



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2021 – 12:08 AM JST

PDB ID : 7CD2  
Title : Crystal structure of the S103F mutant of Bacillus subtilis (natto) YabJ protein.  
Authors : Fujimoto, Z.; Kishine, N.; Kimura, K.  
Deposited on : 2020-06-18  
Resolution : 2.70 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

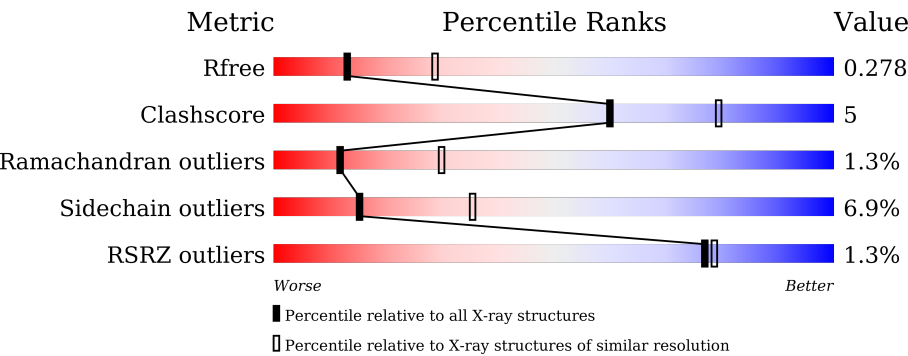
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	125	<div><div></div><div>73%13%•14%</div></div>
1	B	125	<div><div></div><div>73%13%•14%</div></div>
1	C	125	<div><div>%</div><div>78%15%•5%</div></div>
1	D	125	<div><div>6%</div><div>63%22%•14%</div></div>
1	E	125	<div><div></div><div>70%14%•14%</div></div>
1	F	125	<div><div>2%</div><div>63%22%•14%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	125	
1	H	125	
1	I	125	
1	J	125	
1	K	125	
1	L	125	
1	M	125	
1	N	125	
1	O	125	
1	P	125	
1	Q	125	
1	R	125	
1	S	125	
1	T	125	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16863 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 YabJ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			840	537	135	164	4			
1	B	108	Total	C	N	O	S	0	0	0
			840	537	135	164	4			
1	C	119	Total	C	N	O	S	0	0	0
			919	589	149	177	4			
1	D	108	Total	C	N	O	S	0	0	0
			840	537	135	164	4			
1	E	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			
1	F	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			
1	G	108	Total	C	N	O	S	0	1	0
			848	541	137	166	4			
1	H	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			
1	I	107	Total	C	N	O	S	0	2	0
			851	543	137	167	4			
1	J	110	Total	C	N	O	S	0	0	0
			859	551	137	167	4			
1	K	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			
1	L	108	Total	C	N	O	S	0	0	0
			840	537	135	164	4			
1	M	108	Total	C	N	O	S	0	0	0
			840	537	135	164	4			
1	N	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			
1	O	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			
1	P	108	Total	C	N	O	S	0	0	0
			840	537	135	164	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			
1	R	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			
1	S	108	Total	C	N	O	S	0	0	0
			840	537	135	164	4			
1	T	107	Total	C	N	O	S	0	0	0
			834	534	134	162	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	PHE	SER	engineered mutation	UNP D4G3D4
B	103	PHE	SER	engineered mutation	UNP D4G3D4
C	103	PHE	SER	engineered mutation	UNP D4G3D4
D	103	PHE	SER	engineered mutation	UNP D4G3D4
E	103	PHE	SER	engineered mutation	UNP D4G3D4
F	103	PHE	SER	engineered mutation	UNP D4G3D4
G	103	PHE	SER	engineered mutation	UNP D4G3D4
H	103	PHE	SER	engineered mutation	UNP D4G3D4
I	103	PHE	SER	engineered mutation	UNP D4G3D4
J	103	PHE	SER	engineered mutation	UNP D4G3D4
K	103	PHE	SER	engineered mutation	UNP D4G3D4
L	103	PHE	SER	engineered mutation	UNP D4G3D4
M	103	PHE	SER	engineered mutation	UNP D4G3D4
N	103	PHE	SER	engineered mutation	UNP D4G3D4
O	103	PHE	SER	engineered mutation	UNP D4G3D4
P	103	PHE	SER	engineered mutation	UNP D4G3D4
Q	103	PHE	SER	engineered mutation	UNP D4G3D4
R	103	PHE	SER	engineered mutation	UNP D4G3D4
S	103	PHE	SER	engineered mutation	UNP D4G3D4
T	103	PHE	SER	engineered mutation	UNP D4G3D4

