O	2.02	0.59
1:C:262:GLU:HA	1:C:305[B]:TRP:CD1	2.39	0.58
1:C:82:VAL:HG21	1:C:137[A]:ASN:HB2	1.84	0.57
1:G:6:PRO:HG3	1:G:36:MET:HE3	1.85	0.57
1:A:82:VAL:HG21	1:A:137:ASN:HB2	1.87	0.57
1:E:68[C]:ILE:HD13	1:E:129:LYS:HD3	1.83	0.57
1:F:4:MET:HB2	1:G:7[C]:LEU:HD11	1.87	0.57
1:F:181:GLU:HG3	4:F:736:HOH:O	2.04	0.57
1:G:36:MET:HE2	1:G:37:HIS:CE1	2.40	0.56
1:D:305[A]:TRP:HA	1:D:305[A]:TRP:CE3	2.40	0.56
1:E:305:TRP:CE3	1:E:305:TRP:CA	2.81	0.56
1:A:272[B]:THR:HG23	1:A:277:LEU:HB2	1.88	0.56
1:G:78[B]:MET:O	1:G:130[B]:VAL:CG2	2.52	0.56
1:C:186:ASN:OD1	1:C:186:ASN:C	2.48	0.56
1:F:294[A]:GLU:HG3	4:F:841:HOH:O	2.05	0.56
1:B:68[B]:ILE:HD12	1:B:126:PHE:CE1	2.41	0.56
1:E:234[B]:HIS:HE1	1:E:262:GLU:OE1	1.89	0.55
1:E:250[B]:LYS:HD2	4:E:756:HOH:O	2.06	0.55
1:B:128[B]:ASN:ND2	4:B:945:HOH:O	2.38	0.55
1:B:128[B]:ASN:CG	4:B:945:HOH:O	2.40	0.55
1:D:294:GLU:HG3	4:D:758:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:GLN:OE1	1:C:234[B]:HIS:NE2	2.40	0.55
1:A:2:SER:N	4:A:802:HOH:O	2.40	0.54
1:E:250[B]:LYS:NZ	4:E:756:HOH:O	2.30	0.54
1:E:161[B]:GLN:OE1	4:E:904:HOH:O	2.18	0.54
1:H:112[B]:LEU:CD2	1:H:116[B]:ARG:CZ	2.85	0.54
1:A:234[B]:HIS:HE1	4:A:824:HOH:O	1.85	0.54
1:D:232:GLN:OE1	1:D:234[B]:HIS:NE2	2.41	0.54
1:H:112[B]:LEU:HG	1:H:116[B]:ARG:CZ	2.38	0.54
1:H:26:LEU:HD13	1:H:70[B]:LYS:HG2	1.90	0.54
1:E:96:LYS:HE2	4:E:676:HOH:O	2.08	0.53
1:F:99[B]:ASP:OD2	1:H:146[B]:ASN:ND2	2.42	0.53
1:B:44:GLY:HA2	1:B:305[B]:TRP:CH2	2.43	0.52
1:E:199:GLN:NE2	4:E:756:HOH:O	2.41	0.52
1:D:112[B]:LEU:HD21	1:D:170[B]:GLN:HG3	1.92	0.52
1:E:68[C]:ILE:CD1	1:E:129:LYS:CD	2.84	0.52
1:H:186:ASN:OD1	1:H:188[B]:LYS:NZ	2.43	0.52
1:A:36:MET:HE1	1:C:286:ALA:HB1	1.91	0.51
1:B:232:GLN:OE1	1:B:234[B]:HIS:NE2	2.44	0.51
1:B:20:ALA:HB2	1:B:305[B]:TRP:CD1	2.46	0.51
1:F:262:GLU:HG2	1:F:305[A]:TRP:CE3	2.45	0.51
1:H:294[B]:GLU:HG2	1:H:295:HIS:ND1	2.26	0.51
1:F:276:ASN:OD1	1:G:30:ARG:NH2	2.43	0.51
1:E:68[C]:ILE:HD11	1:E:129:LYS:CD	2.38	0.51
1:A:196[B]:GLU:HG3	1:A:231:MET:HE2	1.93	0.50
1:F:112:LEU:HG	1:F:116[B]:ARG:CZ	2.41	0.50
1:A:24:GLU:HG3	4:A:720:HOH:O	2.10	0.50
1:A:270[A]:ASN:N	1:A:270[A]:ASN:OD1	2.44	0.50
1:C:27:GLU:HG3	4:C:616:HOH:O	2.12	0.50
1:D:196[B]:GLU:HG3	1:D:231:MET:HE2	1.93	0.50
