



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:47 AM GMT

PDB ID : 2O3O
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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

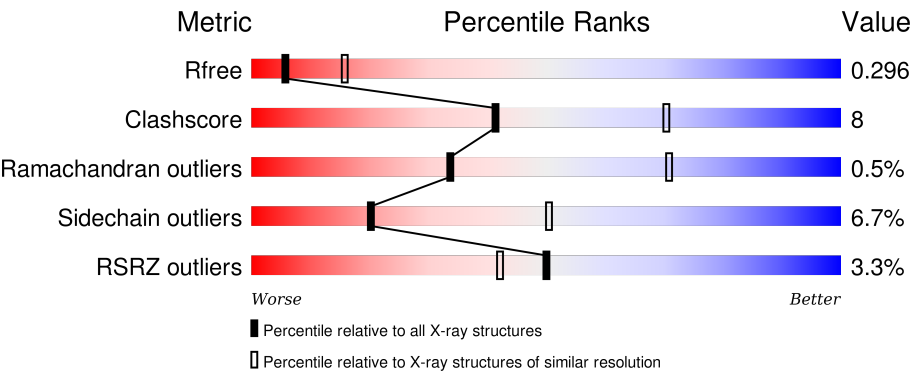
1 Overall quality at a glance i

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))
R _{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	254	
1	B	254	
1	C	254	
1	D	254	
1	E	254	

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Mol	Chain	Length	Quality of chain
1	F	254	<div> <div>4%</div> <div>76%</div> <div>16%</div> <div>6%</div> </div>
1	G	254	<div> <div>4%</div> <div>77%</div> <div>14%</div> <div>7%</div> </div>
1	H	254	<div> <div>4%</div> <div>77%</div> <div>16%</div> <div>5%</div> </div>
1	I	254	<div> <div>2%</div> <div>76%</div> <div>17%</div> <div></div> </div>
1	J	254	<div> <div>%</div> <div>75%</div> <div>16%</div> <div>6%</div> </div>
1	K	254	<div> <div>4%</div> <div>75%</div> <div>16%</div> <div>7%</div> </div>
1	L	254	<div> <div>7%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>

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 (three-letter code: CL) (formula: Cl).

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

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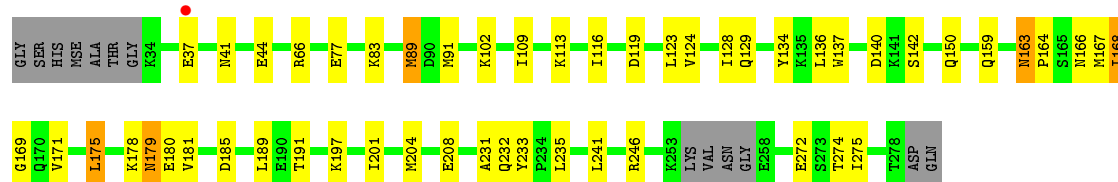
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

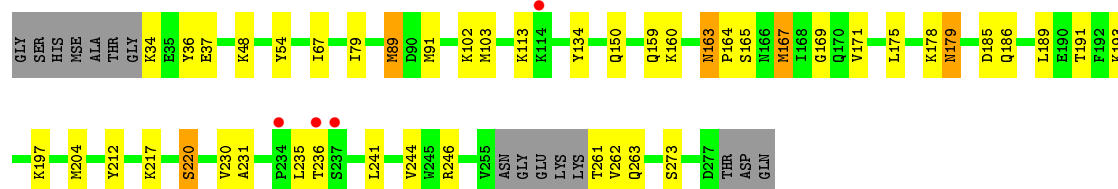
• Molecule 1: YycI protein

Chain A: 




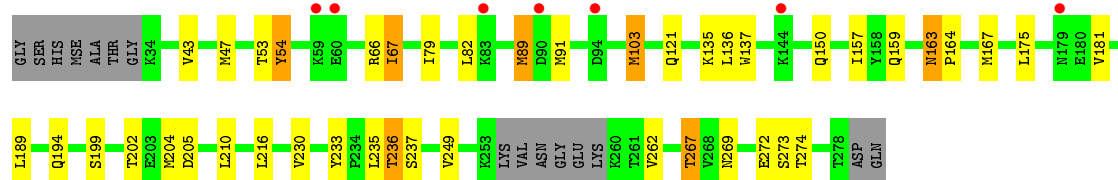
• Molecule 1: YycI protein

Chain B: 



• Molecule 1: YycI protein

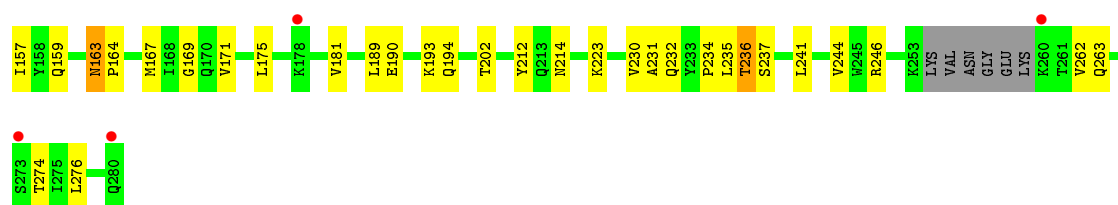
Chain C: 



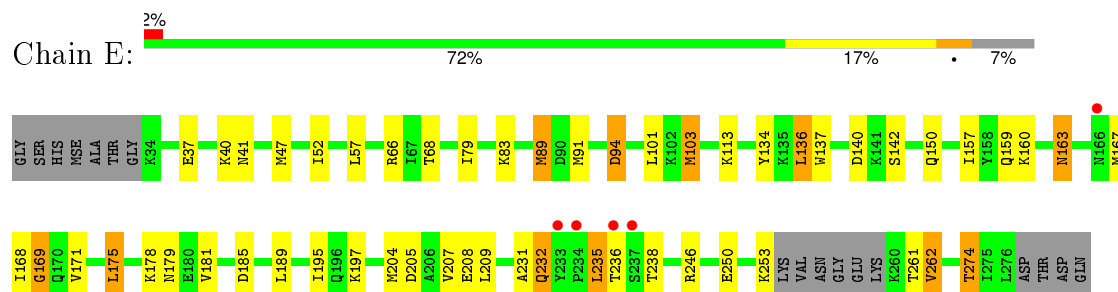
• Molecule 1: YycI protein

Chain D: 

