Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 09:11 am GMT

PDB ID	:	4V4F
Title	:	The structure of the trp RNA-binding attenuation protein (TRAP) bound to a RNA molecule containing UAGAU repeats
Authors	:	Hopcroft, N.H.; Manfredo, A.; Wendt, A.L.; Brzozowski, A.M.; Gollnick, P.; Antson, A.A.
Deposited on	:	2003-12-08
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

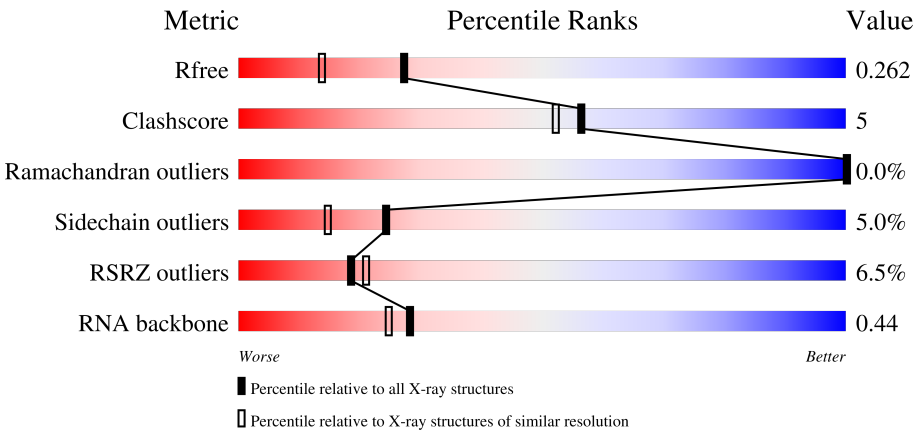
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)
RNA backbone	3102	1013 (2.42-1.38)

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	A0	5	40%; 40%, 20%, 40%
1	A1	5	20%; 40%, 20%, 40%
1	A2	5	40%, 20%, 40%
1	A3	5	20%; 60%, 20%, 20%

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Mol	Chain	Length	Quality of chain
1	A4	5	40% / 40% 20% 40%
1	A5	5	20% / 60% 20% 20%
1	A6	5	40% / 20% 20% 60%
1	A7	5	40% / 60% 40%
1	A8	5	40% 20% 40%
1	A9	5	20% / 40% 20% 40%
1	AZ	5	20% / 20% 20% 20% 40%
1	B0	5	20% / 40% 20% 20% 20%
1	B1	5	60% / 40% 20% 40%
1	B2	5	20% / 20% 20% 60%
1	B3	5	20% / 20% 20% 60%
1	B4	5	40% / 20% 20% 20% 40%
1	B5	5	40% / 40% 20% 40%
1	B6	5	20% / 60% 20% 20%
1	B7	5	20% / 60% 40%
1	B8	5	20% / 40% 20% 40%
1	B9	5	40% 20% 40%
1	BZ	5	40% / 40% 20% 40%
2	AA	74	7% / 88% 5% 5%
2	AB	74	5% / 84% 12%
2	AC	74	5% / 81% 14% 5%
2	AD	74	8% / 81% 12% 5%
2	AE	74	7% / 72% 20% 5%
2	AF	74	4% / 78% 12% 5%
2	AG	74	4% / 86% 5% 5%

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Mol	Chain	Length	Quality of chain
2	AH	74	4% 81% 14% 5%
2	AI	74	4% 84% 11% 5%
2	AJ	74	7% 81% 14% 5%
2	AK	74	3% 82% 14%
2	AL	74	8% 86% 7% 5%
2	AM	74	7% 78% 16%
2	AN	74	5% 82% 12% 5%
2	AO	74	9% 76% 18%
2	AP	74	5% 84% 8% 5%
2	AQ	74	5% 85% 9% 5%
2	AR	74	7% 89% 5% 5%
2	AS	74	5% 80% 15% 5%
2	AT	74	8% 85% 8% 5%
2	AU	74	5% 77% 18% 5%
2	AV	74	5% 86% 8% 5%
2	BA	74	86% 9%
2	BB	74	3% 85% 11%
2	BC	74	% 80% 15% 5%
2	BD	74	5% 78% 14%
2	BE	74	7% 81% 9% 5%
2	BF	74	5% 72% 20% 5%
2	BG	74	4% 78% 14% 5%
2	BH	74	7% 78% 15% 5%
2	BI	74	4% 76% 18% 5%
2	BJ	74	4% 82% 9% 5%

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Mol	Chain	Length	Quality of chain
2	BK	74	7% 72% 20% • 5%
2	BL	74	5% 84% 9% • 5%
2	BM	74	7% 84% 12% •
2	BN	74	5% 78% 15% • 5%
2	BO	74	7% 82% 12% 5%
2	BP	74	5% 78% 16% 5%
2	BQ	74	4% 80% 14% • 5%
2	BR	74	4% 82% 12% 5%
2	BS	74	3% 81% 14% 5%
2	BT	74	5% 81% 14% 5%
2	BU	74	9% 91% • • 5%
2	BV	74	7% 81% 11% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29038 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 RNA chain called 5'-R(*UP*AP*GP*AP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A0	3	48	20	10	15	3	0	0	0
1	A1	3	48	20	10	15	3	0	0	0
1	A2	3	48	20	10	15	3	0	0	0
1	A3	4	68	29	12	23	4	0	0	0
1	A4	3	67	30	15	19	3	0	0	0
1	A5	4	68	29	12	23	4	0	0	0
1	A6	2	45	20	10	13	2	0	0	0
1	A7	3	48	20	10	15	3	0	0	0
1	A8	3	48	20	10	15	3	0	0	0
1	A9	3	48	20	10	15	3	0	0	0
1	AZ	3	48	20	10	15	3	0	0	0
1	B0	4	68	29	12	23	4	0	0	0
1	B1	3	48	20	10	15	3	0	0	0
1	B2	2	41	20	10	10	1	0	0	0
1	B3	2	45	20	10	13	2	0	0	0
1	B4	3	48	20	10	15	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B5	3	48	20	10	15	3	0	0	0
1	B6	4	68	29	12	23	4	0	0	0
1	B7	3	48	20	10	15	3	0	0	0
1	B8	3	48	20	10	15	3	0	0	0
1	B9	3	48	20	10	15	3	0	0	0
1	BZ	3	48	20	10	15	3	0	0	0

- Molecule 2 is a protein called TRANSCRIPTION ATTENUATION PROTEIN MTRB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	AA	70	542	338	99	105	0	0	0
2	AB	71	551	344	101	106	4	0	0
2	AC	70	542	338	99	105	0	0	0
2	AD	70	542	338	99	105	4	0	0
2	AE	70	542	338	99	105	0	0	0
2	AF	70	542	338	99	105	0	0	0
2	AG	70	542	338	99	105	4	0	0
2	AH	70	542	338	99	105	0	0	0
2	AI	70	542	338	99	105	0	0	0
2	AJ	70	542	338	99	105	0	0	0
2	AK	71	551	344	101	106	0	0	0
2	AL	70	542	338	99	105	0	0	0
2	AM	71	551	344	101	106	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	AN	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	AO	71	551	344	101	106	3	0	0
			Total	C	N	O			
2	AP	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	AQ	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	AR	70	542	338	99	105	3	0	0
			Total	C	N	O			
2	AS	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	AT	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	AU	70	542	338	99	105	4	0	0
			Total	C	N	O			
2	AV	70	542	338	99	105	4	0	0
			Total	C	N	O			
2	BA	71	551	344	101	106	0	0	0
			Total	C	N	O			
2	BB	71	551	344	101	106	4	0	0
			Total	C	N	O			
2	BC	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	BD	71	551	344	101	106	0	0	0
			Total	C	N	O			
2	BE	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	BF	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	BG	70	542	338	99	105	4	0	0
			Total	C	N	O			
2	BH	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	BI	70	542	338	99	105	4	0	0
			Total	C	N	O			
2	BJ	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	BK	70	542	338	99	105	0	0	0
			Total	C	N	O			
2	BL	70	542	338	99	105	0	0	0

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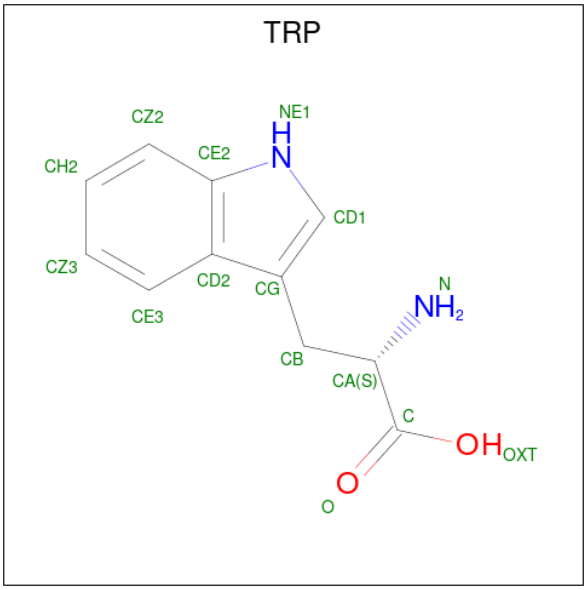
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	BM	71	551	344	101	106	4	0	0
2	BN	70	542	338	99	105	1	0	0
2	BO	70	542	338	99	105	0	0	0
2	BP	70	542	338	99	105	4	0	0
2	BQ	70	542	338	99	105	1	0	0
2	BR	70	542	338	99	105	0	0	0
2	BS	70	542	338	99	105	0	0	0
2	BT	70	542	338	99	105	4	0	0
2	BU	70	542	338	99	105	0	0	0
2	BV	70	542	338	99	105	0	0	0

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	AA	1	15	11	2	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	AB	1	15	11	2	2	0	0
3	AC	1	15	11	2	2	0	0
3	AD	1	15	11	2	2	0	0
3	AE	1	15	11	2	2	0	0
3	AF	1	15	11	2	2	0	0
3	AG	1	15	11	2	2	0	0
3	AH	1	15	11	2	2	0	0
3	AI	1	15	11	2	2	0	0
3	AJ	1	15	11	2	2	0	0
3	AK	1	15	11	2	2	0	0
3	AL	1	15	11	2	2	0	0
3	AM	1	15	11	2	2	0	0
3	AN	1	15	11	2	2	0	0
3	AO	1	15	11	2	2	0	0
3	AP	1	15	11	2	2	0	0
3	AQ	1	15	11	2	2	0	0
3	AR	1	15	11	2	2	0	0
3	AS	1	15	11	2	2	0	0
3	AT	1	15	11	2	2	0	0
3	AU	1	15	11	2	2	0	0
3	AV	1	15	11	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BA	1	Total C N O 15 11 2 2	0	0
3	BB	1	Total C N O 15 11 2 2	0	0
3	BC	1	Total C N O 15 11 2 2	0	0
3	BD	1	Total C N O 15 11 2 2	0	0
3	BE	1	Total C N O 15 11 2 2	0	0
3	BF	1	Total C N O 15 11 2 2	0	0
3	BG	1	Total C N O 15 11 2 2	0	0
3	BH	1	Total C N O 15 11 2 2	0	0
3	BI	1	Total C N O 15 11 2 2	0	0
3	BJ	1	Total C N O 15 11 2 2	0	0
3	BK	1	Total C N O 15 11 2 2	0	0
3	BL	1	Total C N 13 11 2	0	0
3	BM	1	Total C N O 15 11 2 2	0	0
3	BN	1	Total C N O 15 11 2 2	0	0
3	BO	1	Total C N O 15 11 2 2	0	0
3	BP	1	Total C N O 15 11 2 2	0	0
3	BQ	1	Total C N O 15 11 2 2	0	0
3	BR	1	Total C N O 15 11 2 2	0	0
3	BS	1	Total C N O 15 11 2 2	0	0
3	BT	1	Total C N O 15 11 2 2	0	0
3	BU	1	Total C N O 15 11 2 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	BV	1	15	11	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A0	11	11	11	0	0
4	A1	7	7	7	0	0
4	A2	9	9	9	0	0
4	A3	8	8	8	0	0
4	A4	4	4	4	0	0
4	A5	8	8	8	0	0
4	A6	10	10	10	0	0
4	A7	6	6	6	0	0
4	A8	13	13	13	0	0
4	A9	11	11	11	0	0
4	AA	87	87	87	0	0
4	AB	74	74	74	0	0
4	AC	77	77	77	0	0
4	AD	74	74	74	0	0
4	AE	67	67	67	0	0
4	AF	69	69	69	0	0
4	AG	80	80	80	0	0
4	AH	67	67	67	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AI	74	Total O 74 74	0	0
4	AJ	78	Total O 78 78	0	0
4	AK	62	Total O 62 62	0	0
4	AL	70	Total O 70 70	0	0
4	AM	50	Total O 50 50	0	0
4	AN	57	Total O 57 57	0	0
4	AO	71	Total O 71 71	0	0
4	AP	61	Total O 61 61	0	0
4	AQ	69	Total O 69 69	0	0
4	AR	75	Total O 75 75	0	0
4	AS	77	Total O 77 77	0	0
4	AT	78	Total O 78 78	0	0
4	AU	85	Total O 85 85	0	0
4	AV	61	Total O 61 61	0	0
4	AZ	5	Total O 5 5	0	0
4	B0	11	Total O 11 11	0	0
4	B1	6	Total O 6 6	0	0
4	B2	8	Total O 8 8	0	0
4	B3	3	Total O 3 3	0	0
4	B4	14	Total O 14 14	0	0
4	B5	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B6	13	Total O 13 13	0	0
4	B7	6	Total O 6 6	0	0
4	B8	5	Total O 5 5	0	0
4	B9	8	Total O 8 8	0	0
4	BA	67	Total O 67 67	0	0
4	BB	80	Total O 80 80	0	0
4	BC	78	Total O 78 78	0	0
4	BD	80	Total O 80 80	0	0
4	BE	76	Total O 76 76	0	0
4	BF	60	Total O 60 60	0	0
4	BG	71	Total O 71 71	0	0
4	BH	73	Total O 73 73	0	0
4	BI	85	Total O 85 85	0	0
4	BJ	80	Total O 80 80	0	0
4	BK	77	Total O 77 77	0	0
4	BL	72	Total O 72 72	0	0
4	BM	52	Total O 52 52	0	0
4	BN	49	Total O 49 49	0	0
4	BO	63	Total O 63 63	0	0
4	BP	55	Total O 55 55	0	0
4	BQ	75	Total O 75 75	0	0

