



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:31 AM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

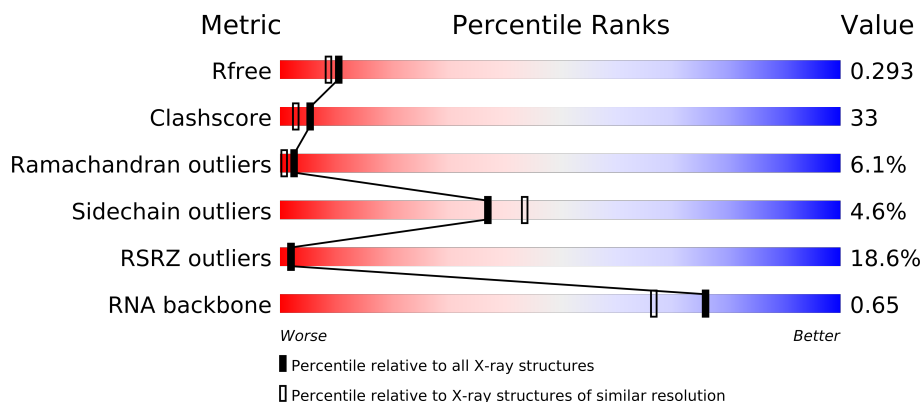
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

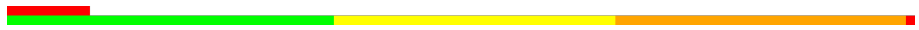

The reported resolution of this entry is 2.20 Å.

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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)
RNA backbone	1838	1120 (3.00-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9386 atoms, of which 0 are hydrogen and 0 are deuterium.

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		

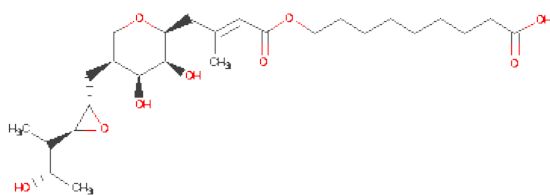
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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.

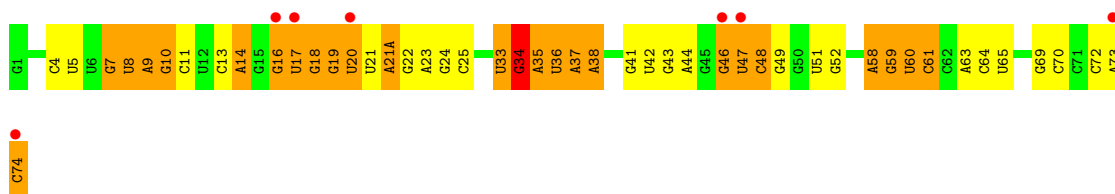
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	208	Total	O	0	0
			208	208		
7	T	120	Total	O	0	0
			120	120		

