



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 06:19 PM UTC

PDB ID : 2O3O / pdb_00002o3o
Title : Crystal Structure of the sensor histidine kinase regulator YycI from *Bacillus subtilis*
Authors : Santelli, E.; Liddington, R.C.
Deposited on : 2006-12-01
Resolution : 2.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

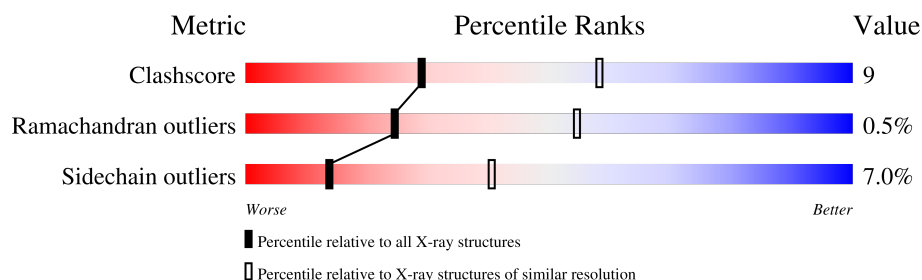
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	254	75% 18% • 5%
1	B	254	74% 17% • 6%
1	C	254	77% 15% • 6%
1	D	254	72% 21% • 5%
1	E	254	72% 18% • 7%
1	F	254	76% 16% • 6%
1	G	254	76% 15% • 7%
1	H	254	77% 15% • 5%

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Mol	Chain	Length	Quality of chain
1	I	254	75% 17%
1	J	254	74% 16% 6%
1	K	254	73% 17% 7%
1	L	254	76% 17% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23401 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 YycI protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	Se	0	0	0
			1965	1251	313	394	1	6			
1	B	239	Total	C	N	O	S	Se	0	0	0
			1947	1241	310	389	1	6			
1	C	239	Total	C	N	O	S	Se	0	0	0
			1947	1240	310	390	1	6			
1	D	241	Total	C	N	O	S	Se	0	0	0
			1965	1249	313	396	1	6			
1	E	237	Total	C	N	O	S	Se	0	0	0
			1932	1232	308	385	1	6			
1	F	240	Total	C	N	O	S	Se	0	0	0
			1958	1248	313	390	1	6			
1	G	237	Total	C	N	O	S	Se	0	0	0
			1929	1228	306	388	1	6			
1	H	241	Total	C	N	O	S	Se	0	0	0
			1965	1249	313	396	1	6			
1	I	244	Total	C	N	O	S	Se	0	0	0
			1986	1264	318	397	1	6			
1	J	238	Total	C	N	O	S	Se	0	0	0
			1941	1238	310	386	1	6			
1	K	235	Total	C	N	O	S	Se	0	0	0
			1913	1219	304	383	1	6			
1	L	239	Total	C	N	O	S	Se	0	0	0
			1947	1237	309	394	1	6			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	cloning artifact	UNP Q45612
A	28	SER	-	cloning artifact	UNP Q45612
A	29	HIS	-	cloning artifact	UNP Q45612
A	30	MSE	-	cloning artifact	UNP Q45612
A	47	MSE	MET	modified residue	UNP Q45612

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Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MSE	MET	modified residue	UNP Q45612
A	91	MSE	MET	modified residue	UNP Q45612
A	103	MSE	MET	modified residue	UNP Q45612
A	167	MSE	MET	modified residue	UNP Q45612
A	204	MSE	MET	modified residue	UNP Q45612
B	27	GLY	-	cloning artifact	UNP Q45612
B	28	SER	-	cloning artifact	UNP Q45612
B	29	HIS	-	cloning artifact	UNP Q45612
B	30	MSE	-	cloning artifact	UNP Q45612
B	47	MSE	MET	modified residue	UNP Q45612
B	89	MSE	MET	modified residue	UNP Q45612
B	91	MSE	MET	modified residue	UNP Q45612
B	103	MSE	MET	modified residue	UNP Q45612
B	167	MSE	MET	modified residue	UNP Q45612
B	204	MSE	MET	modified residue	UNP Q45612
C	27	GLY	-	cloning artifact	UNP Q45612
C	28	SER	-	cloning artifact	UNP Q45612
C	29	HIS	-	cloning artifact	UNP Q45612
C	30	MSE	-	cloning artifact	UNP Q45612
C	47	MSE	MET	modified residue	UNP Q45612
C	89	MSE	MET	modified residue	UNP Q45612
C	91	MSE	MET	modified residue	UNP Q45612
C	103	MSE	MET	modified residue	UNP Q45612
C	167	MSE	MET	modified residue	UNP Q45612
C	204	MSE	MET	modified residue	UNP Q45612
D	27	GLY	-	cloning artifact	UNP Q45612
D	28	SER	-	cloning artifact	UNP Q45612
D	29	HIS	-	cloning artifact	UNP Q45612
D	30	MSE	-	cloning artifact	UNP Q45612
D	47	MSE	MET	modified residue	UNP Q45612
D	89	MSE	MET	modified residue	UNP Q45612
D	91	MSE	MET	modified residue	UNP Q45612
D	103	MSE	MET	modified residue	UNP Q45612
D	167	MSE	MET	modified residue	UNP Q45612
D	204	MSE	MET	modified residue	UNP Q45612
E	27	GLY	-	cloning artifact	UNP Q45612
E	28	SER	-	cloning artifact	UNP Q45612
E	29	HIS	-	cloning artifact	UNP Q45612
E	30	MSE	-	cloning artifact	UNP Q45612
E	47	MSE	MET	modified residue	UNP Q45612
E	89	MSE	MET	modified residue	UNP Q45612
E	91	MSE	MET	modified residue	UNP Q45612

