Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 05:50 PM EDT

PDB ID	:	3MKZ
Title	:	Structure of SopB(155-272)-18mer complex, P21 form
Authors	:	Schumacher, M.A.
Deposited on	:	2010-04-15
Resolution	:	2.98 Å(reported)

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

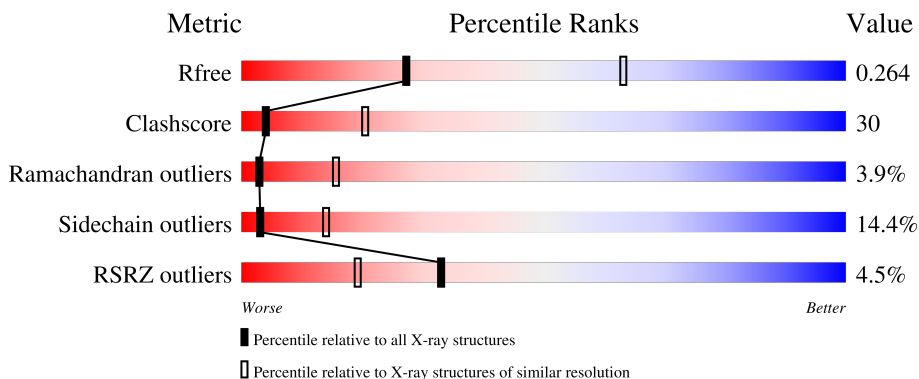|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.98 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	Percentile Ranks	Value
Rfree		0.264
Clashscore		30
Ramachandran outliers		3.9%
Sidechain outliers		14.4%
RSRZ outliers		4.5%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	121	4% — 50% / 34% / 9% / 7%
1	B	121	2% — 45% / 39% / 7% / 8%
1	N	121	3% — 36% / 44% / 10% / · / 9%
1	U	121	10% — 42% / 39% / 11% / 8%
2	C	18	44% / 44% / 11%

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Mol	Chain	Length	Quality of chain
2	D	18	22% 67% 11%
2	Y	18	17% 56% 28%
2	Z	18	33% 61% 6%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4899 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 Protein sopB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	112	Total	C	N	O	S	0	0	0
			861	537	154	169	1			
1	B	111	Total	C	N	O	S	0	0	0
			855	534	153	167	1			
1	U	111	Total	C	N	O	S	0	0	0
			855	534	153	167	1			
1	N	110	Total	C	N	O	S	0	0	0
			848	530	152	165	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLY	-	expression tag	UNP P62558
A	153	SER	-	expression tag	UNP P62558
A	154	HIS	-	expression tag	UNP P62558
A	255	ASP	GLU	conflict	UNP P62558
B	152	GLY	-	expression tag	UNP P62558
B	153	SER	-	expression tag	UNP P62558
B	154	HIS	-	expression tag	UNP P62558
B	255	ASP	GLU	conflict	UNP P62558
U	152	GLY	-	expression tag	UNP P62558
U	153	SER	-	expression tag	UNP P62558
U	154	HIS	-	expression tag	UNP P62558
U	255	ASP	GLU	conflict	UNP P62558
N	152	GLY	-	expression tag	UNP P62558
N	153	SER	-	expression tag	UNP P62558
N	154	HIS	-	expression tag	UNP P62558
N	255	ASP	GLU	conflict	UNP P62558

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*GP*GP*GP*AP*CP*CP*AP*TP* GP*GP*TP*CP*CP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			
2	D	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			
2	Y	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			
2	Z	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	U	1	Total	Ca	0	0
			1	1		
3	Z	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	C	5	Total	O	0	0
			5	5		
4	D	3	Total	O	0	0
			3	3		
4	N	1	Total	O	0	0
			1	1		

3 Residue-property plots ⓘ

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.
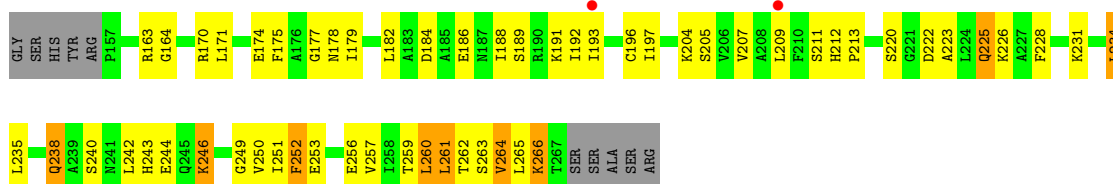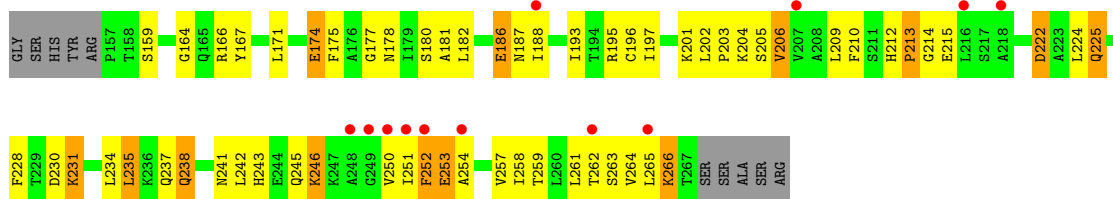
● Molecule 1: Protein sopB