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

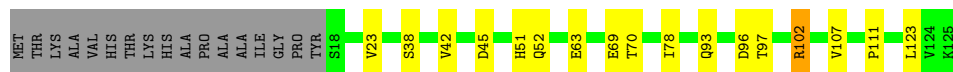
- Molecule 1: YabJ protein

Chain A: 




- Molecule 1: YabJ protein

Chain B: 



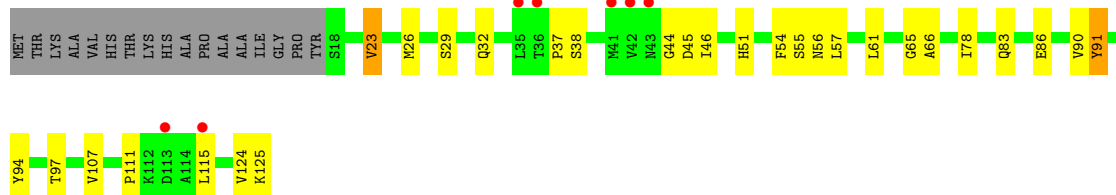
- Molecule 1: YabJ protein

Chain C: 



- Molecule 1: YabJ protein

Chain D: 

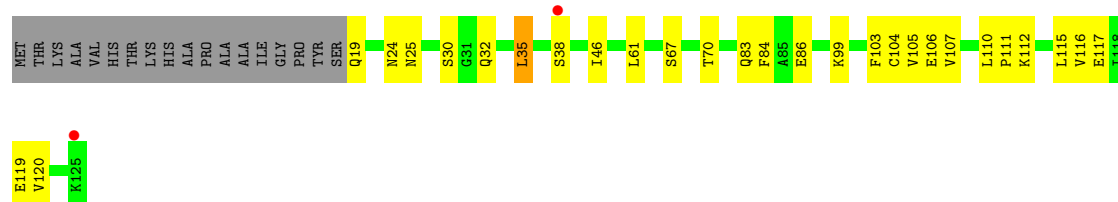


- Molecule 1: YabJ protein

Chain E: 



