



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:12 pm GMT

PDB ID : 1QU2  
Title : INSIGHTS INTO EDITING FROM AN ILE-TRNA SYNTHETASE STRUCTURE WITH TRNA(ILE) AND MUPIROCIN  
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Deposited on : 1999-07-06  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

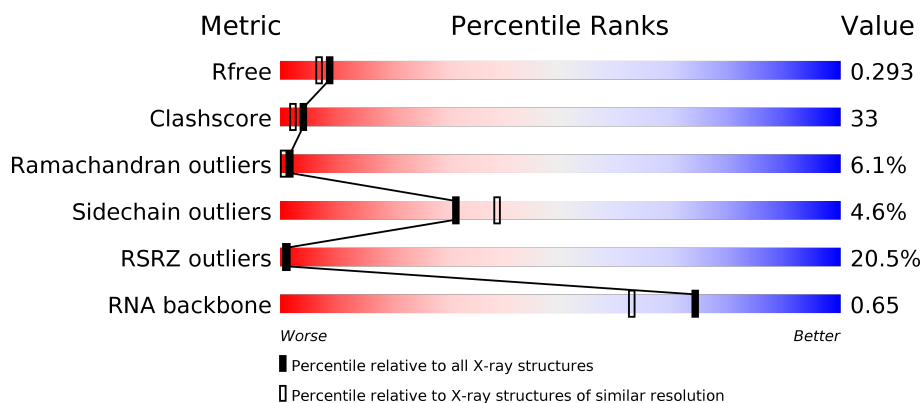
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)
RNA backbone	2435	1007 (2.74-1.66)

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

Mol	Chain	Length	Quality of chain
1	T	75	
2	A	917	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MRC	A	1993	X	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9386 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 ISOLEUCYL-TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	75	Total	C	N	O	P	24	0	0
			1603	715	289	525	74			

- Molecule 2 is a protein called ISOLEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	917	Total	C	N	O	S	0	0	0
			7407	4716	1249	1417	25			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	LYS	CONFLICT	UNP P41972
A	5	LYS	GLU	CONFLICT	UNP P41972
A	295	TRP	TYR	CONFLICT	UNP P41972
A	340	GLN	LYS	CONFLICT	UNP P41972
A	644	ASP	VAL	CONFLICT	UNP P41972

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	1	Total	K	0	0
			1	1		

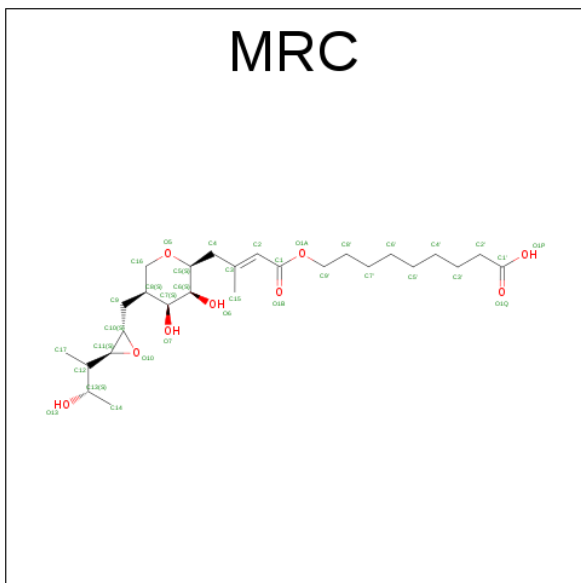
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	10	Total	Mg	0	0
			10	10		

- Molecule 6 is MUPIROCIN (three-letter code: MRC) (formula:  $C_{26}H_{44}O_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			35	26	9		

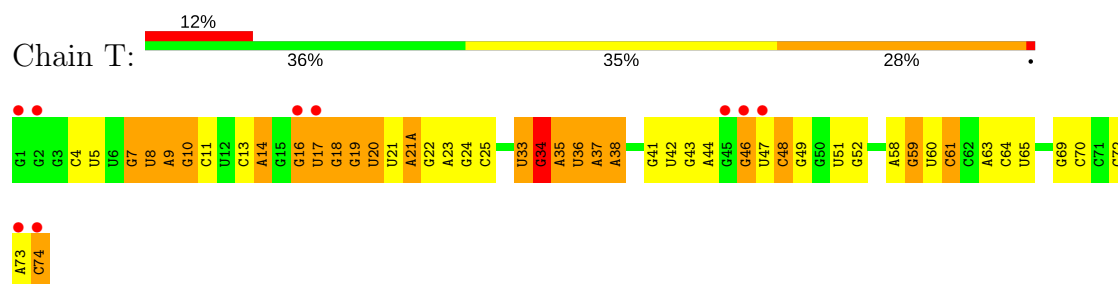
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	208	Total	O	0	0
			208	208		
7	T	120	Total	O	0	0
			120	120		

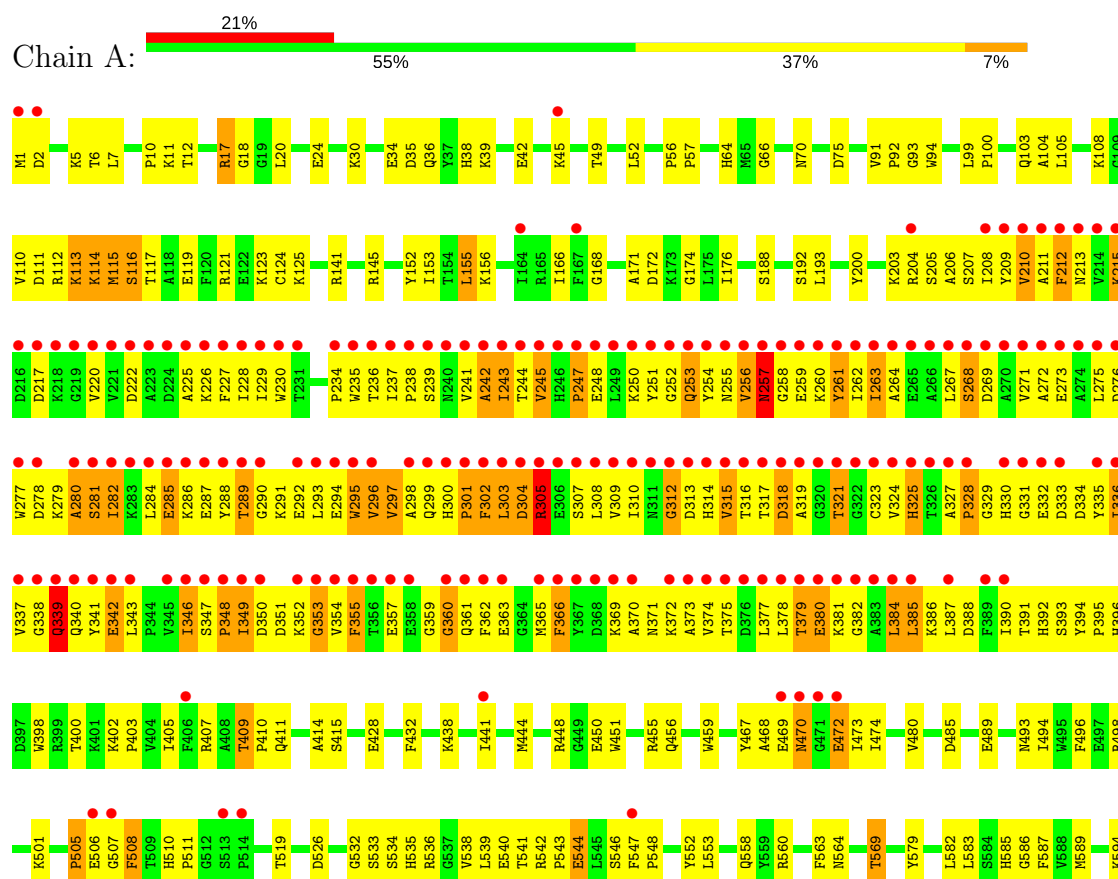
### 3 Residue-property plots [i](#)

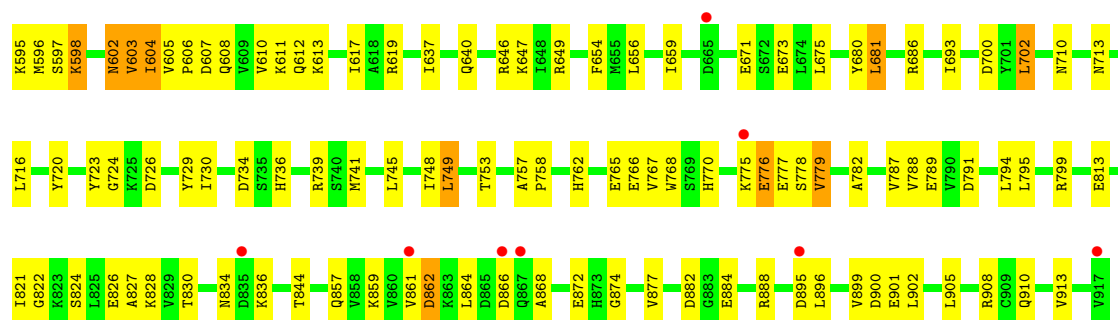
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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: ISOLEUCYL-TRNA