1:E:112[B]:LEU:HG	1:E:116[B]:ARG:CZ	2.42	0.50
1:D:234[B]:HIS:CE1	1:D:262:GLU:OE1	2.64	0.50
1:E:96:LYS:CE	4:E:676:HOH:O	2.60	0.50
1:F:99[B]:ASP:OD2	1:H:146[B]:ASN:CG	2.55	0.50
1:G:3:HIS:CE1	1:G:7[A]:LEU:HD11	2.46	0.50
1:C:250:LYS:NZ	4:C:837:HOH:O	2.33	0.49
1:C:186:ASN:OD1	1:C:186:ASN:O	2.30	0.49
1:F:3:HIS:HB2	1:F:37:HIS:CE1	2.46	0.49
1:G:196[A]:GLU:OE2	1:G:231:MET:HG2	2.12	0.49
1:C:264[B]:ASP:OD1	1:C:264[B]:ASP:O	2.29	0.49
1:G:196[B]:GLU:H	1:G:196[B]:GLU:CD	2.19	0.49
1:H:264:ASP:HB2	1:H:305[B]:TRP:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196[A]:GLU:OE2	1:H:231:MET:HG2	2.13	0.49
1:D:96:LYS:NZ	4:D:792:HOH:O	2.40	0.49
1:A:41[B]:VAL:HG13	1:A:41[B]:VAL:O	2.12	0.49
1:A:272[A]:THR:O	1:A:273[A]:LEU:HB3	2.13	0.49
1:D:29[B]:THR:HG21	4:D:805:HOH:O	2.11	0.49
1:A:3:HIS:CE1	1:A:7[A]:LEU:HD11	2.47	0.48
1:B:245[B]:LYS:HG3	1:B:291:LEU:HD11	1.95	0.48
1:B:186[B]:ASN:ND2	1:B:186[B]:ASN:C	2.54	0.48
1:B:305[A]:TRP:CE3	1:B:305[A]:TRP:CA	2.93	0.48
1:C:69:ASP:CG	4:C:879:HOH:O	2.56	0.48
1:E:112[B]:LEU:HD21	1:E:116[B]:ARG:HH22	1.77	0.48
1:F:3:HIS:CE1	1:F:7[A]:LEU:HD11	2.48	0.48
1:F:10:VAL:HG11	1:G:5:ALA:HB2	1.95	0.48
1:D:232:GLN:OE1	1:D:234[B]:HIS:CE1	2.66	0.47
1:E:223[B]:LYS:NZ	4:E:883:HOH:O	2.18	0.47
1:C:264[B]:ASP:OD1	1:C:264[B]:ASP:C	2.54	0.47
1:A:124:LYS:NZ	4:A:634:HOH:O	2.39	0.47
1:E:156[B]:GLN:HG3	3:E:403:CL:CL	2.52	0.47
1:B:68[B]:ILE:HD12	1:B:126:PHE:CD1	2.49	0.47
1:D:18:GLY:HA2	1:D:40:VAL:O	2.15	0.46
1:E:2:SER:CA	4:E:677:HOH:O	2.64	0.46
1:E:3:HIS:HB2	1:E:37:HIS:CE1	2.50	0.46
1:E:224:LEU:HA	4:E:712:HOH:O	2.13	0.46
1:G:19[B]:ASN:HB2	1:G:38:HIS:CD2	2.50	0.46
1:H:112[B]:LEU:HG	1:H:116[B]:ARG:NH1	2.29	0.46
1:E:36:MET:HE3	1:E:36:MET:HB2	1.82	0.46
1:F:10:VAL:HG11	1:G:5:ALA:CB	2.46	0.46
1:H:50:ASP:OD2	4:H:853:HOH:O	2.21	0.45
1:A:232:GLN:OE1	1:A:234[B]:HIS:NE2	2.50	0.45
1:A:272[A]:THR:O	1:A:273[A]:LEU:HB2	2.16	0.45
1:B:96:LYS:NZ	4:B:744:HOH:O	2.38	0.45
1:H:112[B]:LEU:CG	1:H:116[B]:ARG:CZ	2.95	0.45
1:D:36[B]:MET:HB2	1:D:36[B]:MET:HE3	1.44	0.44
1:F:3:HIS:NE2	1:F:7[A]:LEU:HD11	2.32	0.44
1:G:262:GLU:HA	1:G:305[B]:TRP:HB2	1.99	0.44
1:H:149[A]:ASP:OD1	1:H:149[A]:ASP:C	2.59	0.44
1:B:305[A]:TRP:NE1	4:B:913:HOH:O	2.49	0.44