Chain A:
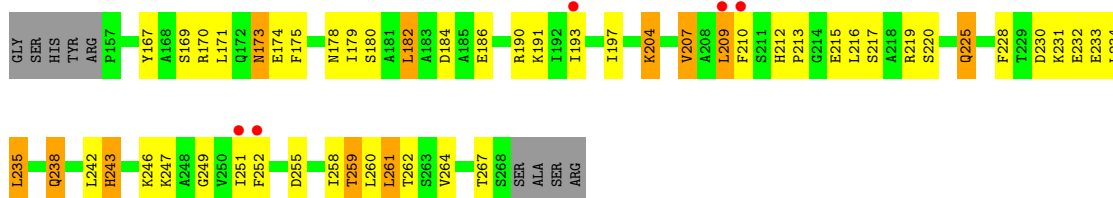
● Molecule 1: Protein sopB

Chain B:

● Molecule 1: Protein sopB

Chain U:

● Molecule 1: Protein sopB

Chain N:
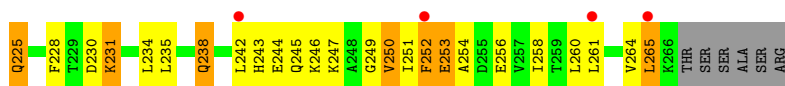
Q225 F228 T229 D230 K231 L234 L235 Q238 L242 H243 E244 Q245 K246 K247 A248 G249 V250 I251 F252 E253 A254 D255 E256 V257 I258 T259 L260 L261 V264 L265 K266 THR SER SER ALA SER ARG

• Molecule 2: DNA (5'-D(*CP*TP*GP*GP*GP*AP*CP*CP*AP*TP*GP*GP*TP*CP*CP*CP*AP*G)-3')

Chain C:

44% 44% 11%

C1 T2 G5 A6 C7 C8 A9 T10 G11 A17 G18

• Molecule 2: DNA (5'-D(*CP*TP*GP*GP*GP*AP*CP*CP*AP*TP*GP*GP*TP*CP*CP*CP*AP*G)-3')

Chain D:

22% 67% 11%

C1 T2 G3 G4 G5 A6 C7 C8 A9 T10 G11 G12 A17 G18

• Molecule 2: DNA (5'-D(*CP*TP*GP*GP*GP*AP*CP*CP*AP*TP*GP*GP*TP*CP*CP*CP*AP*G)-3')

Chain Y:

17% 56% 28%

C1 T2 G3 G4 G5 A6 C7 C8 A9 T10 G11 G12 C16 A17 G18

• Molecule 2: DNA (5'-D(*CP*TP*GP*GP*GP*AP*CP*CP*AP*TP*GP*GP*TP*CP*CP*CP*AP*G)-3')

Chain Z:

33% 61% 6%

C1 T2 G3 A6 C7 C8 A9 T10 G11 G12 T13 C14 A17 G18
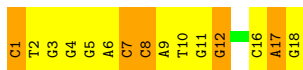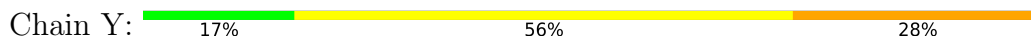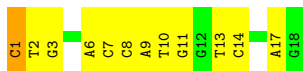
4 Data and refinement statistics ⓘ

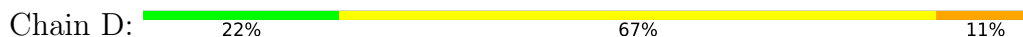| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.38Å 47.12Å 118.23Å 90.00° 115.97° 90.00°	Depositor
Resolution (Å)	50.07 – 2.98 50.07 – 2.98	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.07-2.98) 96.3 (50.07-2.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.213 , 0.264 0.213 , 0.264	Depositor DCC
R_{free} test set	2202 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.989	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4899	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: CA

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	0.57	0/871	0.78	1/1172 (0.1%)
1	B	0.61	0/865	0.77	0/1164
1	N	0.54	0/858	0.72	0/1154
1	U	0.51	0/865	0.66	0/1164
2	C	0.78	0/410	0.87	0/631
2	D	0.89	0/410	0.97	0/631
2	Y	0.76	0/410	0.85	0/631
2	Z	0.76	0/410	0.91	0/631
All	All	0.64	0/5099	0.80	1/7178 (0.0%)

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
2	C	0	3
2	D	0	2
2	Y	0	5
2	Z	0	2
All	All	0	12