#### • Molecule 2: ISOLEUCYL-TRNA SYNTHETASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.00Å 100.00Å 186.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 19.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	75.7 (10.00-2.20) 85.6 (19.97-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 2.19Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.239 , 0.281 0.249 , 0.293	Depositor DCC
$R_{free}$ test set	2908 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ZN, MRC

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	T	0.41	0/1792	0.82	3/2794 (0.1%)
2	A	0.37	0/7586	0.62	0/10282
All	All	0.38	0/9378	0.67	3/13076 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	G	C2'-C3'-O3'	-7.43	93.15	109.50
1	T	7	G	N9-C1'-C2'	5.87	121.64	114.00
1	T	34	G	N9-C1'-C2'	5.39	121.01	114.00

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	T	1603	0	810	62	0
2	A	7407	0	7214	507	0
3	T	1	0	0	0	0
4	A	2	0	0	0	0
5	T	10	0	0	0	0
6	A	35	0	41	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	208	0	0	20	0
7	T	120	0	0	4	0
All	All	9386	0	8065	554	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 33.

All (554) 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)
2:A:821:ILE:HD12	2:A:827:ALA:HB2	1.33	1.09
2:A:210:VAL:HG13	2:A:385:LEU:HD11	1.43	1.00
2:A:346:ILE:HD13	2:A:346:ILE:H	1.28	0.99
2:A:210:VAL:HG23	2:A:229:ILE:HB	1.44	0.97
2:A:400:THR:HG22	2:A:402:LYS:HG2	1.45	0.97
1:T:46:G:H2'	1:T:47:U:H5'	1.46	0.97
2:A:716:LEU:HD11	2:A:748:ILE:HD11	1.49	0.94
2:A:211:ALA:HA	2:A:228:ILE:HA	1.47	0.94
2:A:380:GLU:HB3	2:A:385:LEU:H	1.29	0.94
2:A:336:ILE:HG13	2:A:337:VAL:H	1.30	0.93
2:A:239:SER:HB3	2:A:346:ILE:HG13	1.51	0.93
2:A:208:ILE:HG22	2:A:387:LEU:HA	1.50	0.92
2:A:213:ASN:HD22	2:A:215:LYS:HG3	1.34	0.92
1:T:73:A:H2'	1:T:74:C:H5'	1.50	0.90
2:A:264:ALA:HB3	2:A:267:LEU:HB2	1.50	0.90
1:T:69:G:H5''	2:A:589:MET:CE	2.02	0.89
1:T:13:C:H2'	1:T:14:A:H5''	1.56	0.88
2:A:534:SER:O	2:A:538:VAL:HG13	1.73	0.88
2:A:252:GLY:HA2	2:A:262:ILE:HG23	1.56	0.87
2:A:857:GLN:NE2	2:A:882:ASP:H	1.72	0.86
1:T:69:G:H5''	2:A:589:MET:HE2	1.55	0.86
2:A:234:PRO:HB2	2:A:371:ASN:HB3	1.57	0.86
1:T:9:A:H5'	1:T:10:G:OP2	1.77	0.85
2:A:589:MET:HE3	2:A:594:LYS:C	1.98	0.84
2:A:834:ASN:HB2	2:A:874:GLY:HA2	1.58	0.84
2:A:857:GLN:HE22	2:A:882:ASP:H	1.23	0.84
2:A:309:VAL:HG12	2:A:310:ILE:H	1.43	0.82
2:A:248:GLU:H	2:A:291:LYS:HD3	1.44	0.82
2:A:1:MET:HG2	2:A:2:ASP:H	1.43	0.82
2:A:18:GLY:H	2:A:646:ARG:NH2	1.77	0.82
2:A:749:LEU:O	2:A:753:THR:HG23	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:121:ARG:HH21	2:A:493:ASN:HD22	1.28	0.81
2:A:213:ASN:HA	2:A:226:LYS:HG2	1.61	0.81
2:A:239:SER:HB3	2:A:327:ALA:HB1	1.62	0.78
2:A:468:ALA:HB2	2:A:474:ILE:HD11	1.63	0.78
1:T:13:C:C2'	1:T:14:A:H5''	2.14	0.78
2:A:289:THR:O	2:A:293:LEU:HG	1.84	0.78
2:A:371:ASN:HA	2:A:375:THR:HG22	1.64	0.78
2:A:861:VAL:O	2:A:862:ASP:HB2	1.84	0.77
2:A:872:GLU:H	2:A:872:GLU:CD	1.88	0.77
2:A:208:ILE:HB	2:A:385:LEU:HD12	1.66	0.77
2:A:257:ASN:ND2	2:A:258:GLY:H	1.82	0.76
2:A:366:PHE:CE1	2:A:369:LYS:HB2	2.21	0.76
2:A:336:ILE:HG13	2:A:337:VAL:N	2.01	0.76
2:A:121:ARG:HH21	2:A:493:ASN:ND2	1.83	0.76
1:T:35:A:O2'	1:T:36:U:OP1	2.04	0.75
2:A:377:LEU:HD12	2:A:381:LYS:NZ	2.01	0.75
2:A:237:ILE:HG22	2:A:238:PRO:HD3	1.68	0.74
2:A:597:SER:H	2:A:602:ASN:HD21	1.35	0.74
2:A:300:HIS:O	2:A:304:ASP:HB3	1.86	0.74
2:A:469:GLU:O	2:A:470:ASN:HB3	1.86	0.74
2:A:207:SER:HB2	2:A:230:TRP:HE1	1.52	0.74
2:A:905:LEU:HD13	7:A:2172:HOH:O	1.87	0.74
1:T:63:A:H2'	1:T:64:C:C6	2.23	0.74
2:A:323:CYS:HA	7:A:2149:HOH:O	1.88	0.73
2:A:379:THR:OG1	2:A:385:LEU:HG	1.88	0.73
2:A:380:GLU:HA	2:A:385:LEU:HD23	1.69	0.73
2:A:380:GLU:HB3	2:A:385:LEU:N	2.03	0.73
2:A:209:TYR:HE2	2:A:321:THR:HG21	1.54	0.72
2:A:166:ILE:HD12	2:A:533:SER:HB2	1.71	0.72
2:A:243:ILE:HB	2:A:310:ILE:HG12	1.71	0.72
1:T:47:U:O2'	1:T:48:C:OP2	2.07	0.72
2:A:243:ILE:HA	2:A:325:HIS:HA	1.69	0.72
1:T:58:A:H2'	1:T:60:U:OP2	1.90	0.72
2:A:365:MET:HE2	2:A:374:VAL:HG21	1.70	0.71
2:A:272:ALA:HA	2:A:275:LEU:HD12	1.70	0.71
2:A:331:GLY:HA3	2:A:334:ASP:HB3	1.71	0.71
2:A:360:GLY:O	2:A:363:GLU:HG3	1.91	0.71
2:A:352:LYS:HB2	2:A:354:VAL:HG12	1.70	0.70
2:A:39:LYS:HG3	7:A:2118:HOH:O	1.90	0.70
2:A:730:ILE:O	2:A:888:ARG:NH2	2.25	0.70
1:T:70:C:OP1	2:A:595:LYS:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:209:TYR:C	2:A:385:LEU:HD13	2.12	0.70
2:A:681:LEU:HD22	2:A:720:TYR:CD2	2.27	0.70
2:A:105:LEU:HD22	2:A:110:VAL:HG21	1.74	0.70
2:A:56:PRO:O	6:A:1993:MRC:H143	1.91	0.70
2:A:70:ASN:HD22	2:A:585:HIS:HE1	1.39	0.70
2:A:250:LYS:HG2	2:A:289:THR:HG23	1.72	0.69
2:A:309:VAL:HG12	2:A:310:ILE:N	2.06	0.69
2:A:864:LEU:HD13	2:A:877:VAL:HG23	1.72	0.69
2:A:228:ILE:O	2:A:323:CYS:HB2	1.92	0.69
2:A:113:LYS:O	2:A:114:LYS:HB2	1.92	0.69
2:A:250:LYS:HB3	2:A:289:THR:HA	1.74	0.69
2:A:117:THR:HG21	2:A:496:PHE:CD2	2.27	0.69
2:A:765:GLU:OE1	2:A:778:SER:HA	1.93	0.69
2:A:254:TYR:HD2	2:A:286:LYS:HZ2	1.41	0.69
1:T:41:G:O2'	2:A:813:GLU:HG2	1.91	0.69
2:A:255:ASN:O	2:A:260:LYS:HG2	1.92	0.69
2:A:547:PHE:HB3	2:A:548:PRO:HD3	1.74	0.68
2:A:263:ILE:HG21	2:A:268:SER:HA	1.76	0.68
2:A:242:ALA:HA	2:A:308:LEU:HB3	1.75	0.67
2:A:263:ILE:HG22	2:A:264:ALA:N	2.09	0.67
2:A:212:PHE:HZ	2:A:302:PHE:HB3	1.60	0.67
2:A:241:VAL:HG21	2:A:346:ILE:HD12	1.75	0.67
2:A:910:GLN:HA	7:A:2172:HOH:O	1.92	0.67
2:A:713:ASN:OD1	7:A:2199:HOH:O	2.12	0.66
2:A:348:PRO:HB3	2:A:357:GLU:HG2	1.77	0.66
2:A:210:VAL:HG12	2:A:385:LEU:HD21	1.77	0.66
1:T:9:A:H3'	7:T:1236:HOH:O	1.94	0.66
2:A:18:GLY:N	2:A:646:ARG:NH2	2.43	0.66
2:A:242:ALA:CA	2:A:308:LEU:HB3	2.26	0.66
2:A:239:SER:CB	2:A:327:ALA:HB1	2.26	0.66
2:A:12:THR:HG21	2:A:656:LEU:HB3	1.78	0.65
2:A:302:PHE:O	2:A:378:LEU:HD23	1.96	0.65
2:A:795:LEU:O	2:A:799:ARG:HG3	1.97	0.65
2:A:237:ILE:HG22	2:A:238:PRO:CD	2.27	0.65
1:T:69:G:C5'	2:A:589:MET:HE2	2.26	0.65
2:A:57:PRO:HD2	2:A:93:GLY:O	1.97	0.64
7:T:1321:HOH:O	2:A:702:LEU:HB3	1.97	0.64
2:A:861:VAL:O	2:A:862:ASP:CB	2.45	0.64
2:A:317:THR:O	2:A:318:ASP:HB2	1.97	0.64
2:A:603:VAL:O	2:A:604:ILE:HB	1.96	0.64
2:A:235:TRP:HB3	2:A:371:ASN:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:243:ILE:HG22	2:A:244:THR:H	1.62	0.64
1:T:33:U:H4'	1:T:34:G:O5'	1.98	0.64
2:A:171:ALA:HB2	2:A:176:ILE:HD12	1.79	0.64