- Molecule 1: YabJ protein



- Molecule 1: YabJ protein



- Molecule 1: YabJ protein



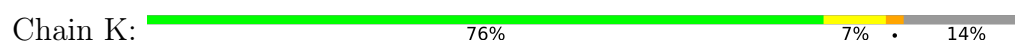
- Molecule 1: YabJ protein



- Molecule 1: YabJ protein



- Molecule 1: YabJ protein

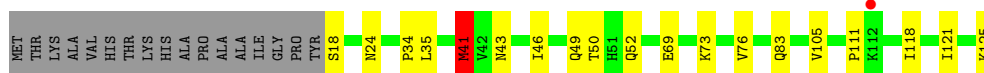


- Molecule 1: YabJ protein





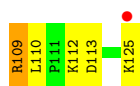
## ● Molecule 1: YabJ protein



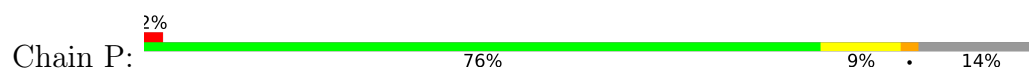
## ● Molecule 1: YabJ protein



## ● Molecule 1: YabJ protein



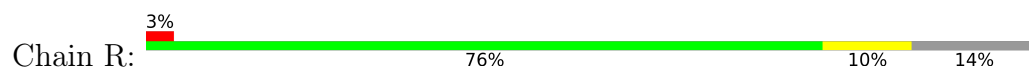
## ● Molecule 1: YabJ protein



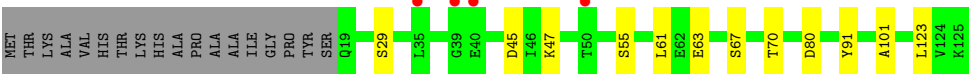
## ● Molecule 1: YabJ protein



## ● Molecule 1: YabJ protein



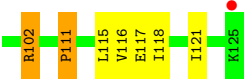




● Molecule 1: YabJ protein



● Molecule 1: YabJ protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.98Å 96.12Å 263.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 2.70 39.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (39.91-2.70) 93.1 (39.91-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.186 , 0.277 0.193 , 0.278	Depositor DCC
$R_{free}$ test set	3166 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.13	1/855 (0.1%)	1.10	2/1157 (0.2%)
1	B	1.06	1/855 (0.1%)	1.08	3/1157 (0.3%)
1	C	1.11	1/938 (0.1%)	1.12	3/1272 (0.2%)
1	D	1.00	1/855 (0.1%)	1.02	1/1157 (0.1%)
1	E	1.06	1/849 (0.1%)	1.10	4/1149 (0.3%)
1	F	1.06	1/849 (0.1%)	1.10	3/1149 (0.3%)
1	G	1.04	1/863 (0.1%)	1.10	4/1168 (0.3%)
1	H	1.05	2/849 (0.2%)	1.05	1/1149 (0.1%)
1	I	1.11	2/866 (0.2%)	1.09	1/1172 (0.1%)
1	J	0.96	0/876	0.99	0/1186
1	K	0.94	0/849	1.09	2/1149 (0.2%)
1	L	1.12	1/855 (0.1%)	1.07	0/1157
1	M	0.94	0/855	1.05	1/1157 (0.1%)
1	N	0.91	0/849	0.97	0/1149
1	O	0.89	0/849	0.93	0/1149
1	P	0.99	1/855 (0.1%)	0.96	0/1157
1	Q	0.98	0/849	1.02	1/1149 (0.1%)
1	R	0.81	0/849	0.90	1/1149 (0.1%)
1	S	1.04	0/855	1.02	1/1157 (0.1%)
1	T	0.93	0/849	1.04	0/1149
All	All	1.01	13/17169 (0.1%)	1.04	28/23238 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	28	TYR	CB-CG	7.41	1.62	1.51
1	F	106	GLU	CD-OE2	7.00	1.33	1.25
1	C	69	GLU	CG-CD	6.53	1.61	1.51
1	H	94	TYR	CE1-CZ	6.38	1.46	1.38
1	I	96	ASP	CB-CG	5.99	1.64	1.51
1	A	48	GLU	CD-OE2	5.99	1.32	1.25
1	H	69	GLU	CG-CD	5.80	1.60	1.51
1	P	45	ASP	CB-CG	5.69	1.63	1.51
1	I	62	GLU	CG-CD	5.68	1.60	1.51
1	L	28	TYR	CE2-CZ	-5.34	1.31	1.38
1	D	91	TYR	CB-CG	5.29	1.59	1.51
1	B	69	GLU	CG-CD	5.22	1.59	1.51
1	G	91	TYR	CZ-OH	5.15	1.46	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	24[A]	ASN	CB-CA-C	6.78	123.95	110.40
1	G	24[B]	ASN	CB-CA-C	6.78	123.95	110.40
1	E	81	MET	CG-SD-CE	-6.70	89.49	100.20
1	F	119	GLU	CB-CA-C	-6.42	97.56	110.40
1	F	35	LEU	CA-CB-CG	6.38	129.97	115.30
1	Q	45	ASP	CB-CG-OD1	6.37	124.03	118.30
1	M	41	MET	CG-SD-CE	6.25	110.21	100.20
1	C	109	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	45	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	45	ASP	CB-CG-OD1	6.13	123.82	118.30
1	E	80	ASP	CB-CG-OD1	6.06	123.76	118.30