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	LEU	CA-CB-CG	6.27	129.73	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Group
2	C	1	DC	Sidechain
2	C	17	DA	Sidechain
2	C	8	DC	Sidechain
2	D	1	DC	Sidechain
2	D	8	DC	Sidechain
2	Y	1	DC	Sidechain
2	Y	12	DG	Sidechain
2	Y	17	DA	Sidechain
2	Y	7	DC	Sidechain
2	Y	8	DC	Sidechain
2	Z	1	DC	Sidechain
2	Z	17	DA	Sidechain

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	861	0	880	43	0
1	B	855	0	875	50	1
1	N	848	0	868	63	0
1	U	855	0	875	67	0
2	C	366	0	203	14	0
2	D	366	0	203	14	0
2	Y	366	0	203	23	1
2	Z	366	0	203	12	0
3	A	1	0	0	0	0
3	U	1	0	0	0	0
3	Z	2	0	0	0	0
4	A	3	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
4	N	1	0	0	0	0
All	All	4899	0	4310	275	1

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 30.

All (275) 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:N:238:GLN:HE21	1:N:264:VAL:HB	1.26	1.00
2:Y:11:DG:H2"	2:Y:12:DG:H5'	1.46	0.97
1:A:246:LYS:NZ	1:A:251:ILE:HD11	1.84	0.93
1:U:238:GLN:HG3	1:U:264:VAL:HG11	1.52	0.91
1:U:202:LEU:HD22	1:U:224:LEU:HD23	1.53	0.91
1:B:225:GLN:HE21	1:B:225:GLN:C	1.76	0.89
1:B:225:GLN:HE21	1:B:226:LYS:N	1.70	0.89
2:Y:11:DG:H2"	2:Y:12:DG:C5'	2.03	0.88
1:A:246:LYS:HZ3	1:A:251:ILE:HD11	1.39	0.86
1:B:171:LEU:HD21	1:B:177:GLY:HA2	1.57	0.86
1:N:230:ASP:O	1:N:231:LYS:HG3	1.77	0.85
1:B:234:LEU:HD21	1:B:264:VAL:HG21	1.57	0.85
1:U:251:ILE:HG22	1:U:252:PHE:H	1.41	0.85
1:N:256:GLU:O	1:N:260:LEU:HG	1.77	0.84
2:C:10:DT:H2"	2:C:11:DG:C8	2.13	0.83
1:N:178:ASN:ND2	1:N:181:ALA:HB2	1.93	0.83
1:N:238:GLN:NE2	1:N:264:VAL:HB	1.92	0.83
1:U:242:LEU:HA	1:U:245:GLN:HG2	1.60	0.82
1:A:219:ARG:HD2	2:C:10:DT:H2'	1.61	0.81
1:A:212:HIS:ND1	1:A:213:PRO:HD2	1.96	0.79
2:C:6:DA:H2"	2:C:7:DC:H5'	1.66	0.77
1:U:215:GLU:HB3	1:U:254:ALA:HB2	1.66	0.77
1:U:178:ASN:HD22	1:U:181:ALA:HB2	1.48	0.77
2:C:5:DG:O6	1:N:191:LYS:HE3	1.86	0.76
1:B:212:HIS:ND1	1:B:213:PRO:HD2	2.01	0.76
1:B:242:LEU:HD21	1:B:260:LEU:HD22	1.68	0.76
1:N:178:ASN:HD22	1:N:181:ALA:HB2	1.47	0.76
1:N:242:LEU:HD22	1:N:252:PHE:CE2	2.21	0.75
2:Y:10:DT:H2"	2:Y:11:DG:C8	2.22	0.74
1:U:212:HIS:ND1	1:U:213:PRO:HD2	2.02	0.74
1:N:171:LEU:CD1	1:N:177:GLY:HA2	2.17	0.74
1:A:169:SER:O	1:A:173:ASN:ND2	2.21	0.73
1:N:206:VAL:O	1:N:209:LEU:HB3	1.89	0.73
1:B:234:LEU:CD2	1:B:264:VAL:HG21	2.18	0.72
2:D:11:DG:N7	1:N:219:ARG:NH1	2.37	0.72
1:N:238:GLN:HG3	1:N:264:VAL:HG11	1.71	0.72
2:Z:6:DA:H2"	2:Z:7:DC:H5"	1.72	0.70
1:U:178:ASN:ND2	1:U:181:ALA:HB2	2.05	0.70
1:B:257:VAL:O	1:B:261:LEU:HB2	1.91	0.70
1:B:234:LEU:HD21	1:B:264:VAL:CG2	2.21	0.70
2:Y:6:DA:H2"	2:Y:7:DC:H5"	1.74	0.69
2:Y:6:DA:H2"	2:Y:7:DC:C5'	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:DC:H2"	2:D:2:DT:H5'	1.73	0.69
1:N:171:LEU:HD13	1:N:177:GLY:HA2	1.75	0.69
1:U:206:VAL:O	1:U:209:LEU:HB2	1.92	0.69
1:A:259:THR:HG22	1:A:260:LEU:HD23	1.75	0.68
2:Z:8:DC:H2"	2:Z:9:DA:C8	2.29	0.67
1:U:228:PHE:CD2	1:U:235:LEU:HB2	2.29	0.67
1:U:203:PRO:HB2	1:U:206:VAL:CG2	2.25	0.66
1:N:242:LEU:HD22	1:N:252:PHE:CZ	2.30	0.66
1:U:234:LEU:HD23	1:U:234:LEU:O	1.95	0.66
2:Z:6:DA:H2"	2:Z:7:DC:C5'	2.25	0.66
2:Y:6:DA:C2'	2:Y:7:DC:H5"	2.27	0.65
2:Y:8:DC:H2"	2:Y:9:DA:C8	2.31	0.65
