



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:54 PM EDT

PDB ID : 6JTI / pdb_00006jti
Title : Crystal structure of native NagZ from Neisseria gonorrhoeae
Authors : Chen, Y.
Deposited on : 2019-04-11
Resolution : 2.20 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

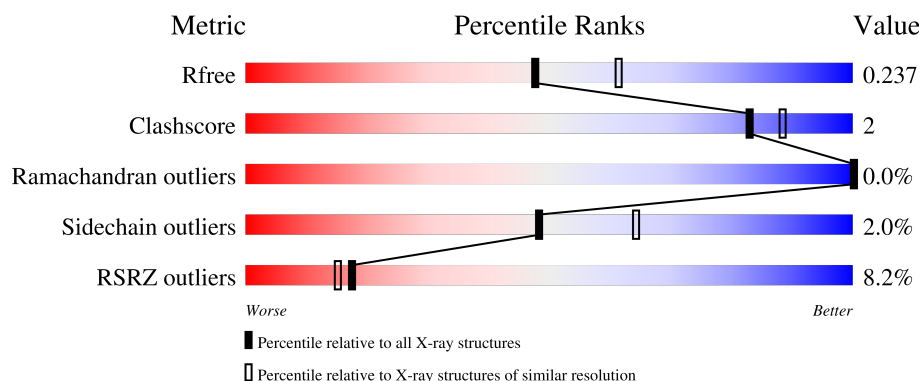
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	397	4% 79% 6% 15%
1	B	397	4% 82% 5% 13%
1	C	397	4% 81% 5% 14%
1	D	397	6% 79% 7% 13%
1	E	397	15% 79% 6% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	397	9% 81% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16208 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 Beta-hexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2599	1642	464	478	15			
1	B	344	Total	C	N	O	S	0	0	0
			2623	1655	469	483	16			
1	C	343	Total	C	N	O	S	0	0	0
			2623	1654	468	485	16			
1	D	344	Total	C	N	O	S	0	0	0
			2625	1656	469	484	16			
1	E	339	Total	C	N	O	S	0	0	0
			2596	1639	464	478	15			
1	F	340	Total	C	N	O	S	0	0	0
			2601	1642	465	479	15			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP Q5FA94
A	-34	GLY	-	expression tag	UNP Q5FA94
A	-33	SER	-	expression tag	UNP Q5FA94
A	-32	SER	-	expression tag	UNP Q5FA94
A	-31	HIS	-	expression tag	UNP Q5FA94
A	-30	HIS	-	expression tag	UNP Q5FA94
A	-29	HIS	-	expression tag	UNP Q5FA94
A	-28	HIS	-	expression tag	UNP Q5FA94
A	-27	HIS	-	expression tag	UNP Q5FA94
A	-26	HIS	-	expression tag	UNP Q5FA94
A	-25	SER	-	expression tag	UNP Q5FA94
A	-24	SER	-	expression tag	UNP Q5FA94
A	-23	GLY	-	expression tag	UNP Q5FA94
A	-22	LEU	-	expression tag	UNP Q5FA94
A	-21	VAL	-	expression tag	UNP Q5FA94
A	-20	PRO	-	expression tag	UNP Q5FA94
A	-19	ARG	-	expression tag	UNP Q5FA94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q5FA94
A	-17	SER	-	expression tag	UNP Q5FA94
A	-16	HIS	-	expression tag	UNP Q5FA94
A	-15	MET	-	expression tag	UNP Q5FA94
A	-14	ALA	-	expression tag	UNP Q5FA94
A	-13	SER	-	expression tag	UNP Q5FA94
A	-12	MET	-	expression tag	UNP Q5FA94
A	-11	THR	-	expression tag	UNP Q5FA94
A	-10	GLY	-	expression tag	UNP Q5FA94
A	-9	GLY	-	expression tag	UNP Q5FA94
A	-8	GLN	-	expression tag	UNP Q5FA94
A	-7	GLN	-	expression tag	UNP Q5FA94
A	-6	MET	-	expression tag	UNP Q5FA94
A	-5	GLY	-	expression tag	UNP Q5FA94
A	-4	ARG	-	expression tag	UNP Q5FA94
A	-3	GLY	-	expression tag	UNP Q5FA94
A	-2	SER	-	expression tag	UNP Q5FA94
A	-1	GLU	-	expression tag	UNP Q5FA94
A	0	PHE	-	expression tag	UNP Q5FA94