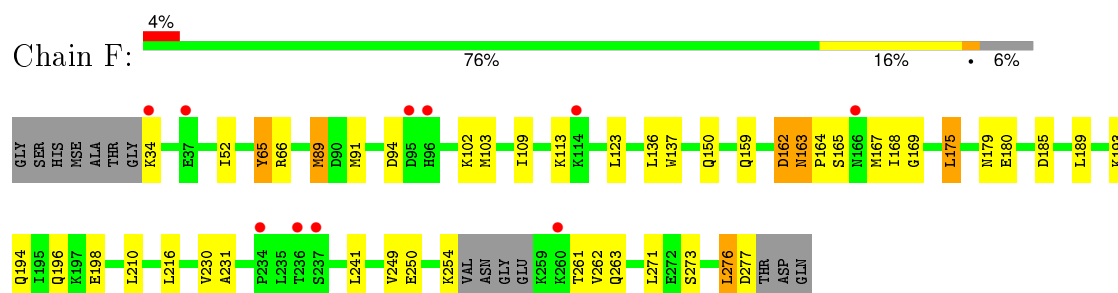




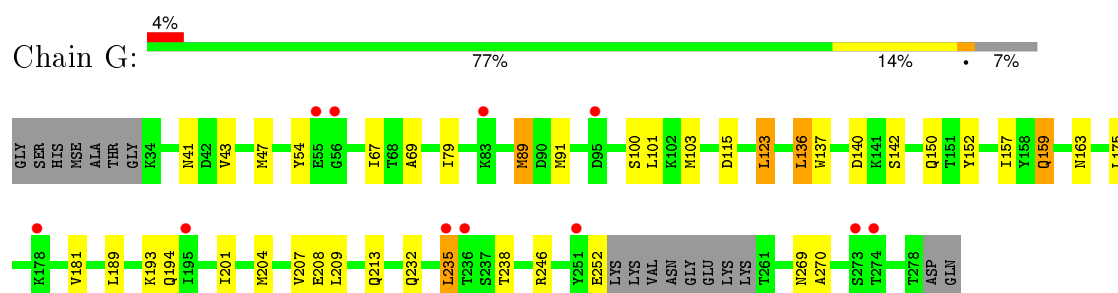
• Molecule 1: YycI protein



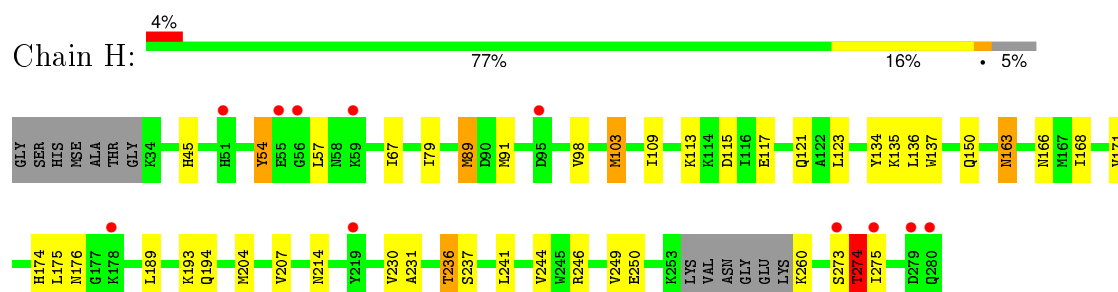
• Molecule 1: YycI protein



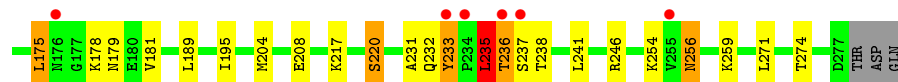
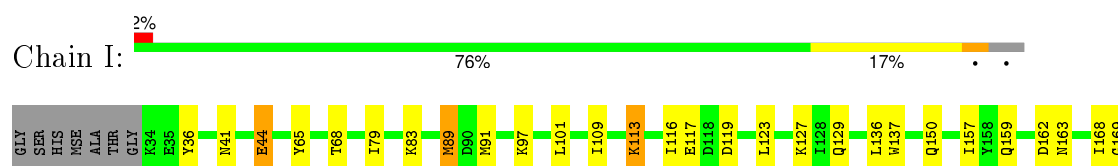
• Molecule 1: YycI protein



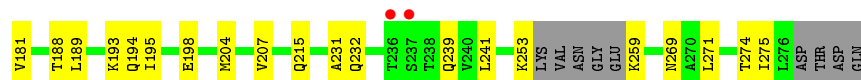
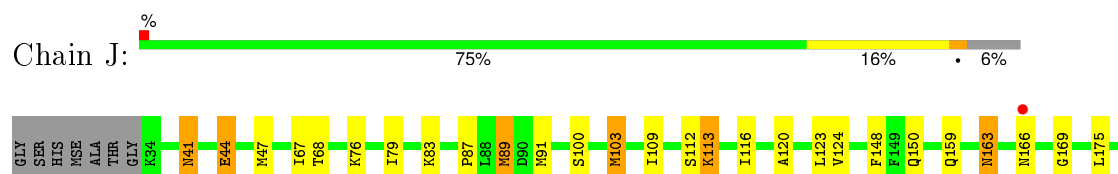
• Molecule 1: YycI protein



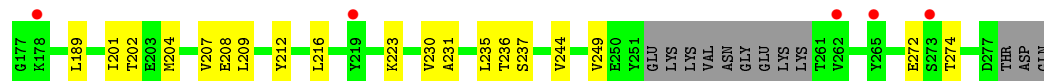
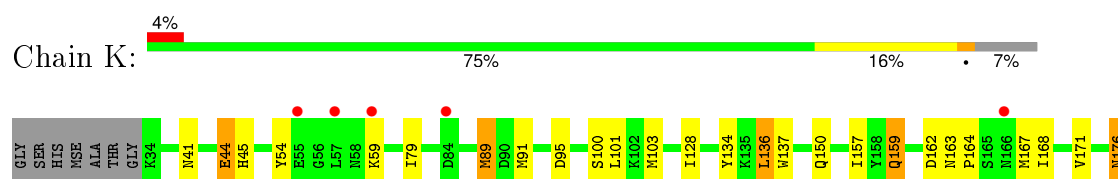
• Molecule 1: YycI protein



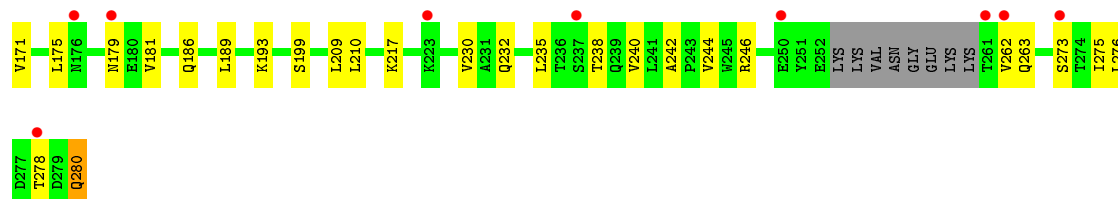
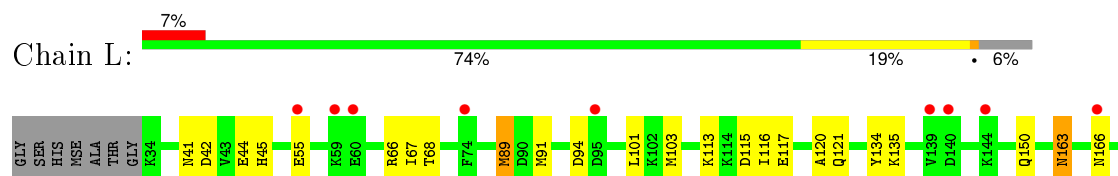
• Molecule 1: YycI protein



• Molecule 1: YycI protein



• Molecule 1: YycI protein



4 Data and refinement statistics

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 48.43 – 2.89	Depositor EDS
% Data completeness (in resolution range)	92.2 (90.00-2.89) 92.2 (48.43-2.89)	Depositor EDS
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 0.255 , 0.296	Depositor DCC
R_{free} test set	3602 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , -10.7	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 71670 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
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, 0.375 respectively for untwinned datasets, and 0.333, 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:
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	0.51	0/1994	0.59	0/2679
1	B	0.50	0/1976	0.61	0/2656
1	C	0.50	0/1976	0.59	0/2656
1	D	0.50	0/1994	0.62	0/2679
1	E	0.50	0/1961	0.60	0/2635
1	F	0.50	0/1987	0.62	0/2668
1	G	0.49	0/1958	0.58	0/2634
1	H	0.47	0/1994	0.57	0/2679
1	I	0.53	0/2016	0.62	0/2709
1	J	0.51	0/1970	0.61	0/2646
1	K	0.48	0/1942	0.58	0/2612
1	L	0.46	0/1976	0.57	0/2657
All	All	0.49	0/23744	0.60	0/31910

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1947	0	1926	30	0
1	C	1947	0	1924	34	0
1	D	1965	0	1936	47	0
1	E	1932	0	1913	44	0
1	F	1958	0	1943	31	0
1	G	1929	0	1898	32	0
1	H	1965	0	1936	33	0
1	I	1986	0	1968	37	0
1	J	1941	0	1926	36	0
1	K	1913	0	1885	36	0
1	L	1947	0	1910	29	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	393	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 8.