1	B	45	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	S	78	ILE	CB-CA-C	-5.90	99.81	111.60
1	C	102	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	23	VAL	CB-CA-C	-5.49	100.98	111.40
1	E	28	TYR	CB-CG-CD2	5.44	124.27	121.00
1	F	105	VAL	CB-CA-C	-5.42	101.09	111.40
1	B	102	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	R	91	TYR	CA-CB-CG	5.41	123.68	113.40
1	E	102	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	G	102	ARG	CG-CD-NE	-5.24	100.80	111.80
1	I	62	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	H	109	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	K	80	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	106	GLU	CA-CB-CG	5.10	124.62	113.40
1	A	45	ASP	CB-CG-OD1	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	42	VAL	CB-CA-C	-5.05	101.80	111.40
1	G	109	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	44	GLY	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	840	0	828	7	0
1	B	840	0	828	7	0
1	C	919	0	907	8	0
1	D	840	0	828	9	0
1	E	834	0	823	8	0
1	F	834	0	823	15	0
1	G	848	0	833	13	0
1	H	834	0	823	8	0
1	I	851	0	833	6	0
1	J	859	0	845	10	0
1	K	834	0	823	5	0
1	L	840	0	828	8	0
1	M	840	0	828	12	0
1	N	834	0	823	12	0
1	O	834	0	823	10	0
1	P	840	0	828	5	0
1	Q	834	0	823	11	0
1	R	834	0	823	3	0
1	S	840	0	828	4	0
1	T	834	0	823	16	0
All	All	16863	0	16621	153	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 5.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:HG3	1:A:32:GLN:HE22	1.37	0.88
1:D:51:HIS:HD1	1:D:94:TYR:HH	1.29	0.80
1:J:98:HIS:CE1	1:K:24:ASN:HD21	2.05	0.74
1:J:98:HIS:CE1	1:K:24:ASN:ND2	2.59	0.71
1:M:43:ASN:OD1	1:Q:43:ASN:ND2	2.28	0.65
1:J:23:VAL:HG21	1:L:107:VAL:HG11	1.79	0.65
1:B:52:GLN:OE1	1:G:93:GLN:NE2	2.28	0.63
1:Q:107:VAL:HG11	1:S:23:VAL:HG21	1.81	0.62
1:O:22:ILE:HD11	1:O:64:ALA:HB1	1.80	0.62
1:T:60:VAL:O	1:T:63:GLU:HG3	2.00	0.62
1:T:73:LYS:HA	1:T:102:ARG:O	2.01	0.59
1:I:84:PHE:CE1	1:I:105:VAL:HG21	2.37	0.59
1:O:106:GLU:HG2	1:P:102:ARG:HD3	1.85	0.59
1:O:73:LYS:HA	1:O:102:ARG:O	2.03	0.59
1:Q:76:VAL:HG22	1:Q:118:ILE:HG12	1.83	0.59
1:S:29:SER:OG	1:S:120:VAL:N	2.29	0.59
1:T:76:VAL:HG22	1:T:118:ILE:HG12	1.85	0.59
1:G:73:LYS:HG3	1:G:74:ALA:N	2.18	0.58
1:O:109:ARG:O	1:O:110:LEU:HD23	2.03	0.58
1:N:58:LYS:O	1:N:59:ALA:C	2.41	0.58
1:Q:24:ASN:HD21	1:T:98:HIS:CE1	2.24	0.55
1:C:78:ILE:O	1:C:107:VAL:HA	2.07	0.55
1:H:19:GLN:HB2	1:H:30:SER:OG	2.06	0.55
1:R:45:ASP:OD1	1:R:47:LYS:N	2.39	0.55
1:F:46:ILE:HD12	1:F:115:LEU:HB3	1.89	0.55
1:S:76:VAL:HG22	1:S:118:ILE:HG12	1.89	0.54
1:N:49:GLN:HE22	1:N:115:LEU:HD12	1.72	0.54
1:B:23:VAL:HG11	1:C:101:ALA:HB2	1.89	0.54
1:D:32:GLN:HG3	1:D:57:LEU:HD23	1.90	0.54
1:T:46:ILE:HD13	1:T:83:GLN:HB3	1.90	0.54
1:L:46:ILE:HD12	1:L:115:LEU:HB3	1.89	0.53
1:Q:36:THR:CG2	1:Q:42:VAL:HG23	2.38	0.53
1:D:46:ILE:HD13	1:D:83:GLN:HB3	1.90	0.52
1:I:78:ILE:HD11	1:I:87:VAL:HG21	1.92	0.52
1:I:24[A]:ASN:O	1:I:24[A]:ASN:OD1	2.28	0.52
1:F:19:GLN:HB3	1:F:30:SER:OG	2.11	0.51
1:G:24[B]:ASN:OD1	1:G:25:ASN:N	2.42	0.51