1:D:196[B]:GLU:HG3	1:D:231:MET:CE	2.47	0.44
1:E:68[C]:ILE:C	1:E:68[C]:ILE:HD12	2.42	0.44
1:C:305[B]:TRP:CE2	4:C:806:HOH:O	2.66	0.44
1:B:305[A]:TRP:CD1	4:B:913:HOH:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LYS:HE2	1:D:36[A]:MET:O	2.17	0.44
1:E:294:GLU:HG3	4:E:734:HOH:O	2.17	0.44
1:A:196[B]:GLU:HG3	1:A:231:MET:CE	2.48	0.43
1:B:196[A]:GLU:OE2	1:B:231:MET:HG2	2.18	0.43
1:C:305[A]:TRP:CE3	1:C:305[A]:TRP:CA	2.92	0.43
1:G:3:HIS:HB2	1:G:37:HIS:CE1	2.53	0.43
1:G:87[B]:GLN:NE2	4:G:683:HOH:O	2.45	0.43
1:C:36[B]:MET:HE2	1:C:36[B]:MET:HB2	1.78	0.43
1:F:98:ASP:HB2	1:H:149[A]:ASP:OD2	2.18	0.43
1:B:224[B]:LEU:HA	4:B:752:HOH:O	2.18	0.43
1:H:250:LYS:CE	4:H:844:HOH:O	2.48	0.43
1:G:269:ASN:ND2	4:G:886:HOH:O	2.43	0.43
1:D:3:HIS:HB2	1:D:37:HIS:CE1	2.54	0.43
1:B:3:HIS:CE1	1:B:7:LEU:HD11	2.54	0.43
1:F:7[C]:LEU:HA	1:F:7[C]:LEU:HD12	1.64	0.43
1:A:3:HIS:HB2	1:A:37:HIS:CE1	2.54	0.43
1:G:262:GLU:HG2	1:G:305[B]:TRP:CE3	2.54	0.42
1:A:272[B]:THR:HG21	1:A:277:LEU:HB2	1.99	0.42
1:C:196[A]:GLU:OE2	1:C:231:MET:HG2	2.19	0.42
1:G:128[B]:ASN:CG	4:G:891:HOH:O	2.59	0.42
1:C:81:HIS:HE1	1:C:137[A]:ASN:ND2	2.17	0.42
1:B:305[B]:TRP:CE2	4:B:753:HOH:O	2.70	0.42
1:H:112[B]:LEU:HD21	1:H:116[B]:ARG:HH22	1.74	0.42
1:C:196[B]:GLU:CG	1:C:231:MET:HE2	2.49	0.42
1:F:196[A]:GLU:OE2	1:F:231:MET:HG2	2.20	0.42
1:G:130[B]:VAL:HG21	1:G:132:SER:O	2.20	0.42
1:H:262:GLU:HG2	1:H:305[C]:TRP:CE3	2.55	0.42
1:H:3:HIS:HB2	1:H:37:HIS:CE1	2.55	0.42
1:A:68[B]:ILE:HD12	1:A:126:PHE:CD1	2.55	0.42
1:G:18:GLY:HA2	1:G:40:VAL:O	2.20	0.42
1:D:27:GLU:HG3	4:D:568:HOH:O	2.20	0.42
1:B:18:GLY:HA2	1:B:40:VAL:O	2.20	0.41
1:G:228:GLY:HA2	1:G:257:GLU:O	2.21	0.41
1:C:264[B]:ASP:CG	4:C:883:HOH:O	2.63	0.41
1:H:132:SER:HB3	1:H:188[B]:LYS:HB2	2.03	0.41
1:A:18:GLY:HA2	1:A:40:VAL:O	2.21	0.41
1:A:232:GLN:HB3	1:A:234[B]:HIS:CD2	2.56	0.41
1:A:294:GLU:HG3	4:A:642:HOH:O	2.21	0.41
1:E:2:SER:HA	4:E:677:HOH:O	2.20	0.41
1:E:196[A]:GLU:OE2	1:E:231:MET:HG2	2.21	0.41
1:G:294:GLU:CD	4:G:826:HOH:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234[B]:HIS:CE1	1:E:262:GLU:OE1	2.71	0.40
1:C:20:ALA:HB2	1:C:305[B]:TRP:CD1	2.56	0.40
1:E:112[B]:LEU:HD21	1:E:116[B]:ARG:CZ	2.50	0.40
1:E:232:GLN:OE1	1:E:234[B]:HIS:NE2	2.54	0.40