1:U:203:PRO:HB2	1:U:206:VAL:HG23	1.79	0.65
1:N:212:HIS:ND1	1:N:213:PRO:HD2	2.12	0.65
1:B:228:PHE:CZ	1:B:265:LEU:HD11	2.32	0.65
1:B:193:ILE:HG22	1:B:197:ILE:HD12	1.78	0.64
1:N:182:LEU:HD23	1:N:182:LEU:O	1.97	0.64
1:B:186:GLU:HB2	1:B:188:ILE:HG22	1.78	0.64
1:U:228:PHE:HD2	1:U:235:LEU:HB2	1.61	0.64
1:B:175:PHE:CD1	1:B:182:LEU:HD23	2.33	0.64
1:U:195:ARG:HA	1:U:222:ASP:HB2	1.80	0.64
1:A:246:LYS:HZ2	1:A:251:ILE:HD11	1.63	0.63
1:A:230:ASP:O	1:A:231:LYS:HG3	1.98	0.63
2:Y:1:DC:H2"	2:Y:2:DT:H5'	1.79	0.63
1:B:225:GLN:C	1:B:225:GLN:NE2	2.50	0.63
2:C:1:DC:H2"	2:C:2:DT:H5'	1.80	0.63
1:B:171:LEU:CD2	1:B:177:GLY:HA2	2.28	0.63
1:U:242:LEU:HA	1:U:245:GLN:CG	2.30	0.62
1:A:175:PHE:CE1	1:A:182:LEU:HD23	2.35	0.62
2:C:1:DC:H2"	2:C:2:DT:C5'	2.30	0.62
2:D:6:DA:H2"	2:D:7:DC:H5'	1.80	0.62
1:B:262:THR:HA	1:B:265:LEU:HD12	1.81	0.62
1:N:182:LEU:HD22	1:N:193:ILE:HD13	1.81	0.61
1:U:252:PHE:N	1:U:252:PHE:CD2	2.68	0.61
1:N:228:PHE:CE2	1:N:265:LEU:HD23	2.35	0.61
1:U:251:ILE:HG22	1:U:252:PHE:N	2.15	0.61
2:Y:11:DG:C2'	2:Y:12:DG:C5'	2.78	0.61
1:A:242:LEU:O	1:A:242:LEU:HD23	2.00	0.60
2:C:1:DC:H3'	1:N:180:SER:OG	2.01	0.60
1:N:246:LYS:HA	1:N:250:VAL:O	2.02	0.60
1:B:182:LEU:CD1	1:B:193:ILE:HD12	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:6:DA:C2'	2:Z:7:DC:H5"	2.31	0.60
2:Y:11:DG:H1'	2:Y:12:DG:H5"	1.84	0.60
2:Z:1:DC:HO5'	2:Z:1:DC:H6	1.49	0.60
1:A:182:LEU:O	1:A:182:LEU:HD22	2.02	0.59
1:U:159:SER:HB3	1:U:213:PRO:O	2.02	0.59
1:U:202:LEU:CD2	1:U:225:GLN:HB2	2.32	0.59
1:A:210:PHE:HB3	1:A:215:GLU:HB2	1.84	0.59
1:B:175:PHE:CE1	1:B:182:LEU:HD23	2.37	0.59
2:Y:18:DG:OP2	2:Y:18:DG:H8	1.86	0.59
1:U:263:SER:C	1:U:265:LEU:H	2.05	0.58
2:Z:10:DT:H2"	2:Z:11:DG:C8	2.38	0.58
1:U:166:ARG:NH1	1:U:186:GLU:OE1	2.36	0.58
1:U:203:PRO:O	1:U:206:VAL:HG23	2.04	0.58
1:A:178:ASN:OD1	1:A:180:SER:HB2	2.04	0.58
1:A:242:LEU:HD13	1:A:261:LEU:CD2	2.34	0.58
1:N:249:GLY:O	1:N:251:ILE:HG13	2.04	0.58
1:U:262:THR:O	1:U:266:LYS:HG3	2.03	0.57
1:U:238:GLN:CG	1:U:264:VAL:HG11	2.31	0.57
1:U:186:GLU:C	1:U:188:ILE:N	2.56	0.57
1:N:171:LEU:HD11	1:N:177:GLY:HA2	1.86	0.57
1:B:170:ARG:HG2	1:B:170:ARG:HH11	1.69	0.57
1:U:202:LEU:CD2	1:U:224:LEU:HD23	2.31	0.57
1:A:212:HIS:H	1:A:215:GLU:HG3	1.70	0.57
1:B:262:THR:O	1:B:265:LEU:HD12	2.05	0.57
1:B:220:SER:O	1:B:223:ALA:HB3	2.06	0.56
1:U:246:LYS:HB2	1:U:251:ILE:HG23	1.85	0.56
1:U:257:VAL:O	1:U:261:LEU:HD23	2.05	0.56
1:N:172:GLN:HG2	1:N:173:ASN:N	2.20	0.56
1:U:171:LEU:CD1	1:U:177:GLY:HA2	2.35	0.56
1:U:186:GLU:O	1:U:188:ILE:N	2.39	0.56
1:B:188:ILE:HD11	1:B:192:ILE:HG13	1.86	0.56
1:U:241:ASN:O	1:U:245:GLN:HG2	2.06	0.55
1:N:164:GLY:HA3	1:N:200:ALA:HB2	1.89	0.55
2:Y:11:DG:C2'	2:Y:12:DG:H5"	2.37	0.55
2:Z:13:DT:H2"	2:Z:14:DC:H5'	1.88	0.55
1:N:228:PHE:CZ	1:N:265:LEU:HD23	2.41	0.55
1:N:202:LEU:HD22	1:N:224:LEU:HD23	1.89	0.55
2:Y:1:DC:H2"	2:Y:2:DT:C5'	2.36	0.55
1:N:203:PRO:HB2	1:N:206:VAL:HG23	1.88	0.55
1:A:212:HIS:HB3	1:A:215:GLU:HG2	1.89	0.54
2:D:17:DA:H2"	2:D:18:DG:OP2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:7:DC:H2"	2:Y:8:DC:H6	1.71	0.54
1:B:209:LEU:HD12	1:B:243:HIS:CE1	2.43	0.54
2:D:6:DA:H1'	2:D:7:DC:H5"	1.89	0.54
2:Y:10:DT:C2'	2:Y:11:DG:C8	2.91	0.54