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Chain	Residue	Modelled	Actual	Comment	Reference
E	103	MSE	MET	modified residue	UNP Q45612
E	167	MSE	MET	modified residue	UNP Q45612
E	204	MSE	MET	modified residue	UNP Q45612
F	27	GLY	-	cloning artifact	UNP Q45612
F	28	SER	-	cloning artifact	UNP Q45612
F	29	HIS	-	cloning artifact	UNP Q45612
F	30	MSE	-	cloning artifact	UNP Q45612
F	47	MSE	MET	modified residue	UNP Q45612
F	89	MSE	MET	modified residue	UNP Q45612
F	91	MSE	MET	modified residue	UNP Q45612
F	103	MSE	MET	modified residue	UNP Q45612
F	167	MSE	MET	modified residue	UNP Q45612
F	204	MSE	MET	modified residue	UNP Q45612
G	27	GLY	-	cloning artifact	UNP Q45612
G	28	SER	-	cloning artifact	UNP Q45612
G	29	HIS	-	cloning artifact	UNP Q45612
G	30	MSE	-	cloning artifact	UNP Q45612
G	47	MSE	MET	modified residue	UNP Q45612
G	89	MSE	MET	modified residue	UNP Q45612
G	91	MSE	MET	modified residue	UNP Q45612
G	103	MSE	MET	modified residue	UNP Q45612
G	167	MSE	MET	modified residue	UNP Q45612
G	204	MSE	MET	modified residue	UNP Q45612
H	27	GLY	-	cloning artifact	UNP Q45612
H	28	SER	-	cloning artifact	UNP Q45612
H	29	HIS	-	cloning artifact	UNP Q45612
H	30	MSE	-	cloning artifact	UNP Q45612
H	47	MSE	MET	modified residue	UNP Q45612
H	89	MSE	MET	modified residue	UNP Q45612
H	91	MSE	MET	modified residue	UNP Q45612
H	103	MSE	MET	modified residue	UNP Q45612
H	167	MSE	MET	modified residue	UNP Q45612
H	204	MSE	MET	modified residue	UNP Q45612
I	27	GLY	-	cloning artifact	UNP Q45612
I	28	SER	-	cloning artifact	UNP Q45612
I	29	HIS	-	cloning artifact	UNP Q45612
I	30	MSE	-	cloning artifact	UNP Q45612
I	47	MSE	MET	modified residue	UNP Q45612
I	89	MSE	MET	modified residue	UNP Q45612
I	91	MSE	MET	modified residue	UNP Q45612
I	103	MSE	MET	modified residue	UNP Q45612
I	167	MSE	MET	modified residue	UNP Q45612