1:E:267:ALA:HB1	1:E:272:THR:HG21	2.03	0.40
1:C:196[B]:GLU:OE2	1:C:231:MET:HB3	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:724:HOH:O	4:E:706:HOH:O[1_655]	2.09	0.11
1:E:30:ARG:NH2	1:H:275[B]:GLU:OE1[2_546]	2.10	0.10
1:D:128[B]:ASN:OD1	4:H:745:HOH:O[2_646]	2.16	0.04

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	321/341 (94%)	313 (98%)	5 (2%)	3 (1%)	14	2
1	B	320/341 (94%)	317 (99%)	3 (1%)	0	100	100
1	C	311/341 (91%)	307 (99%)	4 (1%)	0	100	100
1	D	312/341 (92%)	305 (98%)	7 (2%)	0	100	100
1	E	314/341 (92%)	307 (98%)	7 (2%)	0	100	100
1	F	319/341 (94%)	311 (98%)	8 (2%)	0	100	100
1	G	314/341 (92%)	309 (98%)	5 (2%)	0	100	100
1	H	321/341 (94%)	313 (98%)	8 (2%)	0	100	100
All	All	2532/2728 (93%)	2482 (98%)	47 (2%)	3 (0%)	48	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270[A]	ASN
1	A	270[B]	ASN
1	A	269	ASN

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	277/288 (96%)	274 (99%)	3 (1%)	65	33
1	B	277/288 (96%)	274 (99%)	3 (1%)	65	33
1	C	269/288 (93%)	263 (98%)	6 (2%)	45	12
1	D	272/288 (94%)	270 (99%)	2 (1%)	76	51
1	E	272/288 (94%)	270 (99%)	2 (1%)	76	51
1	F	276/288 (96%)	276 (100%)	0	100	100
1	G	271/288 (94%)	268 (99%)	3 (1%)	65	33
1	H	278/288 (96%)	276 (99%)	2 (1%)	76	51
All	All	2192/2304 (95%)	2171 (99%)	21 (1%)	73	37

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270[A]	ASN
1	A	270[B]	ASN
1	A	305	TRP
1	B	99	ASP
1	B	272	THR
1	B	273	LEU
1	C	99	ASP
1	C	186	ASN
1	C	272	THR
1	C	273	LEU
1	C	305[A]	TRP

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Mol	Chain	Res	Type
1	C	305[B]	TRP
1	D	27	GLU
1	D	221	ASN
1	E	277	LEU
1	E	305	TRP
1	G	87[A]	GLN
1	G	87[B]	GLN
1	G	274	PRO
1	H	305[B]	TRP
1	H	305[C]	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	B	102	ASN
1	D	199	GLN
1	D	238	ASN
1	E	58	ASN
1	E	199	GLN
1	G	3	HIS
1	G	238	ASN
1	H	19	ASN
1	H	102	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 21 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

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 ⓘ

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	304/341 (89%)	-0.23	8 (2%) 57 67	7, 19, 28, 54	24 (7%)
1	B	304/341 (89%)	-0.29	4 (1%) 75 83	7, 18, 27, 55	22 (7%)