All (393) 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:235:LEU:HD13	1:G:235:LEU:HD13	1.49	0.91
1:C:89:MSE:HE2	1:C:91:MSE:CE	2.01	0.90
1:C:150:GLN:HE22	1:C:189:LEU:H	1.20	0.89
1:F:210:LEU:HD23	1:H:275:ILE:HD11	1.55	0.88
1:K:150:GLN:HE22	1:K:189:LEU:H	1.21	0.88
1:A:109:ILE:HD13	1:A:123:LEU:HD11	1.56	0.88
1:L:163:ASN:HD21	1:L:166:ASN:HD22	1.21	0.87
1:I:109:ILE:HG21	1:I:123:LEU:HD13	1.57	0.85
1:K:89:MSE:HE2	1:K:91:MSE:HE1	1.59	0.83
1:H:79:ILE:HG23	1:H:103:MSE:HE1	1.60	0.82
1:H:109:ILE:HD13	1:H:123:LEU:HD11	1.61	0.82
1:K:79:ILE:HG23	1:K:103:MSE:HE1	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:GLN:HE22	1:I:189:LEU:H	1.26	0.81
1:B:150:GLN:HE22	1:B:189:LEU:H	1.28	0.81
1:E:150:GLN:HE22	1:E:189:LEU:H	1.29	0.80
1:F:89:MSE:HE2	1:F:91:MSE:CE	2.12	0.80
1:C:79:ILE:CG2	1:C:103:MSE:HE1	2.12	0.79
1:G:150:GLN:HE22	1:G:189:LEU:H	1.28	0.79
1:J:89:MSE:HE2	1:J:91:MSE:HE1	1.63	0.79
1:F:150:GLN:HE22	1:F:189:LEU:H	1.32	0.78
1:C:89:MSE:CE	1:C:91:MSE:HE1	2.12	0.77
1:F:109:ILE:HD12	1:F:123:LEU:HD11	1.64	0.77
1:E:79:ILE:HG23	1:E:103:MSE:HE1	1.68	0.75
1:J:231:ALA:HA	1:J:241:LEU:HD23	1.66	0.75
1:A:89:MSE:CE	1:A:91:MSE:HE1	2.14	0.74
1:D:91:MSE:HE2	1:D:91:MSE:HA	1.69	0.74
1:K:136:LEU:HD12	1:K:137:TRP:N	2.02	0.74
1:D:89:MSE:HE3	1:D:101:LEU:HD23	1.69	0.74
1:E:160:LYS:HZ1	1:K:176:ASN:HD21	1.33	0.74
1:E:238:THR:HG21	1:G:235:LEU:HD21	1.70	0.73
1:L:150:GLN:HE22	1:L:189:LEU:H	1.36	0.73
1:K:89:MSE:HE2	1:K:91:MSE:CE	2.18	0.73
1:D:79:ILE:HG23	1:D:103:MSE:HE1	1.70	0.72
1:D:124:VAL:HA	1:D:128:ILE:HD12	1.69	0.72
1:D:150:GLN:HE22	1:D:189:LEU:H	1.36	0.72
1:B:89:MSE:HE2	1:B:91:MSE:HE1	1.72	0.71
1:H:163:ASN:HD21	1:H:166:ASN:HD22	1.37	0.71
1:I:79:ILE:HG21	1:I:91:MSE:HE1	1.73	0.71
1:F:89:MSE:HE2	1:F:91:MSE:HE1	1.73	0.70
1:H:150:GLN:HE22	1:H:189:LEU:H	1.39	0.70
1:D:79:ILE:HD13	1:D:91:MSE:HE1	1.74	0.69
1:L:163:ASN:HD21	1:L:166:ASN:ND2	1.91	0.69
1:B:34:LYS:HA	1:D:214:ASN:HD21	1.58	0.69
1:D:164:PRO:HA	1:D:167:MSE:HE2	1.73	0.69
1:E:160:LYS:NZ	1:K:176:ASN:HD21	1.91	0.68
1:K:91:MSE:HE2	1:K:91:MSE:HA	1.75	0.68
1:G:79:ILE:HG23	1:G:103:MSE:HE1	1.74	0.68
1:J:150:GLN:HE22	1:J:189:LEU:H	1.39	0.68
1:H:89:MSE:HE3	1:H:98:VAL:HG11	1.75	0.68
1:J:163:ASN:HD22	1:J:163:ASN:H	1.39	0.67
1:K:204:MSE:HE2	1:K:208:GLU:HG3	1.76	0.67
1:H:109:ILE:HD13	1:H:123:LEU:CD1	2.24	0.67
1:H:91:MSE:HA	1:H:91:MSE:HE2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:MSE:HE2	1:G:208:GLU:HG3	1.76	0.67
1:B:89:MSE:HE2	1:B:91:MSE:CE	2.25	0.66
1:B:235:LEU:HD13	1:D:235:LEU:HD12	1.77	0.66
1:I:109:ILE:HD13	1:I:123:LEU:CD1	2.24	0.66
1:K:216:LEU:CD2	1:K:249:VAL:HG21	2.26	0.66
1:I:136:LEU:HD12	1:I:137:TRP:N	2.11	0.66
1:H:163:ASN:HD21	1:H:166:ASN:ND2	1.94	0.66
1:E:91:MSE:HE2	1:E:91:MSE:HA	1.78	0.66
1:D:231:ALA:HA	1:D:241:LEU:HD23	1.79	0.65
1:F:89:MSE:HE2	1:F:91:MSE:HE2	1.78	0.65
1:F:163:ASN:HD22	1:F:163:ASN:H	1.43	0.65
1:E:136:LEU:HD12	1:E:137:TRP:N	2.12	0.65
1:C:150:GLN:NE2	1:C:189:LEU:H	1.94	0.65
1:K:216:LEU:HD21	1:K:249:VAL:HG21	1.79	0.64
1:I:217:LYS:O	1:I:220:SER:OG	2.16	0.64
1:F:89:MSE:CE	1:F:91:MSE:HE1	2.27	0.64
1:F:109:ILE:HD12	1:F:123:LEU:CD1	2.28	0.64
1:J:47:MSE:HE1	1:J:207:VAL:HG12	1.80	0.64
1:J:89:MSE:HE2	1:J:91:MSE:CE	2.28	0.63
1:G:79:ILE:HD13	1:G:89:MSE:HE1	1.80	0.63
1:G:136:LEU:HD12	1:G:137:TRP:N	2.13	0.63
1:E:68:THR:HG23	1:E:195:ILE:HG21	1.82	0.61
1:L:91:MSE:HE2	1:L:91:MSE:HA	1.81	0.61
1:C:230:VAL:HG11	1:C:267:THR:HG21	1.82	0.61
1:L:280:GLN:C	1:L:280:GLN:HE21	2.04	0.61
1:F:159:GLN:HE22	1:F:169:GLY:H	1.49	0.61
1:H:273:SER:O	1:H:274:THR:HG23	2.00	0.61
1:D:79:ILE:CG2	1:D:103:MSE:HE1	2.30	0.61
1:A:191:THR:O	1:A:191:THR:HG22	2.01	0.61
1:I:232:GLN:O	1:I:233:TYR:HB3	2.01	0.61
1:J:124:VAL:HG21	1:J:148:PHE:CZ	2.36	0.60
1:B:159:GLN:HE22	1:B:169:GLY:H	1.50	0.60
1:J:175:LEU:CD2	1:J:181:VAL:HG22	2.32	0.60
1:A:163:ASN:HD21	1:A:166:ASN:CG	2.04	0.60
1:D:230:VAL:HG13	1:D:244:VAL:HG11	1.83	0.60
1:E:238:THR:HG21	1:G:235:LEU:CD2	2.32	0.59
1:L:89:MSE:HE3	1:L:101:LEU:HD23	1.84	0.59
1:A:150:GLN:HE22	1:A:189:LEU:H	1.50	0.59
1:B:191:THR:HG22	1:B:193:LYS:HE3	1.85	0.59
1:C:91:MSE:HA	1:C:91:MSE:HE2	1.84	0.59
1:C:164:PRO:HA	1:C:167:MSE:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:275:ILE:HG22	1:H:275:ILE:O	2.02	0.59
1:I:109:ILE:CD1	1:I:123:LEU:HD11	2.33	0.59
1:D:175:LEU:CD2	1:D:181:VAL:HG22	2.33	0.58
1:I:123:LEU:HD12	1:I:127:LYS:HD2	1.84	0.58
1:B:160:LYS:NZ	1:H:176:ASN:OD1	2.35	0.58
1:J:79:ILE:HG23	1:J:103:MSE:HE1	1.84	0.58
1:E:238:THR:CG2	1:G:235:LEU:HD21	2.33	0.58
1:E:89:MSE:HE2	1:E:91:MSE:HE1	1.84	0.58
1:E:175:LEU:CD2	1:E:181:VAL:HG22	2.34	0.58
1:H:67:ILE:HD12	1:H:194:GLN:HG2	1.84	0.58
1:E:89:MSE:HE2	1:E:91:MSE:CE	2.34	0.57
1:B:164:PRO:HA	1:B:167:MSE:HE2	1.86	0.57
1:I:150:GLN:NE2	1:I:189:LEU:H	2.01	0.57
1:E:134:TYR:CD2	1:E:171:VAL:HG23	2.40	0.57
1:F:196:GLN:NE2	1:F:198:GLU:OE2	2.37	0.57
1:E:160:LYS:NZ	1:K:176:ASN:ND2	2.52	0.57
1:H:168:ILE:HD13	1:H:231:ALA:HB2	1.86	0.57
1:I:175:LEU:HD23	1:I:181:VAL:HG22	1.87	0.57
1:G:69:ALA:O	1:G:238:THR:HG23	2.05	0.57
1:D:236:THR:HG22	1:D:237:SER:N	2.20	0.56
1:A:89:MSE:HE2	1:A:91:MSE:HE2	1.86	0.56
1:D:89:MSE:HE3	1:D:101:LEU:CD2	2.34	0.56
1:I:109:ILE:HD13	1:I:123:LEU:HD11	1.87	0.56
1:G:204:MSE:HE3	1:G:207:VAL:HB	1.87	0.56
1:E:168:ILE:HD13	1:E:231:ALA:HB2	1.88	0.56
1:B:163:ASN:HD22	1:B:163:ASN:N	2.04	0.56
1:E:168:ILE:CD1	1:E:231:ALA:HB2	2.36	0.56
1:E:66:ARG:HE	1:E:232:GLN:HE22	1.53	0.56
1:K:89:MSE:CE	1:K:91:MSE:HE1	2.34	0.56
1:C:67:ILE:HD12	1:C:194:GLN:HG2	1.88	0.56
1:A:204:MSE:HE3	1:A:208:GLU:HG3	1.88	0.55
1:C:79:ILE:HG23	1:C:103:MSE:CE	2.22	0.55
1:J:44:GLU:OE2	1:J:204:MSE:HE2	2.06	0.55
1:F:34:LYS:HA	1:H:214:ASN:HD21	1.69	0.55
1:C:202:THR:HG23	1:C:205:ASP:OD2	2.06	0.55
1:H:163:ASN:N	1:H:163:ASN:HD22	2.05	0.55
1:K:236:THR:HG22	1:K:237:SER:N	2.22	0.55
1:I:89:MSE:HE2	1:I:91:MSE:CE	2.37	0.55
1:A:159:GLN:HE22	1:A:169:GLY:H	1.54	0.55