1:T:27:PHE:O	1:T:121:ILE:HA	2.11	0.51
1:F:46:ILE:HD13	1:F:83:GLN:HB3	1.92	0.51
1:J:42:VAL:HG22	1:J:43:ASN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:58:LYS:HD2	1:N:68:PHE:CE2	2.46	0.50
1:M:46:ILE:HD13	1:M:83:GLN:HB3	1.92	0.50
1:K:70:THR:HG21	1:K:125:LYS:HE2	1.93	0.50
1:G:70:THR:HB	1:G:123:LEU:HB3	1.94	0.49
1:A:78:ILE:O	1:A:107:VAL:HA	2.12	0.49
1:R:70:THR:HB	1:R:123:LEU:O	2.12	0.49
1:N:53:VAL:HG11	1:N:118:ILE:HG13	1.94	0.49
1:O:61:LEU:O	1:O:66:ALA:HB3	2.11	0.49
1:E:77:PHE:HA	1:E:106:GLU:O	2.12	0.49
1:D:32:GLN:CG	1:D:57:LEU:HD23	2.43	0.48
1:T:83:GLN:HE22	1:T:115:LEU:HD13	1.77	0.48
1:M:73:LYS:HB3	1:M:121:ILE:HD12	1.94	0.48
1:D:46:ILE:HD12	1:D:115:LEU:HB3	1.96	0.48
1:M:34:PRO:HB3	1:M:49:GLN:HG2	1.95	0.47
1:A:53:VAL:HG21	1:A:116:VAL:HG13	1.95	0.47
1:N:95:PHE:O	1:N:99:LYS:HG3	2.14	0.47
1:M:43:ASN:OD1	1:M:43:ASN:N	2.44	0.47
1:J:49:GLN:O	1:J:53:VAL:HG23	2.15	0.47
1:O:55:SER:O	1:O:58:LYS:HB3	2.13	0.47
1:F:110:LEU:O	1:F:111:PRO:C	2.51	0.47
1:B:102:ARG:NH1	1:C:121:ILE:HD11	2.30	0.47
1:O:86:GLU:O	1:O:89:GLU:N	2.48	0.47
1:M:24:ASN:ND2	1:P:72:VAL:HG12	2.30	0.46
1:N:23:VAL:HG11	1:O:101:ALA:HB2	1.97	0.46
1:T:82:GLU:HA	1:T:82:GLU:OE1	2.16	0.46
1:G:106:GLU:HG3	1:H:102:ARG:HG3	1.97	0.46
1:I:73:LYS:HB3	1:I:121:ILE:HD12	1.97	0.46
1:E:24:ASN:O	1:E:25:ASN:HB2	2.15	0.46
1:A:23:VAL:HG12	1:A:24:ASN:HB2	1.98	0.46
1:B:70:THR:HB	1:B:123:LEU:HB3	1.98	0.45
1:N:57:LEU:HD22	1:N:120:VAL:HG22	1.99	0.45
1:P:41:MET:O	1:P:42:VAL:C	2.54	0.45
1:H:53:VAL:HG11	1:H:118:ILE:HG13	1.98	0.45
1:I:84:PHE:CD1	1:I:105:VAL:HG21	2.51	0.45
1:T:53:VAL:O	1:T:56:ASN:HB2	2.16	0.45
1:I:24[A]:ASN:O	1:I:24[A]:ASN:CG	2.55	0.45
1:J:109:ARG:NH1	1:L:20:GLY:O	2.49	0.45
1:L:91:TYR:OH	1:L:100:PRO:HG2	2.17	0.45
1:M:35:LEU:HD23	1:M:41:MET:HE3	1.98	0.45
1:D:78:ILE:O	1:D:107:VAL:HA	2.17	0.45
1:F:67:SER:O	1:F:70:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:78:ILE:HD12	1:L:87:VAL:HG21	1.99	0.45
1:Q:43:ASN:HD22	1:Q:43:ASN:H	1.65	0.45
1:E:70:THR:HG21	1:E:125:LYS:HE2	1.99	0.44
1:M:76:VAL:HG22	1:M:118:ILE:HG12	1.99	0.44
1:T:33:ILE:HB	1:T:34:PRO:CD	2.47	0.44
1:J:74:ALA:O	1:J:103:PHE:HA	2.17	0.44
1:F:84:PHE:HE1	1:F:103:PHE:HZ	1.66	0.44
1:K:102:ARG:HG2	1:L:106:GLU:CB	2.48	0.44
1:T:46:ILE:HD12	1:T:115:LEU:HB3	1.98	0.44
1:D:65:GLY:O	1:D:124:VAL:HG13	2.18	0.44
1:T:51:HIS:CE1	1:T:90:VAL:HG13	2.53	0.44
1:Q:32:GLN:O	1:Q:117:GLU:HG3	2.18	0.44
1:E:34:PRO:HB3	1:E:53:VAL:HG23	2.00	0.44
1:M:35:LEU:HD23	1:M:41:MET:CE	2.47	0.43
1:Q:32:GLN:NE2	1:Q:60:VAL:HG11	2.32	0.43
1:A:95:PHE:O	1:A:99:LYS:HE3	2.18	0.43
1:C:33:ILE:HB	1:C:34:PRO:CD	2.48	0.43
1:S:71:VAL:O	1:S:100:PRO:HB3	2.18	0.43
1:T:84:PHE:CE1	1:T:88:ASN:HB2	2.54	0.43
1:C:102:ARG:HH11	1:C:102:ARG:HG3	1.84	0.43
1:O:103:PHE:CE2	1:P:105:VAL:HG21	2.53	0.43
1:F:32:GLN:NE2	1:F:32:GLN:HA	2.34	0.43
1:J:124:VAL:HG12	1:J:125:LYS:HB3	2.01	0.43
1:N:77:PHE:O	1:N:110:LEU:HD11	2.18	0.43
1:E:23:VAL:HG21	1:G:107:VAL:HG11	2.01	0.43
1:K:70:THR:HG21	1:K:125:LYS:CE	2.49	0.43