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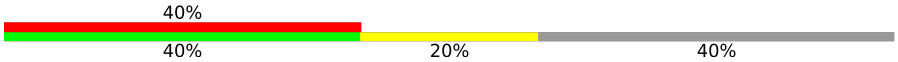
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	BR	76	76	76	0	0
			Total	O		
4	BS	72	72	72	0	0
			Total	O		
4	BT	88	88	88	0	0
			Total	O		
4	BU	71	71	71	0	0
			Total	O		
4	BV	71	71	71	0	0
			Total	O		
4	BZ	6	6	6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

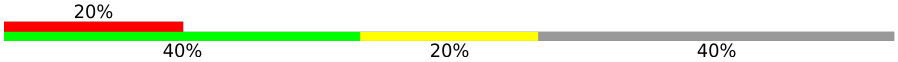
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A0:



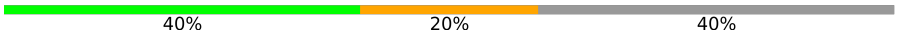
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A1:



• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A2:

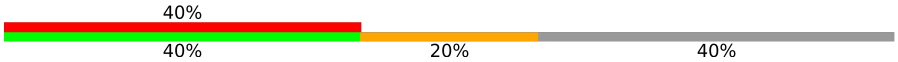


• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A3:

• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A4:



• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A5:

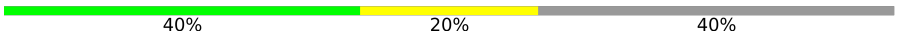
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A6:

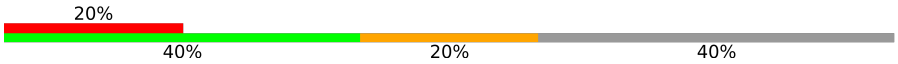
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A7:

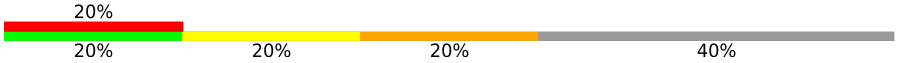
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A8: 

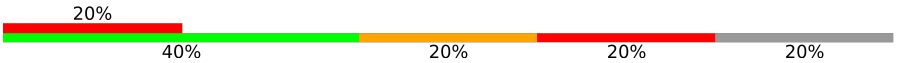
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain A9: 

• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

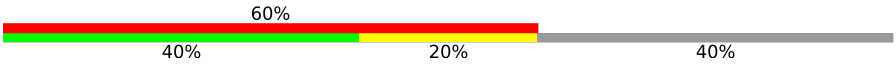
Chain AZ: 

• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain B0: 

• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain B1:



• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

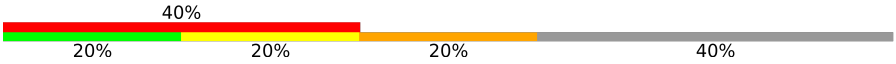
Chain B2:

• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain B3:

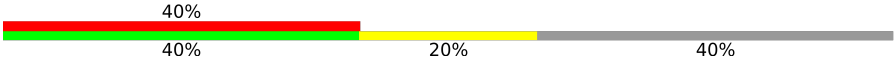
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain B4:



• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain B5:



• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

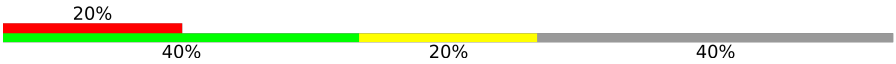
Chain B6:

• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain B7:

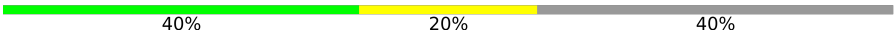
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain B8:



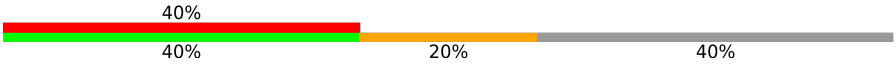
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain B9:



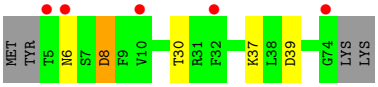
• Molecule 1: 5'-R(*UP*AP*GP*AP*UP)-3'

Chain BZ:



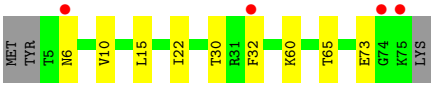
• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AA:



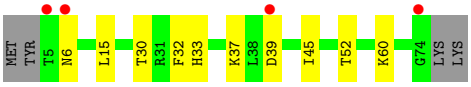
• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AB:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AC:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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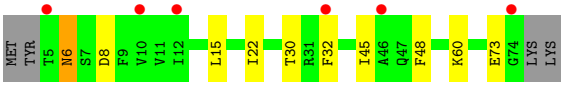
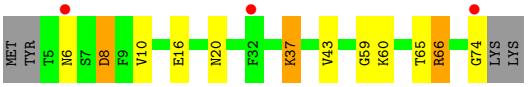


• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AE:

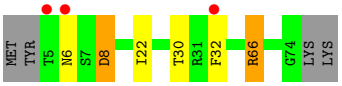
• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AF:



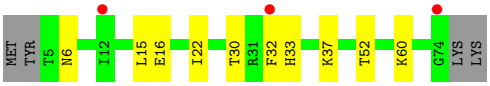
• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AG:



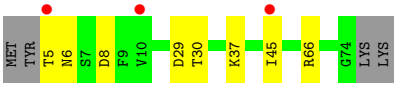
• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AH:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AI:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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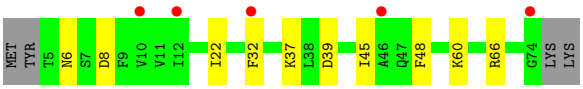
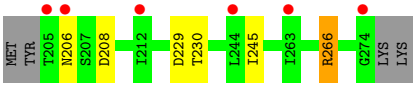


• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AK:

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AL:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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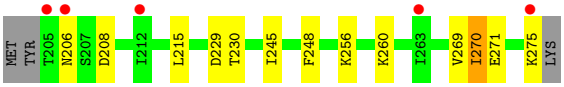
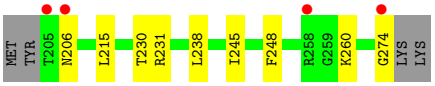


• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AN:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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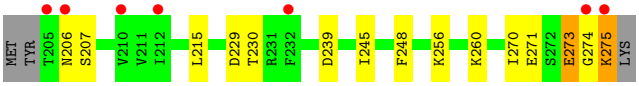


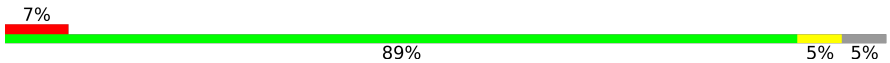
• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

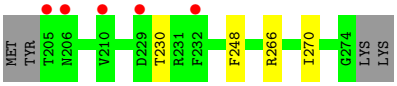
Chain AP:

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AQ:

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain AR: 



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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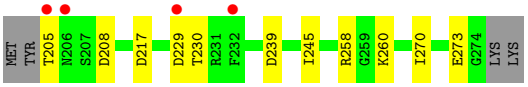

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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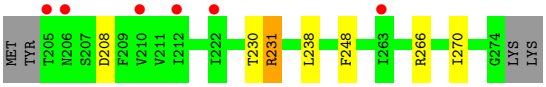

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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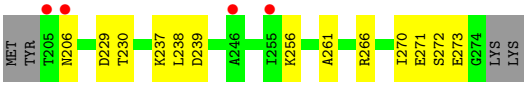

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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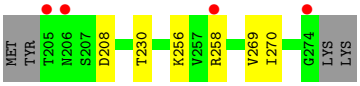
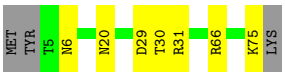


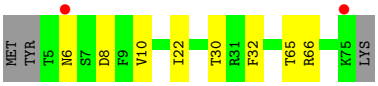
• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BA:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BB:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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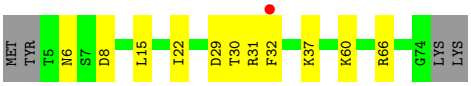

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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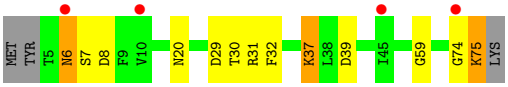
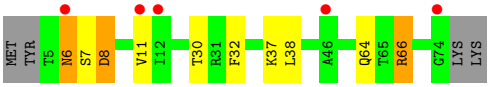


• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BE:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

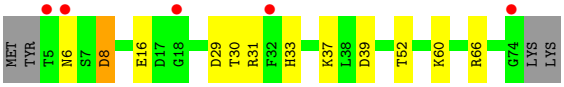
Chain BF:

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BG:

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BH:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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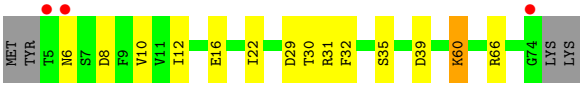

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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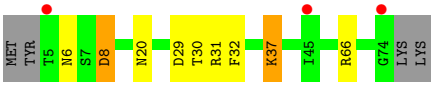

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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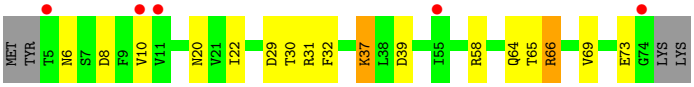

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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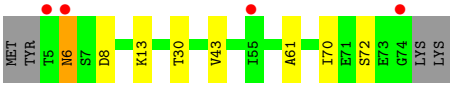

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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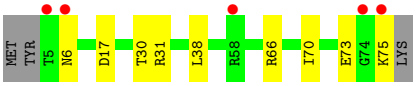

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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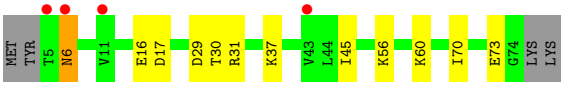

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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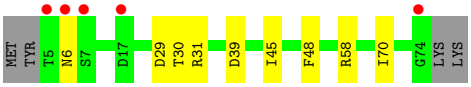
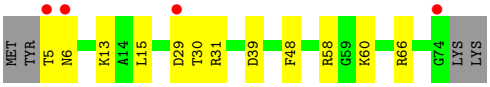


• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BP:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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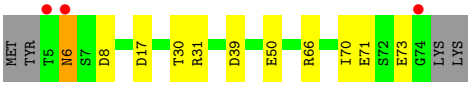
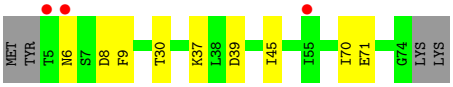


• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BR:

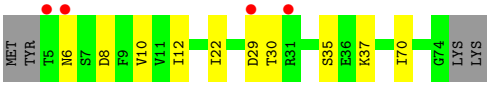


• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BS:

• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BT:



• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

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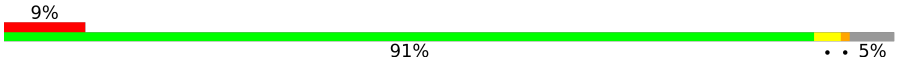
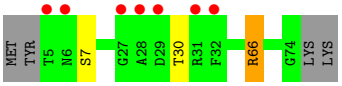
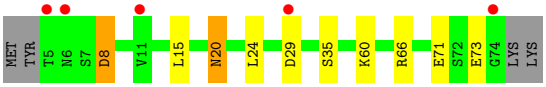