3 Residue-property plots

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

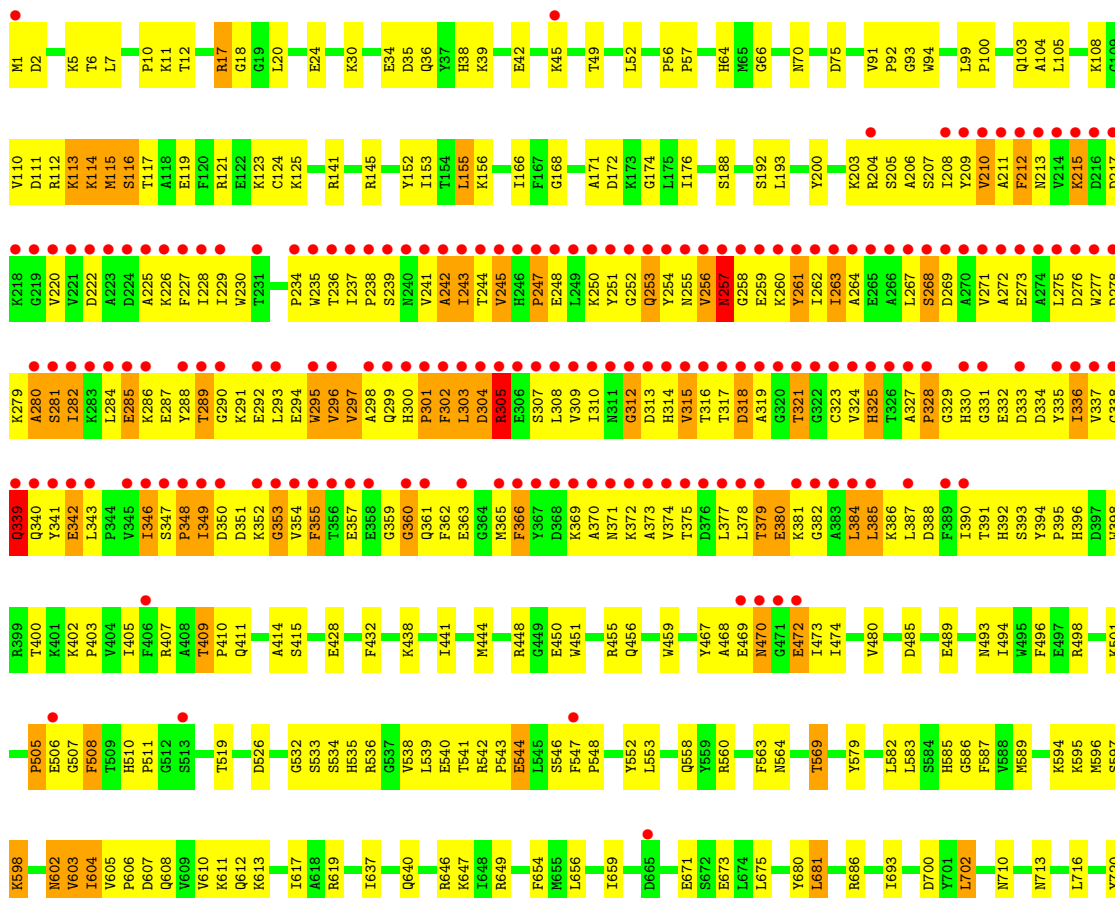
• Molecule 1: ISOLEUCYL-TRNA

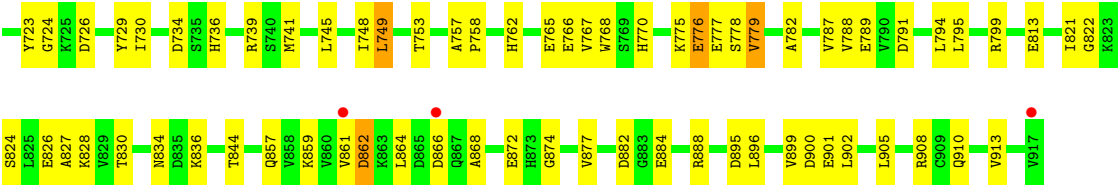
Chain T: 