1:U:186:GLU:C	1:U:188:ILE:H	2.10	0.54
1:B:170:ARG:HG2	1:B:170:ARG:NH1	2.21	0.54
2:C:9:DA:C8	2:C:10:DT:H72	2.43	0.54
2:C:8:DC:H2"	2:C:9:DA:C8	2.43	0.53
1:A:217:SER:HB3	1:A:220:SER:OG	2.09	0.53
1:U:242:LEU:HD23	1:U:245:GLN:HG3	1.91	0.53
2:D:1:DC:H2"	2:D:2:DT:C5'	2.40	0.52
1:U:164:GLY:CA	1:U:196:CYS:HB3	2.39	0.52
1:A:182:LEU:HD13	1:A:193:ILE:HD12	1.91	0.52
1:U:201:LYS:HB2	1:U:225:GLN:HG3	1.91	0.52
1:A:170:ARG:HH11	1:A:170:ARG:HG2	1.75	0.52
1:N:170:ARG:O	1:N:174:GLU:HB3	2.10	0.52
1:A:191:LYS:NZ	2:D:5:DG:N7	2.58	0.51
1:N:209:LEU:HD21	1:N:242:LEU:HD13	1.92	0.51
1:N:250:VAL:HG12	1:N:252:PHE:CD1	2.46	0.51
2:D:6:DA:H2"	2:D:7:DC:C5'	2.40	0.51
1:B:205:SER:O	1:B:209:LEU:HD13	2.11	0.51
1:U:263:SER:C	1:U:265:LEU:N	2.64	0.51
2:C:1:DC:H2"	2:C:2:DT:O5'	2.11	0.51
1:U:182:LEU:HD22	1:U:193:ILE:HG21	1.92	0.51
1:U:180:SER:OG	2:Z:1:DC:H3'	2.10	0.51
1:N:194:THR:HG22	1:N:195:ARG:N	2.25	0.51
1:B:252:PHE:HB3	1:B:256:GLU:OE1	2.10	0.50
2:Y:7:DC:H6	2:Y:7:DC:H5'	1.77	0.50
1:B:249:GLY:O	1:B:251:ILE:HG12	2.11	0.50
1:A:225:GLN:NE2	1:A:225:GLN:C	2.65	0.50
2:Y:1:DC:H2'	2:Y:2:DT:C7	2.42	0.50
1:B:256:GLU:O	1:B:260:LEU:HB2	2.12	0.50
1:B:240:SER:O	1:B:244:GLU:HG3	2.12	0.49
1:B:264:VAL:O	1:B:264:VAL:HG22	2.12	0.49
1:B:225:GLN:NE2	1:B:226:LYS:N	2.51	0.49
1:U:258:ILE:HG13	1:U:259:THR:N	2.27	0.49
1:A:204:LYS:HA	1:A:207:VAL:HG23	1.95	0.49
1:N:186:GLU:O	1:N:187:ASN:C	2.51	0.49
1:N:235:LEU:HD23	1:N:261:LEU:HD12	1.93	0.49
1:A:228:PHE:CD2	1:A:235:LEU:HB2	2.47	0.49
2:D:11:DG:H2"	2:D:12:DG:O5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:205:SER:O	1:U:209:LEU:HD13	2.13	0.49
1:N:242:LEU:HD21	1:N:260:LEU:HD13	1.95	0.48
1:N:197:ILE:O	1:N:200:ALA:HB3	2.13	0.48
1:A:255:ASP:O	1:A:258:ILE:HG22	2.13	0.48
1:U:234:LEU:HD21	1:U:264:VAL:HG22	1.94	0.48
1:A:219:ARG:HG3	2:C:11:DG:OP2	2.14	0.48
2:C:7:DC:H2"	2:C:8:DC:OP2	2.14	0.48
1:N:199:THR:O	1:N:202:LEU:HB2	2.14	0.48
1:B:228:PHE:CE1	1:B:265:LEU:HD11	2.48	0.48
1:U:174:GLU:HB3	1:U:175:PHE:CD1	2.48	0.48
1:N:243:HIS:O	1:N:247:LYS:HB2	2.14	0.48
1:B:171:LEU:HD11	1:B:179:ILE:HG12	1.96	0.47
2:D:8:DC:H2"	2:D:9:DA:C8	2.49	0.47
1:U:251:ILE:CG2	1:U:252:PHE:H	2.21	0.47
1:N:173:ASN:O	1:N:174:GLU:HB2	2.13	0.47
1:N:230:ASP:O	1:N:231:LYS:CG	2.58	0.47
1:N:238:GLN:HE21	1:N:264:VAL:CB	2.12	0.47
1:U:164:GLY:HA2	1:U:196:CYS:HB3	1.96	0.47
1:U:241:ASN:O	1:U:245:GLN:NE2	2.48	0.47
1:N:163:ARG:HA	1:N:166:ARG:HB2	1.97	0.47
1:B:171:LEU:C	1:B:171:LEU:HD23	2.35	0.46
1:N:165:GLN:HE21	1:N:165:GLN:HB2	1.50	0.46
1:N:182:LEU:HD22	1:N:193:ILE:CD1	2.45	0.46
1:A:238:GLN:HG3	1:A:264:VAL:CG1	2.46	0.46
1:B:263:SER:C	1:B:265:LEU:H	2.19	0.46
1:B:263:SER:O	1:B:265:LEU:N	2.48	0.46
1:U:171:LEU:HD11	1:U:177:GLY:HA2	1.98	0.46
1:A:234:LEU:CD2	1:B:238:GLN:HG2	2.45	0.46
1:A:246:LYS:HD2	1:A:246:LYS:O	2.16	0.46
1:U:182:LEU:CD2	1:U:193:ILE:HD12	2.46	0.46
2:Z:1:DC:H2"	2:Z:2:DT:C5'	2.46	0.46
2:Y:7:DC:H2"	2:Y:8:DC:C6	2.51	0.46
1:N:161:TYR:CE1	1:N:207:VAL:HG21	2.50	0.46
1:N:253:GLU:OE1	1:N:256:GLU:HB2	2.15	0.46
1:A:209:LEU:HD12	1:A:243:HIS:CE1	2.51	0.46
1:B:242:LEU:HD12	1:B:261:LEU:HD13	1.97	0.45
2:Z:2:DT:H2"	2:Z:3:DG:C8	2.51	0.45
1:A:182:LEU:CD1	1:A:193:ILE:HD12	2.47	0.45