• Molecule 2: TRANSCRIPTION ATTENUATION PROTEIN MTRB

Chain BV:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.91Å 133.99Å 232.83Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 34.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 93.0 (34.69-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.186 , 0.236 0.230 , 0.262	Depositor DCC
R_{free} test set	1249 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	29038	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8804e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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	A0	0.94	0/53	1.40	1/80 (1.2%)
1	A1	0.69	0/53	1.58	1/80 (1.2%)
1	A2	0.85	0/53	1.79	1/80 (1.2%)
1	A3	0.73	0/75	1.76	1/114 (0.9%)
1	A4	1.07	0/75	1.48	1/115 (0.9%)
1	A5	1.02	0/75	1.53	0/114
1	A6	0.72	0/50	1.46	1/76 (1.3%)
1	A7	0.90	0/53	1.21	0/80
1	A8	0.85	0/53	1.72	1/80 (1.2%)
1	A9	0.86	0/53	2.06	1/80 (1.2%)
1	AZ	0.88	0/53	1.37	1/80 (1.2%)
1	B0	0.95	0/75	1.54	1/114 (0.9%)
1	B1	0.82	0/53	1.40	1/80 (1.2%)
1	B2	1.10	0/46	1.68	1/71 (1.4%)
1	B3	1.00	0/50	1.57	1/76 (1.3%)
1	B4	1.07	0/53	1.75	1/80 (1.2%)
1	B5	0.83	0/53	1.30	0/80
1	B6	0.90	0/75	1.48	1/114 (0.9%)
1	B7	0.72	0/53	1.26	0/80
1	B8	0.85	0/53	1.31	0/80
1	B9	0.86	0/53	1.42	0/80
1	BZ	0.91	0/53	1.62	1/80 (1.2%)
2	AA	0.77	0/549	0.88	1/738 (0.1%)
2	AB	0.75	0/558	0.79	0/749
2	AC	0.70	0/549	0.84	1/738 (0.1%)
2	AD	0.69	0/549	0.86	0/738
2	AE	0.67	0/549	0.83	1/738 (0.1%)
2	AF	0.70	1/549 (0.2%)	0.81	0/738
2	AG	0.73	0/549	0.82	1/738 (0.1%)
2	AH	0.66	0/549	0.85	0/738
2	AI	0.72	0/549	0.84	0/738
2	AJ	0.70	0/549	0.80	1/738 (0.1%)
2	AK	0.70	0/558	0.80	1/749 (0.1%)
2	AL	0.65	0/549	0.82	1/738 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	AM	0.60	0/558	0.78	0/749
2	AN	0.65	0/549	0.82	0/738
2	AO	0.66	0/558	0.78	2/749 (0.3%)
2	AP	0.69	0/549	0.80	0/738
2	AQ	0.69	0/549	0.84	1/738 (0.1%)
2	AR	0.63	0/549	0.80	0/738
2	AS	0.71	0/549	0.83	2/738 (0.3%)
2	AT	0.69	0/549	0.79	0/738
2	AU	0.74	1/549 (0.2%)	0.81	2/738 (0.3%)
2	AV	0.72	0/549	0.78	0/738
2	BA	0.82	0/558	0.84	0/749
2	BB	0.77	0/558	0.84	0/749
2	BC	0.65	0/549	0.83	0/738
2	BD	0.70	0/558	0.83	1/749 (0.1%)
2	BE	0.64	0/549	0.78	0/738
2	BF	0.66	0/549	0.81	2/738 (0.3%)
2	BG	0.69	0/549	0.85	2/738 (0.3%)
2	BH	0.66	0/549	0.82	1/738 (0.1%)
2	BI	0.69	0/549	0.82	1/738 (0.1%)
2	BJ	0.70	0/549	0.84	0/738
2	BK	0.68	0/549	0.80	1/738 (0.1%)
2	BL	0.73	0/549	0.81	0/738
2	BM	0.63	0/558	0.84	1/749 (0.1%)
2	BN	0.98	1/549 (0.2%)	0.95	3/738 (0.4%)
2	BO	0.63	0/549	0.80	2/738 (0.3%)
2	BP	0.66	0/549	0.83	2/738 (0.3%)
2	BQ	0.69	0/549	0.85	3/738 (0.4%)
2	BR	0.75	0/549	0.81	1/738 (0.1%)
2	BS	0.74	0/549	0.83	1/738 (0.1%)
2	BT	0.82	1/549 (0.2%)	0.86	3/738 (0.4%)
2	BU	0.74	0/549	0.79	0/738
2	BV	0.72	0/549	0.79	0/738
All	All	0.72	4/25491 (0.0%)	0.88	54/34474 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BN	37	LYS	CE-NZ	-15.55	1.10	1.49
2	BT	37	LYS	CB-CG	-11.14	1.22	1.52
2	AU	237	LYS	CB-CG	-6.72	1.34	1.52
2	AF	43	VAL	CB-CG1	5.50	1.64	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A9	103	G	O4'-C1'-N9	11.01	117.01	108.20
2	BN	37	LYS	CD-CE-NZ	10.71	136.32	111.70
1	B4	103	G	O4'-C1'-N9	9.91	116.13	108.20
1	B3	103	G	O4'-C1'-N9	8.35	114.88	108.20
1	A2	103	G	O4'-C1'-N9	8.07	114.65	108.20
1	B2	103	G	O4'-C1'-N9	7.88	114.51	108.20
2	AE	39	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A0	103	G	O4'-C1'-N9	6.81	113.65	108.20
1	A4	103	G	O4'-C1'-N9	6.80	113.64	108.20
2	BQ	39	ASP	CB-CG-OD2	6.68	124.31	118.30
2	AL	229	ASP	CB-CG-OD2	6.62	124.25	118.30
2	BM	17	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A6	103	G	O4'-C1'-N9	6.60	113.48	108.20
1	BZ	103	G	O4'-C1'-N9	6.56	113.45	108.20
1	AZ	103	G	O4'-C1'-N9	6.36	113.29	108.20
2	BN	29	ASP	CB-CG-OD2	6.27	123.94	118.30
2	AA	39	ASP	CB-CG-OD2	6.24	123.91	118.30
2	BG	17	ASP	CB-CG-OD2	6.04	123.74	118.30
2	BI	39	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B6	103	G	O4'-C1'-N9	5.89	112.91	108.20
2	BN	17	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A3	103	G	O4'-C1'-N9	5.81	112.85	108.20
2	AC	39	ASP	CB-CG-OD2	5.72	123.44	118.30
2	BK	39	ASP	CB-CG-OD2	5.69	123.42	118.30
2	BP	39	ASP	CB-CG-OD2	5.69	123.42	118.30
2	BG	29	ASP	CB-CG-OD2	5.66	123.39	118.30
2	AU	239	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A1	103	G	O4'-C1'-N9	5.65	112.72	108.20
2	BR	39	ASP	CB-CG-OD2	5.63	123.37	118.30
2	AK	17	ASP	CB-CG-OD2	5.60	123.34	118.30
2	AS	217	ASP	CB-CG-OD2	5.53	123.28	118.30
2	BH	39	ASP	CB-CG-OD2	5.52	123.26	118.30
2	BO	29	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B1	103	G	O4'-C1'-N9	5.49	112.59	108.20
2	BD	39	ASP	CB-CG-OD2	5.46	123.21	118.30
2	AO	229	ASP	CB-CG-OD2	5.39	123.15	118.30
2	AO	239	ASP	CB-CG-OD2	5.38	123.14	118.30
2	AG	8	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A8	103	G	O4'-C1'-N9	5.37	112.49	108.20
2	BF	29	ASP	CB-CG-OD2	5.33	123.10	118.30
2	BS	17	ASP	CB-CG-OD2	5.33	123.09	118.30
2	AS	239	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AQ	239	ASP	CB-CG-OD2	5.26	123.03	118.30
2	BT	37	LYS	CA-CB-CG	5.23	124.91	113.40
2	BP	29	ASP	CB-CG-OD2	5.22	123.00	118.30
2	AJ	39	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B0	101	U	P-O3'-C3'	5.10	125.82	119.70
2	BO	39	ASP	CB-CG-OD2	5.08	122.88	118.30
2	BQ	8	ASP	CB-CG-OD2	5.08	122.87	118.30
2	BT	29	ASP	CB-CG-OD2	5.06	122.85	118.30
2	BQ	17	ASP	CB-CG-OD2	5.05	122.85	118.30
2	BF	39	ASP	CB-CG-OD2	5.03	122.83	118.30
2	AU	229	ASP	CB-CG-OD2	5.02	122.82	118.30
2	BT	8	ASP	CB-CG-OD2	5.02	122.81	118.30