• Molecule 2: ISOLEUCYL-TRNA SYNTHETASE

Chain A: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.19Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.239 , 0.281 0.250 , 0.293	Depositor DCC
R_{free} test set	2908 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 60370 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9386	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	10	0	0	0	0
6	A	35	0	41	3	0
7	A	208	0	0	20	0
7	T	120	0	0	4	0
All	All	9386	0	8065	554	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (554) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:T:69:G:H5''	2:A:589:MET:HE2	1.55	0.86
2:A:857:GLN:NE2	2:A:882:ASP:H	1.72	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	Distance(Å)	Clash(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:366:PHE:CE1	2:A:369:LYS:HB2	2.21	0.76
2:A:257:ASN:ND2	2:A:258:GLY:H	1.82	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:905:LEU:HD13	7:A:2172:HOH:O	1.87	0.74
2:A:207:SER:HB2	2:A:230:TRP:HE1	1.52	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
1:T:70:C:OP1	2:A:595:LYS:HD3	1.91	0.70
2:A:730:ILE:O	2:A:888:ARG:NH2	2.25	0.70
2:A:209:TYR:C	2:A:385:LEU:HD13	2.12	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:250:LYS:HB3	2:A:289:THR:HA	1.74	0.69
2:A:113:LYS:O	2:A:114:LYS:HB2	1.92	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:212:PHE:HZ	2:A:302:PHE:HB3	1.60	0.67
2:A:263:ILE:HG22	2:A:264:ALA:N	2.09	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:17:ARG:CB	2:A:17:ARG:HH11	2.12	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:730:ILE:HG23	2:A:888:ARG:HH21	1.66	0.60
2:A:415:SER:HA	2:A:450:GLU:OE1	2.02	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:535:HIS:NE2	2:A:569:THR:HG23	2.16	0.59
2:A:2:ASP:OD2	2:A:5:LYS:HG3	2.02	0.59
2:A:229:ILE:HD11	2:A:300:HIS:CD2	2.37	0.59
2:A:821:ILE:HG12	2:A:822:GLY:N	2.18	0.59
2:A:295:TRP:HA	2:A:309:VAL:HG13	1.83	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:212:PHE:CE2	2:A:301:PRO:HB2	2.37	0.59
2:A:125:LYS:HG3	2:A:155:LEU:HD22	1.84	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:366:PHE:O	2:A:370:ALA:HB3	2.03	0.58
2:A:305:ARG:HA	2:A:305:ARG:HE	1.69	0.58
2:A:244:THR:OG1	2:A:324:VAL:HB	2.03	0.58
2:A:91:VAL:HG23	2:A:91:VAL:O	2.04	0.58
2:A:607:ASP:O	2:A:611:LYS:HG2	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
1:T:18:G:O2'	1:T:19:G:OP1	2.22	0.57
2:A:777:GLU:O	2:A:778:SER:HB3	2.04	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: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:279:LYS:O	2:A:280:ALA:HB3	2.05	0.57
2:A:236:THR:O	2:A:236:THR:HG22	2.04	0.57
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:209:TYR:CE2	2:A:321:THR:HG21	2.37	0.56
2:A:348:PRO:HG2	2:A:355:PHE:CB	2.36	0.56
2:A:11:LYS:O	2:A:12:THR:HG23	2.05	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:553:LEU:HA	2:A:583:LEU:O	2.07	0.55
2:A:30:LYS:O	2:A:34:GLU:HG2	2.07	0.55
2:A:745:LEU:O	2:A:748:ILE:HG22	2.05	0.55
2:A:390:ILE:HG22	2:A:391:THR:N	2.22	0.55
1:T:23:A:H2'	1:T:24:G:C8	2.41	0.55
2:A:411:GLN:HE22	2:A:456:GLN:HE22	1.54	0.55
2:A:536:ARG:O	2:A:541:THR:HG23	2.06	0.55
2:A:338:GLY:C	2:A:343:LEU:HD12	2.26	0.55
2:A:673:GLU:O	2:A:736:HIS:HE1	1.90	0.55
2:A:726:ASP:O	2:A:908:ARG:NH2	2.39	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
1:T:46:G:C2'	1:T:47:U:H5'	2.28	0.55
2:A:394:TYR:O	2:A:396:HIS:HD2	1.89	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:HG13	2:A:245:VAL:O	2.07	0.54
2:A:400:THR:HG22	2:A:402:LYS:CG	2.28	0.54
2:A:693:ILE:HD12	2:A:787:VAL:CG2	2.38	0.54
2:A:613:LYS:O	2:A:617:ILE:HD12	2.08	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:329:GLY:H	2:A:346:ILE:HD11	1.72	0.54
2:A:153:ILE:HD12	2:A:156:LYS:HE2	1.89	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:245:VAL:CG1	2:A:310:ILE:HG22	2.38	0.53
2:A:309:VAL:CG1	2:A:310:ILE:H	2.19	0.53
2:A:380:GLU:CB	2:A:385:LEU:HB2	2.37	0.53
2:A:913:VAL:HB	7:A:2172:HOH:O	2.07	0.53
2:A:35:ASP:O	2:A:39:LYS:HG2	2.09	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:217:ASP:HA	2:A:220:VAL:HG23	1.90	0.53