2:A:251:TYR:HD2	2:A:253:GLN:HE22	1.46	0.64
2:A:371:ASN:CA	2:A:375:THR:HG22	2.28	0.63
2:A:213:ASN:ND2	2:A:215:LYS:HG3	2.11	0.63
2:A:237:ILE:HA	7:A:2117:HOH:O	1.97	0.63
2:A:261:TYR:C	2:A:262:ILE:HD12	2.18	0.63
2:A:222:ASP:HB3	2:A:288:TYR:CD1	2.33	0.63
2:A:455:ARG:NE	7:A:2178:HOH:O	2.30	0.63
2:A:226:LYS:HB2	2:A:261:TYR:CD1	2.33	0.63
1:T:69:G:H5''	2:A:589:MET:HE1	1.77	0.63
2:A:494:ILE:HD11	2:A:498:ARG:NE	2.14	0.63
2:A:608:GLN:HB3	2:A:612:GLN:NE2	2.14	0.63
2:A:301:PRO:C	2:A:303:LEU:H	2.02	0.62
2:A:141:ARG:HG3	2:A:610:VAL:HG11	1.81	0.62
2:A:768:TRP:HB2	2:A:779:VAL:HG22	1.82	0.62
2:A:2:ASP:HB3	2:A:5:LYS:NZ	2.13	0.62
2:A:681:LEU:HD13	2:A:720:TYR:CD1	2.34	0.62
2:A:64:HIS:HD2	2:A:66:GLY:H	1.47	0.62
2:A:671:GLU:HB2	7:A:2071:HOH:O	2.00	0.62
2:A:17:ARG:CB	2:A:17:ARG:HH11	2.12	0.62
2:A:248:GLU:N	2:A:291:LYS:HD3	2.13	0.62
2:A:380:GLU:HG3	2:A:385:LEU:HB2	1.82	0.62
2:A:213:ASN:HA	2:A:226:LYS:CG	2.30	0.62
1:T:43:G:O2'	1:T:44:A:H5'	1.98	0.62
2:A:243:ILE:HG22	2:A:244:THR:N	2.15	0.61
2:A:378:LEU:HD12	2:A:378:LEU:H	1.63	0.61
2:A:210:VAL:CG1	2:A:385:LEU:HD11	2.26	0.61
2:A:605:VAL:HG13	2:A:606:PRO:HD2	1.82	0.61
2:A:596:MET:SD	2:A:603:VAL:O	2.58	0.61
2:A:220:VAL:O	2:A:220:VAL:HG12	2.00	0.61
2:A:469:GLU:HB3	7:A:2186:HOH:O	1.99	0.61
2:A:209:TYR:O	2:A:385:LEU:HD13	2.01	0.61
2:A:260:LYS:HD2	2:A:286:LYS:HZ1	1.64	0.61
2:A:341:TYR:O	2:A:343:LEU:HG	2.01	0.61
2:A:243:ILE:HB	2:A:310:ILE:CG1	2.31	0.60
1:T:58:A:O2'	1:T:60:U:H5	1.85	0.60
2:A:370:ALA:C	2:A:371:ASN:HD22	2.05	0.60
2:A:243:ILE:HD11	2:A:308:LEU:HB2	1.84	0.60
2:A:415:SER:HA	2:A:450:GLU:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:730:ILE:HG23	2:A:888:ARG:HH21	1.66	0.60
1:T:73:A:C2'	1:T:74:C:H5'	2.29	0.60
2:A:379:THR:HG23	2:A:380:GLU:H	1.66	0.59
2:A:2:ASP:OD2	2:A:5:LYS:HG3	2.02	0.59
2:A:535:HIS:NE2	2:A:569:THR:HG23	2.16	0.59
2:A:229:ILE:HD11	2:A:300:HIS:CD2	2.37	0.59
2:A:295:TRP:HA	2:A:309:VAL:HG13	1.83	0.59
2:A:821:ILE:HG12	2:A:822:GLY:N	2.18	0.59
2:A:377:LEU:HD12	2:A:381:LYS:HZ1	1.67	0.59
2:A:244:THR:HG22	2:A:245:VAL:N	2.16	0.59
2:A:448:ARG:NH1	2:A:564:ASN:HD21	2.01	0.59
2:A:125:LYS:HG3	2:A:155:LEU:HD22	1.84	0.59
2:A:212:PHE:CE2	2:A:301:PRO:HB2	2.37	0.59
2:A:597:SER:O	2:A:598:LYS:HB2	2.02	0.59
2:A:402:LYS:HE3	7:A:2140:HOH:O	2.03	0.58
2:A:259:GLU:HB2	2:A:261:TYR:CE1	2.38	0.58
2:A:333:ASP:HA	2:A:336:ILE:HG12	1.83	0.58
2:A:542:ARG:HB3	2:A:544:GLU:OE1	2.04	0.58
2:A:244:THR:HG23	2:A:313:ASP:OD2	2.04	0.58
2:A:302:PHE:O	2:A:303:LEU:HB2	2.03	0.58
2:A:647:LYS:HE2	7:A:2199:HOH:O	2.02	0.58
2:A:217:ASP:HA	2:A:220:VAL:CG2	2.34	0.58
2:A:532:GLY:O	2:A:569:THR:HG21	2.03	0.58
2:A:828:LYS:HG3	2:A:857:GLN:HG3	1.85	0.58
2:A:305:ARG:HA	2:A:305:ARG:HE	1.69	0.58
2:A:366:PHE:O	2:A:370:ALA:HB3	2.03	0.58
2:A:244:THR:OG1	2:A:324:VAL:HB	2.03	0.58
2:A:607:ASP:O	2:A:611:LYS:HG2	2.04	0.58
2:A:91:VAL:HG23	2:A:91:VAL:O	2.04	0.58
2:A:226:LYS:HB2	2:A:261:TYR:CE1	2.39	0.58
2:A:776:GLU:HG3	2:A:782:ALA:HB2	1.85	0.58
2:A:1:MET:HG2	2:A:2:ASP:N	2.16	0.58
2:A:115:MET:O	2:A:116:SER:CB	2.52	0.57
2:A:339:GLN:N	2:A:343:LEU:HD12	2.19	0.57
2:A:49:THR:HG22	7:A:2114:HOH:O	2.02	0.57
2:A:777:GLU:O	2:A:778:SER:HB3	2.04	0.57
1:T:18:G:O2'	1:T:19:G:OP1	2.22	0.57
2:A:766:GLU:O	2:A:770:HIS:HD2	1.86	0.57
2:A:275:LEU:C	2:A:386:LYS:HE3	2.25	0.57
2:A:236:THR:HG22	2:A:236:THR:O	2.04	0.57
2:A:279:LYS:O	2:A:280:ALA:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:51:U:O2'	1:T:52:G:H5'	2.03	0.57
2:A:64:HIS:HD2	2:A:66:GLY:N	2.03	0.57
2:A:24:GLU:HG2	2:A:762:HIS:CG	2.40	0.56
2:A:213:ASN:CA	2:A:226:LYS:HG2	2.33	0.56
2:A:209:TYR:CE2	2:A:321:THR:HG21	2.37	0.56
2:A:11:LYS:O	2:A:12:THR:HG23	2.05	0.56
2:A:348:PRO:HG2	2:A:355:PHE:CB	2.36	0.56
2:A:263:ILE:HG23	2:A:271:VAL:HG11	1.86	0.56
2:A:250:LYS:CG	2:A:289:THR:HG23	2.36	0.56
2:A:379:THR:HG23	2:A:380:GLU:N	2.21	0.56
2:A:540:GLU:HG2	2:A:547:PHE:HB2	1.87	0.56
2:A:235:TRP:O	2:A:238:PRO:HD2	2.05	0.56
2:A:377:LEU:HD12	2:A:381:LYS:HZ2	1.69	0.56
2:A:346:ILE:HD13	2:A:346:ILE:N	2.10	0.56
2:A:428:GLU:HA	2:A:438:LYS:HE2	1.87	0.56
1:T:42:U:O4'	2:A:813:GLU:HG3	2.05	0.56
2:A:884:GLU:HB2	2:A:896:LEU:HD12	1.88	0.56
2:A:302:PHE:O	2:A:303:LEU:CB	2.54	0.55
2:A:378:LEU:HD12	2:A:378:LEU:N	2.21	0.55
2:A:2:ASP:HB3	2:A:5:LYS:HZ3	1.70	0.55
2:A:299:GLN:O	2:A:301:PRO:HD3	2.05	0.55
2:A:30:LYS:O	2:A:34:GLU:HG2	2.07	0.55
2:A:553:LEU:HA	2:A:583:LEU:O	2.07	0.55
2:A:390:ILE:HG22	2:A:391:THR:N	2.22	0.55
2:A:745:LEU:O	2:A:748:ILE:HG22	2.05	0.55
2:A:411:GLN:HE22	2:A:456:GLN:HE22	1.54	0.55
1:T:23:A:H2'	1:T:24:G:C8	2.41	0.55
2:A:338:GLY:C	2:A:343:LEU:HD12	2.26	0.55
2:A:536:ARG:O	2:A:541:THR:HG23	2.06	0.55
2:A:726:ASP:O	2:A:908:ARG:NH2	2.39	0.55
2:A:673:GLU:O	2:A:736:HIS:HE1	1.90	0.55
2:A:535:HIS:NE2	2:A:569:THR:CG2	2.70	0.55
1:T:58:A:O2'	1:T:59:G:O5'	2.21	0.55
2:A:394:TYR:O	2:A:396:HIS:HD2	1.89	0.55
1:T:46:G:C2'	1:T:47:U:H5'	2.28	0.55
2:A:247:PRO:HA	2:A:291:LYS:HG3	1.89	0.55
2:A:346:ILE:CD1	2:A:346:ILE:H	2.07	0.54
1:T:47:U:O2'	1:T:48:C:P	2.66	0.54
2:A:203:LYS:HG2	2:A:204:ARG:N	2.22	0.54
2:A:52:LEU:C	2:A:52:LEU:HD23	2.27	0.54
2:A:245:VAL:O	2:A:245:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:400:THR:HG22	2:A:402:LYS:CG	2.28	0.54
2:A:613:LYS:O	2:A:617:ILE:HD12	2.08	0.54
2:A:693:ILE:HD12	2:A:787:VAL:CG2	2.38	0.54
2:A:602:ASN:H	2:A:602:ASN:HD22	1.56	0.54
2:A:834:ASN:HD22	2:A:874:GLY:C	2.11	0.54
2:A:153:ILE:HD12	2:A:156:LYS:HE2	1.89	0.54
2:A:329:GLY:H	2:A:346:ILE:HD11	1.72	0.54
2:A:257:ASN:ND2	2:A:258:GLY:N	2.55	0.54
2:A:821:ILE:HG13	2:A:826:GLU:HB2	1.90	0.53
2:A:267:LEU:O	2:A:271:VAL:HG23	2.08	0.53
2:A:309:VAL:CG1	2:A:310:ILE:H	2.19	0.53
2:A:245:VAL:CG1	2:A:310:ILE:HG22	2.38	0.53
2:A:380:GLU:CB	2:A:385:LEU:HB2	2.37	0.53
2:A:35:ASP:O	2:A:39:LYS:HG2	2.09	0.53
2:A:913:VAL:HB	7:A:2172:HOH:O	2.07	0.53
2:A:245:VAL:O	2:A:247:PRO:HD3	2.08	0.53
2:A:380:GLU:CG	2:A:385:LEU:HB2	2.38	0.53
2:A:115:MET:O	2:A:116:SER:OG	2.21	0.53
2:A:217:ASP:HA	2:A:220:VAL:HG23	1.90	0.53
2:A:166:ILE:HD11	2:A:536:ARG:HB2	1.90	0.53
2:A:252:GLY:H	2:A:287:GLU:HB2	1.74	0.53
2:A:252:GLY:O	2:A:262:ILE:HA	2.09	0.53
1:T:64:C:O2'	1:T:65:U:H5'	2.08	0.53
2:A:261:TYR:OH	2:A:384:LEU:HD12	2.09	0.53
2:A:597:SER:H	2:A:602:ASN:ND2	2.05	0.52
2:A:212:PHE:O	2:A:227:PHE:N	2.37	0.52