1:G:67:ILE:HD12	1:G:194:GLN:HG2	1.87	0.54
1:K:59:LYS:O	1:K:202:THR:HG21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168:ILE:HD13	1:K:231:ALA:HB2	1.89	0.54
1:I:68:THR:HG23	1:I:195:ILE:HG21	1.89	0.54
1:E:150:GLN:NE2	1:E:189:LEU:H	2.03	0.54
1:J:68:THR:HG23	1:J:195:ILE:HD13	1.90	0.54
1:L:232:GLN:NE2	1:L:242:ALA:HB2	2.23	0.54
1:B:79:ILE:HG23	1:B:103:MSE:HE1	1.90	0.54
1:K:150:GLN:NE2	1:K:189:LEU:H	1.98	0.53
1:L:116:ILE:HD12	1:L:179:ASN:ND2	2.24	0.53
1:H:89:MSE:HE2	1:H:91:MSE:HE1	1.91	0.53
1:K:134:TYR:CE2	1:K:171:VAL:HG23	2.44	0.53
1:D:89:MSE:HE2	1:D:91:MSE:CE	2.39	0.53
1:C:235:LEU:O	1:C:236:THR:C	2.47	0.53
1:A:178:LYS:O	1:A:180:GLU:N	2.42	0.53
1:J:67:ILE:HG22	1:J:194:GLN:HA	1.90	0.53
1:B:217:LYS:O	1:B:220:SER:OG	2.26	0.53
1:I:238:THR:HG21	1:K:235:LEU:HD22	1.91	0.53
1:I:236:THR:HG22	1:I:237:SER:H	1.74	0.52
1:L:66:ARG:C	1:L:67:ILE:HD13	2.28	0.52
1:F:261:THR:HG22	1:F:261:THR:O	2.10	0.52
1:I:159:GLN:HE22	1:I:169:GLY:H	1.56	0.52
1:C:82:LEU:HD12	1:C:103:MSE:HE2	1.91	0.52
1:K:204:MSE:HE3	1:K:207:VAL:HB	1.91	0.52
1:L:171:VAL:HG22	1:L:186:GLN:HG3	1.91	0.52
1:H:236:THR:HG22	1:H:237:SER:N	2.24	0.52
1:A:91:MSE:HE2	1:A:91:MSE:HA	1.92	0.52
1:L:280:GLN:HE21	1:L:280:GLN:CA	2.23	0.52
1:F:136:LEU:HD12	1:F:137:TRP:N	2.25	0.52
1:E:167:MSE:HE1	1:E:185:ASP:CB	2.40	0.52
1:E:140:ASP:OD1	1:E:142:SER:OG	2.27	0.52
1:H:168:ILE:CD1	1:H:231:ALA:HB2	2.40	0.52
1:D:136:LEU:HD12	1:D:137:TRP:N	2.25	0.51
1:J:215:GLN:HE21	1:L:275:ILE:HD13	1.74	0.51
1:F:175:LEU:HA	1:F:180:GLU:O	2.10	0.51
1:G:150:GLN:NE2	1:G:189:LEU:H	2.04	0.51
1:F:164:PRO:HA	1:F:167:MSE:HE2	1.92	0.51
1:I:178:LYS:O	1:I:179:ASN:C	2.49	0.51
1:E:274:THR:OG1	1:G:213:GLN:NE2	2.43	0.51
1:D:124:VAL:HG22	1:D:128:ILE:CD1	2.40	0.51
1:J:231:ALA:HB1	1:J:239:GLN:NE2	2.26	0.51
1:J:159:GLN:HE22	1:J:169:GLY:H	1.57	0.51
1:I:41:ASN:HA	1:I:44:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:LEU:HD22	1:G:103:MSE:SE	2.60	0.51
1:H:89:MSE:HE2	1:H:91:MSE:CE	2.40	0.51
1:I:231:ALA:HA	1:I:241:LEU:HD23	1.93	0.51
1:G:79:ILE:HD13	1:G:89:MSE:CE	2.39	0.51
1:D:150:GLN:NE2	1:D:189:LEU:H	2.07	0.51
1:E:68:THR:CG2	1:E:195:ILE:HG21	2.40	0.50
1:G:152:TYR:OH	1:G:194:GLN:NE2	2.44	0.50
1:D:92:PRO:HB3	1:D:98:VAL:HG23	1.92	0.50
1:D:89:MSE:CE	1:D:101:LEU:CD2	2.89	0.50
1:D:163:ASN:HB2	1:D:164:PRO:HD2	1.93	0.50
1:E:274:THR:CG2	1:G:209:LEU:HD21	2.42	0.50
1:G:91:MSE:HE2	1:G:91:MSE:HA	1.93	0.50
1:L:68:THR:HG22	1:L:240:VAL:HG22	1.94	0.50
1:J:120:ALA:O	1:J:124:VAL:HG23	2.12	0.50
1:E:167:MSE:HE1	1:E:185:ASP:HB3	1.94	0.50
1:C:235:LEU:O	1:C:237:SER:N	2.45	0.49
1:L:41:ASN:HA	1:L:44:GLU:HB2	1.93	0.49
1:B:91:MSE:HA	1:B:91:MSE:HE2	1.95	0.49
1:E:68:THR:HG23	1:E:195:ILE:CG2	2.42	0.49
1:E:261:THR:O	1:E:261:THR:HG22	2.11	0.49
1:J:163:ASN:H	1:J:163:ASN:ND2	2.10	0.49
1:J:112:SER:OG	1:J:113:LYS:N	2.45	0.49
1:L:175:LEU:CD2	1:L:181:VAL:HG22	2.42	0.49
1:C:136:LEU:HD12	1:C:137:TRP:N	2.27	0.49
1:K:136:LEU:HD12	1:K:136:LEU:C	2.32	0.49
1:J:163:ASN:HD21	1:J:166:ASN:ND2	2.11	0.49
1:L:230:VAL:HG13	1:L:244:VAL:HG21	1.95	0.49
1:B:231:ALA:HA	1:B:241:LEU:HD23	1.95	0.49
1:H:231:ALA:HA	1:H:241:LEU:HD23	1.95	0.49
1:L:134:TYR:CD2	1:L:171:VAL:HG23	2.48	0.49
1:L:262:VAL:HG12	1:L:263:GLN:N	2.27	0.49
1:C:66:ARG:C	1:C:67:ILE:HD13	2.32	0.48
1:C:43:VAL:O	1:C:47:MSE:HG3	2.12	0.48
1:B:36:TYR:HB2	1:D:212:TYR:CE1	2.48	0.48
1:D:67:ILE:HD12	1:D:194:GLN:HG2	1.93	0.48
1:H:150:GLN:NE2	1:H:189:LEU:H	2.09	0.48
1:H:134:TYR:CE2	1:H:171:VAL:HG23	2.48	0.48
1:E:94:ASP:N	1:E:94:ASP:OD1	2.47	0.48
1:A:136:LEU:HD12	1:A:137:TRP:H	1.78	0.48
1:B:261:THR:O	1:B:261:THR:HG22	2.14	0.48
1:I:136:LEU:HD12	1:I:137:TRP:H	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LEU:HD22	1:D:181:VAL:HG22	1.94	0.48
1:E:159:GLN:HE22	1:E:169:GLY:H	1.61	0.48
1:H:136:LEU:HD12	1:H:137:TRP:N	2.29	0.48
1:E:89:MSE:CE	1:E:91:MSE:HE1	2.43	0.48
1:C:54:TYR:CE2	1:C:204:MSE:HE1	2.49	0.48
1:A:163:ASN:HD21	1:A:166:ASN:ND2	2.12	0.48
1:K:157:ILE:O	1:K:159:GLN:HG2	2.14	0.48
1:H:121:GLN:HE22	1:H:135:LYS:HA	1.79	0.48
1:E:40:LYS:HE2	1:E:205:ASP:OD1	2.13	0.48
1:A:163:ASN:HD22	1:A:163:ASN:C	2.17	0.48
1:H:230:VAL:HG13	1:H:244:VAL:HG11	1.94	0.48
1:A:231:ALA:HA	1:A:241:LEU:HD23	1.96	0.48
1:D:124:VAL:HG22	1:D:128:ILE:HD12	1.95	0.48
1:C:175:LEU:HD23	1:C:181:VAL:HA	1.96	0.48
1:B:171:VAL:HG22	1:B:186:GLN:HG3	1.96	0.48
1:C:216:LEU:CD2	1:C:249:VAL:HG21	2.44	0.48
1:K:164:PRO:HB3	1:K:167:MSE:HE2	1.96	0.48
1:F:163:ASN:ND2	1:F:163:ASN:H	2.11	0.47
1:D:163:ASN:C	1:D:163:ASN:HD22	2.18	0.47
1:D:66:ARG:C	1:D:67:ILE:HD13	2.35	0.47
1:D:87:PRO:N	1:D:103:MSE:HE3	2.29	0.47
1:D:157:ILE:O	1:D:159:GLN:HG3	2.14	0.47
1:D:109:ILE:HD12	1:D:123:LEU:HD11	1.96	0.47
1:G:89:MSE:HE2	1:G:91:MSE:CE	2.45	0.47
1:E:157:ILE:O	1:E:159:GLN:HG3	2.14	0.47
1:C:216:LEU:HD21	1:C:249:VAL:HG21	1.95	0.47
1:H:79:ILE:HG23	1:H:103:MSE:CE	2.38	0.47
1:E:57:LEU:HD11	1:E:207:VAL:HG21	1.96	0.47
1:J:150:GLN:NE2	1:J:189:LEU:H	2.09	0.47
1:J:47:MSE:HE1	1:J:207:VAL:CG1	2.44	0.47
1:E:134:TYR:CE2	1:E:171:VAL:HG23	2.50	0.47
1:I:89:MSE:HE2	1:I:91:MSE:HE1	1.97	0.47
1:A:201:ILE:HG22	1:A:272:GLU:HB2	1.97	0.47
1:B:89:MSE:CE	1:B:91:MSE:HE1	2.41	0.47
1:A:178:LYS:O	1:A:179:ASN:C	2.53	0.47
1:B:134:TYR:CE2	1:B:171:VAL:HG23	2.51	0.46
1:G:79:ILE:HG12	1:G:101:LEU:HD21	1.98	0.46
1:C:272:GLU:O	1:C:274:THR:HG23	2.15	0.46
1:F:109:ILE:HG21	1:F:123:LEU:HD13	1.96	0.46
1:G:204:MSE:HE2	1:G:208:GLU:CG	2.44	0.46
1:B:163:ASN:HD22	1:B:163:ASN:H	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:THR:O	1:B:191:THR:HG22	2.16	0.46
1:D:89:MSE:HE2	1:D:91:MSE:HE1	1.97	0.46
1:H:117:GLU:HB3	1:H:136:LEU:HD23	1.97	0.46
1:K:204:MSE:O	1:K:204:MSE:HE3	2.16	0.46
1:E:178:LYS:O	1:E:179:ASN:C	2.55	0.46
1:F:249:VAL:HG12	1:F:250:GLU:N	2.31	0.45
1:F:231:ALA:HA	1:F:241:LEU:HD23	1.98	0.45
1:J:79:ILE:CG2	1:J:103:MSE:HE1	2.46	0.45
1:K:201:ILE:HG22	1:K:272:GLU:HG3	1.97	0.45
1:C:157:ILE:O	1:C:159:GLN:HG3	2.16	0.45