2:A:115:MET:O	2:A:116:SER:OG	2.21	0.53
2:A:166:ILE:HD11	2:A:536:ARG:HB2	1.90	0.53
2:A:252:GLY:O	2:A:262:ILE:HA	2.09	0.53
2:A:252:GLY:H	2:A:287:GLU:HB2	1.74	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
1:T:13:C:H2'	1:T:14:A:C5'	2.33	0.52
2:A:350:ASP:HA	2:A:407:ARG:NH2	2.25	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: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: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
2:A:166:ILE:HD11	2:A:536:ARG:CB	2.39	0.51
2:A:350:ASP:OD1	2:A:351:ASP:N	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:608:GLN:HB3	2:A:612:GLN:HE21	1.75	0.51
2:A:250:LYS:CD	2:A:289:THR:HG23	2.40	0.51
2:A:540:GLU:CG	2:A:547:PHE:HB2	2.41	0.51
2:A:256:VAL:HG12	2:A:257:ASN:N	2.25	0.51
2:A:357:GLU:C	2:A:359:GLY:H	2.14	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:821:ILE:HD11	2:A:824:SER:HA	1.93	0.50
2:A:604:ILE:HA	7:A:2131:HOH:O	2.11	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:276:ASP:HB3	2:A:386:LYS:HZ1	1.77	0.50
2:A:254:TYR:HD2	2:A:286:LYS:NZ	2.07	0.50
1:T:34:G:C2	2:A:7:LEU:HD21	2.46	0.50
2:A:245:VAL:HG12	2:A:310:ILE:HG22	1.94	0.50
2:A:267:LEU:HB3	2:A:271:VAL:HG21	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
2:A:444:MET:CE	2:A:448:ARG:HB2	2.43	0.49
2:A:200:TYR:CE2	2:A:395:PRO:HG3	2.48	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:558:GLN:HG3	6:A:1993:MRC:H172	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:745:LEU:O	2:A:748:ILE:CG2	2.62	0.48
2:A:166:ILE:HD12	2:A:533:SER:CB	2.40	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: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:342:GLU:O	2:A:343:LEU:HD23	2.13	0.48
2:A:213:ASN:OD1	2:A:301:PRO:HG2	2.14	0.48
1:T:9:A:C3'	7:T:1236:HOH:O	2.56	0.48
2:A:680:TYR:HA	2:A:794:LEU:HD21	1.95	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: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:110:VAL:O	2:A:111:ASP:HB3	2.13	0.48
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:17:ARG:HB3	2:A:17:ARG:NH1	2.29	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:538:VAL:HG22	2:A:539:LEU:N	2.29	0.47
2:A:409:THR:HG23	2:A:410:PRO:HD2	1.95	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
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:542:ARG:HA	2:A:543:PRO:HD3	1.80	0.47
2:A:49:THR:HG23	7:A:2012:HOH:O	2.15	0.47
2:A:637:ILE:O	2:A:640:GLN:HB2	2.14	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:539:LEU:HD13	2:A:547:PHE:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:58:A:O2'	1:T:59:G:P	2.73	0.47
2:A:441:ILE:O	2:A:444:MET:HB3	2.15	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:272:ALA:HA	2:A:275:LEU:HB2	1.97	0.47
2:A:254:TYR:CZ	2:A:288:TYR:HD1	2.33	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:506:GLU:O	2:A:506:GLU:HG3	2.14	0.46
2:A:298:ALA:N	2:A:307:SER:HB3	2.30	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:380:GLU:HB3	2:A:385:LEU:HB2	1.97	0.46
2:A:1:MET:HB3	2:A:902:LEU:CD2	2.44	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: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
2:A:153:ILE:HG22	2:A:155:LEU:HG	1.98	0.46
1:T:72:C:H4'	2:A:560:ARG:NH2	2.30	0.46
2:A:241:VAL:HA	2:A:308:LEU:HD22	1.97	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
1:T:60:U:O2'	1:T:61:C:OP1	2.30	0.46
2:A:432:PHE:HE2	2:A:582:LEU:HD23	1.81	0.46
2:A:284:LEU:HD12	2:A:285:GLU:N	2.31	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:248:GLU:N	2:A:291:LYS:HB2	2.32	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:280:ALA:O	2:A:282:ILE:N	2.50	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
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:799:ARG:HD2	7:A:2141:HOH:O	2.15	0.45
2:A:210:VAL:O	2:A:229:ILE:HB	2.17	0.45
2:A:247:PRO:HA	2:A:291:LYS:CB	2.47	0.45
2:A:263:ILE:HG22	2:A:264:ALA:H	1.78	0.45
2:A:75:ASP:OD2	2:A:619:ARG:NH2	2.36	0.45
2:A:724:GLY:HA3	2:A:741:MET:CE	2.47	0.45
2:A:377:LEU:HB3	2:A:378:LEU:HD12	1.97	0.45
2:A:267:LEU:HB3	2:A:271:VAL:CG2	2.47	0.45
2:A:105:LEU:HD11	2:A:124:CYS:HA	1.99	0.45