2:A:243:ILE:HB	2:A:310:ILE:CD1	2.39	0.52
2:A:301:PRO:O	2:A:303:LEU:N	2.40	0.52
1:T:9:A:C5'	1:T:10:G:OP2	2.56	0.52
1:T:41:G:O2'	2:A:813:GLU:CG	2.58	0.52
2:A:350:ASP:HA	2:A:407:ARG:NH2	2.25	0.52
1:T:13:C:H2'	1:T:14:A:C5'	2.33	0.52
2:A:340:GLN:HB2	2:A:341:TYR:CD1	2.45	0.52
2:A:414:ALA:HB3	2:A:451:TRP:HB3	1.91	0.52
2:A:836:LYS:HE2	2:A:872:GLU:HA	1.92	0.52
1:T:18:G:O2'	1:T:19:G:P	2.68	0.52
2:A:212:PHE:CG	2:A:301:PRO:HD2	2.45	0.52
2:A:821:ILE:CD1	2:A:827:ALA:HB2	2.22	0.52
1:T:42:U:C4'	2:A:813:GLU:HG3	2.39	0.52
2:A:370:ALA:O	2:A:374:VAL:HB	2.09	0.52
2:A:587:PHE:HA	6:A:1993:MRC:H152	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:ASP:OD1	2:A:351:ASP:N	2.39	0.51
2:A:166:ILE:HD11	2:A:536:ARG:CB	2.39	0.51
2:A:111:ASP:OD2	2:A:114:LYS:HE2	2.10	0.51
2:A:341:TYR:N	2:A:341:TYR:CD1	2.77	0.51
2:A:369:LYS:C	2:A:371:ASN:H	2.13	0.51
2:A:716:LEU:HD21	2:A:748:ILE:CD1	2.40	0.51
2:A:608:GLN:HB3	2:A:612:GLN:HE21	1.75	0.51
2:A:256:VAL:HG12	2:A:257:ASN:N	2.25	0.51
2:A:250:LYS:CD	2:A:289:THR:HG23	2.40	0.51
2:A:357:GLU:C	2:A:359:GLY:H	2.14	0.51
2:A:540:GLU:CG	2:A:547:PHE:HB2	2.41	0.51
2:A:589:MET:CE	2:A:595:LYS:N	2.74	0.51
2:A:589:MET:HE3	2:A:595:LYS:N	2.25	0.51
1:T:16:G:H5'	1:T:17:U:OP2	2.10	0.51
2:A:352:LYS:HE3	2:A:354:VAL:CG1	2.41	0.51
2:A:884:GLU:HB2	2:A:896:LEU:CD1	2.41	0.51
2:A:241:VAL:CA	2:A:308:LEU:HD22	2.41	0.51
2:A:324:VAL:O	2:A:325:HIS:HB3	2.11	0.51
2:A:365:MET:HG3	2:A:370:ALA:HB2	1.93	0.51
2:A:56:PRO:HD3	2:A:152:TYR:OH	2.11	0.51
2:A:348:PRO:HG2	2:A:355:PHE:HB2	1.93	0.51
2:A:604:ILE:HA	7:A:2131:HOH:O	2.11	0.50
2:A:821:ILE:HD11	2:A:824:SER:HA	1.93	0.50
2:A:314:HIS:O	2:A:315:VAL:HB	2.11	0.50
2:A:352:LYS:C	2:A:354:VAL:H	2.14	0.50
2:A:734:ASP:HA	2:A:739:ARG:HE	1.76	0.50
2:A:248:GLU:H	2:A:291:LYS:HB2	1.77	0.50
2:A:789:GLU:HG2	7:A:2103:HOH:O	2.11	0.50
1:T:24:G:H5'	2:A:710:ASN:OD1	2.12	0.50
2:A:730:ILE:CG2	2:A:888:ARG:HH21	2.25	0.50
2:A:254:TYR:HD2	2:A:286:LYS:NZ	2.07	0.50
2:A:276:ASP:HB3	2:A:386:LYS:HZ1	1.77	0.50
1:T:34:G:C2	2:A:7:LEU:HD21	2.46	0.50
2:A:267:LEU:HB3	2:A:271:VAL:HG21	1.94	0.50
2:A:245:VAL:HG12	2:A:310:ILE:HG22	1.94	0.50
2:A:585:HIS:HD2	2:A:586:GLY:O	1.95	0.50
2:A:112:ARG:O	2:A:114:LYS:N	2.45	0.49
2:A:864:LEU:HD13	2:A:877:VAL:CG2	2.40	0.49
2:A:327:ALA:O	2:A:329:GLY:N	2.45	0.49
1:T:19:G:O2'	1:T:20:U:OP1	2.24	0.49
2:A:333:ASP:CA	2:A:336:ILE:HG12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:200:TYR:CE2	2:A:395:PRO:HG3	2.48	0.49
2:A:444:MET:CE	2:A:448:ARG:HB2	2.43	0.49
2:A:243:ILE:N	2:A:243:ILE:HD12	2.27	0.49
2:A:379:THR:HG23	2:A:380:GLU:CD	2.33	0.49
2:A:558:GLN:HG3	6:A:1993:MRC:H172	1.94	0.49
2:A:213:ASN:HA	2:A:226:LYS:CB	2.42	0.49
2:A:316:THR:HG23	2:A:324:VAL:HG21	1.94	0.49
2:A:1:MET:HB2	2:A:901:GLU:HG3	1.94	0.49
2:A:248:GLU:H	2:A:291:LYS:CD	2.20	0.48
2:A:493:ASN:N	2:A:493:ASN:HD22	2.09	0.48
2:A:244:THR:CG2	2:A:245:VAL:N	2.76	0.48
2:A:263:ILE:HG23	2:A:271:VAL:HG21	1.94	0.48
2:A:166:ILE:HD12	2:A:533:SER:CB	2.40	0.48
2:A:745:LEU:O	2:A:748:ILE:CG2	2.62	0.48
2:A:309:VAL:CG1	2:A:310:ILE:N	2.77	0.48
1:T:13:C:H4'	2:A:702:LEU:HD21	1.94	0.48
1:T:9:A:OP2	7:T:1329:HOH:O	2.20	0.48
2:A:301:PRO:HA	2:A:304:ASP:OD1	2.14	0.48
2:A:342:GLU:O	2:A:343:LEU:HD23	2.13	0.48
2:A:348:PRO:O	2:A:349:ILE:HB	2.14	0.48
2:A:768:TRP:CE3	2:A:779:VAL:HG13	2.48	0.48
2:A:213:ASN:OD1	2:A:301:PRO:HG2	2.14	0.48
2:A:680:TYR:HA	2:A:794:LEU:HD21	1.95	0.48
1:T:9:A:C3'	7:T:1236:HOH:O	2.56	0.48
2:A:228:ILE:HG22	2:A:229:ILE:N	2.28	0.48
2:A:348:PRO:HG2	2:A:355:PHE:HB3	1.96	0.48
2:A:110:VAL:O	2:A:111:ASP:HB3	2.13	0.48
2:A:212:PHE:CE1	2:A:302:PHE:HD2	2.31	0.48
2:A:366:PHE:CZ	2:A:369:LYS:HB2	2.48	0.48
1:T:69:G:H2'	1:T:70:C:C6	2.49	0.48
2:A:17:ARG:HB3	2:A:17:ARG:NH1	2.29	0.47
2:A:328:PRO:HB3	2:A:335:TYR:HD1	1.78	0.47
2:A:336:ILE:CG1	2:A:337:VAL:H	2.14	0.47
1:T:35:A:C2	2:A:654:PHE:HB2	2.48	0.47
2:A:693:ILE:HD12	2:A:787:VAL:HG23	1.96	0.47
2:A:700:ASP:HB3	7:A:2060:HOH:O	2.14	0.47
2:A:241:VAL:HG11	2:A:328:PRO:CD	2.44	0.47
2:A:409:THR:HG23	2:A:410:PRO:HD2	1.95	0.47
2:A:538:VAL:HG22	2:A:539:LEU:N	2.29	0.47
2:A:237:ILE:H	2:A:238:PRO:CD	2.27	0.47
2:A:371:ASN:HA	2:A:375:THR:CG2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:49:THR:HG23	7:A:2012:HOH:O	2.15	0.47
2:A:542:ARG:HA	2:A:543:PRO:HD3	1.80	0.47
2:A:637:ILE:O	2:A:640:GLN:HB2	2.14	0.47
1:T:19:G:H4'	1:T:20:U:OP2	2.15	0.47
1:T:58:A:H1'	1:T:60:U:C5	2.50	0.47
2:A:245:VAL:HB	2:A:310:ILE:HG21	1.97	0.47
2:A:313:ASP:OD1	2:A:314:HIS:N	2.48	0.47
2:A:441:ILE:O	2:A:444:MET:HB3	2.15	0.47
2:A:539:LEU:HD13	2:A:547:PHE:O	2.14	0.47
1:T:58:A:O2'	1:T:59:G:P	2.73	0.47
2:A:104:ALA:O	2:A:108:LYS:HB2	2.14	0.47
2:A:247:PRO:O	2:A:248:GLU:HB3	2.15	0.47
2:A:39:LYS:HA	2:A:42:GLU:HG2	1.96	0.47
2:A:1:MET:HB3	2:A:902:LEU:HD23	1.97	0.47
2:A:254:TYR:CZ	2:A:288:TYR:HD1	2.33	0.47
2:A:272:ALA:HA	2:A:275:LEU:HB2	1.97	0.47
2:A:340:GLN:HB2	2:A:341:TYR:CE1	2.49	0.47
2:A:296:VAL:HG12	2:A:296:VAL:O	2.14	0.46
2:A:298:ALA:N	2:A:307:SER:HB3	2.30	0.46
2:A:506:GLU:O	2:A:506:GLU:HG3	2.14	0.46
2:A:329:GLY:N	2:A:346:ILE:HD11	2.31	0.46
2:A:99:LEU:O	2:A:103:GLN:HG3	2.15	0.46
1:T:37:A:O2'	1:T:38:A:OP2	2.26	0.46
2:A:613:LYS:HB3	2:A:617:ILE:CD1	2.45	0.46
2:A:1:MET:HB3	2:A:902:LEU:CD2	2.44	0.46
2:A:380:GLU:HB3	2:A:385:LEU:HB2	1.97	0.46
2:A:210:VAL:HG23	2:A:229:ILE:CB	2.31	0.46
2:A:250:LYS:O	2:A:251:TYR:HB2	2.15	0.46
2:A:293:LEU:HB3	2:A:296:VAL:HG21	1.97	0.46
2:A:753:THR:HG21	2:A:767:VAL:HG11	1.97	0.46
2:A:18:GLY:H	2:A:646:ARG:HH22	1.61	0.46
2:A:256:VAL:HG12	2:A:257:ASN:H	1.81	0.46
2:A:35:ASP:OD2	2:A:38:HIS:HB2	2.15	0.46
2:A:686:ARG:HD3	2:A:788:VAL:CG2	2.45	0.46
2:A:375:THR:C	2:A:377:LEU:H	2.19	0.46
2:A:597:SER:O	2:A:598:LYS:CB	2.64	0.46
1:T:58:A:H4'	1:T:59:G:OP1	2.15	0.46
2:A:153:ILE:HG22	2:A:155:LEU:HG	1.98	0.46
2:A:250:LYS:CA	2:A:290:GLY:H	2.29	0.46
1:T:48:C:OP2	1:T:48:C:H6	1.98	0.46
1:T:72:C:H4'	2:A:560:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:241:VAL:HA	2:A:308:LEU:HD22	1.97	0.46
2:A:284:LEU:HD12	2:A:285:GLU:N	2.31	0.46
2:A:250:LYS:HB3	2:A:290:GLY:H	1.80	0.46
2:A:294:GLU:HG2	2:A:295:TRP:HE3	1.81	0.46
2:A:432:PHE:HE2	2:A:582:LEU:HD23	1.81	0.46
1:T:60:U:O2'	1:T:61:C:OP1	2.30	0.46
2:A:237:ILE:N	2:A:238:PRO:CD	2.79	0.45
2:A:141:ARG:CG	2:A:610:VAL:HG11	2.46	0.45