1:T:116:VAL:HG22	1:T:117:GLU:N	2.34	0.43
1:Q:43:ASN:HD22	1:Q:43:ASN:N	2.17	0.42
1:C:36:THR:HB	1:C:37:PRO:CD	2.49	0.42
1:F:61:LEU:HD21	1:F:120:VAL:HG21	2.00	0.42
1:C:42:VAL:HB	1:C:52:GLN:HG2	1.99	0.42
1:J:71:VAL:HG12	1:J:100:PRO:HB3	2.02	0.42
1:A:47:LYS:NZ	1:A:89:GLU:OE1	2.38	0.42
1:B:78:ILE:O	1:B:107:VAL:HA	2.19	0.42
1:D:54:PHE:CD2	1:D:94:TYR:CD2	3.07	0.42
1:E:103:PHE:O	1:F:104:CYS:HA	2.19	0.42
1:E:28:TYR:CD1	1:H:102:ARG:NH1	2.88	0.42
1:F:84:PHE:CE1	1:F:103:PHE:HZ	2.37	0.42
1:G:77:PHE:HA	1:G:106:GLU:O	2.20	0.42
1:R:61:LEU:HD13	1:R:67:SER:O	2.20	0.42
1:J:70:THR:CG2	1:J:123:LEU:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:VAL:HG11	1:H:23:VAL:HG21	2.01	0.41
1:L:27:PHE:O	1:L:121:ILE:HA	2.20	0.41
1:D:61:LEU:HB3	1:D:66:ALA:O	2.21	0.41
1:F:46:ILE:CG2	1:F:86:GLU:OE1	2.69	0.41
1:G:101:ALA:O	1:H:107:VAL:HG23	2.21	0.41
1:L:91:TYR:OH	1:L:100:PRO:CG	2.69	0.41
1:N:60:VAL:HA	1:N:63:GLU:HG3	2.02	0.41
1:E:82:GLU:OE2	1:F:99:LYS:HE3	2.21	0.41
1:G:77:PHE:HB2	1:G:117:GLU:HB3	2.03	0.41
1:N:78:ILE:HD11	1:N:83:GLN:HB2	2.01	0.41
1:T:33:ILE:HB	1:T:34:PRO:HD2	2.02	0.41
1:A:106:GLU:HG2	1:B:102:ARG:HG2	2.01	0.41
1:F:111:PRO:O	1:F:112:LYS:C	2.59	0.41
1:M:34:PRO:CB	1:M:49:GLN:HG2	2.51	0.41
1:M:49:GLN:O	1:M:50:THR:C	2.59	0.41
1:H:95:PHE:HB3	1:H:98:HIS:O	2.20	0.41
1:Q:70:THR:HB	1:Q:123:LEU:HB3	2.02	0.41
1:B:51:HIS:CG	1:G:51:HIS:CE1	3.08	0.41
1:G:50:THR:HG22	1:G:90:VAL:HG11	2.03	0.41
1:O:32:GLN:HG3	1:O:57:LEU:HD23	2.03	0.41
1:F:116:VAL:HG22	1:F:117:GLU:N	2.36	0.41
1:H:81:MET:O	1:H:82:GLU:C	2.59	0.41
1:M:49:GLN:O	1:M:52:GLN:N	2.54	0.41
1:Q:36:THR:HB	1:Q:37:PRO:CD	2.50	0.41
1:C:14:ILE:HD11	1:C:59:ALA:HB1	2.03	0.40
1:N:58:LYS:CD	1:N:68:PHE:CE2	3.04	0.40
1:G:78:ILE:HD12	1:G:81:MET:HA	2.04	0.40
1:N:54:PHE:HA	1:N:57:LEU:HD12	2.03	0.40
1:T:79:ALA:HB3	1:T:115:LEU:HD23	2.03	0.40
1:G:36:THR:OG1	1:G:40:GLU:HB2	2.21	0.40
1:P:50:THR:OG1	1:P:116:VAL:HG11	2.21	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	106/125 (85%)	101 (95%)	5 (5%)	0	100	100
1	B	106/125 (85%)	100 (94%)	5 (5%)	1 (1%)	17	40
1	C	117/125 (94%)	106 (91%)	10 (8%)	1 (1%)	17	40
1	D	106/125 (85%)	96 (91%)	5 (5%)	5 (5%)	2	4
1	E	105/125 (84%)	96 (91%)	9 (9%)	0	100	100
1	F	105/125 (84%)	90 (86%)	15 (14%)	0	100	100
1	G	107/125 (86%)	98 (92%)	9 (8%)	0	100	100
1	H	105/125 (84%)	91 (87%)	14 (13%)	0	100	100
1	I	107/125 (86%)	100 (94%)	6 (6%)	1 (1%)	17	40
1	J	108/125 (86%)	96 (89%)	12 (11%)	0	100	100
1	K	105/125 (84%)	98 (93%)	5 (5%)	2 (2%)	8	20
1	L	106/125 (85%)	95 (90%)	10 (9%)	1 (1%)	17	40
1	M	106/125 (85%)	96 (91%)	9 (8%)	1 (1%)	17	40
1	N	105/125 (84%)	91 (87%)	11 (10%)	3 (3%)	4	10
1	O	105/125 (84%)	88 (84%)	15 (14%)	2 (2%)	8	20
1	P	106/125 (85%)	98 (92%)	7 (7%)	1 (1%)	17	40
1	Q	105/125 (84%)	97 (92%)	5 (5%)	3 (3%)	4	10
1	R	105/125 (84%)	91 (87%)	12 (11%)	2 (2%)	8	20
1	S	106/125 (85%)	94 (89%)	10 (9%)	2 (2%)	8	20
1	T	105/125 (84%)	95 (90%)	7 (7%)	3 (3%)	4	10
All	All	2126/2500 (85%)	1917 (90%)	181 (8%)	28 (1%)	12	30