1:N:249:GLY:O	1:N:250:VAL:C	2.54	0.45
1:U:234:LEU:O	1:U:238:GLN:HB2	2.17	0.45
2:Y:11:DG:C1'	2:Y:12:DG:H5"	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:252:PHE:CD1	1:N:252:PHE:N	2.85	0.45
1:U:167:TYR:HB3	1:U:197:ILE:HD11	1.97	0.45
1:N:209:LEU:HD21	1:N:242:LEU:CD1	2.46	0.45
1:N:234:LEU:HD23	1:N:234:LEU:O	2.17	0.45
1:N:235:LEU:CD2	1:N:261:LEU:HD12	2.47	0.45
1:B:182:LEU:HD12	1:B:193:ILE:HG21	1.99	0.44
1:U:210:PHE:CE2	1:U:254:ALA:HA	2.52	0.44
1:U:262:THR:O	1:U:262:THR:HG22	2.17	0.44
2:Y:1:DC:H2'	2:Y:2:DT:C6	2.52	0.44
2:Z:1:DC:H2"	2:Z:2:DT:H5'	1.99	0.44
1:U:202:LEU:HD21	1:U:225:GLN:HB2	1.98	0.44
1:N:186:GLU:O	1:N:188:ILE:N	2.50	0.44
1:N:206:VAL:O	1:N:209:LEU:CB	2.64	0.44
2:D:10:DT:C2'	2:D:11:DG:C8	3.00	0.44
1:U:235:LEU:C	1:U:237:GLN:N	2.71	0.44
1:A:193:ILE:O	1:A:197:ILE:HG13	2.18	0.44
1:B:188:ILE:HG13	1:B:189:SER:N	2.33	0.44
1:U:186:GLU:HB2	1:U:188:ILE:HG22	1.98	0.44
1:U:262:THR:HG22	1:U:266:LYS:HE2	1.99	0.44
1:A:247:LYS:HD2	1:A:247:LYS:O	2.17	0.44
1:U:228:PHE:CD2	1:U:235:LEU:HD12	2.53	0.44
1:B:170:ARG:NH1	1:B:174:GLU:OE2	2.51	0.43
1:A:170:ARG:HE	1:A:174:GLU:CD	2.22	0.43
1:N:250:VAL:HG12	1:N:252:PHE:HD1	1.83	0.43
1:A:247:LYS:C	1:A:249:GLY:H	2.20	0.43
2:C:9:DA:H2"	2:C:10:DT:OP2	2.19	0.43
1:N:194:THR:HG23	1:N:198:ASN:ND2	2.33	0.43
1:A:233:GLU:OE1	1:A:233:GLU:HA	2.19	0.43
2:D:18:DG:OP2	2:D:18:DG:H8	2.02	0.43
1:B:262:THR:HG22	1:B:266:LYS:NZ	2.33	0.43
1:B:246:LYS:HA	1:B:250:VAL:O	2.19	0.43
1:U:180:SER:OG	2:Z:2:DT:OP2	2.32	0.43
1:N:238:GLN:HG3	1:N:264:VAL:CG1	2.44	0.42
1:N:161:TYR:CD1	1:N:207:VAL:HG21	2.53	0.42
1:U:186:GLU:CB	1:U:188:ILE:HG22	2.49	0.42
1:U:230:ASP:C	1:U:231:LYS:HD3	2.39	0.42
1:U:171:LEU:HD13	1:U:177:GLY:HA2	2.00	0.42
1:A:210:PHE:CE1	1:A:216:LEU:HB2	2.54	0.42
2:C:2:DT:OP2	1:N:179:ILE:HB	2.20	0.42
1:N:220:SER:O	1:N:223:ALA:HB3	2.19	0.42
1:A:167:TYR:HE2	1:A:186:GLU:OE2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:N	1:A:261:LEU:HD23	2.34	0.42
1:U:253:GLU:HG2	1:U:254:ALA:N	2.35	0.42
1:N:244:GLU:O	1:N:247:LYS:HB3	2.20	0.42
1:A:238:GLN:HG3	1:A:264:VAL:HG11	2.02	0.41
1:A:238:GLN:HA	1:A:238:GLN:NE2	2.35	0.41
1:U:182:LEU:HD21	1:U:193:ILE:HD12	2.02	0.41
1:N:192:ILE:HD13	1:N:192:ILE:HA	1.85	0.41
2:D:3:DG:H2"	2:D:4:DG:C8	2.55	0.41
1:B:252:PHE:CD2	1:B:252:PHE:N	2.88	0.41
1:N:220:SER:HB2	1:N:258:ILE:HD13	2.01	0.41
1:U:212:HIS:O	1:U:214:GLY:N	2.54	0.41
1:U:264:VAL:HG22	1:U:264:VAL:O	2.20	0.41
1:N:245:GLN:O	1:N:250:VAL:HB	2.20	0.41
1:B:178:ASN:OD1	1:B:178:ASN:C	2.59	0.41
1:N:224:LEU:O	1:N:225:GLN:C	2.57	0.41
1:A:175:PHE:CD1	1:A:182:LEU:HD23	2.56	0.41
1:A:212:HIS:H	1:A:215:GLU:CG	2.32	0.41
1:B:189:SER:HB2	1:B:192:ILE:HG12	2.03	0.41
1:B:250:VAL:O	1:B:251:ILE:HD13	2.21	0.41
2:Y:3:DG:H2"	2:Y:4:DG:C8	2.55	0.41
2:Y:6:DA:H1'	2:Y:7:DC:H5"	2.02	0.41
1:U:258:ILE:HG13	1:U:259:THR:H	1.85	0.40
2:Y:16:DC:H2"	2:Y:17:DA:C8	2.56	0.40
1:A:234:LEU:HD22	1:B:238:GLN:HG2	2.03	0.40
1:B:164:GLY:HA2	1:B:196:CYS:HB3	2.02	0.40
2:D:10:DT:H2"	2:D:11:DG:C8	2.56	0.40
1:B:163:ARG:HH22	1:B:192:ILE:HG21	1.86	0.40
1:U:225:GLN:CD	1:U:225:GLN:O	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:NZ	2:Y:5:DG:O6[1_556]	2.09	0.11

