Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 12:53 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

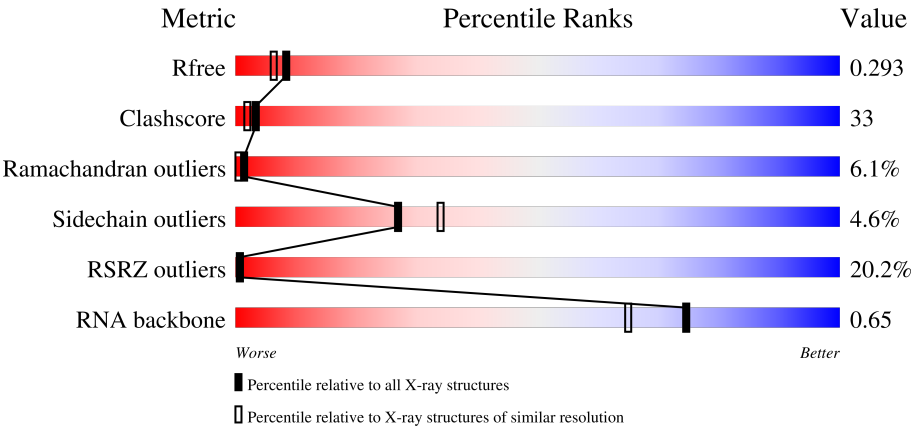
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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	T	75	12% 36% 31% 32% .
2	A	917	21% 55% 37% 7%

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	-	-	-

2 Entry composition (i)

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		

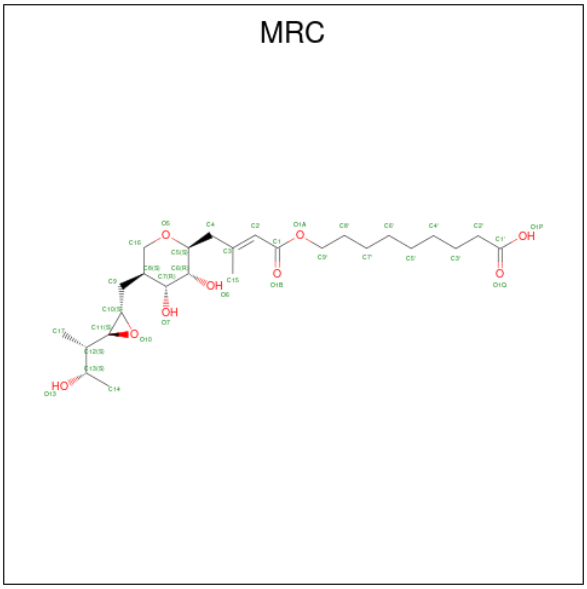
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- 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 35 26 9	0	0

- Molecule 7 is water.

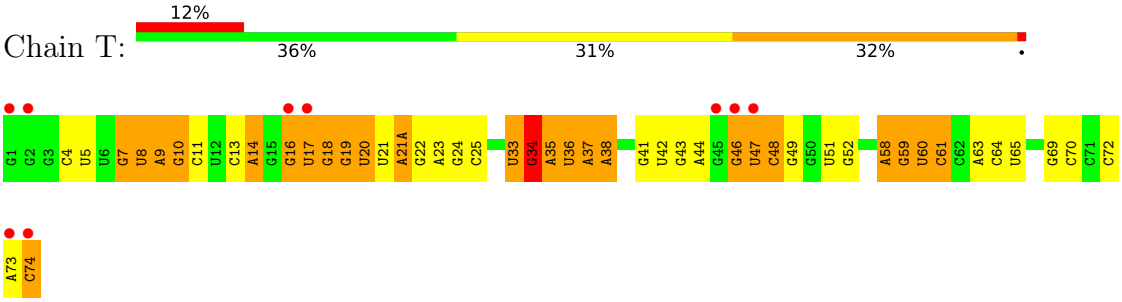
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	120	Total O 120 120	0	0
7	A	208	Total O 208 208	0	0

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.