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:209:TYR:O	2:A:385:LEU:HD22	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:192:SER:O	2:A:193:LEU:HD23	2.17	0.44
2:A:535:HIS:O	2:A:539:LEU:HB2	2.18	0.44
2:A:119:GLU:O	2:A:123:LYS:HG2	2.17	0.44
2:A:602:ASN:H	2:A:602:ASN:ND2	2.15	0.44
2:A:36:GLN:HE21	2:A:145:ARG:HH11	1.65	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
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:353:GLY:O	2:A:366:PHE:HA	2.17	0.44
2:A:271:VAL:O	2:A:275:LEU:HG	2.18	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:243:ILE:HB	2:A:310:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:T:19:G:OP1	1:T:60:U:N3	2.45	0.44
2:A:205:SER:OG	2:A:392:HIS:HE1	2.01	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: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:269:ASP:O	2:A:273:GLU:HB2	2.17	0.43
2:A:247:PRO:HA	2:A:291:LYS:CG	2.48	0.43
1:T:37:A:O2'	1:T:38:A:P	2.77	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
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: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:17:ARG:HH11	2:A:17:ARG:HB2	1.81	0.43
2:A:899:VAL:O	2:A:900:ASP:HB2	2.18	0.43
2:A:290:GLY:O	2:A:291:LYS:C	2.57	0.43
2:A:93:GLY:HA2	2:A:152:TYR:O	2.18	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:287:GLU:HG3	2:A:287:GLU:O	2.19	0.43
2:A:279:LYS:O	2:A:280:ALA:CB	2.66	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:748:ILE:HG23	2:A:749:LEU:N	2.34	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
2:A:716:LEU:HD21	2:A:748:ILE:HD12	2.01	0.42
2:A:312:GLY:O	2:A:337:VAL:HG21	2.19	0.42
2:A:547:PHE:CB	2:A:548:PRO:HD3	2.45	0.42
2:A:409:THR:HG23	2:A:410:PRO:CD	2.49	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:646:ARG:HH21	2:A:649:ARG:HD3	1.85	0.42
2:A:493:ASN:ND2	2:A:493:ASN:N	2.68	0.42
2:A:242:ALA:N	2:A:308:LEU:HD22	2.35	0.42
2:A:275:LEU:C	2:A:277:TRP:H	2.23	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:757:ALA:HB3	2:A:758:PRO:HD3	2.00	0.42
2:A:302:PHE:CD1	2:A:302:PHE:C	2.93	0.42
2:A:255:ASN:ND2	2:A:282:ILE:O	2.51	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:370:ALA:C	2:A:374:VAL:HB	2.40	0.42
2:A:361:GLN:OE1	2:A:361:GLN:N	2.45	0.42
2:A:225:ALA:HB1	2:A:260:LYS:O	2.20	0.41
2:A:141:ARG:HD3	7:A:2100:HOH:O	2.19	0.41
2:A:64:HIS:CD2	2:A:66:GLY:H	2.33	0.41
2:A:342:GLU:CD	2:A:342:GLU:H	2.24	0.41
2:A:245:VAL:O	2:A:245:VAL:CG1	2.68	0.41
2:A:303:LEU:HG	2:A:303:LEU:O	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: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:99:LEU:HB3	2:A:100:PRO:HD3	2.01	0.41
2:A:250:LYS:CB	2:A:290:GLY:H	2.34	0.41
1:T:21(A):A:N6	1:T:46:G:H2'	2.35	0.41
2:A:333:ASP:O	2:A:336:ILE:HG12	2.19	0.41
2:A:124:CYS:HB3	2:A:459:TRP:CE2	2.55	0.41
2:A:338:GLY:O	2:A:339:GLN:HB2	2.20	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:602:ASN:N	2:A:602:ASN:HD22	2.15	0.41
2:A:281:SER:O	2:A:282:ILE:C	2.59	0.41
2:A:830:THR:HA	2:A:859:LYS:O	2.21	0.41
2:A:289:THR:HG21	2:A:292:GLU:CG	2.50	0.41
2:A:1:MET:HB2	2:A:901:GLU:CG	2.51	0.41
2:A:396:HIS:CE1	2:A:403:PRO:HG3	2.55	0.41
2:A:330:HIS:NE2	2:A:347:SER:CB	2.83	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
1:T:63:A:H2'	1:T:64:C:H6	1.77	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
2:A:379:THR:CG2	2:A:380:GLU:H	2.29	0.41
2:A:359:GLY:O	2:A:363:GLU:HG2	2.21	0.41
2:A:295:TRP:O	2:A:297:VAL:N	2.47	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:300:HIS:O	2:A:301:PRO:O	2.38	0.41
2:A:188:SER:HB3	2:A:400:THR:HG21	2.01	0.41
2:A:394:TYR:HA	2:A:395:PRO:HD3	1.92	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:6:THR:OG1	2:A:888:ARG:HD2	2.20	0.41
2:A:36:GLN:NE2	2:A:145:ARG:HH11	2.19	0.41
2:A:510:HIS:CD2	2:A:511:PRO:HD2	2.56	0.41
2:A:237:ILE:HA	2:A:237:ILE:HD12	1.94	0.40
2:A:172:ASP:C	2:A:174:GLY:H	2.24	0.40
2:A:10:PRO:HD3	2:A:729:TYR:CE1	2.56	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:91:VAL:HA	2:A:92:PRO:HD3	1.95	0.40
2:A:206:ALA:HA	2:A:388:ASP:O	2.21	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 1