2:A:242:ALA:C	2:A:243:ILE:HD12	2.37	0.45
2:A:248:GLU:N	2:A:291:LYS:HB2	2.32	0.45
2:A:280:ALA:O	2:A:282:ILE:N	2.50	0.45
2:A:350:ASP:C	2:A:352:LYS:H	2.19	0.45
2:A:432:PHE:CE2	2:A:582:LEU:HD23	2.51	0.45
2:A:209:TYR:O	2:A:385:LEU:HA	2.17	0.45
2:A:902:LEU:HB3	2:A:905:LEU:HD11	1.99	0.45
2:A:734:ASP:HA	2:A:739:ARG:NE	2.31	0.45
1:T:4:C:O2'	1:T:5:U:H5'	2.16	0.45
2:A:799:ARG:HD2	7:A:2141:HOH:O	2.15	0.45
1:T:46:G:H2'	1:T:47:U:C5'	2.30	0.45
1:T:58:A:C2'	1:T:60:U:OP2	2.63	0.45
2:A:210:VAL:O	2:A:229:ILE:HB	2.17	0.45
2:A:263:ILE:HG22	2:A:264:ALA:H	1.78	0.45
2:A:247:PRO:HA	2:A:291:LYS:CB	2.47	0.45
2:A:724:GLY:HA3	2:A:741:MET:CE	2.47	0.45
2:A:75:ASP:OD2	2:A:619:ARG:NH2	2.36	0.45
2:A:105:LEU:HD11	2:A:124:CYS:HA	1.99	0.45
2:A:267:LEU:HB3	2:A:271:VAL:CG2	2.47	0.45
2:A:377:LEU:HB3	2:A:378:LEU:HD12	1.97	0.45
2:A:209:TYR:O	2:A:385:LEU:HD22	2.17	0.44
2:A:243:ILE:CG2	2:A:244:THR:H	2.25	0.44
2:A:262:ILE:N	2:A:262:ILE:HD12	2.32	0.44
2:A:192:SER:O	2:A:193:LEU:HD23	2.17	0.44
2:A:296:VAL:O	2:A:297:VAL:C	2.55	0.44
2:A:448:ARG:NH1	2:A:564:ASN:ND2	2.65	0.44
2:A:119:GLU:O	2:A:123:LYS:HG2	2.17	0.44
2:A:535:HIS:O	2:A:539:LEU:HB2	2.18	0.44
2:A:36:GLN:HE21	2:A:145:ARG:HH11	1.65	0.44
2:A:602:ASN:H	2:A:602:ASN:ND2	2.15	0.44
2:A:558:GLN:O	2:A:563:PHE:HB2	2.17	0.44
2:A:659:ILE:C	2:A:659:ILE:HD12	2.37	0.44
2:A:213:ASN:ND2	2:A:215:LYS:HE3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:247:PRO:O	2:A:248:GLU:CB	2.66	0.44
2:A:432:PHE:CE1	2:A:438:LYS:HG3	2.53	0.44
1:T:8:U:H6	1:T:8:U:O5'	2.01	0.44
2:A:235:TRP:CH2	2:A:405:ILE:HB	2.53	0.44
2:A:271:VAL:O	2:A:275:LEU:HG	2.18	0.44
2:A:353:GLY:O	2:A:366:PHE:HA	2.17	0.44
2:A:768:TRP:CB	2:A:779:VAL:HG22	2.48	0.44
2:A:328:PRO:N	2:A:346:ILE:HD11	2.33	0.44
2:A:365:MET:HG3	2:A:370:ALA:CB	2.48	0.44
2:A:205:SER:OG	2:A:392:HIS:HE1	2.01	0.44
2:A:243:ILE:HB	2:A:310:ILE:HD11	1.98	0.44
1:T:19:G:OP1	1:T:60:U:N3	2.45	0.44
2:A:276:ASP:HB3	2:A:386:LYS:NZ	2.33	0.43
2:A:200:TYR:HB3	2:A:393:SER:OG	2.18	0.43
2:A:269:ASP:O	2:A:273:GLU:HB2	2.17	0.43
2:A:371:ASN:O	2:A:373:ALA:N	2.51	0.43
1:T:47:U:HO2'	1:T:48:C:P	2.35	0.43
2:A:247:PRO:HA	2:A:291:LYS:CG	2.48	0.43
2:A:467:TYR:HB2	2:A:519:THR:HB	2.00	0.43
2:A:168:GLY:HA3	2:A:480:VAL:HG11	2.00	0.43
1:T:37:A:O2'	1:T:38:A:P	2.77	0.43
2:A:17:ARG:CB	2:A:17:ARG:NH1	2.80	0.43
2:A:284:LEU:C	2:A:284:LEU:HD12	2.38	0.43
2:A:560:ARG:HG3	2:A:560:ARG:O	2.18	0.43
2:A:17:ARG:HB2	2:A:17:ARG:HH11	1.81	0.43
2:A:247:PRO:HA	2:A:291:LYS:HB2	2.00	0.43
2:A:348:PRO:HB3	2:A:357:GLU:CG	2.45	0.43
2:A:563:PHE:CZ	2:A:582:LEU:HD11	2.53	0.43
2:A:899:VAL:O	2:A:900:ASP:HB2	2.18	0.43
2:A:93:GLY:HA2	2:A:152:TYR:O	2.18	0.43
2:A:290:GLY:O	2:A:291:LYS:C	2.57	0.43
2:A:318:ASP:CG	2:A:319:ALA:H	2.21	0.43
2:A:210:VAL:HA	2:A:385:LEU:CD2	2.49	0.43
2:A:279:LYS:O	2:A:280:ALA:CB	2.66	0.43
2:A:287:GLU:HG3	2:A:287:GLU:O	2.19	0.43
2:A:241:VAL:HG11	2:A:328:PRO:HD2	2.01	0.42
2:A:301:PRO:C	2:A:303:LEU:N	2.71	0.42
2:A:681:LEU:HD22	2:A:720:TYR:CG	2.53	0.42
2:A:207:SER:HB2	2:A:230:TRP:NE1	2.29	0.42
2:A:467:TYR:CD2	2:A:472:GLU:HB2	2.54	0.42
2:A:505:PRO:HD3	7:A:2013:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:748:ILE:HG23	2:A:749:LEU:N	2.34	0.42
2:A:312:GLY:O	2:A:337:VAL:HG21	2.19	0.42
2:A:409:THR:HG23	2:A:410:PRO:CD	2.49	0.42
2:A:547:PHE:CB	2:A:548:PRO:HD3	2.45	0.42
2:A:716:LEU:HD21	2:A:748:ILE:HD12	2.01	0.42
2:A:350:ASP:C	2:A:352:LYS:N	2.72	0.42
2:A:552:TYR:CD1	2:A:579:TYR:HB3	2.54	0.42
2:A:493:ASN:ND2	2:A:493:ASN:N	2.68	0.42
2:A:646:ARG:HH21	2:A:649:ARG:HD3	1.85	0.42
2:A:275:LEU:C	2:A:277:TRP:H	2.23	0.42
2:A:242:ALA:N	2:A:308:LEU:HD22	2.35	0.42
2:A:757:ALA:HB3	2:A:758:PRO:HD3	2.00	0.42
2:A:255:ASN:ND2	2:A:282:ILE:O	2.51	0.42
2:A:302:PHE:CD1	2:A:302:PHE:C	2.93	0.42
2:A:380:GLU:C	2:A:382:GLY:H	2.22	0.42
2:A:469:GLU:O	2:A:470:ASN:CB	2.61	0.42
2:A:264:ALA:HB3	2:A:267:LEU:CB	2.36	0.42
2:A:56:PRO:HA	2:A:57:PRO:HD2	2.00	0.42
2:A:361:GLN:OE1	2:A:361:GLN:N	2.45	0.42
2:A:370:ALA:C	2:A:374:VAL:HB	2.40	0.42
2:A:141:ARG:HD3	7:A:2100:HOH:O	2.19	0.41
2:A:225:ALA:HB1	2:A:260:LYS:O	2.20	0.41
2:A:342:GLU:CD	2:A:342:GLU:H	2.24	0.41
2:A:64:HIS:CD2	2:A:66:GLY:H	2.33	0.41
2:A:245:VAL:O	2:A:245:VAL:CG1	2.68	0.41
2:A:303:LEU:O	2:A:303:LEU:HG	2.20	0.41
2:A:327:ALA:C	2:A:329:GLY:H	2.23	0.41
1:T:24:G:H2'	1:T:25:C:O4'	2.20	0.41
2:A:99:LEU:HB3	2:A:100:PRO:HD3	2.01	0.41
2:A:2:ASP:HB3	2:A:5:LYS:HZ2	1.85	0.41
2:A:868:ALA:HB2	2:A:877:VAL:HG22	2.01	0.41
2:A:124:CYS:HB3	2:A:459:TRP:CE2	2.55	0.41
2:A:250:LYS:CB	2:A:290:GLY:H	2.34	0.41
2:A:333:ASP:O	2:A:336:ILE:HG12	2.19	0.41
2:A:338:GLY:O	2:A:339:GLN:HB2	2.20	0.41
1:T:21(A):A:N6	1:T:46:G:H2'	2.35	0.41
2:A:241:VAL:HB	2:A:327:ALA:HA	2.02	0.41
2:A:263:ILE:CG2	2:A:271:VAL:HG21	2.51	0.41
2:A:281:SER:O	2:A:282:ILE:C	2.59	0.41
2:A:602:ASN:N	2:A:602:ASN:HD22	2.15	0.41
2:A:830:THR:HA	2:A:859:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:MET:HB2	2:A:901:GLU:CG	2.51	0.41
2:A:289:THR:HG21	2:A:292:GLU:CG	2.50	0.41
2:A:330:HIS:NE2	2:A:347:SER:CB	2.83	0.41
2:A:396:HIS:CE1	2:A:403:PRO:HG3	2.55	0.41
2:A:267:LEU:O	2:A:268:SER:C	2.59	0.41
2:A:275:LEU:O	2:A:386:LYS:HE3	2.21	0.41
2:A:349:ILE:HA	2:A:354:VAL:O	2.20	0.41
2:A:506:GLU:O	2:A:508:PHE:N	2.54	0.41
1:T:63:A:H2'	1:T:64:C:H6	1.77	0.41
2:A:359:GLY:O	2:A:363:GLU:HG2	2.21	0.41
2:A:379:THR:CG2	2:A:380:GLU:H	2.29	0.41
2:A:295:TRP:O	2:A:297:VAL:N	2.47	0.41
2:A:300:HIS:O	2:A:301:PRO:O	2.38	0.41
2:A:394:TYR:HA	2:A:395:PRO:HD3	1.92	0.41
2:A:188:SER:HB3	2:A:400:THR:HG21	2.01	0.41
2:A:36:GLN:NE2	2:A:145:ARG:HH11	2.19	0.41
2:A:237:ILE:C	2:A:239:SER:H	2.25	0.41
2:A:468:ALA:O	2:A:470:ASN:ND2	2.54	0.41
2:A:510:HIS:CD2	2:A:511:PRO:HD2	2.56	0.41
2:A:6:THR:OG1	2:A:888:ARG:HD2	2.20	0.41
2:A:10:PRO:HD3	2:A:729:TYR:CE1	2.56	0.40
2:A:172:ASP:C	2:A:174:GLY:H	2.24	0.40
2:A:237:ILE:HA	2:A:237:ILE:HD12	1.94	0.40
2:A:247:PRO:CD	2:A:313:ASP:H	2.35	0.40
2:A:872:GLU:N	2:A:872:GLU:CD	2.65	0.40
1:T:58:A:O2'	1:T:60:U:C5	2.70	0.40
2:A:206:ALA:HA	2:A:388:ASP:O	2.21	0.40
2:A:91:VAL:HA	2:A:92:PRO:HD3	1.95	0.40
2:A:791:ASP:C	2:A:791:ASP:OD1	2.59	0.40
2:A:250:LYS:HE3	2:A:289:THR:HG23	2.03	0.40
1:T:11:C:O2	2:A:640:GLN:NE2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	915/917 (100%)	763 (83%)	96 (10%)	56 (6%)	2 0