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	A0	48	0	22	0	0
1	A1	48	0	22	0	0
1	A2	48	0	22	3	0
1	A3	68	0	32	2	0
1	A4	67	0	34	2	0
1	A5	68	0	32	0	0
1	A6	45	0	23	1	0
1	A7	48	0	22	0	0
1	A8	48	0	22	0	0
1	A9	48	0	22	1	0
1	AZ	48	0	22	1	0
1	B0	68	0	32	3	0
1	B1	48	0	22	0	0
1	B2	41	0	21	1	0
1	B3	45	0	23	1	0
1	B4	48	0	22	3	0
1	B5	48	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B6	68	0	32	2	0
1	B7	48	0	22	0	0
1	B8	48	0	22	2	0
1	B9	48	0	22	1	0
1	BZ	48	0	22	1	0
2	AA	542	0	541	2	0
2	AB	551	0	554	7	0
2	AC	542	0	541	6	0
2	AD	542	0	541	10	0
2	AE	542	0	541	15	0
2	AF	542	0	541	11	0
2	AG	542	0	541	6	0
2	AH	542	0	541	8	0
2	AI	542	0	541	5	0
2	AJ	542	0	541	7	0
2	AK	551	0	554	6	0
2	AL	542	0	541	4	0
2	AM	551	0	554	7	0
2	AN	542	0	541	6	0
2	AO	551	0	554	9	0
2	AP	542	0	541	4	0
2	AQ	542	0	541	2	0
2	AR	542	0	541	2	0
2	AS	542	0	541	5	0
2	AT	542	0	541	6	0
2	AU	542	0	541	6	0
2	AV	542	0	541	4	0
2	BA	551	0	554	2	0
2	BB	551	0	554	6	0
2	BC	542	0	541	6	0
2	BD	551	0	554	9	0
2	BE	542	0	541	13	0
2	BF	542	0	541	15	0
2	BG	542	0	541	9	0
2	BH	542	0	541	6	0
2	BI	542	0	541	10	0
2	BJ	542	0	541	5	0
2	BK	542	0	541	11	0
2	BL	542	0	541	6	0
2	BM	551	0	554	5	0
2	BN	542	0	541	5	0
2	BO	542	0	541	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BP	542	0	541	6	0
2	BQ	542	0	541	3	0
2	BR	542	0	541	6	0
2	BS	542	0	541	9	0
2	BT	542	0	541	3	0
2	BU	542	0	541	3	0
2	BV	542	0	541	5	0
3	AA	15	0	9	1	0
3	AB	15	0	9	1	0
3	AC	15	0	9	1	0
3	AD	15	0	9	1	0
3	AE	15	0	9	1	0
3	AF	15	0	9	0	0
3	AG	15	0	9	1	0
3	AH	15	0	9	1	0
3	AI	15	0	9	1	0
3	AJ	15	0	9	0	0
3	AK	15	0	9	1	0
3	AL	15	0	9	1	0
3	AM	15	0	9	1	0
3	AN	15	0	9	1	0
3	AO	15	0	9	1	0
3	AP	15	0	9	1	0
3	AQ	15	0	9	1	0
3	AR	15	0	9	1	0
3	AS	15	0	9	1	0
3	AT	15	0	9	1	0
3	AU	15	0	9	1	0
3	AV	15	0	9	1	0
3	BA	15	0	9	1	0
3	BB	15	0	9	1	0
3	BC	15	0	9	1	0
3	BD	15	0	9	1	0
3	BE	15	0	9	1	0
3	BF	15	0	9	1	0
3	BG	15	0	9	1	0
3	BH	15	0	9	1	0
3	BI	15	0	9	1	0
3	BJ	15	0	9	1	0
3	BK	15	0	9	1	0
3	BL	13	0	9	1	0
3	BM	15	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BN	15	0	9	1	0
3	BO	15	0	9	1	0
3	BP	15	0	9	1	0
3	BQ	15	0	9	1	0
3	BR	15	0	9	1	0
3	BS	15	0	9	1	0
3	BT	15	0	9	1	0
3	BU	15	0	9	1	0
3	BV	15	0	9	0	0
4	A0	11	0	0	0	0
4	A1	7	0	0	0	0
4	A2	9	0	0	1	0
4	A3	8	0	0	0	0
4	A4	4	0	0	0	0
4	A5	8	0	0	0	0
4	A6	10	0	0	0	0
4	A7	6	0	0	0	0
4	A8	13	0	0	0	0
4	A9	11	0	0	0	0
4	AA	87	0	0	4	0
4	AB	74	0	0	0	0
4	AC	77	0	0	0	0
4	AD	74	0	0	1	0
4	AE	67	0	0	4	0
4	AF	69	0	0	4	0
4	AG	80	0	0	0	0
4	AH	67	0	0	0	0
4	AI	74	0	0	1	0
4	AJ	78	0	0	1	0
4	AK	62	0	0	1	0
4	AL	70	0	0	1	0
4	AM	50	0	0	2	0
4	AN	57	0	0	1	0
4	AO	71	0	0	3	0
4	AP	61	0	0	0	0
4	AQ	69	0	0	0	0
4	AR	75	0	0	0	0
4	AS	77	0	0	3	0
4	AT	78	0	0	1	0
4	AU	85	0	0	1	0
4	AV	61	0	0	1	0
4	AZ	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B0	11	0	0	0	0
4	B1	6	0	0	0	0
4	B2	8	0	0	0	0
4	B3	3	0	0	0	0
4	B4	14	0	0	1	0
4	B5	12	0	0	0	0
4	B6	13	0	0	0	0
4	B7	6	0	0	0	0
4	B8	5	0	0	0	0
4	B9	8	0	0	0	0
4	BA	67	0	0	1	0
4	BB	80	0	0	0	0
4	BC	78	0	0	0	0
4	BD	80	0	0	1	0
4	BE	76	0	0	2	0
4	BF	60	0	0	2	0
4	BG	71	0	0	2	0
4	BH	73	0	0	0	0
4	BI	85	0	0	2	0
4	BJ	80	0	0	1	0
4	BK	77	0	0	3	0
4	BL	72	0	0	3	0
4	BM	52	0	0	2	0
4	BN	49	0	0	1	0
4	BO	63	0	0	1	0
4	BP	55	0	0	1	0
4	BQ	75	0	0	1	0
4	BR	76	0	0	1	0
4	BS	72	0	0	1	0
4	BT	88	0	0	1	0
4	BU	71	0	0	1	0
4	BV	71	0	0	2	0
4	BZ	6	0	0	0	0
All	All	29038	0	24841	252	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 (252) 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)
4:BL:2047:HOH:O	2:BM:66:ARG:HD3	1.55	1.05
2:BL:8:ASP:HB2	4:BL:2003:HOH:O	1.66	0.93
4:AF:241:HOH:O	2:AG:66:ARG:HD3	1.74	0.86
2:AL:208:ASP:HB2	4:AL:2117:HOH:O	1.76	0.84
2:AH:16:GLU:HG2	2:AH:60:LYS:HB3	1.64	0.79
2:BJ:8:ASP:OD1	2:BJ:66:ARG:NH1	2.18	0.75
2:AF:16:GLU:HG2	2:AF:60:LYS:HB2	1.70	0.74
2:BF:7:SER:O	4:BF:206:HOH:O	2.07	0.72
1:B0:101:U:H5'	2:BK:37:LYS:HE2	1.72	0.71
2:BE:66:ARG:HH22	2:BF:66:ARG:HD3	1.55	0.70
2:BG:8:ASP:OD1	4:BG:210:HOH:O	2.09	0.69
2:AJ:22:ILE:HG21	2:AJ:32:PHE:CE1	2.28	0.69
4:AA:2009:HOH:O	2:AB:73:GLU:HG3	1.94	0.68
2:AE:6:ASN:ND2	2:AF:8:ASP:H	1.94	0.66
4:AA:2009:HOH:O	2:AB:73:GLU:CD	2.34	0.65
2:AD:73:GLU:OE1	4:AD:259:HOH:O	2.14	0.65
2:AP:215:LEU:HB2	2:AP:260:LYS:HG2	1.78	0.65
2:BS:30:THR:HG1	3:BS:101:TRP:N	1.94	0.65
2:AM:215:LEU:HB2	2:AM:260:LYS:HG2	1.80	0.64
2:AO:230:THR:HG1	3:AO:301:TRP:N	1.96	0.64
2:AH:22:ILE:HG21	2:AH:32:PHE:CE1	2.33	0.64
2:BE:7:SER:O	4:BE:209:HOH:O	2.15	0.63
2:AG:6:ASN:ND2	2:AH:6:ASN:O	2.32	0.63
2:AO:271:GLU:OE2	4:AO:2065:HOH:O	2.15	0.63
2:BV:20:ASN:ND2	2:BV:35:SER:OG	2.28	0.63
2:AB:15:LEU:HB2	2:AB:60:LYS:HG2	1.81	0.63
2:BK:6:ASN:HA	4:BK:209:HOH:O	2.00	0.62
2:AO:274:GLY:O	2:AO:275:LYS:HB3	1.97	0.62
2:BR:30:THR:HG1	3:BR:101:TRP:N	1.97	0.61
2:AC:15:LEU:HB2	2:AC:60:LYS:HG2	1.82	0.61
2:BH:30:THR:HG1	3:BH:101:TRP:N	1.98	0.61
2:BK:58:ARG:HD2	4:BK:247:HOH:O	1.99	0.61
2:AV:256:LYS:HD3	2:AV:258:ARG:HE	1.65	0.61
2:BN:6:ASN:HB3	4:BN:203:HOH:O	2.01	0.61
2:AU:271:GLU:OE2	4:AU:476:HOH:O	2.16	0.61
1:A9:103:G:C6	2:AJ:32:PHE:CZ	2.90	0.60
2:BO:30:THR:HG1	3:BO:101:TRP:N	2.00	0.60
2:AE:66:ARG:HH22	2:AF:66:ARG:HE	1.49	0.60
2:AS:230:THR:HG1	3:AS:301:TRP:N	2.00	0.60
2:BN:30:THR:HG1	3:BN:101:TRP:N	1.98	0.60
2:BM:30:THR:HG1	3:BM:101:TRP:N	2.00	0.60
2:BU:30:THR:HG1	3:BU:101:TRP:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AC:30:THR:HG1	3:AC:101:TRP:N	2.00	0.60
2:AM:230:THR:HG1	3:AM:301:TRP:N	2.00	0.60
2:BF:15:LEU:HB2	2:BF:60:LYS:HG2	1.83	0.60
2:BE:30:THR:HG1	3:BE:101:TRP:N	2.00	0.60
2:BV:15:LEU:HB2	2:BV:60:LYS:HG2	1.84	0.59
2:BI:6:ASN:HB3	4:BI:207:HOH:O	2.02	0.59
2:BB:66:ARG:HH22	2:BC:66:ARG:HD2	1.68	0.59
2:AV:230:THR:HG1	3:AV:301:TRP:N	2.00	0.59
2:AE:5:THR:N	4:AE:205:HOH:O	2.35	0.58
2:AK:30:THR:HG1	3:AK:101:TRP:N	2.01	0.58
2:BM:31:ARG:NH1	4:BM:226:HOH:O	2.27	0.58
2:AI:6:ASN:HA	4:AJ:207:HOH:O	2.01	0.58
2:BT:30:THR:HG1	3:BT:101:TRP:N	2.02	0.58
2:BE:66:ARG:NH2	2:BF:66:ARG:HD3	2.19	0.58
2:AL:230:THR:HG1	3:AL:301:TRP:N	2.02	0.58
2:AT:230:THR:HG1	3:AT:301:TRP:N	2.02	0.58
2:BK:20:ASN:OD1	2:BK:37:LYS:HD2	2.03	0.58
2:BJ:29:ASP:OD2	2:BJ:31:ARG:HD3	2.04	0.58
2:BI:6:ASN:HA	4:BJ:214:HOH:O	2.04	0.57
2:BK:29:ASP:OD2	2:BK:31:ARG:HD3	2.04	0.57
2:BL:8:ASP:CB	4:BL:2003:HOH:O	2.37	0.57
4:AA:2009:HOH:O	2:AB:73:GLU:CG	2.52	0.57
2:AJ:22:ILE:HG21	2:AJ:32:PHE:CZ	2.39	0.57
2:BA:29:ASP:OD2	2:BA:31:ARG:HD3	2.04	0.57
2:BV:8:ASP:OD1	2:BV:66:ARG:HD2	2.05	0.57
2:AQ:230:THR:HG1	3:AQ:301:TRP:N	2.03	0.56
2:AE:30:THR:HG1	3:AE:101:TRP:N	2.03	0.56
2:AN:245:ILE:HG22	2:AO:248:PHE:HZ	1.71	0.56
2:AU:230:THR:HG1	3:AU:301:TRP:N	2.04	0.56
2:AF:59:GLY:HA2	2:AF:74:GLY:HA2	1.87	0.55
2:BC:22:ILE:HG21	2:BC:32:PHE:CE1	2.42	0.55
2:AR:230:THR:HG1	3:AR:301:TRP:N	2.04	0.55
2:AS:245:ILE:HG22	2:AT:248:PHE:HZ	1.72	0.55
2:BV:66:ARG:HD3	4:BV:206:HOH:O	2.07	0.55
2:AO:260:LYS:NZ	4:AO:2055:HOH:O	2.40	0.55
2:BN:45:ILE:HG22	2:BO:48:PHE:HZ	1.72	0.55
1:A2:103:G:C6	2:AC:32:PHE:CZ	2.95	0.55
2:BQ:30:THR:HG1	3:BQ:101:TRP:N	2.05	0.54
2:BP:30:THR:HG1	3:BP:101:TRP:N	2.06	0.54
2:BU:7:SER:O	4:BU:204:HOH:O	2.18	0.54
2:AA:8:ASP:HB2	4:AA:2005:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BH:16:GLU:HG2	2:BH:60:LYS:HB3	1.90	0.54
2:AN:238:LEU:HD23	2:AO:256:LYS:HE3	1.90	0.54
1:B5:103:G:C6	2:BF:32:PHE:CZ	2.96	0.54
2:BL:30:THR:HG1	3:BL:101:TRP:N	2.06	0.53
2:BD:7:SER:O	4:BD:210:HOH:O	2.18	0.53
2:AJ:66:ARG:HH22	2:AK:66:ARG:HE	1.56	0.53
1:B5:103:G:C5	2:BF:32:PHE:CZ	2.96	0.53
2:AN:230:THR:HG1	3:AN:301:TRP:N	2.06	0.52
2:AD:30:THR:HG1	3:AD:101:TRP:N	2.08	0.52
2:BD:59:GLY:HA2	2:BD:74:GLY:HA3	1.91	0.52
1:A2:103:G:N7	4:A2:2002:HOH:O	2.34	0.52
2:AM:269:VAL:HG22	4:AM:440:HOH:O	2.08	0.52
2:BF:30:THR:HG1	3:BF:101:TRP:N	2.08	0.51
2:AT:231:ARG:NH1	4:AT:435:HOH:O	2.38	0.51
2:AM:256:LYS:NZ	4:AM:433:HOH:O	2.43	0.51
1:B6:103:G:C6	2:BG:32:PHE:CZ	2.99	0.51
2:AF:74:GLY:HA3	4:AF:210:HOH:O	2.09	0.51
2:BS:6:ASN:HA	4:BT:208:HOH:O	2.10	0.51
2:AF:20:ASN:OD1	2:AF:37:LYS:HE2	2.11	0.50
1:B3:103:G:C6	2:BD:32:PHE:CZ	2.99	0.50
2:BB:30:THR:HG1	3:BB:101:TRP:N	2.09	0.50
2:BF:13:LYS:HB2	2:BG:70:ILE:HD11	1.93	0.50
2:BT:22:ILE:HG12	2:BT:35:SER:OG	2.10	0.50
2:AH:30:THR:HG1	3:AH:101:TRP:N	2.10	0.50
2:AO:215:LEU:HB2	2:AO:260:LYS:HG2	1.93	0.49
2:AM:245:ILE:HG22	2:AN:248:PHE:HZ	1.76	0.49
2:AJ:60:LYS:HE3	4:BF:253:HOH:O	2.11	0.49
2:BS:6:ASN:CG	2:BS:6:ASN:O	2.51	0.49
2:AK:18:GLY:HA2	2:AK:37:LYS:HE3	1.94	0.49
2:AL:245:ILE:HG22	2:AM:248:PHE:HZ	1.77	0.49
2:AD:22:ILE:HG21	2:AD:32:PHE:CE1	2.48	0.49
2:AG:30:THR:HG1	3:AG:101:TRP:N	2.09	0.49
2:BK:30:THR:HG1	3:BK:101:TRP:N	2.11	0.49
2:BL:13:LYS:HG3	2:BL:43:VAL:HG22	1.94	0.49
2:BK:64:GLN:HG2	2:BK:69:VAL:HG12	1.95	0.49
2:AT:238:LEU:CD2	2:AU:256:LYS:HE3	2.43	0.49
2:AD:60:LYS:HE3	4:BA:254:HOH:O	2.12	0.48
2:AF:74:GLY:CA	4:AF:210:HOH:O	2.61	0.48
2:AK:5:THR:N	4:AK:209:HOH:O	2.46	0.48
2:AH:33:HIS:CE1	2:AH:52:THR:HG1	2.29	0.48
2:AQ:245:ILE:HG22	2:AR:248:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:30:THR:HG1	3:AB:101:TRP:N	2.12	0.48
2:AE:33:HIS:NE2	2:AE:52:THR:OG1	2.45	0.48
2:AP:230:THR:HG1	3:AP:301:TRP:N	2.11	0.48
2:BG:5:THR:N	4:BG:206:HOH:O	2.47	0.48
2:AO:273:GLU:HB3	4:AO:2055:HOH:O	2.14	0.48
2:BE:66:ARG:HH22	2:BF:66:ARG:CD	2.26	0.48
2:BK:66:ARG:NH1	4:BK:211:HOH:O	2.45	0.48
2:BI:30:THR:HG1	3:BI:101:TRP:N	2.12	0.48
2:AP:220:ASN:HD21	2:AP:235:SER:CB	2.27	0.48
1:B0:101:U:H4'	1:B0:102:A:C5	2.48	0.48
2:AT:238:LEU:HD23	2:AU:256:LYS:HE3	1.95	0.48
2:BG:29:ASP:OD2	2:BG:31:ARG:HD3	2.14	0.48
2:BR:45:ILE:HG22	2:BS:48:PHE:HZ	1.78	0.47
2:AH:33:HIS:NE2	2:AH:52:THR:OG1	2.40	0.47
2:AE:60:LYS:HE3	4:AE:245:HOH:O	2.14	0.47
2:AN:274:GLY:HA3	4:AN:419:HOH:O	2.14	0.47
4:AS:423:HOH:O	2:AT:266:ARG:HD3	2.15	0.47
2:BH:8:ASP:OD2	2:BH:66:ARG:NE	2.38	0.47
2:BI:29:ASP:OD2	2:BI:31:ARG:HD3	2.14	0.47
2:BK:10:VAL:HG12	2:BK:65:THR:HG22	1.97	0.47
2:BT:10:VAL:HG23	2:BT:12:ILE:HD11	1.95	0.47
2:AI:30:THR:HG1	3:AI:101:TRP:N	2.13	0.47
1:B2:102:A:C5	1:B2:103:G:C6	3.03	0.47
2:AD:45:ILE:HG22	2:AE:48:PHE:HZ	1.80	0.47
2:BC:30:THR:HG1	3:BC:101:TRP:N	2.13	0.47
2:AL:208:ASP:OD2	2:AL:266:ARG:NE	2.48	0.46
2:BD:29:ASP:OD2	2:BD:31:ARG:HD3	2.15	0.46
1:A4:103:G:C6	2:AE:32:PHE:CZ	3.03	0.46
2:AH:15:LEU:HB2	2:AH:60:LYS:HG2	1.96	0.46
2:AI:5:THR:N	4:AI:204:HOH:O	2.48	0.46
2:BA:30:THR:HG1	3:BA:101:TRP:N	2.13	0.46
1:B6:103:G:C5	2:BG:32:PHE:CZ	3.03	0.46
2:BF:45:ILE:HG22	2:BG:48:PHE:HZ	1.80	0.46
2:AE:22:ILE:HG21	2:AE:32:PHE:CE1	2.51	0.46
2:BF:29:ASP:OD2	2:BF:31:ARG:HD3	2.16	0.46
2:AA:30:THR:HG1	3:AA:101:TRP:N	2.13	0.46
1:B4:103:G:C6	2:BE:32:PHE:CZ	3.04	0.46
2:BS:10:VAL:CG2	2:BS:12:ILE:HD11	2.46	0.46
2:AC:33:HIS:NE2	2:AC:52:THR:OG1	2.39	0.46
2:BM:38:LEU:HD23	2:BN:56:LYS:HE3	1.98	0.46
2:BR:9:PHE:CE1	2:BS:67:HIS:CD2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:103:G:C6	2:AD:32:PHE:CZ	3.04	0.46
1:A6:103:G:C6	2:AG:32:PHE:CZ	3.04	0.45
1:B9:103:G:C6	2:BJ:32:PHE:CZ	3.05	0.45
2:AV:269:VAL:HG22	4:AV:455:HOH:O	2.15	0.45
2:AI:29:ASP:OD2	2:AS:260:LYS:NZ	2.50	0.45
2:BG:30:THR:HG1	3:BG:101:TRP:N	2.14	0.45
2:BU:66:ARG:HH11	2:BU:66:ARG:HB2	1.81	0.45
2:AS:205:THR:HA	4:AS:422:HOH:O	2.17	0.45
2:BH:6:ASN:CG	2:BH:6:ASN:O	2.56	0.45
2:BK:22:ILE:HG21	2:BK:32:PHE:CE1	2.52	0.45
1:A3:103:G:C5	2:AD:32:PHE:CZ	3.05	0.44
2:AM:270:ILE:HG13	2:AM:271:GLU:N	2.32	0.44
2:BD:74:GLY:O	2:BD:75:LYS:HB3	2.18	0.44
2:BF:16:GLU:HA	2:BF:40:LYS:HG3	2.00	0.44
2:BM:31:ARG:HD2	4:BM:227:HOH:O	2.18	0.44
2:AD:15:LEU:HB2	2:AD:60:LYS:HG2	1.99	0.44
2:BD:20:ASN:OD1	2:BD:37:LYS:HE2	2.17	0.44
2:BE:11:VAL:HB	2:BE:64:GLN:HB2	1.98	0.44
2:AC:45:ILE:HG22	2:AD:48:PHE:HZ	1.82	0.44
2:BS:10:VAL:HG23	2:BS:12:ILE:CD1	2.47	0.44
2:AE:74:GLY:C	4:AE:247:HOH:O	2.57	0.44
1:B8:103:G:C5	2:BI:32:PHE:CZ	3.05	0.44
2:BE:6:ASN:ND2	2:BF:8:ASP:H	2.16	0.44
2:BS:58:ARG:NH1	4:BS:241:HOH:O	2.48	0.44
2:BQ:6:ASN:ND2	4:BQ:204:HOH:O	2.36	0.43
2:AB:10:VAL:HG22	2:AB:65:THR:HG22	2.00	0.43
2:BI:22:ILE:HG21	2:BI:32:PHE:CE1	2.54	0.43
2:AF:10:VAL:HG22	2:AF:65:THR:HG22	2.00	0.43
2:AK:74:GLY:O	2:AK:75:LYS:HB3	2.18	0.43
2:AU:261:ALA:HB3	2:AU:272:SER:OG	2.19	0.43
2:BS:10:VAL:HG23	2:BS:12:ILE:HD11	1.99	0.43
2:BI:6:ASN:CB	4:BI:207:HOH:O	2.64	0.43
2:AN:215:LEU:HB2	2:AN:260:LYS:HG2	2.00	0.43
2:AJ:45:ILE:HG22	2:AK:48:PHE:HZ	1.83	0.43
1:B0:101:U:H4'	1:B0:102:A:C4	2.54	0.43
1:B4:102:A:C5	1:B4:103:G:C6	3.06	0.43
2:BD:30:THR:HG1	3:BD:101:TRP:N	2.17	0.43
2:AG:8:ASP:OD1	2:AG:66:ARG:NH1	2.49	0.43
2:BE:8:ASP:OD1	4:BE:210:HOH:O	2.21	0.43
2:BP:15:LEU:HB2	2:BP:60:LYS:HG2	1.99	0.43
2:AD:6:ASN:HA	4:AE:209:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:6:ASN:CG	2:BB:6:ASN:O	2.56	0.43
2:BB:22:ILE:HG21	2:BB:32:PHE:CE1	2.53	0.43
2:AE:66:ARG:NH2	2:AF:66:ARG:HE	2.15	0.43
1:B8:103:G:C6	2:BI:32:PHE:CZ	3.07	0.43
2:BK:32:PHE:CZ	1:BZ:103:G:C5	3.05	0.43
2:BO:45:ILE:HG22	2:BP:48:PHE:HZ	1.84	0.43
2:BE:38:LEU:HD23	2:BF:56:LYS:HE3	2.00	0.42
2:BJ:30:THR:HG1	3:BJ:101:TRP:N	2.16	0.42
2:BJ:20:ASN:OD1	2:BJ:37:LYS:HG3	2.19	0.42
2:BL:61:ALA:HB3	2:BL:72:SER:OG	2.20	0.42
2:BR:8:ASP:OD2	4:BR:206:HOH:O	2.22	0.42
2:AS:258:ARG:NH2	4:AS:462:HOH:O	2.53	0.42
1:B4:102:A:H5"	4:B4:2009:HOH:O	2.18	0.42
2:BD:6:ASN:CG	2:BE:7:SER:HA	2.40	0.42
2:BE:6:ASN:CG	2:BF:7:SER:HA	2.39	0.42
4:BO:232:HOH:O	2:BP:58:ARG:CZ	2.67	0.42
2:AE:6:ASN:HD21	2:AF:8:ASP:H	1.66	0.42
1:A2:103:G:C5	2:AC:32:PHE:CZ	3.07	0.42
2:AF:66:ARG:NH1	4:AF:241:HOH:O	2.48	0.42
2:BI:16:GLU:HG2	2:BI:60:LYS:HB2	2.00	0.42
2:BR:6:ASN:O	2:BR:6:ASN:ND2	2.53	0.42
2:BP:5:THR:N	4:BP:204:HOH:O	2.53	0.42
2:BP:13:LYS:HE3	2:BQ:71:GLU:O	2.20	0.42
1:AZ:102:A:C5	1:AZ:103:G:C6	3.09	0.41
2:BG:22:ILE:HG21	2:BG:32:PHE:CE1	2.55	0.41
2:BB:66:ARG:NH2	2:BC:66:ARG:HD2	2.32	0.41
2:BC:15:LEU:HB2	2:BC:60:LYS:HG2	2.01	0.41
2:BH:33:HIS:NE2	2:BH:52:THR:OG1	2.51	0.41
2:BI:10:VAL:HG23	2:BI:12:ILE:HD11	2.02	0.41
2:AE:22:ILE:HG22	2:AE:24:LEU:HD12	2.03	0.41
2:AG:22:ILE:HG21	2:AG:32:PHE:CE1	2.55	0.41
2:BH:29:ASP:OD2	2:BH:31:ARG:HD3	2.20	0.41
1:A4:103:G:C5	2:AE:32:PHE:CZ	3.08	0.41
2:BR:70:ILE:HG13	2:BR:71:GLU:N	2.36	0.41
2:AB:22:ILE:HG21	2:AB:32:PHE:CE1	2.55	0.41
2:AH:22:ILE:HG21	2:AH:32:PHE:CD1	2.55	0.41
2:AE:29:ASP:OD2	2:AE:31:ARG:HD3	2.21	0.41
2:AO:245:ILE:HG22	2:AP:248:PHE:HZ	1.85	0.41
2:AI:45:ILE:HG22	2:AJ:48:PHE:HZ	1.86	0.41
2:BC:29:ASP:OD2	2:BC:31:ARG:HD3	2.20	0.41
2:BL:6:ASN:O	2:BL:6:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BV:71:GLU:OE2	4:BV:258:HOH:O	2.21	0.40
2:AU:238:LEU:HD23	2:AV:256:LYS:HE2	2.02	0.40
2:BB:10:VAL:HG12	2:BB:65:THR:HG22	2.04	0.40
2:BN:16:GLU:HG2	2:BN:60:LYS:HB3	2.03	0.40
2:BD:6:ASN:ND2	2:BE:8:ASP:H	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AB	69/74 (93%)	69 (100%)	0	0	100	100
2	AC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AD	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AE	68/74 (92%)	68 (100%)	0	0	100	100
2	AF	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AG	68/74 (92%)	68 (100%)	0	0	100	100
2	AH	68/74 (92%)	68 (100%)	0	0	100	100
2	AI	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AJ	68/74 (92%)	68 (100%)	0	0	100	100
2	AK	69/74 (93%)	68 (99%)	1 (1%)	0	100	100
2	AL	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AM	69/74 (93%)	68 (99%)	1 (1%)	0	100	100
2	AN	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AO	69/74 (93%)	68 (99%)	0	1 (1%)	11	3
2	AP	68/74 (92%)	68 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AQ	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AR	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AS	68/74 (92%)	68 (100%)	0	0	100	100
2	AT	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	AU	68/74 (92%)	68 (100%)	0	0	100	100
2	AV	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	BA	69/74 (93%)	69 (100%)	0	0	100	100
2	BB	69/74 (93%)	69 (100%)	0	0	100	100
2	BC	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	BD	69/74 (93%)	67 (97%)	2 (3%)	0	100	100
2	BE	68/74 (92%)	68 (100%)	0	0	100	100
2	BF	68/74 (92%)	68 (100%)	0	0	100	100
2	BG	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
2	BH	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	BI	68/74 (92%)	68 (100%)	0	0	100	100
2	BJ	68/74 (92%)	68 (100%)	0	0	100	100
2	BK	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	BL	68/74 (92%)	68 (100%)	0	0	100	100
2	BM	69/74 (93%)	68 (99%)	1 (1%)	0	100	100
2	BN	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	BO	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
2	BP	68/74 (92%)	68 (100%)	0	0	100	100
2	BQ	68/74 (92%)	68 (100%)	0	0	100	100
2	BR	68/74 (92%)	68 (100%)	0	0	100	100
2	BS	68/74 (92%)	68 (100%)	0	0	100	100
2	BT	68/74 (92%)	68 (100%)	0	0	100	100
2	BU	68/74 (92%)	68 (100%)	0	0	100	100
2	BV	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
All	All	3000/3256 (92%)	2975 (99%)	24 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AO	207	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	AB	59/62 (95%)	58 (98%)	1 (2%)	60	57
2	AC	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	AD	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	AE	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	AF	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	AG	58/62 (94%)	57 (98%)	1 (2%)	60	57
2	AH	58/62 (94%)	57 (98%)	1 (2%)	60	57
2	AI	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	AJ	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	AK	59/62 (95%)	58 (98%)	1 (2%)	60	57
2	AL	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	AM	59/62 (95%)	54 (92%)	5 (8%)	10	4
2	AN	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	AO	59/62 (95%)	55 (93%)	4 (7%)	16	7
2	AP	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	AQ	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	AR	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	AS	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	AT	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	AU	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	AV	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	BA	59/62 (95%)	55 (93%)	4 (7%)	16	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BB	59/62 (95%)	58 (98%)	1 (2%)	60	57
2	BC	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	BD	59/62 (95%)	55 (93%)	4 (7%)	16	7
2	BE	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	BF	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	BG	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	BH	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	BI	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	BJ	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	BK	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	BL	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	BM	59/62 (95%)	55 (93%)	4 (7%)	16	7
2	BN	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	BO	58/62 (94%)	54 (93%)	4 (7%)	15	7
2	BP	58/62 (94%)	55 (95%)	3 (5%)	23	14
2	BQ	58/62 (94%)	52 (90%)	6 (10%)	7	2
2	BR	58/62 (94%)	57 (98%)	1 (2%)	60	57
2	BS	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	BT	58/62 (94%)	56 (97%)	2 (3%)	37	28
2	BU	58/62 (94%)	57 (98%)	1 (2%)	60	57
2	BV	58/62 (94%)	53 (91%)	5 (9%)	10	4
All	All	2560/2728 (94%)	2430 (95%)	130 (5%)	24	14