B	-35	MET	-	expression tag	UNP Q5FA94
B	-34	GLY	-	expression tag	UNP Q5FA94
B	-33	SER	-	expression tag	UNP Q5FA94
B	-32	SER	-	expression tag	UNP Q5FA94
B	-31	HIS	-	expression tag	UNP Q5FA94
B	-30	HIS	-	expression tag	UNP Q5FA94
B	-29	HIS	-	expression tag	UNP Q5FA94
B	-28	HIS	-	expression tag	UNP Q5FA94
B	-27	HIS	-	expression tag	UNP Q5FA94
B	-26	HIS	-	expression tag	UNP Q5FA94
B	-25	SER	-	expression tag	UNP Q5FA94
B	-24	SER	-	expression tag	UNP Q5FA94
B	-23	GLY	-	expression tag	UNP Q5FA94
B	-22	LEU	-	expression tag	UNP Q5FA94
B	-21	VAL	-	expression tag	UNP Q5FA94
B	-20	PRO	-	expression tag	UNP Q5FA94
B	-19	ARG	-	expression tag	UNP Q5FA94
B	-18	GLY	-	expression tag	UNP Q5FA94
B	-17	SER	-	expression tag	UNP Q5FA94
B	-16	HIS	-	expression tag	UNP Q5FA94
B	-15	MET	-	expression tag	UNP Q5FA94
B	-14	ALA	-	expression tag	UNP Q5FA94
B	-13	SER	-	expression tag	UNP Q5FA94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	MET	-	expression tag	UNP Q5FA94
B	-11	THR	-	expression tag	UNP Q5FA94
B	-10	GLY	-	expression tag	UNP Q5FA94
B	-9	GLY	-	expression tag	UNP Q5FA94
B	-8	GLN	-	expression tag	UNP Q5FA94
B	-7	GLN	-	expression tag	UNP Q5FA94
B	-6	MET	-	expression tag	UNP Q5FA94
B	-5	GLY	-	expression tag	UNP Q5FA94
B	-4	ARG	-	expression tag	UNP Q5FA94
B	-3	GLY	-	expression tag	UNP Q5FA94
B	-2	SER	-	expression tag	UNP Q5FA94
B	-1	GLU	-	expression tag	UNP Q5FA94
B	0	PHE	-	expression tag	UNP Q5FA94
C	-35	MET	-	expression tag	UNP Q5FA94
C	-34	GLY	-	expression tag	UNP Q5FA94
C	-33	SER	-	expression tag	UNP Q5FA94
C	-32	SER	-	expression tag	UNP Q5FA94
C	-31	HIS	-	expression tag	UNP Q5FA94
C	-30	HIS	-	expression tag	UNP Q5FA94
C	-29	HIS	-	expression tag	UNP Q5FA94
C	-28	HIS	-	expression tag	UNP Q5FA94
C	-27	HIS	-	expression tag	UNP Q5FA94
C	-26	HIS	-	expression tag	UNP Q5FA94
C	-25	SER	-	expression tag	UNP Q5FA94
C	-24	SER	-	expression tag	UNP Q5FA94
C	-23	GLY	-	expression tag	UNP Q5FA94
C	-22	LEU	-	expression tag	UNP Q5FA94
C	-21	VAL	-	expression tag	UNP Q5FA94
C	-20	PRO	-	expression tag	UNP Q5FA94
C	-19	ARG	-	expression tag	UNP Q5FA94
C	-18	GLY	-	expression tag	UNP Q5FA94
C	-17	SER	-	expression tag	UNP Q5FA94
C	-16	HIS	-	expression tag	UNP Q5FA94
C	-15	MET	-	expression tag	UNP Q5FA94
C	-14	ALA	-	expression tag	UNP Q5FA94
C	-13	SER	-	expression tag	UNP Q5FA94
C	-12	MET	-	expression tag	UNP Q5FA94
C	-11	THR	-	expression tag	UNP Q5FA94
C	-10	GLY	-	expression tag	UNP Q5FA94
C	-9	GLY	-	expression tag	UNP Q5FA94