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	110/121 (91%)	100 (91%)	8 (7%)	2 (2%)	8	35
1	B	109/121 (90%)	100 (92%)	6 (6%)	3 (3%)	5	23
1	N	108/121 (89%)	80 (74%)	21 (19%)	7 (6%)	1	6
1	U	109/121 (90%)	84 (77%)	20 (18%)	5 (5%)	2	12
All	All	436/484 (90%)	364 (84%)	55 (13%)	17 (4%)	3	15

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	THR
1	N	172	GLN
1	N	174	GLU
1	N	187	ASN
1	N	231	LYS
1	U	187	ASN
1	U	250	VAL
1	N	250	VAL
1	N	254	ALA
1	A	209	LEU
1	U	266	LYS
1	N	158	THR
1	B	264	VAL
1	B	266	LYS
1	B	231	LYS
1	U	174	GLU
1	U	213	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	93/100 (93%)	77 (83%)	16 (17%)	2	9
1	B	92/100 (92%)	77 (84%)	15 (16%)	2	10
1	N	91/100 (91%)	81 (89%)	10 (11%)	6	23
1	U	92/100 (92%)	80 (87%)	12 (13%)	4	17
All	All	368/400 (92%)	315 (86%)	53 (14%)	3	14

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	179	ILE
1	A	182	LEU
1	A	184	ASP
1	A	190	ARG
1	A	204	LYS
1	A	207	VAL
1	A	225	GLN
1	A	232	GLU
1	A	235	LEU
1	A	238	GLN
1	A	243	HIS
1	A	252	PHE
1	A	259	THR
1	A	261	LEU
1	A	262	THR
1	B	184	ASP
1	B	204	LYS
1	B	207	VAL
1	B	211	SER
1	B	222	ASP
1	B	225	GLN
1	B	234	LEU
1	B	235	LEU
1	B	238	GLN
1	B	246	LYS
1	B	252	PHE
1	B	253	GLU