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	6	ASN
2	AA	8	ASP
2	AA	37	LYS
2	AB	6	ASN
2	AC	6	ASN
2	AC	37	LYS
2	AD	6	ASN
2	AD	8	ASP
2	AE	6	ASN

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Mol	Chain	Res	Type
2	AE	35	SER
2	AE	37	LYS
2	AE	66	ARG
2	AF	6	ASN
2	AF	8	ASP
2	AF	37	LYS
2	AF	66	ARG
2	AG	66	ARG
2	AH	37	LYS
2	AI	8	ASP
2	AI	37	LYS
2	AI	66	ARG
2	AJ	6	ASN
2	AJ	8	ASP
2	AJ	37	LYS
2	AK	8	ASP
2	AL	206	ASN
2	AL	266	ARG
2	AM	206	ASN
2	AM	208	ASP
2	AM	229	ASP
2	AM	270	ILE
2	AM	275	LYS
2	AN	206	ASN
2	AN	231	ARG
2	AO	206	ASN
2	AO	270	ILE
2	AO	273	GLU
2	AO	275	LYS
2	AP	206	ASN
2	AP	220	ASN
2	AP	224	LEU
2	AP	235	SER
2	AQ	206	ASN
2	AQ	237	LYS
2	AQ	266	ARG
2	AQ	273	GLU
2	AR	266	ARG
2	AR	270	ILE
2	AS	208	ASP
2	AS	229	ASP
2	AS	270	ILE