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	81	MET
1	Q	42	VAL
1	C	45	ASP
1	I	111	PRO
1	L	38	SER
1	N	24	ASN
1	Q	45	ASP
1	R	101	ALA

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Mol	Chain	Res	Type
1	S	42	VAL
1	O	24	ASN
1	R	63	GLU
1	S	117	GLU
1	T	25	ASN
1	D	111	PRO
1	K	112	LYS
1	T	42	VAL
1	B	111	PRO
1	D	45	ASP
1	D	91	TYR
1	K	24	ASN
1	M	111	PRO
1	D	90	VAL
1	N	111	PRO
1	P	42	VAL
1	D	37	PRO
1	N	46	ILE
1	T	111	PRO
1	Q	111	PRO

### 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	92/104 (88%)	89 (97%)	3 (3%)	38	67
1	B	92/104 (88%)	86 (94%)	6 (6%)	17	38
1	C	99/104 (95%)	94 (95%)	5 (5%)	24	50
1	D	92/104 (88%)	83 (90%)	9 (10%)	8	18
1	E	91/104 (88%)	86 (94%)	5 (6%)	21	46
1	F	91/104 (88%)	87 (96%)	4 (4%)	28	56
1	G	93/104 (89%)	88 (95%)	5 (5%)	22	47
1	H	91/104 (88%)	83 (91%)	8 (9%)	10	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	93/104 (89%)	86 (92%)	7 (8%)	13	31
1	J	94/104 (90%)	87 (93%)	7 (7%)	13	32
1	K	91/104 (88%)	84 (92%)	7 (8%)	13	30
1	L	92/104 (88%)	87 (95%)	5 (5%)	22	47
1	M	92/104 (88%)	87 (95%)	5 (5%)	22	47
1	N	91/104 (88%)	82 (90%)	9 (10%)	8	18
1	O	91/104 (88%)	80 (88%)	11 (12%)	5	11
1	P	92/104 (88%)	86 (94%)	6 (6%)	17	38
1	Q	91/104 (88%)	84 (92%)	7 (8%)	13	30
1	R	91/104 (88%)	88 (97%)	3 (3%)	38	67
1	S	92/104 (88%)	83 (90%)	9 (10%)	8	18
1	T	91/104 (88%)	86 (94%)	5 (6%)	21	46
All	All	1842/2080 (89%)	1716 (93%)	126 (7%)	15	36

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	19	GLN
1	A	38	SER
1	B	38	SER
1	B	42	VAL
1	B	63	GLU
1	B	93	GLN
1	B	96	ASP
1	B	97	THR
1	C	7	THR
1	C	8	LYS
1	C	38	SER
1	C	42	VAL
1	C	125	LYS
1	D	23	VAL
1	D	26	MET
1	D	29	SER
1	D	38	SER
1	D	55	SER
1	D	56	ASN
1	D	86	GLU

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Mol	Chain	Res	Type
1	D	97	THR
1	D	125	LYS
1	E	29	SER
1	E	38	SER
1	E	73	LYS
1	E	112	LYS
1	E	125	LYS
1	F	24	ASN
1	F	25	ASN
1	F	35	LEU
1	F	38	SER
1	G	18	SER
1	G	25	ASN
1	G	78	ILE
1	G	89	GLU
1	G	112	LYS
1	H	19	GLN
1	H	35	LEU
1	H	55	SER
1	H	78	ILE
1	H	89	GLU
1	H	109	ARG
1	H	113	ASP
1	H	119	GLU
1	I	38	SER
1	I	55	SER
1	I	62	GLU
1	I	63	GLU
1	I	80	ASP
1	I	96	ASP
1	I	103	PHE
1	J	35	LEU
1	J	38	SER
1	J	58	LYS
1	J	70	THR
1	J	80	ASP
1	J	83	GLN
1	J	103	PHE
1	K	36	THR
1	K	42	VAL
1	K	55	SER
1	K	78	ILE