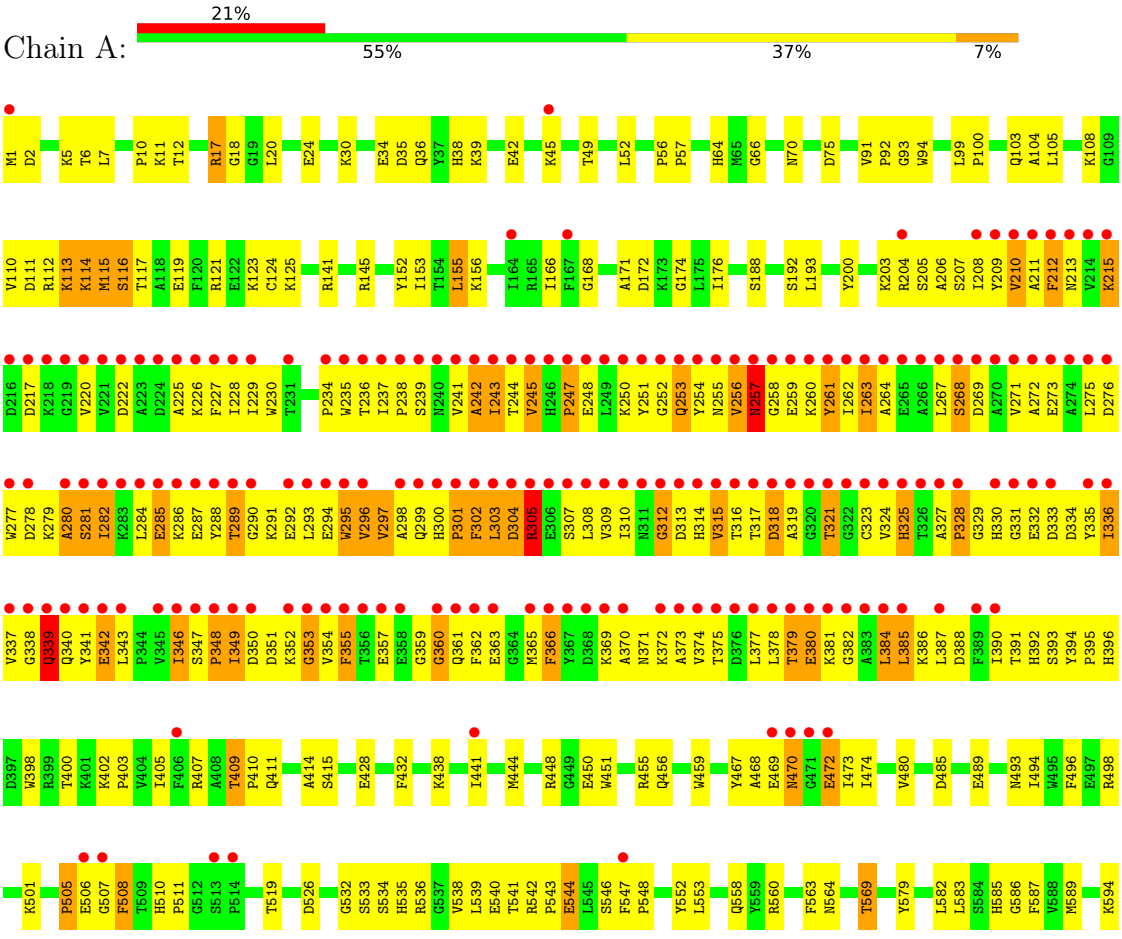
• Molecule 1: ISOLEUCYL-TRNA

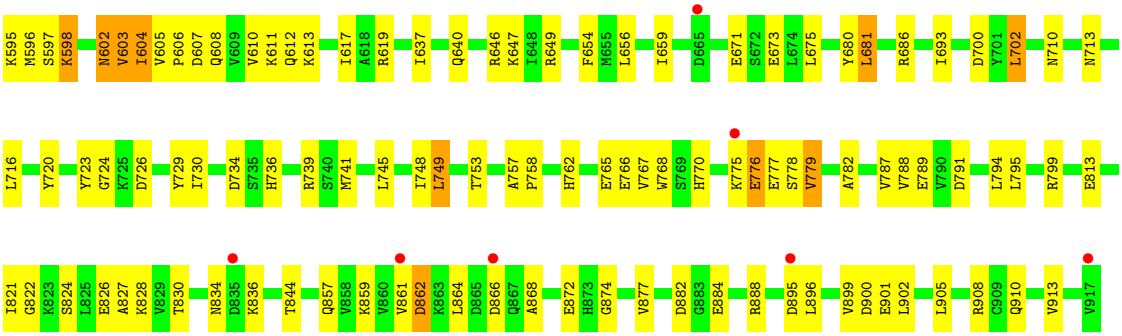
Chain T:



• Molecule 2: ISOLEUCYL-TRNA SYNTHETASE

Chain A:




K595 M596 S597 K598 N602 V603 I604 V605 P606 D607 Q608 V609 V610 K611 Q612 K613 I617 A618 R619 I637 Q640 R646 K647 I648 R649 F654 M655 L656 I659 D665 E671 S672 E673 L674 L675 Y680 L681 R686 I693 D700 Y701 L702 N710 N713
L716 Y720 Y723 G724 K725 D726 Y729 I730 D734 S735 H736 R739 S740 M741 L745 I748 L749 T753 A757 P758 H762 E765 E766 V767 W768 S769 H770 K775 E776 E777 S778 V779 A782 V787 V788 E789 V790 D791 L794 L795 R799 E813
I821 G822 K823 S824 L825 E826 A827 K828 V829 T830 N834 D835 K836 T844 Q857 V858 K859 V860 V861 D862 K863 L864 D865 D866 Q867 A868 E872 H873 G874 V877 D882 Q883 E884 R888 D895 L896 V899 D900 E901 L902 L905 R908 C909 Q910 V913 V917

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	4.21 (at 2.19Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.239 , 0.281 0.247 , 0.293	Depositor DCC
R_{free} test set	3016 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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^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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, K, 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(^{o})	Ideal(^{o})
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

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	T	10	0	0	0	0
5	A	2	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
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	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:CD	2:A:872:GLU:H	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
1:T:63:A:H2'	1:T:64:C:C6	2.23	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
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:39:LYS:HG3	7:A:2118:HOH:O	1.90	0.70
2:A:352:LYS:HB2	2:A:354:VAL:HG12	1.70	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