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Mol	Chain	Res	Type
2	AS	273	GLU
2	AT	208	ASP
2	AT	231	ARG
2	AT	270	ILE
2	AU	206	ASN
2	AU	266	ARG
2	AU	270	ILE
2	AU	273	GLU
2	AV	208	ASP
2	AV	270	ILE
2	BA	6	ASN
2	BA	20	ASN
2	BA	66	ARG
2	BA	75	LYS
2	BB	8	ASP
2	BC	6	ASN
2	BC	8	ASP
2	BC	37	LYS
2	BD	6	ASN
2	BD	8	ASP
2	BD	37	LYS
2	BD	75	LYS
2	BE	6	ASN
2	BE	8	ASP
2	BE	37	LYS
2	BE	66	ARG
2	BF	6	ASN
2	BF	8	ASP
2	BF	37	LYS
2	BG	8	ASP
2	BG	66	ARG
2	BG	73	GLU
2	BH	8	ASP
2	BH	37	LYS
2	BI	8	ASP
2	BI	35	SER
2	BI	60	LYS
2	BI	66	ARG
2	BJ	6	ASN
2	BJ	8	ASP
2	BJ	37	LYS
2	BK	8	ASP

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Mol	Chain	Res	Type
2	BK	37	LYS
2	BK	66	ARG
2	BK	73	GLU
2	BL	6	ASN
2	BL	70	ILE
2	BM	6	ASN
2	BM	70	ILE
2	BM	73	GLU
2	BM	75	LYS
2	BN	6	ASN
2	BN	31	ARG
2	BN	70	ILE
2	BN	73	GLU
2	BO	6	ASN
2	BO	31	ARG
2	BO	58	ARG
2	BO	70	ILE
2	BP	6	ASN
2	BP	31	ARG
2	BP	66	ARG
2	BQ	6	ASN
2	BQ	31	ARG
2	BQ	50	GLU
2	BQ	66	ARG
2	BQ	70	ILE
2	BQ	73	GLU
2	BR	37	LYS
2	BS	31	ARG
2	BS	70	ILE
2	BT	6	ASN
2	BT	70	ILE
2	BU	66	ARG
2	BV	8	ASP
2	BV	20	ASN
2	BV	24	LEU
2	BV	29	ASP
2	BV	73	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	6	ASN

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Mol	Chain	Res	Type
2	AD	6	ASN
2	AD	20	ASN
2	AE	6	ASN
2	AF	6	ASN
2	AG	6	ASN
2	AI	6	ASN
2	AJ	6	ASN
2	AL	206	ASN
2	AM	220	ASN
2	AP	220	ASN
2	AQ	206	ASN
2	AT	206	ASN
2	AU	206	ASN
2	AU	220	ASN
2	AV	220	ASN
2	BD	6	ASN
2	BE	6	ASN
2	BF	6	ASN
2	BJ	6	ASN
2	BL	6	ASN
2	BM	6	ASN
2	BT	20	ASN
2	BV	20	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A0	1/5 (20%)	0	0
1	A1	1/5 (20%)	0	0
1	A2	1/5 (20%)	0	0
1	A3	2/5 (40%)	0	0
1	A4	2/5 (40%)	0	0
1	A5	2/5 (40%)	1 (50%)	0
1	A6	1/5 (20%)	0	0
1	A7	1/5 (20%)	0	0
1	A8	1/5 (20%)	0	0
1	A9	1/5 (20%)	0	0
1	AZ	1/5 (20%)	0	0
1	B0	3/5 (60%)	1 (33%)	1 (33%)
1	B1	1/5 (20%)	0	0
1	B2	1/5 (20%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B3	1/5 (20%)	0	0
1	B4	1/5 (20%)	0	0
1	B5	1/5 (20%)	0	0
1	B6	2/5 (40%)	0	0
1	B7	1/5 (20%)	0	0
1	B8	1/5 (20%)	0	0
1	B9	1/5 (20%)	0	0
1	BZ	1/5 (20%)	0	0
All	All	28/110 (25%)	2 (7%)	1 (3%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A5	102	A
1	B0	102	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B0	101	U

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)

44 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TRP	BT	101	-	14,16,16	1.10	2 (14%)	16,22,22	1.16	2 (12%)
3	TRP	BA	101	-	14,16,16	0.69	0	16,22,22	1.23	1 (6%)
3	TRP	BG	101	-	14,16,16	0.87	0	16,22,22	1.19	2 (12%)
3	TRP	BO	101	-	14,16,16	0.94	0	16,22,22	1.48	2 (12%)
3	TRP	BF	101	-	14,16,16	0.83	0	16,22,22	1.24	2 (12%)
3	TRP	BH	101	-	14,16,16	0.81	0	16,22,22	1.15	2 (12%)
3	TRP	BE	101	-	14,16,16	0.85	0	16,22,22	1.19	2 (12%)
3	TRP	AM	301	-	14,16,16	0.95	1 (7%)	16,22,22	1.36	2 (12%)
3	TRP	AE	101	-	14,16,16	0.86	0	16,22,22	1.17	2 (12%)
3	TRP	AI	101	-	14,16,16	0.97	1 (7%)	16,22,22	1.03	1 (6%)
3	TRP	AJ	101	-	14,16,16	1.06	1 (7%)	16,22,22	1.22	2 (12%)
3	TRP	BP	101	-	14,16,16	0.83	0	16,22,22	1.03	1 (6%)
3	TRP	AF	101	-	14,16,16	0.75	0	16,22,22	1.41	2 (12%)
3	TRP	AC	101	-	14,16,16	0.73	0	16,22,22	1.21	2 (12%)
3	TRP	AP	301	-	14,16,16	0.85	0	16,22,22	1.05	1 (6%)
3	TRP	BV	101	-	14,16,16	0.98	1 (7%)	16,22,22	0.91	0
3	TRP	AG	101	-	14,16,16	0.94	1 (7%)	16,22,22	1.46	2 (12%)
3	TRP	BK	101	-	14,16,16	0.78	0	16,22,22	1.17	2 (12%)
3	TRP	BN	101	-	14,16,16	1.06	2 (14%)	16,22,22	1.11	2 (12%)
3	TRP	BB	101	-	14,16,16	0.83	0	16,22,22	1.13	2 (12%)
3	TRP	BL	101	-	13,14,16	0.89	0	13,19,22	0.85	0
3	TRP	AB	101	-	14,16,16	0.91	1 (7%)	16,22,22	1.15	2 (12%)
3	TRP	AH	101	-	14,16,16	0.66	0	16,22,22	1.22	2 (12%)
3	TRP	AN	301	-	14,16,16	0.80	1 (7%)	16,22,22	1.44	3 (18%)
3	TRP	AQ	301	-	14,16,16	0.92	0	16,22,22	1.10	1 (6%)
3	TRP	BJ	101	-	14,16,16	0.90	1 (7%)	16,22,22	1.14	2 (12%)
3	TRP	BU	101	-	14,16,16	0.75	0	16,22,22	1.24	2 (12%)
3	TRP	AD	101	-	14,16,16	0.88	0	16,22,22	0.91	1 (6%)
3	TRP	AK	101	-	14,16,16	0.77	0	16,22,22	1.18	1 (6%)
3	TRP	AS	301	-	14,16,16	1.19	2 (14%)	16,22,22	1.10	1 (6%)
3	TRP	AO	301	-	14,16,16	0.92	0	16,22,22	0.87	0
3	TRP	BM	101	-	14,16,16	0.95	0	16,22,22	0.92	0
3	TRP	AA	101	-	14,16,16	0.87	1 (7%)	16,22,22	1.38	2 (12%)
3	TRP	BI	101	-	14,16,16	0.89	1 (7%)	16,22,22	1.24	2 (12%)
3	TRP	AT	301	-	14,16,16	0.82	0	16,22,22	1.20	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TRP	BR	101	-	14,16,16	0.90	1 (7%)	16,22,22	0.86	0
3	TRP	BC	101	-	14,16,16	1.00	2 (14%)	16,22,22	1.15	2 (12%)
3	TRP	BD	101	-	14,16,16	0.84	0	16,22,22	1.16	2 (12%)
3	TRP	AL	301	-	14,16,16	0.95	1 (7%)	16,22,22	0.94	0
3	TRP	AV	301	-	14,16,16	0.88	0	16,22,22	1.36	3 (18%)
3	TRP	AR	301	-	14,16,16	0.98	1 (7%)	16,22,22	0.99	1 (6%)
3	TRP	BS	101	-	14,16,16	0.93	1 (7%)	16,22,22	1.07	2 (12%)
3	TRP	BQ	101	-	14,16,16	0.92	1 (7%)	16,22,22	1.10	2 (12%)
3	TRP	AU	301	-	14,16,16	1.01	2 (14%)	16,22,22	1.25	2 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	BT	101	-	-	0/7/8/8	0/2/2/2
3	TRP	BA	101	-	-	1/7/8/8	0/2/2/2
3	TRP	BG	101	-	-	1/7/8/8	0/2/2/2
3	TRP	BO	101	-	-	0/7/8/8	0/2/2/2
3	TRP	BF	101	-	-	1/7/8/8	0/2/2/2
3	TRP	BH	101	-	-	1/7/8/8	0/2/2/2
3	TRP	BE	101	-	-	0/7/8/8	0/2/2/2
3	TRP	AM	301	-	-	0/7/8/8	0/2/2/2
3	TRP	AE	101	-	-	1/7/8/8	0/2/2/2
3	TRP	AI	101	-	-	1/7/8/8	0/2/2/2
3	TRP	AJ	101	-	-	0/7/8/8	0/2/2/2
3	TRP	BP	101	-	-	2/7/8/8	0/2/2/2
3	TRP	AF	101	-	-	0/7/8/8	0/2/2/2
3	TRP	AC	101	-	-	1/7/8/8	0/2/2/2
3	TRP	AP	301	-	-	1/7/8/8	0/2/2/2
3	TRP	BV	101	-	-	2/7/8/8	0/2/2/2
3	TRP	AG	101	-	-	0/7/8/8	0/2/2/2
3	TRP	BK	101	-	-	1/7/8/8	0/2/2/2
3	TRP	BN	101	-	-	0/7/8/8	0/2/2/2
3	TRP	BB	101	-	-	1/7/8/8	0/2/2/2
3	TRP	BL	101	-	-	0/3/4/8	0/2/2/2
3	TRP	AB	101	-	-	1/7/8/8	0/2/2/2
3	TRP	AH	101	-	-	0/7/8/8	0/2/2/2
3	TRP	AN	301	-	-	0/7/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	AQ	301	-	-	1/7/8/8	0/2/2/2
3	TRP	BJ	101	-	-	1/7/8/8	0/2/2/2
3	TRP	BU	101	-	-	2/7/8/8	0/2/2/2
3	TRP	AD	101	-	-	0/7/8/8	0/2/2/2
3	TRP	AK	101	-	-	1/7/8/8	0/2/2/2
3	TRP	AS	301	-	-	0/7/8/8	0/2/2/2
3	TRP	AO	301	-	-	1/7/8/8	0/2/2/2
3	TRP	BM	101	-	-	0/7/8/8	0/2/2/2
3	TRP	AA	101	-	-	0/7/8/8	0/2/2/2
3	TRP	BI	101	-	-	1/7/8/8	0/2/2/2
3	TRP	AT	301	-	-	1/7/8/8	0/2/2/2
3	TRP	BR	101	-	-	0/7/8/8	0/2/2/2
3	TRP	BC	101	-	-	1/7/8/8	0/2/2/2
3	TRP	BD	101	-	-	1/7/8/8	0/2/2/2
3	TRP	AL	301	-	-	0/7/8/8	0/2/2/2
3	TRP	AV	301	-	-	1/7/8/8	0/2/2/2
3	TRP	AR	301	-	-	0/7/8/8	0/2/2/2
3	TRP	BS	101	-	-	2/7/8/8	0/2/2/2
3	TRP	BQ	101	-	-	1/7/8/8	0/2/2/2
3	TRP	AU	301	-	-	1/7/8/8	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BT	101	TRP	CZ3-CE3	3.05	1.43	1.36
3	AS	301	TRP	CZ3-CE3	2.65	1.42	1.36
3	AL	301	TRP	OXT-C	-2.64	1.21	1.30
3	AS	301	TRP	OXT-C	-2.62	1.22	1.30
3	BN	101	TRP	OXT-C	-2.52	1.22	1.30
3	AJ	101	TRP	CZ3-CE3	2.46	1.42	1.36
3	AI	101	TRP	OXT-C	-2.39	1.22	1.30
3	AB	101	TRP	OXT-C	-2.33	1.22	1.30
3	AM	301	TRP	OXT-C	-2.31	1.23	1.30
3	AG	101	TRP	OXT-C	-2.29	1.23	1.30
3	BR	101	TRP	OXT-C	-2.26	1.23	1.30
3	AU	301	TRP	CZ3-CE3	2.25	1.41	1.36
3	BC	101	TRP	OXT-C	-2.24	1.23	1.30
3	BS	101	TRP	OXT-C	-2.23	1.23	1.30
3	AA	101	TRP	OXT-C	-2.20	1.23	1.30
3	AU	301	TRP	OXT-C	-2.19	1.23	1.30
3	BQ	101	TRP	OXT-C	-2.19	1.23	1.30
3	BI	101	TRP	OXT-C	-2.14	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BN	101	TRP	CZ3-CE3	2.14	1.41	1.36
3	BC	101	TRP	CH2-CZ3	2.07	1.43	1.38
3	AR	301	TRP	OXT-C	-2.06	1.23	1.30
3	BV	101	TRP	CZ3-CE3	2.03	1.41	1.36
3	AN	301	TRP	OXT-C	-2.02	1.23	1.30
3	BT	101	TRP	OXT-C	-2.02	1.23	1.30
3	BJ	101	TRP	OXT-C	-2.01	1.24	1.30