C	-8	GLN	-	expression tag	UNP Q5FA94
C	-7	GLN	-	expression tag	UNP Q5FA94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	expression tag	UNP Q5FA94
C	-5	GLY	-	expression tag	UNP Q5FA94
C	-4	ARG	-	expression tag	UNP Q5FA94
C	-3	GLY	-	expression tag	UNP Q5FA94
C	-2	SER	-	expression tag	UNP Q5FA94
C	-1	GLU	-	expression tag	UNP Q5FA94
C	0	PHE	-	expression tag	UNP Q5FA94
D	-35	MET	-	expression tag	UNP Q5FA94
D	-34	GLY	-	expression tag	UNP Q5FA94
D	-33	SER	-	expression tag	UNP Q5FA94
D	-32	SER	-	expression tag	UNP Q5FA94
D	-31	HIS	-	expression tag	UNP Q5FA94
D	-30	HIS	-	expression tag	UNP Q5FA94
D	-29	HIS	-	expression tag	UNP Q5FA94
D	-28	HIS	-	expression tag	UNP Q5FA94
D	-27	HIS	-	expression tag	UNP Q5FA94
D	-26	HIS	-	expression tag	UNP Q5FA94
D	-25	SER	-	expression tag	UNP Q5FA94
D	-24	SER	-	expression tag	UNP Q5FA94
D	-23	GLY	-	expression tag	UNP Q5FA94
D	-22	LEU	-	expression tag	UNP Q5FA94
D	-21	VAL	-	expression tag	UNP Q5FA94
D	-20	PRO	-	expression tag	UNP Q5FA94
D	-19	ARG	-	expression tag	UNP Q5FA94
D	-18	GLY	-	expression tag	UNP Q5FA94
D	-17	SER	-	expression tag	UNP Q5FA94
D	-16	HIS	-	expression tag	UNP Q5FA94
D	-15	MET	-	expression tag	UNP Q5FA94
D	-14	ALA	-	expression tag	UNP Q5FA94
D	-13	SER	-	expression tag	UNP Q5FA94
D	-12	MET	-	expression tag	UNP Q5FA94
D	-11	THR	-	expression tag	UNP Q5FA94
D	-10	GLY	-	expression tag	UNP Q5FA94
D	-9	GLY	-	expression tag	UNP Q5FA94
D	-8	GLN	-	expression tag	UNP Q5FA94
D	-7	GLN	-	expression tag	UNP Q5FA94
D	-6	MET	-	expression tag	UNP Q5FA94
D	-5	GLY	-	expression tag	UNP Q5FA94
D	-4	ARG	-	expression tag	UNP Q5FA94
D	-3	GLY	-	expression tag	UNP Q5FA94
D	-2	SER	-	expression tag	UNP Q5FA94
D	-1	GLU	-	expression tag	UNP Q5FA94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PHE	-	expression tag	UNP Q5FA94
E	-35	MET	-	expression tag	UNP Q5FA94
E	-34	GLY	-	expression tag	UNP Q5FA94
E	-33	SER	-	expression tag	UNP Q5FA94
E	-32	SER	-	expression tag	UNP Q5FA94
E	-31	HIS	-	expression tag	UNP Q5FA94
E	-30	HIS	-	expression tag	UNP Q5FA94
E	-29	HIS	-	expression tag	UNP Q5FA94
E	-28	HIS	-	expression tag	UNP Q5FA94
E	-27	HIS	-	expression tag	UNP Q5FA94
E	-26	HIS	-	expression tag	UNP Q5FA94
E	-25	SER	-	expression tag	UNP Q5FA94
E	-24	SER	-	expression tag	UNP Q5FA94
E	-23	GLY	-	expression tag	UNP Q5FA94
E	-22	LEU	-	expression tag	UNP Q5FA94
E	-21	VAL	-	expression tag	UNP Q5FA94
E	-20	PRO	-	expression tag	UNP Q5FA94
E	-19	ARG	-	expression tag	UNP Q5FA94
E	-18	GLY	-	expression tag	UNP Q5FA94