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	114	LYS
2	A	215	LYS
2	A	242	ALA
2	A	261	TYR
2	A	281	SER
2	A	289	THR
2	A	301	PRO
2	A	303	LEU
2	A	332	GLU
2	A	348	PRO
2	A	384	LEU
2	A	472	GLU
2	A	473	ILE
2	A	508	PHE
2	A	113	LYS
2	A	245	VAL
2	A	256	VAL
2	A	297	VAL
2	A	302	PHE
2	A	304	ASP
2	A	305	ARG
2	A	318	ASP
2	A	328	PRO
2	A	339	GLN
2	A	342	GLU
2	A	372	LYS
2	A	470	ASN
2	A	505	PRO
2	A	598	LYS
2	A	862	ASP
2	A	45	LYS
2	A	243	ILE
2	A	278	ASP
2	A	280	ALA
2	A	296	VAL

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Mol	Chain	Res	Type
2	A	312	GLY
2	A	116	SER
2	A	257	ASN
2	A	349	ILE
2	A	379	THR
2	A	507	GLY
2	A	604	ILE
2	A	775	LYS
2	A	263	ILE
2	A	268	SER
2	A	282	ILE
2	A	285	GLU
2	A	315	VAL
2	A	321	THR
2	A	360	GLY
2	A	115	MET
2	A	253	GLN
2	A	353	GLY
2	A	336	ILE
2	A	247	PRO
2	A	603	VAL