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Chain	Residue	Modelled	Actual	Comment	Reference
I	204	MSE	MET	modified residue	UNP Q45612
J	27	GLY	-	cloning artifact	UNP Q45612
J	28	SER	-	cloning artifact	UNP Q45612
J	29	HIS	-	cloning artifact	UNP Q45612
J	30	MSE	-	cloning artifact	UNP Q45612
J	47	MSE	MET	modified residue	UNP Q45612
J	89	MSE	MET	modified residue	UNP Q45612
J	91	MSE	MET	modified residue	UNP Q45612
J	103	MSE	MET	modified residue	UNP Q45612
J	167	MSE	MET	modified residue	UNP Q45612
J	204	MSE	MET	modified residue	UNP Q45612
K	27	GLY	-	cloning artifact	UNP Q45612
K	28	SER	-	cloning artifact	UNP Q45612
K	29	HIS	-	cloning artifact	UNP Q45612
K	30	MSE	-	cloning artifact	UNP Q45612
K	47	MSE	MET	modified residue	UNP Q45612
K	89	MSE	MET	modified residue	UNP Q45612
K	91	MSE	MET	modified residue	UNP Q45612
K	103	MSE	MET	modified residue	UNP Q45612
K	167	MSE	MET	modified residue	UNP Q45612
K	204	MSE	MET	modified residue	UNP Q45612
L	27	GLY	-	cloning artifact	UNP Q45612
L	28	SER	-	cloning artifact	UNP Q45612
L	29	HIS	-	cloning artifact	UNP Q45612
L	30	MSE	-	cloning artifact	UNP Q45612
L	47	MSE	MET	modified residue	UNP Q45612
L	89	MSE	MET	modified residue	UNP Q45612
L	91	MSE	MET	modified residue	UNP Q45612
L	103	MSE	MET	modified residue	UNP Q45612
L	167	MSE	MET	modified residue	UNP Q45612
L	204	MSE	MET	modified residue	UNP Q45612

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	1	Total 1	Cl 1	0	0
2	L	1	Total 1	Cl 1	0	0

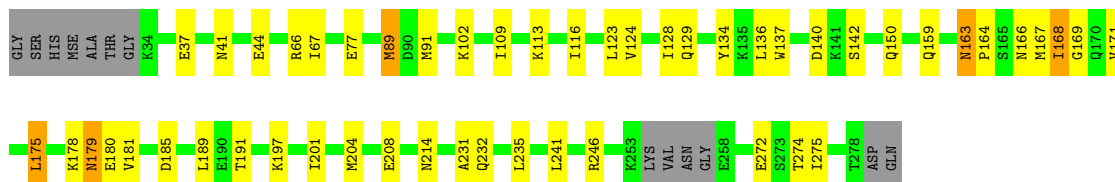
3 Residue-property plots [i](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

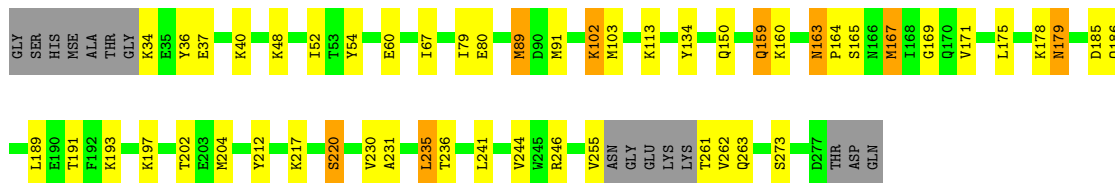
• Molecule 1: YycI protein

Chain A: 



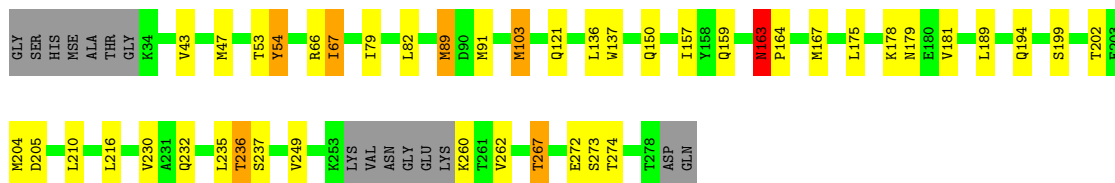
• Molecule 1: YycI protein

Chain B: 



• Molecule 1: YycI protein

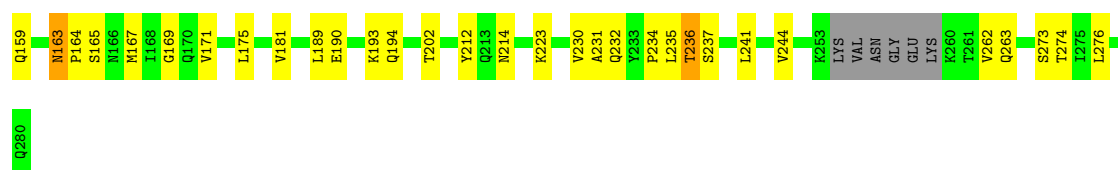
Chain C: 



• Molecule 1: YycI protein

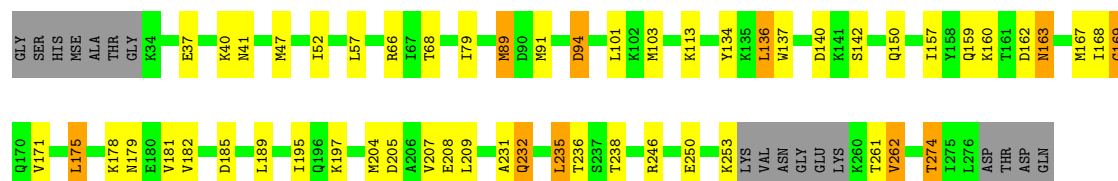
Chain D: 