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BO	101	TRP	OXT-C-O	-4.40	114.09	124.09
3	AG	101	TRP	OXT-C-O	-3.87	115.31	124.09
3	AN	301	TRP	OXT-C-O	-3.66	115.77	124.09
3	AF	101	TRP	OXT-C-O	-3.54	116.05	124.09
3	AA	101	TRP	OXT-C-O	-3.52	116.09	124.09
3	AM	301	TRP	OXT-C-O	-3.50	116.14	124.09
3	AV	301	TRP	OXT-C-O	-3.31	116.58	124.09
3	AF	101	TRP	OXT-C-CA	3.30	124.62	113.38
3	AG	101	TRP	OXT-C-CA	3.18	124.21	113.38
3	BA	101	TRP	OXT-C-CA	3.11	123.99	113.38
3	AJ	101	TRP	OXT-C-O	-3.06	117.15	124.09
3	AB	101	TRP	OXT-C-O	-3.04	117.18	124.09
3	BF	101	TRP	OXT-C-CA	2.95	123.44	113.38
3	BI	101	TRP	OXT-C-O	-2.95	117.39	124.09
3	AV	301	TRP	OXT-C-CA	2.91	123.31	113.38
3	BE	101	TRP	OXT-C-O	-2.88	117.54	124.09
3	AM	301	TRP	OXT-C-CA	2.88	123.20	113.38
3	AE	101	TRP	OXT-C-O	-2.84	117.65	124.09
3	AA	101	TRP	OXT-C-CA	2.84	123.04	113.38
3	BH	101	TRP	OXT-C-CA	2.82	123.00	113.38
3	BU	101	TRP	OXT-C-CA	2.82	123.00	113.38
3	AS	301	TRP	OXT-C-O	-2.81	117.71	124.09
3	AH	101	TRP	OXT-C-CA	2.74	122.72	113.38
3	AC	101	TRP	OXT-C-CA	2.74	122.70	113.38
3	BC	101	TRP	OXT-C-O	-2.73	117.88	124.09
3	AJ	101	TRP	OXT-C-CA	2.73	122.67	113.38
3	BD	101	TRP	OXT-C-CA	2.73	122.67	113.38
3	AK	101	TRP	OXT-C-CA	2.72	122.65	113.38
3	BG	101	TRP	OXT-C-O	-2.70	117.97	124.09
3	BT	101	TRP	OXT-C-O	-2.69	117.98	124.09
3	BK	101	TRP	OXT-C-CA	2.69	122.53	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AU	301	TRP	OXT-C-CA	2.68	122.50	113.38
3	AU	301	TRP	OXT-C-O	-2.68	118.01	124.09
3	BU	101	TRP	OXT-C-O	-2.67	118.02	124.09
3	BJ	101	TRP	OXT-C-CA	2.66	122.45	113.38
3	AN	301	TRP	OXT-C-CA	2.62	122.30	113.38
3	AE	101	TRP	OXT-C-CA	2.61	122.27	113.38
3	BI	101	TRP	OXT-C-CA	2.60	122.25	113.38
3	AT	301	TRP	OXT-C-CA	2.57	122.15	113.38
3	BG	101	TRP	OXT-C-CA	2.56	122.10	113.38
3	BQ	101	TRP	OXT-C-O	-2.52	118.38	124.09
3	AQ	301	TRP	OXT-C-CA	2.50	121.91	113.38
3	AT	301	TRP	OXT-C-O	-2.50	118.41	124.09
3	BO	101	TRP	OXT-C-CA	2.49	121.86	113.38
3	BB	101	TRP	OXT-C-CA	2.48	121.82	113.38
3	BD	101	TRP	OXT-C-O	-2.44	118.55	124.09
3	AP	301	TRP	OXT-C-CA	2.42	121.64	113.38
3	BF	101	TRP	OXT-C-O	-2.42	118.59	124.09
3	BN	101	TRP	OXT-C-O	-2.36	118.72	124.09
3	BP	101	TRP	OXT-C-CA	2.33	121.31	113.38
3	BS	101	TRP	OXT-C-O	-2.31	118.83	124.09
3	BE	101	TRP	OXT-C-CA	2.31	121.25	113.38
3	BS	101	TRP	OXT-C-CA	2.30	121.23	113.38
3	BJ	101	TRP	OXT-C-O	-2.29	118.89	124.09
3	AH	101	TRP	CH2-CZ2-CE2	-2.27	116.81	120.08
3	AB	101	TRP	OXT-C-CA	2.26	121.09	113.38
3	BC	101	TRP	OXT-C-CA	2.25	121.04	113.38
3	BK	101	TRP	OXT-C-O	-2.22	119.06	124.09
3	AR	301	TRP	OXT-C-O	-2.15	119.21	124.09
3	BH	101	TRP	OXT-C-O	-2.15	119.21	124.09
3	BQ	101	TRP	OXT-C-CA	2.14	120.68	113.38
3	BN	101	TRP	OXT-C-CA	2.13	120.64	113.38
3	AI	101	TRP	OXT-C-CA	2.08	120.46	113.38
3	BT	101	TRP	OXT-C-CA	2.07	120.45	113.38
3	AN	301	TRP	CH2-CZ2-CE2	-2.05	117.13	120.08
3	BB	101	TRP	CH2-CZ2-CE2	-2.04	117.14	120.08
3	AD	101	TRP	OXT-C-CA	2.03	120.29	113.38
3	AC	101	TRP	CH2-CZ2-CE2	-2.02	117.17	120.08
3	AV	301	TRP	CH2-CZ2-CE2	-2.00	117.20	120.08

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BU	101	TRP	OXT-C-CA-N
3	BS	101	TRP	OXT-C-CA-N
3	AB	101	TRP	OXT-C-CA-N
3	BH	101	TRP	OXT-C-CA-N
3	BQ	101	TRP	OXT-C-CA-N
3	BK	101	TRP	OXT-C-CA-N
3	BP	101	TRP	OXT-C-CA-N
3	BV	101	TRP	OXT-C-CA-N
3	BA	101	TRP	OXT-C-CA-N
3	BP	101	TRP	O-C-CA-N
3	BS	101	TRP	O-C-CA-N
3	BU	101	TRP	O-C-CA-N
3	BV	101	TRP	O-C-CA-N
3	BI	101	TRP	OXT-C-CA-N
3	AI	101	TRP	OXT-C-CA-N
3	AK	101	TRP	OXT-C-CA-N
3	AO	301	TRP	OXT-C-CA-N
3	AQ	301	TRP	OXT-C-CA-N
3	AT	301	TRP	OXT-C-CA-N
3	AV	301	TRP	OXT-C-CA-N
3	BB	101	TRP	OXT-C-CA-N
3	BG	101	TRP	OXT-C-CA-N
3	BJ	101	TRP	OXT-C-CA-N
3	AC	101	TRP	OXT-C-CA-N
3	AE	101	TRP	OXT-C-CA-N
3	AP	301	TRP	OXT-C-CA-N
3	AU	301	TRP	OXT-C-CA-N
3	BC	101	TRP	OXT-C-CA-N
3	BD	101	TRP	OXT-C-CA-N
3	BF	101	TRP	OXT-C-CA-N

There are no ring outliers.

41 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BT	101	TRP	1	0
3	BA	101	TRP	1	0
3	BG	101	TRP	1	0
3	BO	101	TRP	1	0
3	BF	101	TRP	1	0
3	BH	101	TRP	1	0
3	BE	101	TRP	1	0
3	AM	301	TRP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AE	101	TRP	1	0
3	AI	101	TRP	1	0
3	BP	101	TRP	1	0
3	AC	101	TRP	1	0
3	AP	301	TRP	1	0
3	AG	101	TRP	1	0
3	BK	101	TRP	1	0
3	BN	101	TRP	1	0
3	BB	101	TRP	1	0
3	BL	101	TRP	1	0
3	AB	101	TRP	1	0
3	AH	101	TRP	1	0
3	AN	301	TRP	1	0
3	AQ	301	TRP	1	0
3	BJ	101	TRP	1	0
3	BU	101	TRP	1	0
3	AD	101	TRP	1	0
3	AK	101	TRP	1	0
3	AS	301	TRP	1	0
3	AO	301	TRP	1	0
3	BM	101	TRP	1	0
3	AA	101	TRP	1	0
3	BI	101	TRP	1	0
3	AT	301	TRP	1	0
3	BR	101	TRP	1	0
3	BC	101	TRP	1	0
3	BD	101	TRP	1	0
3	AL	301	TRP	1	0
3	AV	301	TRP	1	0
3	AR	301	TRP	1	0
3	BS	101	TRP	1	0
3	BQ	101	TRP	1	0
3	AU	301	TRP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	A0	3/5 (60%)	1.97	2 (66%)	0	0	14, 14, 16, 32	0
1	A1	3/5 (60%)	1.91	1 (33%)	0	0	13, 13, 16, 26	0
1	A2	3/5 (60%)	1.50	0	100	100	13, 13, 15, 20	0
1	A3	4/5 (80%)	1.75	1 (25%)	0	0	13, 14, 19, 21	0
1	A4	3/5 (60%)	2.94	2 (66%)	0	0	12, 12, 17, 29	0
1	A5	4/5 (80%)	1.50	1 (25%)	0	0	12, 14, 21, 28	0
1	A6	2/5 (40%)	2.96	2 (100%)	0	0	16, 16, 16, 18	0
1	A7	3/5 (60%)	2.86	2 (66%)	0	0	15, 15, 18, 32	0
1	A8	3/5 (60%)	1.38	0	100	100	15, 15, 16, 22	0
1	A9	3/5 (60%)	2.03	1 (33%)	0	0	11, 11, 17, 27	0
1	AZ	3/5 (60%)	1.63	1 (33%)	0	0	12, 12, 15, 28	0
1	B0	4/5 (80%)	1.83	1 (25%)	0	0	9, 11, 18, 23	0
1	B1	3/5 (60%)	3.80	3 (100%)	0	0	14, 14, 16, 32	0
1	B2	2/5 (40%)	2.07	1 (50%)	0	0	15, 15, 15, 20	0
1	B3	2/5 (40%)	2.29	1 (50%)	0	0	15, 15, 15, 17	0
1	B4	3/5 (60%)	2.37	2 (66%)	0	0	15, 15, 19, 23	0
1	B5	3/5 (60%)	2.40	2 (66%)	0	0	13, 13, 16, 16	0
1	B6	4/5 (80%)	1.66	1 (25%)	0	0	9, 12, 15, 18	0
1	B7	3/5 (60%)	1.84	1 (33%)	0	0	14, 14, 16, 28	0
1	B8	3/5 (60%)	2.01	1 (33%)	0	0	16, 16, 16, 22	0
1	B9	3/5 (60%)	1.08	0	100	100	15, 15, 15, 24	0
1	BZ	3/5 (60%)	2.04	2 (66%)	0	0	14, 14, 17, 26	0
2	AA	70/74 (94%)	0.28	5 (7%)	16	17	5, 10, 17, 22	0
2	AB	71/74 (95%)	0.38	4 (5%)	24	27	5, 9, 18, 25	1 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	AC	70/74 (94%)	0.19	4 (5%)	23	26	4, 8, 15, 20	0
2	AD	70/74 (94%)	0.22	6 (8%)	10	12	4, 8, 16, 23	1 (1%)
2	AE	70/74 (94%)	0.35	5 (7%)	16	17	5, 8, 15, 21	0
2	AF	70/74 (94%)	0.15	3 (4%)	35	38	5, 9, 16, 19	0
2	AG	70/74 (94%)	0.14	3 (4%)	35	38	3, 9, 15, 20	1 (1%)
2	AH	70/74 (94%)	0.22	3 (4%)	35	38	5, 9, 16, 21	0
2	AI	70/74 (94%)	0.15	3 (4%)	35	38	4, 8, 16, 23	0
2	AJ	70/74 (94%)	0.41	5 (7%)	16	17	4, 8, 15, 21	0
2	AK	71/74 (95%)	0.26	2 (2%)	53	56	4, 8, 14, 23	0
2	AL	70/74 (94%)	0.47	6 (8%)	10	12	4, 8, 18, 25	0
2	AM	71/74 (95%)	0.48	5 (7%)	16	18	5, 8, 17, 25	1 (1%)
2	AN	70/74 (94%)	0.33	4 (5%)	23	26	4, 8, 17, 25	0
2	AO	71/74 (95%)	0.37	7 (9%)	7	8	4, 8, 18, 26	1 (1%)
2	AP	70/74 (94%)	0.26	4 (5%)	23	26	5, 8, 16, 28	0
2	AQ	70/74 (94%)	0.47	4 (5%)	23	26	5, 8, 17, 28	0
2	AR	70/74 (94%)	0.55	5 (7%)	16	17	4, 9, 18, 27	1 (1%)
2	AS	70/74 (94%)	0.54	4 (5%)	23	26	5, 9, 19, 26	0
2	AT	70/74 (94%)	0.49	6 (8%)	10	12	5, 8, 17, 28	0
2	AU	70/74 (94%)	0.29	4 (5%)	23	26	5, 8, 17, 25	1 (1%)
2	AV	70/74 (94%)	0.30	4 (5%)	23	26	4, 8, 18, 27	1 (1%)
2	BA	71/74 (95%)	0.13	0	100	100	4, 9, 15, 19	0
2	BB	71/74 (95%)	0.14	2 (2%)	53	56	4, 9, 15, 22	1 (1%)
2	BC	70/74 (94%)	0.09	1 (1%)	75	77	4, 9, 15, 19	0
2	BD	71/74 (95%)	0.24	4 (5%)	24	27	4, 8, 17, 21	0
2	BE	70/74 (94%)	0.49	5 (7%)	16	17	4, 8, 15, 20	0
2	BF	70/74 (94%)	0.21	4 (5%)	23	26	4, 8, 15, 20	0
2	BG	70/74 (94%)	0.11	3 (4%)	35	38	4, 9, 16, 19	1 (1%)
2	BH	70/74 (94%)	0.35	5 (7%)	16	17	4, 9, 17, 24	0
2	BI	70/74 (94%)	0.10	3 (4%)	35	38	4, 8, 17, 22	1 (1%)
2	BJ	70/74 (94%)	0.07	3 (4%)	35	38	5, 8, 17, 22	0
2	BK	70/74 (94%)	0.37	5 (7%)	16	17	4, 8, 15, 24	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	BL	70/74 (94%)	0.23	4 (5%)	23	26	4, 8, 18, 26	0
2	BM	71/74 (95%)	0.34	5 (7%)	16	18	5, 9, 18, 24	1 (1%)
2	BN	70/74 (94%)	0.37	4 (5%)	23	26	4, 9, 18, 22	1 (1%)
2	BO	70/74 (94%)	0.41	5 (7%)	16	17	4, 8, 17, 24	0
2	BP	70/74 (94%)	0.27	4 (5%)	23	26	4, 8, 17, 28	1 (1%)
2	BQ	70/74 (94%)	0.39	3 (4%)	35	38	5, 8, 18, 22	1 (1%)
2	BR	70/74 (94%)	0.21	3 (4%)	35	38	4, 8, 17, 26	0
2	BS	70/74 (94%)	0.23	2 (2%)	51	54	4, 8, 17, 29	0
2	BT	70/74 (94%)	0.40	4 (5%)	23	26	4, 9, 16, 27	1 (1%)
2	BU	70/74 (94%)	0.58	7 (10%)	7	8	4, 9, 18, 26	0
2	BV	70/74 (94%)	0.31	5 (7%)	16	17	4, 8, 16, 24	0
All	All	3155/3366 (93%)	0.34	205 (6%)	18	21	3, 8, 18, 32	16 (0%)