1:A:164:PRO:HB3	1:A:167:MSE:HE2	1.98	0.45
1:F:136:LEU:HD12	1:F:137:TRP:H	1.81	0.45
1:H:57:LEU:HD11	1:H:207:VAL:HG21	1.98	0.45
1:F:163:ASN:N	1:F:163:ASN:HD22	2.09	0.45
1:A:275:ILE:HD11	1:C:210:LEU:HD23	1.98	0.45
1:A:175:LEU:HD22	1:A:181:VAL:HG22	1.99	0.45
1:E:150:GLN:HE22	1:E:189:LEU:N	2.07	0.45
1:D:234:PRO:O	1:D:235:LEU:HD23	2.17	0.45
1:G:201:ILE:HG23	1:G:270:ALA:O	2.16	0.45
1:C:79:ILE:HD13	1:C:89:MSE:CE	2.46	0.45
1:I:116:ILE:HG23	1:I:117:GLU:N	2.31	0.45
1:I:233:TYR:HE1	1:I:235:LEU:HD12	1.81	0.45
1:C:136:LEU:HD12	1:C:137:TRP:H	1.82	0.45
1:B:150:GLN:NE2	1:B:189:LEU:H	2.07	0.45
1:D:134:TYR:CE2	1:D:171:VAL:HG23	2.52	0.45
1:K:41:ASN:HA	1:K:44:GLU:HB2	1.99	0.45
1:H:163:ASN:N	1:H:163:ASN:ND2	2.65	0.44
1:G:140:ASP:OD1	1:G:142:SER:OG	2.30	0.44
1:G:123:LEU:HD12	1:G:123:LEU:O	2.18	0.44
1:L:89:MSE:CE	1:L:101:LEU:CD2	2.96	0.44
1:C:67:ILE:N	1:C:67:ILE:HD13	2.32	0.44
1:L:117:GLU:O	1:L:120:ALA:HB3	2.18	0.44
1:K:216:LEU:HD22	1:K:249:VAL:HG21	2.00	0.44
1:I:68:THR:HG23	1:I:195:ILE:CG2	2.46	0.44
1:I:274:THR:HB	1:K:209:LEU:HD21	1.99	0.44
1:B:212:TYR:CE1	1:D:36:TYR:HA	2.52	0.44
1:A:233:TYR:HH	1:C:233:TYR:HH	1.57	0.44
1:A:140:ASP:OD1	1:A:142:SER:OG	2.32	0.44
1:H:54:TYR:HB2	1:H:57:LEU:HD12	1.98	0.44
1:B:54:TYR:CZ	1:B:204:MSE:HE1	2.52	0.44
1:E:204:MSE:HE2	1:E:208:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:HD12	1:A:179:ASN:ND2	2.33	0.43
1:K:89:MSE:HE3	1:K:101:LEU:HD23	2.00	0.43
1:J:87:PRO:CB	1:J:91:MSE:HE1	2.48	0.43
1:J:198:GLU:OE1	1:J:271:LEU:HD22	2.18	0.43
1:F:91:MSE:HA	1:F:91:MSE:HE2	2.00	0.43
1:E:160:LYS:HZ3	1:K:176:ASN:ND2	2.17	0.43
1:J:163:ASN:HD22	1:J:163:ASN:N	2.06	0.43
1:I:89:MSE:HE3	1:I:101:LEU:CD2	2.48	0.43
1:G:43:VAL:O	1:G:47:MSE:HG3	2.18	0.43
1:B:102:LYS:HG3	1:B:185:ASP:OD1	2.19	0.43
1:J:274:THR:HB	1:L:209:LEU:HD21	2.01	0.43
1:C:163:ASN:N	1:C:163:ASN:HD22	2.14	0.43
1:G:157:ILE:O	1:G:159:GLN:HG2	2.19	0.43
1:B:230:VAL:HG13	1:B:244:VAL:HG11	1.99	0.43
1:D:163:ASN:HB2	1:D:164:PRO:CD	2.48	0.43
1:C:272:GLU:O	1:C:274:THR:N	2.52	0.43
1:D:61:ALA:HA	1:D:202:THR:HG22	2.01	0.43
1:J:150:GLN:HE22	1:J:188:THR:HA	1.83	0.43
1:E:89:MSE:HE3	1:E:101:LEU:HD23	2.00	0.43
1:E:175:LEU:HD22	1:E:181:VAL:HG22	2.01	0.43
1:A:102:LYS:HG3	1:A:185:ASP:OD1	2.18	0.43
1:I:109:ILE:HD12	1:I:123:LEU:HD11	2.00	0.43
1:F:102:LYS:HG3	1:F:185:ASP:OD1	2.19	0.43
1:L:235:LEU:O	1:L:238:THR:N	2.48	0.42
1:J:79:ILE:HG23	1:J:103:MSE:CE	2.48	0.42
1:J:275:ILE:HD11	1:L:210:LEU:HD23	2.01	0.42
1:C:89:MSE:O	1:C:91:MSE:HE3	2.19	0.42
1:G:67:ILE:HD13	1:G:67:ILE:N	2.34	0.42
1:D:67:ILE:HD13	1:D:67:ILE:N	2.34	0.42
1:J:253:LYS:C	1:J:259:LYS:HA	2.40	0.42
1:G:175:LEU:HD23	1:G:181:VAL:HG22	2.01	0.42
1:D:159:GLN:HE22	1:D:169:GLY:H	1.67	0.42
1:B:178:LYS:O	1:B:179:ASN:C	2.57	0.42
1:D:136:LEU:C	1:D:136:LEU:HD12	2.40	0.42
1:E:47:MSE:HE3	1:E:52:ILE:HG21	2.02	0.42
1:I:113:LYS:NZ	1:I:178:LYS:HE3	2.35	0.42
1:J:109:ILE:HD13	1:J:123:LEU:HD13	2.01	0.42
1:A:124:VAL:O	1:A:128:ILE:HB	2.20	0.42
1:J:87:PRO:HB2	1:J:91:MSE:HE1	2.01	0.41
1:E:142:SER:CB	1:K:164:PRO:HG2	2.50	0.41
1:B:67:ILE:HG13	1:B:241:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ASP:N	1:D:94:ASP:OD1	2.52	0.41
1:I:89:MSE:HE2	1:I:91:MSE:HE2	2.01	0.41
1:I:117:GLU:HG2	1:I:136:LEU:HD21	2.01	0.41
1:L:89:MSE:HE2	1:L:91:MSE:CE	2.50	0.41
1:L:275:ILE:C	1:L:276:LEU:HD23	2.41	0.41
1:H:174:HIS:C	1:H:175:LEU:HD23	2.41	0.41
1:D:65:TYR:HB2	1:D:67:ILE:HD11	2.02	0.41
1:C:54:TYR:CD2	1:C:204:MSE:HE1	2.55	0.41
1:G:123:LEU:HD12	1:G:123:LEU:C	2.41	0.41
1:F:262:VAL:HG12	1:F:263:GLN:N	2.36	0.41
1:A:136:LEU:HD12	1:A:137:TRP:N	2.35	0.41
1:L:121:GLN:HE22	1:L:135:LYS:HA	1.84	0.41
1:B:89:MSE:HE2	1:B:91:MSE:HE2	2.01	0.41
1:F:66:ARG:HG3	1:F:271:LEU:HD11	2.01	0.41
1:D:230:VAL:HG13	1:D:244:VAL:CG1	2.50	0.41
1:D:230:VAL:CG1	1:D:244:VAL:HG11	2.48	0.41
1:I:254:LYS:HA	1:I:259:LYS:HA	2.03	0.41
1:K:230:VAL:HG13	1:K:244:VAL:HG11	2.01	0.41
1:A:159:GLN:NE2	1:A:169:GLY:H	2.18	0.41
1:A:168:ILE:CD1	1:A:231:ALA:HB2	2.51	0.41
1:I:204:MSE:HE2	1:I:208:GLU:HG3	2.03	0.41
1:J:175:LEU:HD21	1:J:181:VAL:HG22	1.99	0.41
1:K:134:TYR:CD2	1:K:171:VAL:HG23	2.56	0.41
1:G:175:LEU:CD2	1:G:181:VAL:HG22	2.50	0.41
1:I:36:TYR:HB3	1:K:212:TYR:O	2.20	0.41
1:I:271:LEU:HD23	1:I:271:LEU:HA	1.96	0.41
1:G:89:MSE:HE2	1:G:91:MSE:HE2	2.02	0.41
1:K:128:ILE:HD13	1:K:171:VAL:HG11	2.03	0.41
1:D:72:LYS:HD3	1:D:190:GLU:OE2	2.21	0.41
1:B:262:VAL:HG12	1:B:263:GLN:N	2.36	0.41
1:I:150:GLN:HE22	1:I:189:LEU:N	2.04	0.41
1:K:159:GLN:HE22	1:K:168:ILE:H	1.69	0.41
1:H:249:VAL:HG12	1:H:250:GLU:N	2.36	0.41
1:E:250:GLU:HB2	1:E:262:VAL:O	2.21	0.41
1:L:134:TYR:CE2	1:L:171:VAL:HG23	2.56	0.40
1:F:168:ILE:CD1	1:F:231:ALA:HB2	2.51	0.40
1:F:162:ASP:N	1:F:162:ASP:OD1	2.55	0.40
1:A:134:TYR:CE2	1:A:171:VAL:HG23	2.57	0.40
1:F:210:LEU:HD13	1:F:216:LEU:HD21	2.04	0.40
1:J:41:ASN:HA	1:J:44:GLU:HB2	2.03	0.40
1:F:276:LEU:HD23	1:F:276:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:150:GLN:HE22	1:J:189:LEU:N	2.13	0.40
1:F:65:TYR:CZ	1:F:194:GLN:NE2	2.90	0.40
1:D:235:LEU:O	1:D:236:THR:C	2.57	0.40
1:L:66:ARG:O	1:L:67:ILE:HD13	2.21	0.40
1:I:157:ILE:O	1:I:159:GLN:HG3	2.22	0.40
1:D:262:VAL:HG12	1:D:263:GLN:N	2.36	0.40
1:J:231:ALA:CA	1:J:241:LEU:HD23	2.46	0.40
1:L:175:LEU:HD22	1:L:181:VAL:HG22	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	237/254 (93%)	224 (94%)	12 (5%)	1 (0%)	39	74
1	B	235/254 (92%)	219 (93%)	15 (6%)	1 (0%)	39	74
1	C	235/254 (92%)	220 (94%)	13 (6%)	2 (1%)	21	57
1	D	237/254 (93%)	221 (93%)	15 (6%)	1 (0%)	39	74
1	E	233/254 (92%)	215 (92%)	16 (7%)	2 (1%)	21	57
1	F	236/254 (93%)	219 (93%)	16 (7%)	1 (0%)	39	74
1	G	233/254 (92%)	217 (93%)	16 (7%)	0	100	100
1	H	237/254 (93%)	223 (94%)	12 (5%)	2 (1%)	24	60
1	I	242/254 (95%)	223 (92%)	15 (6%)	4 (2%)	11	38
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%)	39	74
All	All	2825/3048 (93%)	2642 (94%)	168 (6%)	15 (0%)	34	71