E	-17	SER	-	expression tag	UNP Q5FA94
E	-16	HIS	-	expression tag	UNP Q5FA94
E	-15	MET	-	expression tag	UNP Q5FA94
E	-14	ALA	-	expression tag	UNP Q5FA94
E	-13	SER	-	expression tag	UNP Q5FA94
E	-12	MET	-	expression tag	UNP Q5FA94
E	-11	THR	-	expression tag	UNP Q5FA94
E	-10	GLY	-	expression tag	UNP Q5FA94
E	-9	GLY	-	expression tag	UNP Q5FA94
E	-8	GLN	-	expression tag	UNP Q5FA94
E	-7	GLN	-	expression tag	UNP Q5FA94
E	-6	MET	-	expression tag	UNP Q5FA94
E	-5	GLY	-	expression tag	UNP Q5FA94
E	-4	ARG	-	expression tag	UNP Q5FA94
E	-3	GLY	-	expression tag	UNP Q5FA94
E	-2	SER	-	expression tag	UNP Q5FA94
E	-1	GLU	-	expression tag	UNP Q5FA94
E	0	PHE	-	expression tag	UNP Q5FA94
F	-35	MET	-	expression tag	UNP Q5FA94
F	-34	GLY	-	expression tag	UNP Q5FA94
F	-33	SER	-	expression tag	UNP Q5FA94
F	-32	SER	-	expression tag	UNP Q5FA94
F	-31	HIS	-	expression tag	UNP Q5FA94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	expression tag	UNP Q5FA94
F	-29	HIS	-	expression tag	UNP Q5FA94
F	-28	HIS	-	expression tag	UNP Q5FA94
F	-27	HIS	-	expression tag	UNP Q5FA94
F	-26	HIS	-	expression tag	UNP Q5FA94
F	-25	SER	-	expression tag	UNP Q5FA94
F	-24	SER	-	expression tag	UNP Q5FA94
F	-23	GLY	-	expression tag	UNP Q5FA94
F	-22	LEU	-	expression tag	UNP Q5FA94
F	-21	VAL	-	expression tag	UNP Q5FA94
F	-20	PRO	-	expression tag	UNP Q5FA94
F	-19	ARG	-	expression tag	UNP Q5FA94
F	-18	GLY	-	expression tag	UNP Q5FA94
F	-17	SER	-	expression tag	UNP Q5FA94
F	-16	HIS	-	expression tag	UNP Q5FA94
F	-15	MET	-	expression tag	UNP Q5FA94
F	-14	ALA	-	expression tag	UNP Q5FA94
F	-13	SER	-	expression tag	UNP Q5FA94
F	-12	MET	-	expression tag	UNP Q5FA94
F	-11	THR	-	expression tag	UNP Q5FA94
F	-10	GLY	-	expression tag	UNP Q5FA94
F	-9	GLY	-	expression tag	UNP Q5FA94
F	-8	GLN	-	expression tag	UNP Q5FA94
F	-7	GLN	-	expression tag	UNP Q5FA94
F	-6	MET	-	expression tag	UNP Q5FA94
F	-5	GLY	-	expression tag	UNP Q5FA94
F	-4	ARG	-	expression tag	UNP Q5FA94
F	-3	GLY	-	expression tag	UNP Q5FA94
F	-2	SER	-	expression tag	UNP Q5FA94
F	-1	GLU	-	expression tag	UNP Q5FA94
F	0	PHE	-	expression tag	UNP Q5FA94

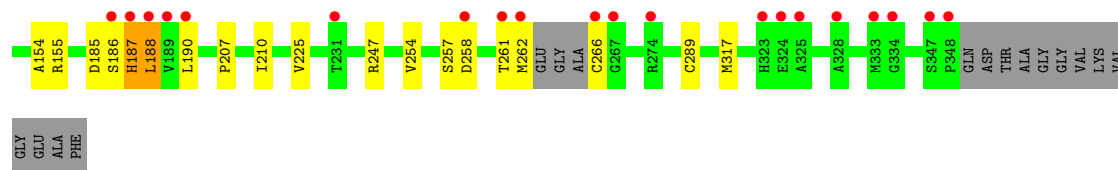
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	128	Total O 128 128	0	0
2	B	124	Total O 124 124	0	0
2	C	114	Total O 114 114	0	0
2	D	67	Total O 67 67	0	0

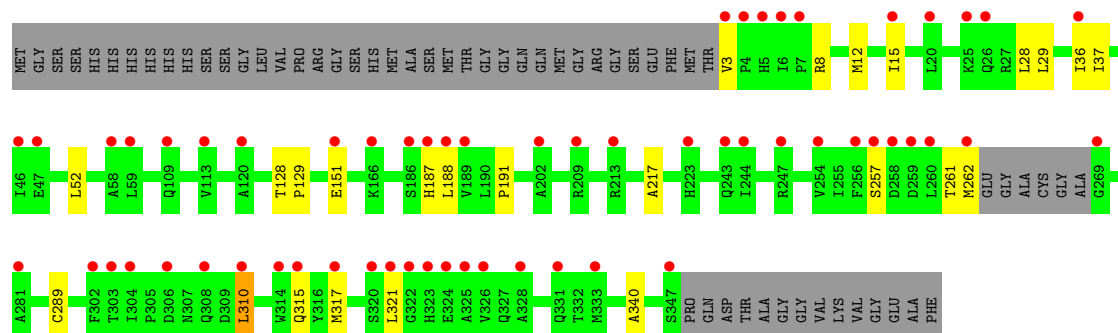
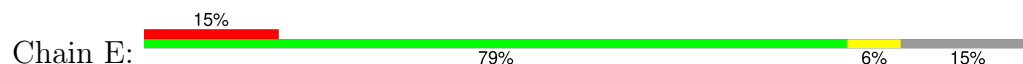
Continued on next page...

Continued from previous page...