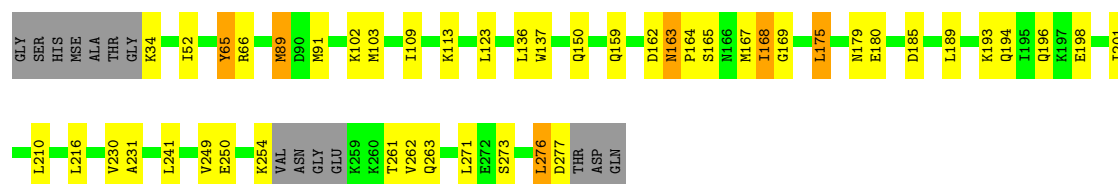
- Molecule 1: YycI protein

Chain E: 72% 18% 7%



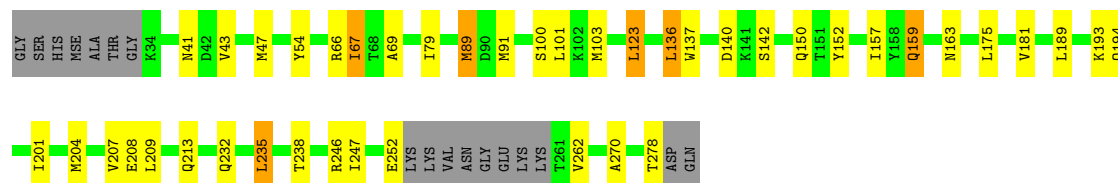
- Molecule 1: YycI protein

Chain F: 76% 16% 6%



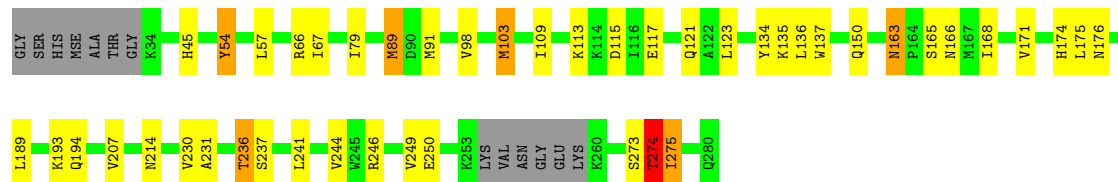
- Molecule 1: YycI protein

Chain G: 76% 15% 7%



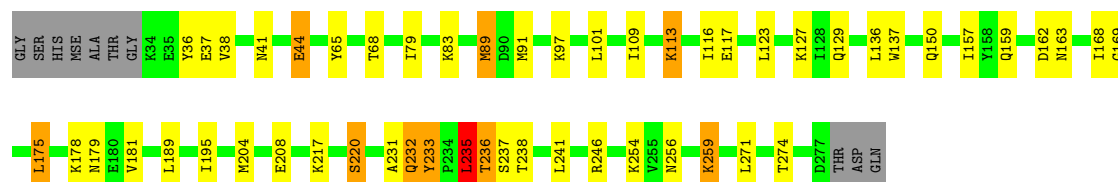
- Molecule 1: YycI protein

Chain H: 77% 15% 5%



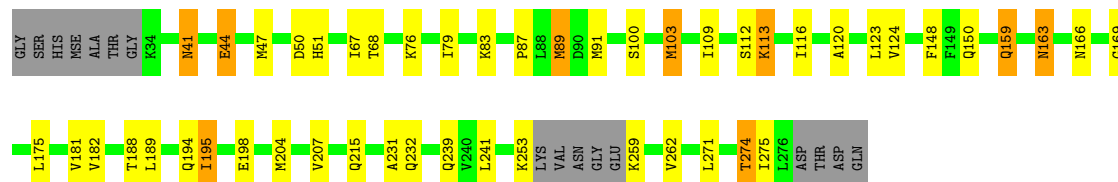
- Molecule 1: YycI protein

Chain I: 75% 17%



• Molecule 1: YycI protein

Chain J: 74% 16% 6%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.79Å 161.92Å 180.16Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	90.00 – 2.89	Depositor
% Data completeness (in resolution range)	92.2 (90.00-2.89)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.262	Depositor
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.245	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
Total number of atoms	23401	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.67% 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:
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	0.60	0/1994	0.75	0/2679
1	B	0.62	0/1976	0.79	1/2656 (0.0%)
1	C	0.60	0/1976	0.78	1/2656 (0.0%)
1	D	0.62	0/1994	0.80	0/2679
1	E	0.61	0/1961	0.77	0/2635
1	F	0.61	0/1987	0.77	1/2668 (0.0%)
1	G	0.58	0/1958	0.78	0/2634
1	H	0.56	0/1994	0.75	0/2679
1	I	0.65	0/2016	0.79	0/2709
1	J	0.62	0/1970	0.76	0/2646
1	K	0.59	0/1942	0.78	1/2612 (0.0%)
1	L	0.57	0/1976	0.75	0/2657
All	All	0.60	0/23744	0.77	4/31910 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	201	ILE	N-CA-C	-5.80	103.73	110.05
1	B	102	LYS	N-CA-C	-5.39	100.39	109.07
1	C	163	ASN	N-CA-C	5.10	112.61	108.07
1	K	273	SER	N-CA-C	5.03	117.75	109.76

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	1965	0	1943	29	0
1	B	1947	0	1926	31	0
1	C	1947	0	1924	34	0
1	D	1965	0	1936	48	0
1	E	1932	0	1913	44	0
1	F	1958	0	1943	30	0
1	G	1929	0	1898	33	0
1	H	1965	0	1936	34	0
1	I	1986	0	1968	39	0
1	J	1941	0	1926	37	0
1	K	1913	0	1885	38	0
1	L	1947	0	1910	31	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
All	All	23401	0	23108	403	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 9.