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	37	43

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	12 (16%)

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
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

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Mol	Chain	Res	Type
1	T	46	G
1	T	48	C
1	T	49	G
1	T	59	G
1	T	61	C
1	T	74	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	T	7	G
1	T	18	G
1	T	19	G
1	T	33	U
1	T	34	G
1	T	35	A
1	T	36	U
1	T	37	A
1	T	47	U
1	T	48	C
1	T	58	A
1	T	60	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	-	36,36,36	2.27	10 (27%)	48,48,48	2.26	10 (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	0/32/54/54	0/1/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1993	MRC	C11-C10	-7.20	1.36	1.46
6	A	1993	MRC	C8-C7	5.85	1.60	1.53
6	A	1993	MRC	C9-C8	3.78	1.61	1.53
6	A	1993	MRC	O1A-C1	3.26	1.42	1.34
6	A	1993	MRC	C16-C8	3.03	1.56	1.51
6	A	1993	MRC	C2-C1	-2.91	1.39	1.47
6	A	1993	MRC	C9-C10	2.57	1.57	1.52
6	A	1993	MRC	C2-C3	2.57	1.39	1.33
6	A	1993	MRC	C4-C5	2.32	1.57	1.53
6	A	1993	MRC	C4-C3	2.05	1.54	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1993	MRC	C16-C8-C7	-6.10	103.25	108.72
6	A	1993	MRC	C9-C8-C7	5.73	121.20	113.19
6	A	1993	MRC	C11-O10-C10	-5.22	57.46	60.59
6	A	1993	MRC	C11-C12-C13	4.89	121.96	110.71
6	A	1993	MRC	O1A-C1-C2	4.26	119.58	110.65
6	A	1993	MRC	C12-C11-C10	3.95	131.46	123.28
6	A	1993	MRC	C17-C12-C11	3.68	118.50	111.46
6	A	1993	MRC	C8-C9-C10	3.67	122.20	115.07
6	A	1993	MRC	C9'-O1A-C1	-3.51	110.30	116.64
6	A	1993	MRC	C17-C12-C13	2.83	118.92	112.94