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Mol	Chain	Res	Type
1	K	109	ARG
1	K	113	ASP
1	K	125	LYS
1	L	38	SER
1	L	46	ILE
1	L	80	ASP
1	L	99	LYS
1	L	102	ARG
1	M	18	SER
1	M	41	MET
1	M	69	GLU
1	M	105	VAL
1	M	125	LYS
1	N	19	GLN
1	N	24	ASN
1	N	41	MET
1	N	45	ASP
1	N	58	LYS
1	N	96	ASP
1	N	97	THR
1	N	120	VAL
1	N	125	LYS
1	O	29	SER
1	O	36	THR
1	O	58	LYS
1	O	62	GLU
1	O	89	GLU
1	O	99	LYS
1	O	103	PHE
1	O	109	ARG
1	O	112	LYS
1	O	113	ASP
1	O	125	LYS
1	P	38	SER
1	P	45	ASP
1	P	55	SER
1	P	97	THR
1	P	99	LYS
1	P	112	LYS
1	Q	42	VAL
1	Q	43	ASN
1	Q	48	GLU

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Mol	Chain	Res	Type
1	Q	55	SER
1	Q	78	ILE
1	Q	97	THR
1	Q	102	ARG
1	R	29	SER
1	R	55	SER
1	R	80	ASP
1	S	36	THR
1	S	46	ILE
1	S	69	GLU
1	S	72	VAL
1	S	78	ILE
1	S	83	GLN
1	S	89	GLU
1	S	112	LYS
1	S	125	LYS
1	T	29	SER
1	T	55	SER
1	T	63	GLU
1	T	102	ARG
1	T	111	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	B	43	ASN
1	C	83	GLN
1	D	19	GLN
1	E	51	HIS
1	F	19	GLN
1	F	24	ASN
1	H	19	GLN
1	J	32	GLN
1	J	83	GLN
1	K	24	ASN
1	M	24	ASN
1	T	98	HIS

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	108/125 (86%)	-0.68	0 100 100	23, 33, 58, 64	0
1	B	108/125 (86%)	-0.46	0 100 100	26, 40, 76, 106	0
1	C	119/125 (95%)	-0.41	1 (0%) 86 87	25, 41, 67, 118	0
1	D	108/125 (86%)	0.15	7 (6%) 18 17	28, 56, 95, 113	0
1	E	107/125 (85%)	-0.33	0 100 100	30, 49, 86, 97	0
1	F	107/125 (85%)	-0.43	2 (1%) 66 69	22, 43, 76, 97	0
1	G	108/125 (86%)	-0.35	0 100 100	27, 45, 85, 108	0
1	H	107/125 (85%)	-0.39	0 100 100	30, 46, 71, 85	0
1	I	107/125 (85%)	-0.57	0 100 100	27, 39, 64, 89	0
1	J	110/125 (88%)	-0.44	0 100 100	31, 48, 82, 98	0
1	K	107/125 (85%)	-0.29	0 100 100	33, 53, 80, 100	0
1	L	108/125 (86%)	-0.41	0 100 100	24, 42, 81, 91	0
1	M	108/125 (86%)	-0.11	1 (0%) 84 85	30, 52, 83, 111	0
1	N	107/125 (85%)	0.15	5 (4%) 31 30	41, 67, 101, 114	0
1	O	107/125 (85%)	0.02	2 (1%) 66 69	44, 75, 101, 109	0
1	P	108/125 (86%)	-0.26	2 (1%) 66 69	32, 50, 86, 101	0
1	Q	107/125 (85%)	-0.18	1 (0%) 84 85	41, 61, 88, 107	0
1	R	107/125 (85%)	0.12	4 (3%) 41 41	48, 68, 104, 138	0
1	S	108/125 (86%)	-0.01	1 (0%) 84 85	46, 66, 88, 107	0
1	T	107/125 (85%)	-0.15	2 (1%) 66 69	41, 66, 93, 104	0
All	All	2163/2500 (86%)	-0.25	28 (1%) 77 78	22, 52, 90, 138	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	THR	3.9
1	P	18	SER	3.7
1	N	37	PRO	3.2
1	T	125	LYS	3.2
1	D	41	MET	3.2
1	D	42	VAL	3.1
1	D	113	ASP	3.0
1	R	40	GLU	2.9
1	N	36	THR	2.9
1	D	35	LEU	2.8
1	N	35	LEU	2.8
1	D	36	THR	2.8
1	D	43	ASN	2.6
1	N	40	GLU	2.6
1	M	112	LYS	2.5
1	R	50	THR	2.5
1	T	43	ASN	2.4
1	O	125	LYS	2.4
1	R	39	GLY	2.4
1	S	125	LYS	2.3
1	R	35	LEU	2.2
1	F	38	SER	2.2
1	N	43	ASN	2.2
1	D	115	LEU	2.2
1	Q	63	GLU	2.1
1	O	38	SER	2.1
1	F	125	LYS	2.0
1	P	125	LYS	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 monosaccharides 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.