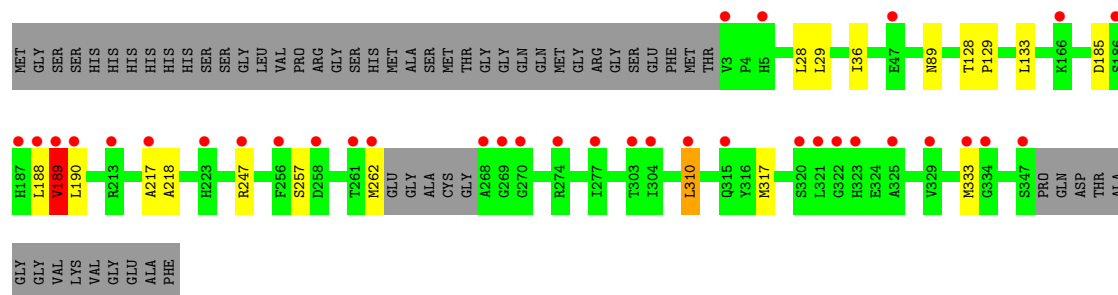
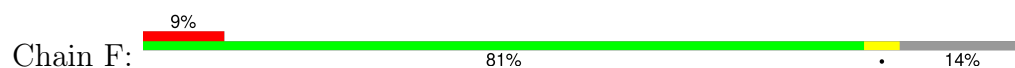
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	45	Total	O	0	0
			45	45		
2	F	63	Total	O	0	0
			63	63		



• Molecule 1: Beta-hexosaminidase



• Molecule 1: Beta-hexosaminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.02Å 124.09Å 189.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.88 – 2.20 103.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (103.88-2.20) 100.0 (103.88-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.214 , 0.233 0.218 , 0.237	Depositor DCC
R_{free} test set	6172 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16208	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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	0.75	0/2649	0.91	4/3582 (0.1%)
1	B	0.75	0/2673	0.90	1/3614 (0.0%)
1	C	0.75	0/2672	0.91	3/3612 (0.1%)
1	D	0.69	0/2675	0.89	3/3617 (0.1%)
1	E	0.67	0/2645	0.87	3/3575 (0.1%)
1	F	0.73	1/2650 (0.0%)	0.93	4/3582 (0.1%)
All	All	0.72	1/15964 (0.0%)	0.90	18/21582 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	189	VAL	C-O	-9.36	1.12	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	333	MET	N-CA-C	-11.00	92.81	110.20
1	D	257	SER	N-CA-C	8.49	123.42	112.89
1	C	265	ALA	N-CA-C	8.15	121.28	111.82
1	F	189	VAL	CA-C-O	-8.05	110.72	120.78
1	A	257	SER	N-CA-C	-6.77	100.50	110.52
1	C	257	SER	N-CA-C	6.70	119.17	110.53
1	F	257	SER	N-CA-C	-6.70	100.61	110.52
1	E	257	SER	N-CA-C	-6.66	100.66	110.52
1	E	310	LEU	CD1-CG-CD2	6.38	124.83	110.80
1	C	258	ASP	N-CA-C	-6.29	98.96	108.96
1	A	192	GLU	CB-CA-C	6.25	122.20	109.76
1	F	310	LEU	CD1-CG-CD2	6.18	124.39	110.80
1	B	257	SER	N-CA-C	-5.79	101.95	110.52
1	A	186	SER	N-CA-C	5.71	120.09	113.18
1	D	155	ARG	CB-CG-CD	5.46	123.85	111.30
1	E	151	GLU	CB-CG-CD	5.26	121.55	112.60
1	D	258	ASP	N-CA-CB	5.25	119.36	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	MET	CB-CG-SD	5.17	128.20	112.70

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	2599	0	2595	13	0
1	B	2623	0	2616	17	0
1	C	2623	0	2614	13	0
1	D	2625	0	2618	14	0
1	E	2596	0	2591	17	0
1	F	2601	0	2596	14	0
2	A	128	0	0	1	0
2	B	124	0	0	0	0
2	C	114	0	0	1	0
2	D	67	0	0	0	0
2	E	45	0	0	0	0
2	F	63	0	0	0	0
All	All	16208	0	15630	74	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 2.