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	75/75 (100%)	0.36	7 (9%) 9 8	18, 32, 72, 99	2 (2%)
2	A	917/917 (100%)	0.88	179 (19%) 2 1	10, 29, 99, 100	0
All	All	992/992 (100%)	0.84	186 (18%) 2 2	10, 30, 99, 100	2 (0%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	219	GLY	15.5
2	A	288	TYR	15.1
2	A	315	VAL	14.4
2	A	280	ALA	13.0
2	A	337	VAL	12.0
2	A	289	THR	11.7
2	A	214	VAL	10.7
2	A	225	ALA	9.5
1	T	74	C	9.5
2	A	324	VAL	9.2
2	A	254	TYR	9.1
2	A	284	LEU	9.0
2	A	345	VAL	8.9
2	A	241	VAL	8.8
2	A	298	ALA	8.4
2	A	317	THR	8.3
2	A	267	LEU	8.1
2	A	242	ALA	7.7
2	A	268	SER	7.5
2	A	252	GLY	7.4
2	A	383	ALA	7.3
2	A	314	HIS	7.3
2	A	290	GLY	7.2
2	A	215	LYS	7.1

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Mol	Chain	Res	Type	RSRZ
2	A	245	VAL	7.0
2	A	262	ILE	6.8
2	A	379	THR	6.8
2	A	917	VAL	6.7
2	A	283	LYS	6.7
2	A	366	PHE	6.6
2	A	384	LEU	6.5
2	A	285	GLU	6.2
2	A	269	ASP	6.2
2	A	372	LYS	6.2
2	A	270	ALA	6.0
2	A	319	ALA	6.0
2	A	228	ILE	5.9
2	A	223	ALA	5.8
2	A	250	LYS	5.7
2	A	265	GLU	5.7
2	A	311	ASN	5.6
2	A	247	PRO	5.5
2	A	1	MET	5.5
2	A	216	ASP	5.5
2	A	251	TYR	5.5
2	A	248	GLU	5.4
2	A	217	ASP	5.3
2	A	276	ASP	5.3
2	A	323	CYS	5.2
2	A	281	SER	5.2
2	A	221	VAL	5.1
2	A	227	PHE	5.1
2	A	382	GLY	5.0
2	A	243	ILE	5.0
2	A	226	LYS	5.0
2	A	307	SER	4.9
2	A	327	ALA	4.9
2	A	255	ASN	4.8
2	A	346	ILE	4.8
2	A	218	LYS	4.8
2	A	373	ALA	4.8
2	A	354	VAL	4.7
2	A	256	VAL	4.7
2	A	275	LEU	4.7
2	A	304	ASP	4.7
2	A	263	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	T	17	U	4.6
2	A	213	ASN	4.6
2	A	292	GLU	4.6
2	A	249	LEU	4.6
2	A	220	VAL	4.6
2	A	339	GLN	4.5
2	A	318	ASP	4.5
2	A	335	TYR	4.5
2	A	347	SER	4.4
2	A	293	LEU	4.2
2	A	360	GLY	4.2
2	A	286	LYS	4.2
2	A	309	VAL	4.1
2	A	513	SER	4.1
1	T	16	G	4.1
2	A	299	GLN	4.1
2	A	340	GLN	4.1
2	A	316	THR	4.1
2	A	381	LYS	4.1
2	A	302	PHE	4.0
2	A	355	PHE	4.0
2	A	257	ASN	4.0
2	A	547	PHE	4.0
2	A	338	GLY	4.0
2	A	390	ILE	4.0
2	A	224	ASP	4.0
2	A	306	GLU	3.9
2	A	370	ALA	3.9
2	A	374	VAL	3.9
2	A	336	ILE	3.9
2	A	308	LEU	3.9
2	A	353	GLY	3.8
2	A	210	VAL	3.8
2	A	264	ALA	3.8
2	A	312	GLY	3.8
2	A	295	TRP	3.8