### 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
2	A	806/806 (100%)	769 (95%)	37 (5%)	31 39

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	ARG
2	A	20	LEU
2	A	94	TRP
2	A	155	LEU
2	A	210	VAL

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Mol	Chain	Res	Type
2	A	212	PHE
2	A	257	ASN
2	A	295	TRP
2	A	305	ARG
2	A	325	HIS
2	A	339	GLN
2	A	346	ILE
2	A	355	PHE
2	A	362	PHE
2	A	366	PHE
2	A	380	GLU
2	A	385	LEU
2	A	398	TRP
2	A	409	THR
2	A	485	ASP
2	A	489	GLU
2	A	501	LYS
2	A	526	ASP
2	A	544	GLU
2	A	546	SER
2	A	569	THR
2	A	602	ASN
2	A	675	LEU
2	A	681	LEU
2	A	702	LEU
2	A	723	TYR
2	A	749	LEU
2	A	776	GLU
2	A	779	VAL
2	A	844	THR
2	A	866	ASP
2	A	895	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	GLN
2	A	60	ASN
2	A	62	ASN
2	A	64	HIS
2	A	97	HIS
2	A	253	GLN

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Mol	Chain	Res	Type
2	A	257	ASN
2	A	299	GLN
2	A	300	HIS
2	A	311	ASN
2	A	339	GLN
2	A	392	HIS
2	A	396	HIS
2	A	411	GLN
2	A	470	ASN
2	A	493	ASN
2	A	510	HIS
2	A	564	ASN
2	A	585	HIS
2	A	602	ASN
2	A	608	GLN
2	A	612	GLN
2	A	650	ASN
2	A	706	GLN
2	A	713	ASN
2	A	732	GLN
2	A	736	HIS
2	A	742	GLN
2	A	770	HIS
2	A	809	ASN
2	A	834	ASN
2	A	857	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	T	74/75 (98%)	25 (33%)	0

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	T	7	G
1	T	8	U
1	T	9	A
1	T	10	G
1	T	14	A
1	T	16	G

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Mol	Chain	Res	Type
1	T	17	U
1	T	18	G
1	T	19	G
1	T	20	U
1	T	21	U
1	T	21(A)	A
1	T	22	G
1	T	33	U
1	T	34	G
1	T	35	A
1	T	36	U
1	T	37	A
1	T	38	A
1	T	46	G
1	T	48	C
1	T	49	G
1	T	59	G
1	T	61	C
1	T	74	C

There are no RNA pucker outliers to report.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 13 are monoatomic - leaving 1 for Mogul analysis.