All (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
1	D	236	THR
1	F	179	ASN
1	I	235	LEU
1	H	236	THR
1	L	273	SER
1	I	256	ASN
1	E	163	ASN
1	H	274	THR
1	I	162	ASP
1	E	169	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/224 (99%)	203 (92%)	18 (8%)	15	39
1	B	219/224 (98%)	206 (94%)	13 (6%)	24	58
1	C	219/224 (98%)	207 (94%)	12 (6%)	27	61
1	D	221/224 (99%)	207 (94%)	14 (6%)	22	54
1	E	217/224 (97%)	198 (91%)	19 (9%)	12	35
1	F	220/224 (98%)	204 (93%)	16 (7%)	17	45
1	G	217/224 (97%)	202 (93%)	15 (7%)	19	48
1	H	221/224 (99%)	209 (95%)	12 (5%)	27	62
1	I	223/224 (100%)	207 (93%)	16 (7%)	18	46
1	J	218/224 (97%)	205 (94%)	13 (6%)	24	57
1	K	215/224 (96%)	202 (94%)	13 (6%)	24	57
1	L	219/224 (98%)	204 (93%)	15 (7%)	20	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2630/2688 (98%)	2454 (93%)	176 (7%)	20	50

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	41	ASN
1	A	44	GLU
1	A	66	ARG
1	A	77	GLU
1	A	83	LYS
1	A	89	MSE
1	A	113	LYS
1	A	119	ASP
1	A	129	GLN
1	A	163	ASN
1	A	168	ILE
1	A	175	LEU
1	A	197	LYS
1	A	232	GLN
1	A	235	LEU
1	A	246	ARG
1	A	274	THR
1	B	37	GLU
1	B	48	LYS
1	B	89	MSE
1	B	113	LYS
1	B	163	ASN
1	B	165	SER
1	B	167	MSE
1	B	175	LEU
1	B	197	LYS
1	B	220	SER
1	B	236	THR
1	B	246	ARG
1	B	273	SER
1	C	53	THR
1	C	54	TYR
1	C	67	ILE
1	C	89	MSE
1	C	103	MSE
1	C	121	GLN