2	A	246	HIS	3.8
2	A	234	PRO	3.7
2	A	282	ILE	3.8
2	A	303	LEU	3.7
2	A	204	ARG	3.7
2	A	300	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	358	GLU	3.7
2	A	350	ASP	3.7
2	A	343	LEU	3.6
2	A	240	ASN	3.6
2	A	357	GLU	3.6
2	A	253	GLN	3.6
2	A	363	GLU	3.6
2	A	266	ALA	3.6
2	A	274	ALA	3.6
2	A	222	ASP	3.6
2	A	277	TRP	3.5
2	A	341	TYR	3.5
2	A	385	LEU	3.5
2	A	229	ILE	3.5
2	A	861	VAL	3.5
2	A	310	ILE	3.4
2	A	321	THR	3.4
2	A	506	GLU	3.4
2	A	378	LEU	3.3
2	A	361	GLN	3.3
2	A	305	ARG	3.3
2	A	389	PHE	3.2
2	A	866	ASP	3.2
2	A	212	PHE	3.2
2	A	296	VAL	3.1
2	A	231	THR	3.1
2	A	469	GLU	3.0
2	A	367	TYR	3.0
2	A	271	VAL	3.0
2	A	261	TYR	3.0
2	A	356	THR	3.0
2	A	209	TYR	3.0
2	A	387	LEU	3.0
2	A	211	ALA	2.9
2	A	208	ILE	2.9
2	A	278	ASP	2.9
2	A	328	PRO	2.9
2	A	259	GLU	2.9
2	A	470	ASN	2.9
2	A	313	ASP	2.8
2	A	368	ASP	2.8
2	A	365	MET	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	239	SER	2.7
1	T	73	A	2.7
2	A	326	THR	2.7
2	A	273	GLU	2.7
2	A	333	ASP	2.7
2	A	236	THR	2.6
2	A	471	GLY	2.6
2	A	348	PRO	2.6
2	A	244	THR	2.6
2	A	331	GLY	2.6
2	A	377	LEU	2.6
2	A	238	PRO	2.6
2	A	349	ILE	2.6
2	A	235	TRP	2.6
2	A	258	GLY	2.6
2	A	322	GLY	2.6
2	A	301	PRO	2.5
1	T	46	G	2.5
1	T	47	U	2.5
2	A	320	GLY	2.4
2	A	260	LYS	2.4
2	A	342	GLU	2.4
2	A	45	LYS	2.4
2	A	472	GLU	2.4
2	A	272	ALA	2.4
2	A	369	LYS	2.3
2	A	237	ILE	2.3
2	A	376	ASP	2.2
2	A	325	HIS	2.2
2	A	352	LYS	2.2
2	A	665	ASP	2.2
2	A	330	HIS	2.2
2	A	371	ASN	2.2
2	A	406	PHE	2.1
2	A	375	THR	2.1
1	T	20	U	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MG	T	1202	1/1	0.17	-	54,54,54,54	0
5	MG	T	1209	1/1	0.18	-	45,45,45,45	0
5	MG	T	1206	1/1	0.24	-	37,37,37,37	0
4	ZN	A	1992	1/1	0.03	-	26,26,26,26	0
5	MG	T	1208	1/1	0.43	-	33,33,33,33	0
3	K	T	301	1/1	0.06	-	26,26,26,26	0
5	MG	T	1201	1/1	0.09	-	37,37,37,37	0
5	MG	T	1205	1/1	0.15	-	29,29,29,29	0
5	MG	T	1210	1/1	0.20	-	36,36,36,36	0
5	MG	T	1204	1/1	0.17	-	30,30,30,30	0
6	MRC	A	1993	35/35	0.21	-	14,29,54,55	0
5	MG	T	1203	1/1	0.22	-	37,37,37,37	0
5	MG	T	1207	1/1	0.11	-	37,37,37,37	0
4	ZN	A	1001	1/1	0.04	-	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.