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
6	MRC	A	1993	-	32,36,36	2.33	8 (25%)	35,48,48	2.19	7 (20%)

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
6	MRC	A	1993	-	1/1/11/12	0/30/54/54	0/1/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1993	MRC	C11-C10	-6.91	1.36	1.46
6	A	1993	MRC	C2-C1	-3.05	1.39	1.46
6	A	1993	MRC	C9-C10	2.53	1.57	1.52
6	A	1993	MRC	C2-C3	2.88	1.39	1.33
6	A	1993	MRC	C16-C8	3.23	1.56	1.51
6	A	1993	MRC	O1A-C1	3.27	1.42	1.34
6	A	1993	MRC	C9-C8	3.94	1.61	1.53
6	A	1993	MRC	C8-C7	5.84	1.60	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1993	MRC	C11-O10-C10	-4.94	57.46	60.58
6	A	1993	MRC	C9'-O1A-C1	-3.53	110.30	116.49
6	A	1993	MRC	O1A-C1-O1B	-2.13	117.78	122.93
6	A	1993	MRC	C17-C12-C11	3.84	118.50	111.43
6	A	1993	MRC	O1A-C1-C2	4.04	119.58	110.61
6	A	1993	MRC	C9-C8-C7	5.54	121.20	113.32
6	A	1993	MRC	C11-C12-C13	6.12	121.96	110.78

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1993	MRC	C12

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1993	MRC	3	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	T	75/75 (100%)	0.53	9 (12%) <b>5</b> <b>4</b>	18, 32, 72, 99	2 (2%)
2	A	917/917 (100%)	1.11	194 (21%) <b>1</b> <b>1</b>	10, 29, 99, 100	0
All	All	992/992 (100%)	1.06	203 (20%) <b>1</b> <b>1</b>	10, 30, 99, 100	2 (0%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	288	TYR	17.3
2	A	219	GLY	15.9
2	A	289	THR	15.6
2	A	280	ALA	13.9
2	A	315	VAL	13.2
2	A	214	VAL	13.0
2	A	241	VAL	11.9
2	A	337	VAL	11.7
2	A	254	TYR	11.2
2	A	225	ALA	10.6
2	A	262	ILE	10.5
2	A	283	LYS	10.1
2	A	290	GLY	9.5
1	T	74	C	9.3
2	A	267	LEU	9.3
2	A	317	THR	9.1
2	A	324	VAL	8.8
2	A	298	ALA	8.6
2	A	314	HIS	8.5
2	A	383	ALA	8.5
2	A	284	LEU	8.4
2	A	245	VAL	8.3
2	A	268	SER	8.1
2	A	379	THR	8.1

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Mol	Chain	Res	Type	RSRZ
2	A	366	PHE	7.8
2	A	917	VAL	7.7
2	A	221	VAL	7.6
2	A	248	GLU	7.5
2	A	345	VAL	7.4
2	A	215	LYS	7.3
2	A	270	ALA	7.1
2	A	242	ALA	6.9
2	A	281	SER	6.9
2	A	307	SER	6.7
2	A	227	PHE	6.7
2	A	282	ILE	6.6
2	A	319	ALA	6.6
2	A	276	ASP	6.6
2	A	269	ASP	6.4
2	A	223	ALA	6.4
2	A	228	ILE	6.3
2	A	286	LYS	6.2
2	A	302	PHE	6.2
2	A	213	ASN	6.1
2	A	285	GLU	6.0
2	A	222	ASP	6.0
2	A	293	LEU	5.8
2	A	304	ASP	5.7
2	A	217	ASP	5.7
2	A	327	ALA	5.7
2	A	339	GLN	5.7
2	A	292	GLU	5.6
2	A	220	VAL	5.6
2	A	513	SER	5.6
2	A	252	GLY	5.6
2	A	303	LEU	5.5
2	A	263	ILE	5.5
2	A	318	ASP	5.5
2	A	251	TYR	5.4
2	A	311	ASN	5.4
2	A	210	VAL	5.2
2	A	323	CYS	5.2
2	A	247	PRO	5.1
2	A	274	ALA	5.1
2	A	347	SER	5.0
2	A	249	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
2	A	340	GLN	4.9
2	A	373	ALA	4.9
2	A	255	ASN	4.9
2	A	372	LYS	4.9
2	A	211	ALA	4.9
2	A	309	VAL	4.9
2	A	250	LYS	4.8
2	A	357	GLU	4.8
2	A	335	TYR	4.7
2	A	226	LYS	4.7
2	A	346	ILE	4.7
1	T	17	U	4.7
2	A	265	GLU	4.7
2	A	1	MET	4.7
2	A	216	ASP	4.6
2	A	384	LEU	4.6
2	A	275	LEU	4.6
2	A	374	VAL	4.5
2	A	361	GLN	4.5
2	A	208	ILE	4.5
2	A	387	LEU	4.4
2	A	243	ILE	4.4
2	A	328	PRO	4.4
2	A	257	ASN	4.4
2	A	354	VAL	4.3
2	A	866	ASP	4.3
2	A	336	ILE	4.3
2	A	355	PHE	4.3
2	A	321	THR	4.3
2	A	506	GLU	4.3
2	A	299	GLN	4.2
2	A	358	GLU	4.2
2	A	218	LYS	4.2
2	A	390	ILE	4.1
2	A	295	TRP	4.1
2	A	224	ASP	4.0
2	A	305	ARG	4.0
2	A	350	ASP	4.0
2	A	338	GLY	4.0
2	A	234	PRO	3.9
2	A	326	THR	3.9
2	A	363	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	A	382	GLY	3.9
2	A	547	PHE	3.8
2	A	306	GLU	3.8
2	A	861	VAL	3.8
2	A	370	ALA	3.8
2	A	356	THR	3.8
2	A	343	LEU	3.8
1	T	16	G	3.8
2	A	240	ASN	3.7
2	A	333	ASP	3.7
2	A	360	GLY	3.7
2	A	308	LEU	3.7
2	A	244	THR	3.7
2	A	261	TYR	3.6
2	A	271	VAL	3.6
2	A	229	ILE	3.6
2	A	313	ASP	3.6
2	A	246	HIS	3.5
2	A	353	GLY	3.5
2	A	266	ALA	3.5
2	A	369	LYS	3.5
2	A	367	TYR	3.5
2	A	341	TYR	3.5
2	A	204	ARG	3.4
2	A	259	GLU	3.4
2	A	300	HIS	3.4
2	A	389	PHE	3.3
2	A	469	GLU	3.3
1	T	47	U	3.2
2	A	209	TYR	3.2
2	A	256	VAL	3.2
2	A	231	THR	3.2
2	A	294	GLU	3.2
2	A	381	LYS	3.1
2	A	287	GLU	3.1
2	A	253	GLN	3.1
2	A	322	GLY	3.1
2	A	235	TRP	3.1
2	A	368	ASP	3.0
1	T	1	G	3.0
2	A	365	MET	3.0
2	A	470	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	385	LEU	3.0
2	A	301	PRO	3.0
2	A	278	ASP	3.0
2	A	349	ILE	3.0
2	A	212	PHE	3.0
2	A	352	LYS	2.9
2	A	273	GLU	2.9
2	A	310	ILE	2.9
2	A	296	VAL	2.9
2	A	835	ASP	2.9
2	A	377	LEU	2.8
2	A	348	PRO	2.8
2	A	471	GLY	2.8
2	A	665	ASP	2.8
2	A	316	THR	2.8
2	A	378	LEU	2.7
2	A	342	GLU	2.7
2	A	380	GLU	2.7
2	A	332	GLU	2.7
2	A	239	SER	2.6
2	A	331	GLY	2.6
2	A	375	THR	2.6
1	T	46	G	2.6
1	T	73	A	2.6
2	A	507	GLY	2.6
2	A	277	TRP	2.5
2	A	45	LYS	2.5
2	A	167	PHE	2.5
2	A	238	PRO	2.5
2	A	272	ALA	2.5
2	A	325	HIS	2.5
1	T	45	G	2.4
2	A	264	ALA	2.4
2	A	260	LYS	2.4
2	A	258	GLY	2.4
2	A	312	GLY	2.4
2	A	406	PHE	2.4
2	A	236	THR	2.4
2	A	362	PHE	2.4
2	A	472	GLU	2.3
2	A	164	ILE	2.3
2	A	775	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	237	ILE	2.3
2	A	895	ASP	2.2
2	A	441	ILE	2.2
2	A	514	PRO	2.2
2	A	2	ASP	2.1
2	A	376	ASP	2.1
1	T	2	G	2.1
2	A	320	GLY	2.1
2	A	230	TRP	2.0
2	A	330	HIS	2.0
2	A	867	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MRC	A	1993	35/35	0.81	0.22	2.40	14,29,54,55	0
5	MG	T	1207	1/1	0.96	0.14	-0.73	37,37,37,37	0
4	ZN	A	1992	1/1	0.99	0.04	-2.96	26,26,26,26	0
3	K	T	301	1/1	0.97	0.05	-2.98	26,26,26,26	0
4	ZN	A	1001	1/1	0.99	0.04	-3.52	26,26,26,26	0
5	MG	T	1209	1/1	0.87	0.19	-	45,45,45,45	0
5	MG	T	1201	1/1	0.86	0.07	-	37,37,37,37	0
5	MG	T	1205	1/1	0.68	0.17	-	29,29,29,29	0
5	MG	T	1210	1/1	0.84	0.16	-	36,36,36,36	0
5	MG	T	1204	1/1	0.87	0.17	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	T	1206	1/1	0.64	0.31	-	37,37,37,37	0
5	MG	T	1203	1/1	0.80	0.23	-	37,37,37,37	0
5	MG	T	1202	1/1	0.56	0.19	-	54,54,54,54	0
5	MG	T	1208	1/1	0.93	0.42	-	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.