All (74) 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:B:347:SER:HB2	1:B:348:PRO:HD2	1.36	1.04
1:B:188:LEU:HD13	1:F:262:MET:C	1.83	1.04
1:B:347:SER:CB	1:B:348:PRO:HD2	1.97	0.94
1:E:12:MET:CE	1:E:37:ILE:HB	2.00	0.91
1:D:188:LEU:HG	1:E:188:LEU:HB3	1.52	0.90
1:C:112:ARG:NH1	2:C:401:HOH:O	1.96	0.89
1:B:188:LEU:CD1	1:F:262:MET:C	2.46	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:SER:HB2	1:B:348:PRO:CD	2.03	0.87
1:F:217:ALA:O	1:F:317:MET:HE1	1.84	0.78
1:D:188:LEU:CG	1:E:188:LEU:HB3	2.15	0.75
1:E:8:ARG:HH12	1:E:315:GLN:HE21	1.34	0.73
1:F:217:ALA:C	1:F:317:MET:HE1	2.14	0.72
1:B:347:SER:CB	1:B:348:PRO:CD	2.66	0.71
1:E:12:MET:HE3	1:E:37:ILE:HB	1.71	0.71
1:A:231:THR:HG21	1:E:340:ALA:HB3	1.77	0.66
1:E:12:MET:HE2	1:E:37:ILE:HB	1.81	0.63
1:E:217:ALA:HB1	1:E:317:MET:SD	2.39	0.63
1:B:155:ARG:NH1	1:D:99:GLY:HA2	2.13	0.63
1:C:190:LEU:HD22	1:C:225:VAL:HG23	1.81	0.62
1:A:231:THR:HG21	1:E:340:ALA:CB	2.28	0.62
1:D:154:ALA:HB1	1:D:210:ILE:HG21	1.83	0.61
1:F:217:ALA:HB1	1:F:317:MET:SD	2.41	0.60
1:D:188:LEU:HD22	1:E:262:MET:HE2	1.83	0.60
1:F:189:VAL:HG23	1:F:190:LEU:H	1.67	0.60
1:C:223:HIS:HE1	1:C:260:LEU:HD22	1.67	0.59
1:E:261:THR:HG21	1:E:289:CYS:O	2.03	0.59
1:E:8:ARG:HH12	1:E:315:GLN:NE2	2.01	0.58
1:A:217:ALA:HB1	1:A:317:MET:SD	2.44	0.57
1:C:15:ILE:HD11	1:C:52:LEU:HD21	1.87	0.56
1:D:261:THR:HG21	1:D:289:CYS:O	2.05	0.55
1:D:190:LEU:HD11	1:D:225:VAL:HG23	1.89	0.55
1:C:243:GLN:O	1:C:247:ARG:CG	2.56	0.55
1:B:188:LEU:HD12	1:F:262:MET:C	2.32	0.54
1:A:15:ILE:HD11	1:A:52:LEU:HD21	1.90	0.54
1:E:15:ILE:HD11	1:E:52:LEU:HD21	1.89	0.53
1:B:188:LEU:HD12	1:F:262:MET:O	2.09	0.53
1:D:207:PRO:HA	1:D:210:ILE:HG22	1.91	0.53
1:D:188:LEU:CD2	1:E:188:LEU:HB3	2.40	0.52
1:A:190:LEU:O	1:A:190:LEU:HG	2.11	0.51
1:C:243:GLN:O	1:C:247:ARG:HG2	2.13	0.49
1:C:243:GLN:O	1:C:247:ARG:HG3	2.13	0.48
1:B:12:MET:HB3	1:B:287:LEU:HD22	1.95	0.48
1:B:188:LEU:CD1	1:F:262:MET:O	2.61	0.47
1:C:243:GLN:HA	1:C:247:ARG:HG2	1.97	0.47
1:C:223:HIS:CE1	1:C:260:LEU:HD22	2.48	0.47
1:F:218:ALA:HB2	1:F:317:MET:HE3	1.96	0.46
1:B:347:SER:OG	1:B:348:PRO:HD2	2.15	0.46
1:B:261:THR:O	1:B:274:ARG:NH1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD22	1:A:36:ILE:HD11	1.99	0.44
1:F:218:ALA:HB2	1:F:317:MET:CE	2.48	0.43
1:A:254:VAL:HG11	1:A:256:PHE:CE1	2.52	0.43
1:F:28:LEU:HD22	1:F:36:ILE:HD11	2.00	0.43
1:F:188:LEU:O	1:F:189:VAL:HG22	2.18	0.43
1:E:28:LEU:HD22	1:E:36:ILE:HD11	2.00	0.43
1:B:128:THR:OG1	1:B:129:PRO:HA	2.19	0.42
1:A:120:ALA:HA	1:A:326:VAL:HG11	2.01	0.42
1:A:128:THR:OG1	1:A:129:PRO:HA	2.19	0.42
1:A:74:ARG:HH21	1:C:134:ASP:CG	2.27	0.42
1:C:28:LEU:HD22	1:C:36:ILE:HD11	2.02	0.42
1:D:128:THR:OG1	1:D:129:PRO:HA	2.20	0.42
1:E:128:THR:OG1	1:E:129:PRO:HA	2.19	0.42
1:C:128:THR:OG1	1:C:129:PRO:HA	2.20	0.42