1	C	302/341 (88%)	-0.25	4 (1%) 75 83	7, 18, 29, 54	21 (6%)
1	D	301/341 (88%)	-0.14	2 (0%) 84 90	8, 19, 31, 56	24 (7%)
1	E	301/341 (88%)	-0.24	5 (1%) 69 79	6, 18, 30, 67	22 (7%)
1	F	304/341 (89%)	-0.21	5 (1%) 70 80	8, 19, 30, 46	23 (7%)
1	G	304/341 (89%)	-0.01	6 (1%) 65 74	9, 21, 31, 46	20 (6%)
1	H	304/341 (89%)	0.06	6 (1%) 65 74	9, 22, 32, 43	26 (8%)
All	All	2424/2728 (88%)	-0.16	40 (1%) 69 79	6, 19, 30, 67	182 (7%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	305[B]	TRP	12.5
1	E	305	TRP	5.7
1	G	305[A]	TRP	5.6
1	D	305[A]	TRP	5.4
1	C	305[A]	TRP	5.3
1	B	269	ASN	5.1
1	B	271	TYR	4.8
1	G	268	GLY	4.6
1	B	305[A]	TRP	4.5
1	E	273	LEU	4.5
1	A	269	ASN	4.4
1	A	271[A]	TYR	4.3
1	A	270[A]	ASN	4.2
1	C	1	GLY	3.9
1	A	305	TRP	3.9
1	F	269	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	272	THR	3.4
1	F	305[A]	TRP	3.4
1	H	268	GLY	3.2
1	E	2	SER	3.2
1	F	2	SER	3.1
1	G	269	ASN	2.7
1	A	273[A]	LEU	2.7
1	A	272[A]	THR	2.6
1	H	270	ASN	2.6
1	D	273	LEU	2.6
1	F	4	MET	2.6
1	H	269[A]	ASN	2.4
1	G	4	MET	2.4
1	E	268	GLY	2.4
1	B	270	ASN	2.4
1	H	271	TYR	2.2
1	H	68[A]	ILE	2.1
1	G	2	SER	2.1
1	C	272	THR	2.1
1	A	275	GLU	2.1
1	G	5	ALA	2.1
1	C	268	GLY	2.0
1	A	13[A]	ASN	2.0
1	F	3	HIS	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($\text{\AA}^2$)	Q<0.9
2	MG	E	404	1/1	0.97	0.07	33,33,33,33	0
2	MG	B	403	1/1	0.99	0.03	23,23,23,23	0
2	MG	C	401[A]	1/1	0.99	0.03	14,14,14,14	1
2	MG	C	401[B]	1/1	0.99	0.03	25,25,25,25	1
2	MG	A	403	1/1	0.99	0.03	27,27,27,27	0
2	MG	F	401	1/1	0.99	0.02	20,20,20,20	0
2	MG	G	401	1/1	0.99	0.07	27,27,27,27	0
2	MG	H	401	1/1	0.99	0.10	25,25,25,25	0
3	CL	E	403	1/1	0.99	0.09	38,38,38,38	0
2	MG	A	401	1/1	1.00	0.02	18,18,18,18	0
2	MG	D	401	1/1	1.00	0.05	21,21,21,21	0
2	MG	E	401	1/1	1.00	0.06	20,20,20,20	0
3	CL	A	402[A]	1/1	1.00	0.02	15,15,15,15	1
3	CL	B	402[A]	1/1	1.00	0.02	14,14,14,14	1
3	CL	C	402[A]	1/1	1.00	0.05	17,17,17,17	1
3	CL	D	402[A]	1/1	1.00	0.06	22,22,22,22	1
3	CL	E	402[A]	1/1	1.00	0.03	16,16,16,16	1
2	MG	B	401	1/1	1.00	0.05	19,19,19,19	0
3	CL	F	402[A]	1/1	1.00	0.05	18,18,18,18	1
3	CL	G	402[A]	1/1	1.00	0.02	18,18,18,18	1
3	CL	H	402[A]	1/1	1.00	0.02	18,18,18,18	1

6.5 Other polymers

There are no such residues in this entry.