The worst 5 of 403 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:C:89:MSE:HE2	1:C:91:MSE:HE1	1.22	1.12
1:C:79:ILE:HG23	1:C:103:MSE:HE1	1.33	1.06
1:A:89:MSE:HE2	1:A:91:MSE:HE1	1.34	1.05
1:A:89:MSE:HE2	1:A:91:MSE:CE	1.93	0.97
1:E:160:LYS:HZ1	1:K:176:ASN:HD21	1.12	0.97

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	237/254 (93%)	224 (94%)	12 (5%)	1 (0%)	30	59
1	B	235/254 (92%)	219 (93%)	15 (6%)	1 (0%)	30	59
1	C	235/254 (92%)	220 (94%)	13 (6%)	2 (1%)	14	41
1	D	237/254 (93%)	221 (93%)	15 (6%)	1 (0%)	30	59
1	E	233/254 (92%)	215 (92%)	16 (7%)	2 (1%)	14	41
1	F	236/254 (93%)	219 (93%)	16 (7%)	1 (0%)	30	59
1	G	233/254 (92%)	217 (93%)	16 (7%)	0	100	100
1	H	237/254 (93%)	223 (94%)	12 (5%)	2 (1%)	16	44
1	I	242/254 (95%)	223 (92%)	15 (6%)	4 (2%)	7	26
1	J	234/254 (92%)	221 (94%)	13 (6%)	0	100	100
1	K	231/254 (91%)	218 (94%)	13 (6%)	0	100	100
1	L	235/254 (92%)	222 (94%)	12 (5%)	1 (0%)	30	59
All	All	2825/3048 (93%)	2642 (94%)	168 (6%)	15 (0%)	24	54

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	C	236	THR
1	C	273	SER
1	I	233	TYR
1	B	179	ASN

5.3.2 Protein sidechains [i](#)

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	221/224 (99%)	203 (92%)	18 (8%)	11	33
1	B	219/224 (98%)	200 (91%)	19 (9%)	9	30
1	C	219/224 (98%)	207 (94%)	12 (6%)	19	50
1	D	221/224 (99%)	206 (93%)	15 (7%)	14	42
1	E	217/224 (97%)	198 (91%)	19 (9%)	9	29
1	F	220/224 (98%)	204 (93%)	16 (7%)	13	38
1	G	217/224 (97%)	200 (92%)	17 (8%)	11	35
1	H	221/224 (99%)	209 (95%)	12 (5%)	20	51
1	I	223/224 (100%)	207 (93%)	16 (7%)	13	39
1	J	218/224 (97%)	202 (93%)	16 (7%)	13	38
1	K	215/224 (96%)	203 (94%)	12 (6%)	19	50
1	L	219/224 (98%)	208 (95%)	11 (5%)	22	53
All	All	2630/2688 (98%)	2447 (93%)	183 (7%)	14	40

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	278	THR
1	I	259	LYS
1	H	103	MSE
1	I	83	LYS
1	J	103	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	159	GLN
1	I	194	GLN
1	H	166	ASN
1	I	71	GLN
1	J	214	ASN

5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 6 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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.