1:D:28:LEU:HD22	1:D:36:ILE:HD11	2.01	0.42
1:F:128:THR:OG1	1:F:129:PRO:HA	2.20	0.42
1:B:14:ASP:O	1:B:15:ILE:HD13	2.20	0.41
1:B:28:LEU:HD22	1:B:36:ILE:HD11	2.02	0.41
1:B:103:ALA:HB1	1:B:156:LEU:HD21	2.03	0.41
1:D:254:VAL:HG21	1:D:317:MET:HE2	2.01	0.41
1:D:14:ASP:O	1:D:15:ILE:HD13	2.21	0.41
1:A:256:PHE:HD2	1:A:287:LEU:HD11	1.86	0.41
1:C:168:GLY:HA2	1:C:320:SER:OG	2.20	0.40
1:A:27:ARG:NH2	2:A:403:HOH:O	2.43	0.40
1:A:326:VAL:O	1:A:329:VAL:HG12	2.22	0.40
1:D:187:HIS:CE1	1:E:191:PRO:HG2	2.56	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	335/397 (84%)	323 (96%)	12 (4%)	0	100	100
1	B	340/397 (86%)	329 (97%)	11 (3%)	0	100	100
1	C	339/397 (85%)	329 (97%)	10 (3%)	0	100	100
1	D	340/397 (86%)	328 (96%)	12 (4%)	0	100	100
1	E	335/397 (84%)	322 (96%)	13 (4%)	0	100	100
1	F	336/397 (85%)	322 (96%)	13 (4%)	1 (0%)	36	42
All	All	2025/2382 (85%)	1953 (96%)	71 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	189	VAL

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	269/309 (87%)	266 (99%)	3 (1%)	65	79
1	B	270/309 (87%)	265 (98%)	5 (2%)	50	66
1	C	271/309 (88%)	267 (98%)	4 (2%)	57	73
1	D	271/309 (88%)	261 (96%)	10 (4%)	30	41
1	E	268/309 (87%)	263 (98%)	5 (2%)	50	66
1	F	268/309 (87%)	262 (98%)	6 (2%)	45	61
All	All	1617/1854 (87%)	1584 (98%)	33 (2%)	48	64

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	185	ASP
1	A	326	VAL
1	B	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	151	GLU
1	B	274	ARG
1	B	287	LEU
1	B	329	VAL
1	C	2	THR
1	C	29	LEU
1	C	190	LEU
1	C	327	GLN
1	D	2	THR
1	D	26	GLN
1	D	29	LEU
1	D	185	ASP
1	D	186	SER
1	D	187	HIS
1	D	188	LEU
1	D	247	ARG
1	D	262	MET
1	D	266	CYS
1	E	3	VAL
1	E	29	LEU
1	E	187	HIS
1	E	310	LEU
1	E	321	LEU
1	F	29	LEU
1	F	89	ASN
1	F	133	LEU
1	F	185	ASP
1	F	247	ARG
1	F	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	161	GLN
1	B	161	GLN
1	B	331	GLN
1	B	336	GLN
1	C	161	GLN
1	C	187	HIS
1	C	327	GLN
1	D	44	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	161	GLN
1	D	187	HIS
1	D	336	GLN
1	E	44	GLN
1	E	161	GLN
1	E	228	GLN
1	E	315	GLN
1	E	331	GLN
1	F	93	GLN
1	F	161	GLN
1	F	336	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	339/397 (85%)	0.24	14 (4%)	41	38	22, 33, 57, 90	0
1	B	344/397 (86%)	0.22	17 (4%)	35	31	22, 33, 57, 94	0
1	C	343/397 (86%)	0.38	17 (4%)	34	31	21, 34, 60, 93	0
1	D	344/397 (86%)	0.63	25 (7%)	21	18	26, 40, 69, 104	0
1	E	339/397 (85%)	1.20	59 (17%)	4	3	29, 50, 73, 118	0
1	F	340/397 (85%)	0.85	35 (10%)	12	9	27, 45, 72, 126	0
All	All	2049/2382 (86%)	0.58	167 (8%)	17	15	21, 39, 68, 126	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	188	LEU	8.7
1	D	187	HIS	7.9
1	E	187	HIS	7.4
1	F	189	VAL	7.3
1	C	265	ALA	6.7
1	D	262	MET	6.0
1	B	188	LEU	5.9
1	A	190	LEU	5.7
1	E	188	LEU	5.7
1	A	348	PRO	5.5