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Mol	Chain	Res	Type
1	C	135	LYS
1	C	163	ASN
1	C	199	SER
1	C	262	VAL
1	C	267	THR
1	C	269	ASN
1	D	83	LYS
1	D	89	MSE
1	D	94	ASP
1	D	103	MSE
1	D	113	LYS
1	D	115	ASP
1	D	136	LEU
1	D	163	ASN
1	D	193	LYS
1	D	223	LYS
1	D	232	GLN
1	D	246	ARG
1	D	274	THR
1	D	276	LEU
1	E	37	GLU
1	E	41	ASN
1	E	83	LYS
1	E	89	MSE
1	E	94	ASP
1	E	103	MSE
1	E	113	LYS
1	E	136	LEU
1	E	163	ASN
1	E	175	LEU
1	E	197	LYS
1	E	209	LEU
1	E	232	GLN
1	E	235	LEU
1	E	236	THR
1	E	246	ARG
1	E	253	LYS
1	E	262	VAL
1	E	274	THR
1	F	52	ILE
1	F	65	TYR
1	F	89	MSE

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Mol	Chain	Res	Type
1	F	94	ASP
1	F	103	MSE
1	F	113	LYS
1	F	162	ASP
1	F	163	ASN
1	F	165	SER
1	F	175	LEU
1	F	193	LYS
1	F	230	VAL
1	F	254	LYS
1	F	273	SER
1	F	276	LEU
1	F	277	ASP
1	G	41	ASN
1	G	54	TYR
1	G	89	MSE
1	G	100	SER
1	G	115	ASP
1	G	123	LEU
1	G	136	LEU
1	G	159	GLN
1	G	163	ASN
1	G	193	LYS
1	G	232	GLN
1	G	235	LEU
1	G	246	ARG
1	G	252	GLU
1	G	269	ASN
1	H	45	HIS
1	H	54	TYR
1	H	89	MSE
1	H	103	MSE
1	H	113	LYS
1	H	115	ASP
1	H	163	ASN
1	H	193	LYS
1	H	204	MSE
1	H	246	ARG
1	H	260	LYS
1	H	274	THR
1	I	44	GLU
1	I	65	TYR

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Mol	Chain	Res	Type
1	I	83	LYS
1	I	89	MSE
1	I	97	LYS
1	I	113	LYS
1	I	119	ASP
1	I	129	GLN
1	I	163	ASN
1	I	168	ILE
1	I	175	LEU
1	I	220	SER
1	I	235	LEU
1	I	236	THR
1	I	246	ARG
1	I	256	ASN
1	J	41	ASN
1	J	44	GLU
1	J	76	LYS
1	J	83	LYS
1	J	89	MSE
1	J	100	SER
1	J	103	MSE
1	J	113	LYS
1	J	116	ILE
1	J	163	ASN
1	J	193	LYS
1	J	232	GLN
1	J	269	ASN
1	K	44	GLU
1	K	45	HIS
1	K	54	TYR
1	K	89	MSE
1	K	95	ASP
1	K	100	SER
1	K	136	LEU
1	K	159	GLN
1	K	162	ASP
1	K	163	ASN
1	K	176	ASN
1	K	223	LYS
1	K	274	THR
1	L	42	ASP
1	L	45	HIS