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AR	205	THR	9.4
2	BT	5	THR	8.1
2	AO	205	THR	7.7
2	AQ	205	THR	7.4
2	BS	5	THR	7.2
2	BP	5	THR	6.8
2	AN	205	THR	6.5
2	BU	5	THR	6.3
2	BV	5	THR	6.2
2	AM	205	THR	6.1
2	AP	205	THR	6.0
2	AQ	206	ASN	5.4
2	BU	6	ASN	5.4
1	B1	104	A	5.4
2	BR	5	THR	5.3
2	AT	205	THR	5.2
2	AS	205	THR	5.2
2	BO	5	THR	5.0
2	BM	5	THR	5.0
1	A4	104	A	4.9
2	BM	6	ASN	4.8
2	AN	206	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
2	AA	6	ASN	4.7
2	AL	206	ASN	4.7
2	AJ	32	PHE	4.6
2	AH	32	PHE	4.5
2	AG	32	PHE	4.4
2	BQ	5	THR	4.4
2	AB	75	LYS	4.4
1	A7	104	A	4.4
2	AC	6	ASN	4.4
2	AL	205	THR	4.3
2	BN	6	ASN	4.2
2	BQ	74	GLY	4.2
2	BN	5	THR	4.2
2	BS	6	ASN	4.0
2	AV	205	THR	4.0
2	AO	206	ASN	4.0
2	AM	206	ASN	3.9
2	AK	6	ASN	3.7
2	AS	206	ASN	3.7
2	AS	229	ASP	3.6
1	A6	103	G	3.6
2	AV	206	ASN	3.6
2	BQ	6	ASN	3.6
2	AP	206	ASN	3.6
2	AS	232	PHE	3.6
2	BK	5	THR	3.6
2	AD	74	GLY	3.5
1	B1	103	G	3.5
2	BV	6	ASN	3.5
2	AE	74	GLY	3.5
2	BD	74	GLY	3.5
2	BR	6	ASN	3.5
2	AU	205	THR	3.5
2	AV	274	GLY	3.4
2	BJ	74	GLY	3.4
2	BU	27	GLY	3.4
1	A9	104	A	3.4
2	AT	206	ASN	3.4
2	AJ	74	GLY	3.4
1	B4	103	G	3.3
2	BM	58	ARG	3.3
2	BO	6	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	AE	10	VAL	3.3
2	BP	6	ASN	3.2
2	BL	74	GLY	3.2
2	AC	74	GLY	3.2
2	BF	74	GLY	3.2
2	AF	74	GLY	3.2
1	B6	104	A	3.2
2	AV	258	ARG	3.1
2	AG	6	ASN	3.1
2	BG	5	THR	3.1
1	A3	101	U	3.1
2	AU	206	ASN	3.1
1	B5	103	G	3.1
2	AH	74	GLY	3.0
2	AN	274	GLY	3.0
2	BM	75	LYS	3.0
2	BK	55	ILE	3.0
1	B3	102	A	3.0
2	AR	206	ASN	3.0
1	A4	103	G	2.9
2	AA	5	THR	2.9
2	AT	212	ILE	2.9
2	BP	74	GLY	2.9
2	AE	55	ILE	2.9
2	AE	32	PHE	2.9
2	AO	275	LYS	2.9
1	A7	103	G	2.9
1	B0	101	U	2.9
2	AQ	274	GLY	2.9
2	AG	5	THR	2.8
2	BB	6	ASN	2.8
2	BU	29	ASP	2.8
2	BI	6	ASN	2.8
2	BH	32	PHE	2.8
2	AB	74	GLY	2.8
2	BI	74	GLY	2.8
2	BH	6	ASN	2.8
2	AT	263	ILE	2.7
2	BT	29	ASP	2.7
2	AF	6	ASN	2.7
2	BU	31	ARG	2.7
2	BI	5	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	AR	229	ASP	2.7
2	BE	74	GLY	2.7
2	AC	5	THR	2.7
2	AA	32	PHE	2.7
2	AO	274	GLY	2.7
2	BH	5	THR	2.7
2	BU	32	PHE	2.6
2	BT	6	ASN	2.6
1	B5	102	A	2.6
2	AF	32	PHE	2.6
2	AI	5	THR	2.6
2	AK	5	THR	2.6
2	BB	75	LYS	2.6
2	AN	258	ARG	2.6
2	BL	5	THR	2.6
2	BM	74	GLY	2.6
2	BV	74	GLY	2.6
2	AU	255	ILE	2.6
2	BE	11	VAL	2.6
2	BU	28	ALA	2.5
1	B8	102	A	2.5
2	BF	6	ASN	2.5
2	AL	212	ILE	2.5
2	BK	11	VAL	2.5
1	AZ	103	G	2.5
2	BD	6	ASN	2.5
2	BP	29	ASP	2.5
2	BE	12	ILE	2.5
1	B2	103	G	2.5
1	A0	104	A	2.5
1	B1	102	A	2.5
2	BJ	5	THR	2.5
2	BL	6	ASN	2.5
2	BD	45	ILE	2.5
2	BJ	45	ILE	2.5
2	AM	275	LYS	2.5
2	BF	5	THR	2.4
2	BK	10	VAL	2.4
2	AJ	12	ILE	2.4
2	BN	43	VAL	2.4
2	BG	74	GLY	2.4
2	BE	46	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	BO	17	ASP	2.4
2	AL	263	ILE	2.4
2	BG	6	ASN	2.4
2	BH	74	GLY	2.4
2	AB	32	PHE	2.4
2	AC	39	ASP	2.4
2	AE	12	ILE	2.4
2	AA	74	GLY	2.3
1	A1	103	G	2.3
1	B4	102	A	2.3
2	AM	212	ILE	2.3
2	AP	210	VAL	2.3
1	A6	102	A	2.3
2	BO	7	SER	2.3
2	BV	11	VAL	2.3
1	BZ	104	A	2.3
2	AR	210	VAL	2.3
2	AB	6	ASN	2.3
2	AD	32	PHE	2.2
2	BC	32	PHE	2.2
2	AM	263	ILE	2.2
2	BR	55	ILE	2.2
1	B7	102	A	2.2
1	BZ	102	A	2.2
2	AD	5	THR	2.2
2	AO	212	ILE	2.2
2	AJ	46	ALA	2.2
2	AL	244	LEU	2.1
2	BO	74	GLY	2.1
2	AD	12	ILE	2.1
2	AL	274	GLY	2.1
2	AR	232	PHE	2.1
2	AO	210	VAL	2.1
2	AQ	210	VAL	2.1
2	BN	11	VAL	2.1
2	BE	6	ASN	2.1
2	BV	29	ASP	2.1
2	AO	232	PHE	2.1
2	BT	31	ARG	2.1
2	AU	246	ALA	2.1
2	BF	55	ILE	2.1
2	BL	55	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	BH	18	GLY	2.1
2	AJ	10	VAL	2.1
2	AP	246	ALA	2.1
2	AI	45	ILE	2.1
2	AT	222	ILE	2.1
1	A0	103	G	2.0
1	A5	101	U	2.0
2	AA	10	VAL	2.0
2	AI	10	VAL	2.0
2	AT	210	VAL	2.0
2	BD	10	VAL	2.0
2	BK	74	GLY	2.0
2	AH	12	ILE	2.0
2	AD	10	VAL	2.0
2	AD	46	ALA	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)

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	TRP	BL	101	13/15	0.84	0.14	3,6,11,11	0
3	TRP	AN	301	15/15	0.90	0.12	4,6,10,10	0
3	TRP	BN	101	15/15	0.91	0.12	3,5,11,12	0
3	TRP	AQ	301	15/15	0.92	0.09	3,5,9,11	0
3	TRP	AS	301	15/15	0.92	0.10	3,6,9,10	0
3	TRP	BP	101	15/15	0.92	0.10	4,6,9,10	0
3	TRP	AT	301	15/15	0.93	0.12	3,5,8,9	0
3	TRP	AU	301	15/15	0.93	0.11	2,5,9,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TRP	AP	301	15/15	0.93	0.10	2,5,8,11	0
3	TRP	BM	101	15/15	0.93	0.10	4,7,10,10	0
3	TRP	AH	101	15/15	0.93	0.09	3,6,10,11	0
3	TRP	BO	101	15/15	0.93	0.09	2,5,8,10	0
3	TRP	AO	301	15/15	0.93	0.10	5,7,9,11	0
3	TRP	BR	101	15/15	0.93	0.10	2,5,9,9	0
3	TRP	BV	101	15/15	0.93	0.10	3,6,8,8	0
3	TRP	AL	301	15/15	0.94	0.09	3,6,9,10	0
3	TRP	AM	301	15/15	0.94	0.09	4,5,8,9	0
3	TRP	AC	101	15/15	0.94	0.13	2,5,9,9	0
3	TRP	AG	101	15/15	0.94	0.09	5,7,9,10	0
3	TRP	BQ	101	15/15	0.94	0.08	3,5,9,11	0
3	TRP	BA	101	15/15	0.94	0.12	2,7,10,11	0
3	TRP	BS	101	15/15	0.94	0.09	4,6,9,9	0
3	TRP	AA	101	15/15	0.94	0.11	3,6,9,10	0
3	TRP	AD	101	15/15	0.95	0.09	2,5,9,10	0
3	TRP	AR	301	15/15	0.95	0.09	3,5,11,12	0
3	TRP	AV	301	15/15	0.95	0.09	4,6,9,11	0
3	TRP	AB	101	15/15	0.95	0.12	5,6,9,9	0
3	TRP	BB	101	15/15	0.95	0.08	4,6,11,11	0
3	TRP	BF	101	15/15	0.95	0.13	5,7,9,11	0
3	TRP	BG	101	15/15	0.95	0.10	4,6,9,10	0
3	TRP	BH	101	15/15	0.95	0.09	3,6,9,11	0
3	TRP	BT	101	15/15	0.95	0.09	5,7,9,11	0
3	TRP	BI	101	15/15	0.95	0.12	3,5,10,10	0
3	TRP	BE	101	15/15	0.96	0.08	5,6,8,9	0
3	TRP	AF	101	15/15	0.96	0.10	3,6,9,10	0
3	TRP	AK	101	15/15	0.96	0.15	4,7,10,10	0
3	TRP	AE	101	15/15	0.96	0.10	3,5,8,9	0
3	TRP	BU	101	15/15	0.96	0.07	3,5,11,12	0
3	TRP	BD	101	15/15	0.96	0.07	5,6,8,10	0
3	TRP	BJ	101	15/15	0.97	0.08	4,6,9,10	0
3	TRP	AI	101	15/15	0.97	0.07	2,5,9,10	0
3	TRP	AJ	101	15/15	0.97	0.08	2,5,8,9	0
3	TRP	BC	101	15/15	0.97	0.10	4,7,10,11	0
3	TRP	BK	101	15/15	0.98	0.09	3,4,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.