1	B	348	PRO	5.3
1	D	348	PRO	5.3
1	D	188	LEU	5.3
1	E	3	VAL	5.1
1	D	189	VAL	5.1
1	C	266	CYS	5.1
1	F	3	VAL	5.0
1	F	262	MET	5.0
1	F	187	HIS	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	269	GLY	4.8
1	D	186	SER	4.6
1	D	2	THR	4.5
1	E	262	MET	4.5
1	F	186	SER	4.4
1	B	262	MET	4.4
1	A	188	LEU	4.3
1	E	189	VAL	4.1
1	A	189	VAL	4.1
1	F	268	ALA	4.0
1	F	347	SER	4.0
1	C	264	GLY	4.0
1	E	310	LEU	3.9
1	A	333	MET	3.8
1	E	256	PHE	3.8
1	D	266	CYS	3.8
1	A	191	PRO	3.7
1	C	270	GLY	3.7
1	B	189	VAL	3.7
1	A	324	GLU	3.7
1	C	261	THR	3.7
1	F	334	GLY	3.7
1	D	258	ASP	3.7
1	E	151	GLU	3.6
1	C	260	LEU	3.6
1	C	2	THR	3.6
1	E	323	HIS	3.4
1	A	256	PHE	3.4
1	D	328	ALA	3.4
1	E	258	ASP	3.4
1	F	323	HIS	3.3
1	B	258	ASP	3.3
1	D	333	MET	3.3
1	E	186	SER	3.3
1	D	323	HIS	3.3
1	E	320	SER	3.3
1	D	325	ALA	3.3
1	A	223	HIS	3.3
1	E	321	LEU	3.2
1	E	6	ILE	3.2
1	C	3	VAL	3.1
1	B	187	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	333	MET	3.0
1	E	47	GLU	3.0
1	F	223	HIS	3.0
1	C	262	MET	3.0
1	F	321	LEU	3.0
1	E	347	SER	3.0
1	E	326	VAL	2.9
1	C	263	GLU	2.9
1	E	304	ILE	2.9
1	F	166	LYS	2.9
1	E	314	TRP	2.9
1	F	217	ALA	2.9
1	E	20	LEU	2.9
1	E	259	ASP	2.8
1	E	247	ARG	2.8
1	D	267	GLY	2.7
1	D	324	GLU	2.7
1	C	188	LEU	2.7
1	E	59	LEU	2.7
1	E	223	HIS	2.7
1	E	333	MET	2.7
1	B	265	ALA	2.7
1	F	5	HIS	2.7
1	E	15	ILE	2.7
1	F	277	ILE	2.7
1	E	317	MET	2.6
1	F	256	PHE	2.6
1	E	25	LYS	2.6
1	D	80	GLU	2.6
1	F	325	ALA	2.6
1	E	209	ARG	2.6
1	E	254	VAL	2.6
1	B	3	VAL	2.5
1	E	36	ILE	2.5
1	A	323	HIS	2.5
1	C	347	SER	2.5
1	A	327	GLN	2.5
1	E	243	GLN	2.5
1	A	328	ALA	2.5
1	E	257	SER	2.4
1	B	333	MET	2.4
1	C	274	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	190	LEU	2.4
1	E	5	HIS	2.4
1	F	310	LEU	2.4
1	D	47	GLU	2.4
1	F	304	ILE	2.4
1	F	329	VAL	2.4
1	E	306	ASP	2.3
1	F	270	GLY	2.3
1	E	58	ALA	2.3
1	E	202	ALA	2.3
1	D	261	THR	2.3
1	F	213	ARG	2.3
1	D	190	LEU	2.3
1	F	261	THR	2.3
1	B	323	HIS	2.3
1	D	3	VAL	2.3
1	E	302	PHE	2.3
1	E	7	PRO	2.3
1	D	334	GLY	2.3
1	D	231	THR	2.3
1	B	347	SER	2.3
1	E	46	ILE	2.3
1	A	329	VAL	2.3
1	B	26	GLN	2.2
1	E	303	THR	2.2
1	D	97	LYS	2.2
1	E	213	ARG	2.2
1	F	247	ARG	2.2
1	F	322	GLY	2.2
1	B	5	HIS	2.2
1	E	109	GLN	2.2
1	E	166	LYS	2.2
1	D	347	SER	2.2
1	B	266	CYS	2.2
1	F	47	GLU	2.2
1	C	26	GLN	2.2
1	E	315	GLN	2.2
1	F	315	GLN	2.2
1	C	328	ALA	2.1
1	F	320	SER	2.1
1	B	321	LEU	2.1
1	E	260	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	324	GLU	2.1
1	E	328	ALA	2.1
1	E	26	GLN	2.1
1	E	331	GLN	2.1
1	E	113	VAL	2.1
1	B	322	GLY	2.1
1	E	322	GLY	2.1
1	A	97	LYS	2.1
1	E	325	ALA	2.1
1	C	15	ILE	2.1
1	E	308	GLN	2.1
1	F	269	GLY	2.1
1	C	209	ARG	2.1
1	B	261	THR	2.0
1	E	120	ALA	2.0
1	E	281	ALA	2.0
1	F	303	THR	2.0
1	F	258	ASP	2.0
1	D	274	ARG	2.0
1	E	4	PRO	2.0
1	E	244	ILE	2.0
1	F	274	ARG	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.