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Mol	Chain	Res	Type
1	L	55	GLU
1	L	89	MSE
1	L	94	ASP
1	L	103	MSE
1	L	113	LYS
1	L	115	ASP
1	L	163	ASN
1	L	193	LYS
1	L	199	SER
1	L	217	LYS
1	L	246	ARG
1	L	278	THR
1	L	280	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	121	GLN
1	A	150	GLN
1	A	159	GLN
1	A	163	ASN
1	A	166	ASN
1	A	214	ASN
1	A	232	GLN
1	B	107	ASN
1	B	150	GLN
1	B	159	GLN
1	B	163	ASN
1	B	170	GLN
1	B	232	GLN
1	B	269	ASN
1	C	71	GLN
1	C	150	GLN
1	C	159	GLN
1	C	194	GLN
1	C	232	GLN
1	C	269	ASN
1	D	71	GLN
1	D	129	GLN
1	D	150	GLN
1	D	159	GLN

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Mol	Chain	Res	Type
1	D	163	ASN
1	D	166	ASN
1	D	194	GLN
1	D	232	GLN
1	D	269	ASN
1	E	150	GLN
1	E	159	GLN
1	E	232	GLN
1	F	71	GLN
1	F	150	GLN
1	F	159	GLN
1	F	163	ASN
1	F	196	GLN
1	F	213	GLN
1	F	232	GLN
1	G	71	GLN
1	G	129	GLN
1	G	150	GLN
1	G	159	GLN
1	G	163	ASN
1	G	194	GLN
1	G	213	GLN
1	G	232	GLN
1	G	239	GLN
1	G	269	ASN
1	H	71	GLN
1	H	121	GLN
1	H	150	GLN
1	H	159	GLN
1	H	163	ASN
1	H	214	ASN
1	H	269	ASN
1	I	71	GLN
1	I	129	GLN
1	I	150	GLN
1	I	159	GLN
1	I	163	ASN
1	I	194	GLN
1	I	232	GLN
1	J	150	GLN
1	J	159	GLN
1	J	163	ASN

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Mol	Chain	Res	Type
1	J	215	GLN
1	J	232	GLN
1	J	239	GLN
1	J	269	ASN
1	K	71	GLN
1	K	150	GLN
1	K	159	GLN
1	K	176	ASN
1	K	232	GLN
1	K	269	ASN
1	L	150	GLN
1	L	159	GLN
1	L	163	ASN
1	L	232	GLN
1	L	280	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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	235/254 (92%)	0.38	1 (0%) 93 92	18, 29, 45, 54	0
1	B	233/254 (91%)	0.40	4 (1%) 73 70	16, 29, 45, 55	0
1	C	233/254 (91%)	0.41	7 (3%) 54 47	15, 28, 46, 58	0
1	D	235/254 (92%)	0.33	6 (2%) 59 54	14, 29, 45, 56	0
1	E	231/254 (90%)	0.40	5 (2%) 65 60	17, 29, 45, 56	0
1	F	234/254 (92%)	0.40	10 (4%) 39 32	17, 29, 45, 58	0
1	G	231/254 (90%)	0.39	11 (4%) 34 28	16, 28, 46, 55	0
1	H	235/254 (92%)	0.43	11 (4%) 35 29	14, 29, 48, 61	0
1	I	238/254 (93%)	0.45	6 (2%) 61 55	17, 29, 46, 56	0
1	J	232/254 (91%)	0.38	3 (1%) 79 78	17, 29, 44, 55	0
1	K	229/254 (90%)	0.47	10 (4%) 38 32	15, 28, 46, 55	0
1	L	233/254 (91%)	0.47	18 (7%) 16 11	13, 29, 47, 61	0
All	All	2799/3048 (91%)	0.41	92 (3%) 50 42	13, 29, 46, 61	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	55	GLU	4.7
1	E	236	THR	4.5
1	B	236	THR	4.3
1	I	237	SER	4.1
1	L	261	THR	4.0
1	K	57	LEU	3.9
1	G	274	THR	3.9
1	H	219	TYR	3.7
1	H	55	GLU	3.7
1	B	234	PRO	3.5
1	F	234	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	237	SER	3.5
1	G	273	SER	3.4
1	J	237	SER	3.3
1	I	234	PRO	3.3
1	K	273	SER	3.3
1	C	59	LYS	3.3
1	C	60	GLU	3.1
1	G	55	GLU	3.0
1	F	95	ASP	3.0
1	F	34	LYS	2.9
1	G	236	THR	2.9
1	L	59	LYS	2.9
1	I	236	THR	2.9
1	E	233	TYR	2.8
1	L	250	GLU	2.8
1	K	84	ASP	2.8
1	K	178	LYS	2.8
1	C	83	LYS	2.8
1	L	278	THR	2.7
1	D	178	LYS	2.7
1	L	273	SER	2.7
1	L	166	ASN	2.6
1	G	235	LEU	2.6
1	J	236	THR	2.6
1	H	273	SER	2.6
1	K	262	VAL	2.6
1	D	260	LYS	2.6
1	I	233	TYR	2.6
1	I	255	VAL	2.6
1	J	166	ASN	2.6
1	L	139	VAL	2.6
1	F	166	ASN	2.5
1	L	144	LYS	2.5
1	A	37	GLU	2.5
1	K	166	ASN	2.5
1	K	219	TYR	2.5
1	L	95	ASP	2.5
1	L	140	ASP	2.4
1	L	74	PHE	2.4
1	L	179	ASN	2.4
1	F	114	LYS	2.4
1	E	166	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	273	SER	2.4
1	E	237	SER	2.4
1	C	94	ASP	2.3
1	F	260	LYS	2.3
1	L	176	ASN	2.3
1	H	280	GLN	2.3
1	G	56	GLY	2.3
1	E	234	PRO	2.3
1	H	51	HIS	2.3
1	G	251	TYR	2.3
1	H	59	LYS	2.3
1	L	262	VAL	2.3
1	H	56	GLY	2.3
1	K	265	TYR	2.2
1	K	59	LYS	2.2
1	L	60	GLU	2.2
1	H	275	ILE	2.2
1	H	178	LYS	2.2
1	H	95	ASP	2.2
1	G	178	LYS	2.2
1	D	280	GLN	2.2
1	G	95	ASP	2.2
1	L	237	SER	2.1
1	B	114	LYS	2.1
1	G	195	ILE	2.1
1	F	37	GLU	2.1
1	C	144	LYS	2.1
1	H	279	ASP	2.1
1	F	237	SER	2.1
1	C	90	ASP	2.0
1	D	51	HIS	2.0
1	C	179	ASN	2.0
1	G	83	LYS	2.0
1	L	223	LYS	2.0
1	L	55	GLU	2.0
1	F	236	THR	2.0
1	I	176	ASN	2.0
1	F	96	HIS	2.0
1	D	56	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	CL	L	10	1/1	0.94	0.21	-0.51	2,2,2,2	0
2	CL	A	1	1/1	0.97	0.19	-0.69	4,4,4,4	0
2	CL	E	5	1/1	0.86	0.08	-2.27	20,20,20,20	0
2	CL	D	2	1/1	0.89	0.16	-8.73	25,25,25,25	0
2	CL	K	9	1/1	0.83	0.10	-	50,50,50,50	0
2	CL	F	6	1/1	0.91	0.13	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.