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Mol	Chain	Res	Type
1	B	259	THR
1	B	260	LEU
1	B	261	LEU
1	U	186	GLU
1	U	204	LYS
1	U	206	VAL
1	U	222	ASP
1	U	225	GLN
1	U	231	LYS
1	U	235	LEU
1	U	238	GLN
1	U	243	HIS
1	U	246	LYS
1	U	252	PHE
1	U	253	GLU
1	N	166	ARG
1	N	173	ASN
1	N	187	ASN
1	N	194	THR
1	N	211	SER
1	N	225	GLN
1	N	238	GLN
1	N	252	PHE
1	N	253	GLU
1	N	265	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	173	ASN
1	A	225	GLN
1	A	241	ASN
1	B	165	GLN
1	B	225	GLN
1	B	238	GLN
1	B	241	ASN
1	U	165	GLN
1	U	178	ASN
1	U	187	ASN
1	U	225	GLN
1	N	165	GLN

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Mol	Chain	Res	Type
1	N	172	GLN
1	N	178	ASN
1	N	198	ASN
1	N	225	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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(Å²)	Q<0.9
1	A	112/121 (92%)	0.47	5 (4%)	33	19	38, 69, 124, 136	0
1	B	111/121 (91%)	0.27	2 (1%)	68	48	40, 61, 116, 128	0
1	N	110/121 (90%)	0.47	4 (3%)	42	26	67, 92, 121, 126	0
1	U	111/121 (91%)	0.60	12 (10%)	5	3	67, 98, 143, 149	0
2	C	18/18 (100%)	0.08	0	100	100	48, 64, 80, 82	0
2	D	18/18 (100%)	0.09	0	100	100	44, 64, 83, 84	0
2	Y	18/18 (100%)	0.00	0	100	100	46, 62, 77, 78	0
2	Z	18/18 (100%)	-0.02	0	100	100	50, 66, 76, 76	0
All	All	516/556 (92%)	0.39	23 (4%)	33	19	38, 77, 128, 149	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	249	GLY	3.8
1	U	250	VAL	3.5
1	A	252	PHE	2.8
1	N	252	PHE	2.6
1	N	261	LEU	2.5
1	U	252	PHE	2.5
1	U	254	ALA	2.5
1	U	216	LEU	2.4
1	N	265	LEU	2.4
1	U	188	ILE	2.4
1	A	210	PHE	2.4
1	A	209	LEU	2.4
1	A	251	ILE	2.2
1	A	193	ILE	2.2
1	U	207	VAL	2.1
1	U	248	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	251	ILE	2.1
1	B	209	LEU	2.1
1	B	193	ILE	2.1
1	U	218	ALA	2.1
1	N	242	LEU	2.0
1	U	262	THR	2.0
1	U	265	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	Z	20	1/1	0.86	0.10	101,101,101,101	0
3	CA	Z	19	1/1	0.88	0.11	98,98,98,98	0
3	CA	U	2	1/1	0.90	0.20	104,104,104,104	0
3	CA	A	1	1/1	0.94	0.06	98,98,98,98	0

6.5 Other polymers ⓘ

There are no such residues in this entry.