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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
1:T:41:G:O2'	2:A:813:GLU:HG2	1.91	0.69
2:A:254:TYR:HD2	2:A:286:LYS:HZ2	1.41	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
1:T:9:A:H3'	7:T:1236:HOH:O	1.94	0.66
2:A:210:VAL:HG12	2:A:385:LEU:HD21	1.77	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
1:T:69:G:C5'	2:A:589:MET:HE2	2.26	0.65
2:A:237:ILE:HG22	2:A:238:PRO:CD	2.27	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
1:T:33:U:H4'	1:T:34:G:O5'	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:T:69:G:H5"	2:A:589:MET:HE1	1.77	0.63
2:A:226:LYS:HB2	2:A:261:TYR:CD1	2.33	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:141:ARG:HG3	2:A:610:VAL:HG11	1.81	0.62
2:A:301:PRO:C	2:A:303:LEU:H	2.02	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:HH11	2:A:17:ARG:CB	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
1:T:43:G:O2'	1:T:44:A:H5'	1.98	0.62
2:A:213:ASN:HA	2:A:226:LYS:CG	2.30	0.62
2:A:210:VAL:CG1	2:A:385:LEU:HD11	2.26	0.61
2:A:243:ILE:HG22	2:A:244:THR:N	2.15	0.61
2:A:378:LEU:H	2:A:378:LEU:HD12	1.63	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:HG12	2:A:220:VAL:O	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
1:T:58:A:O2'	1:T:60:U:H5	1.85	0.60
2:A:243:ILE:HB	2:A:310:ILE:CG1	2.31	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:HE	2:A:305:ARG:HA	1.69	0.58
2:A:366:PHE:O	2:A:370:ALA:HB3	2.03	0.58
2:A:91:VAL:HG23	2:A:91:VAL:O	2.04	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: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:49:THR:HG22	7:A:2114:HOH:O	2.02	0.57
2:A:339:GLN:N	2:A:343:LEU:HD12	2.19	0.57
2:A:777:GLU:O	2:A:778:SER:HB3	2.04	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
1:T:51:U:O2'	1:T:52:G:H5'	2.03	0.57
2:A:236:THR:O	2:A:236:THR:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:279:LYS:O	2:A:280:ALA:HB3	2.05	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
1:T:42:U:O4’	2:A:813:GLU:HG3	2.05	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
2:A:884:GLU:HB2	2:A:896:LEU:HD12	1.88	0.56
2:A:2:ASP:HB3	2:A:5:LYS:HZ3	1.70	0.55
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:30:LYS:O	2:A:34:GLU:HG2	2.07	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: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
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: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: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
1:T:47:U:O2’	1:T:48:C:P	2.66	0.54
2:A:346:ILE:H	2:A:346:ILE:CD1	2.07	0.54
2:A:52:LEU:C	2:A:52:LEU:HD23	2.27	0.54
2:A:203:LYS:HG2	2:A:204:ARG:N	2.22	0.54
2:A:245:VAL:HG13	2:A:245:VAL:O	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:HD22	2:A:602:ASN:H	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:35:ASP:O	2:A:39:LYS:HG2	2.09	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: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
1:T:64:C:O2'	1:T:65:U:H5'	2.08	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
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
1:T:9:A:C5'	1:T:10:G:OP2	2.56	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: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
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:836:LYS:HE2	2:A:872:GLU:HA	1.92	0.52
2:A:212:PHE:CG	2:A:301:PRO:HD2	2.45	0.52
1:T:42:U:C4'	2:A:813:GLU:HG3	2.39	0.52
2:A:821:ILE:CD1	2:A:827:ALA:HB2	2.22	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: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:CD1	2:A:341:TYR:N	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:250:LYS:CD	2:A:289:THR:HG23	2.40	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:540:GLU:CG	2:A:547:PHE:HB2	2.41	0.51
1:T:16:G:H5'	1:T:17:U:OP2	2.10	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
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:56:PRO:HD3	2:A:152:TYR:OH	2.11	0.51
2:A:365:MET:HG3	2:A:370:ALA:HB2	1.93	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
1:T:34:G:C2	2:A:7:LEU:HD21	2.46	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
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
1:T:19:G:O2'	1:T:20:U:OP1	2.24	0.49
2:A:327:ALA:O	2:A:329:GLY:N	2.45	0.49
2:A:200:TYR:CE2	2:A:395:PRO:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1:MET:HB2	2:A:901:GLU:HG3	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: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:HD22	2:A:493:ASN:N	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
1:T:9:A:OP2	7:T:1329:HOH:O	2.20	0.48
1:T:13:C:H4'	2:A:702:LEU:HD21	1.94	0.48
2:A:309:VAL:CG1	2:A:310:ILE:N	2.77	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
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
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: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:35:A:C2	2:A:654:PHE:HB2	2.48	0.47
2:A:17:ARG:NH1	2:A:17:ARG:HB3	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
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
1:T:19:G:H4'	1:T:20:U:OP2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:58:A:H1'	1:T:60:U:C5	2.50	0.47
2:A:49:THR:HG23	7:A:2012:HOH:O	2.15	0.47
2:A:371:ASN:HA	2:A:375:THR:CG2	2.40	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
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
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: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
2:A:39:LYS:HA	2:A:42:GLU:HG2	1.96	0.47
2:A:247:PRO:O	2:A:248:GLU:HB3	2.15	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
1:T:37:A:O2'	1:T:38:A:OP2	2.26	0.46
2:A:99:LEU:O	2:A:103:GLN:HG3	2.15	0.46
2:A:329:GLY:N	2:A:346:ILE:HD11	2.31	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:35:ASP:OD2	2:A:38:HIS:HB2	2.15	0.46
2:A:256:VAL:HG12	2:A:257:ASN:H	1.81	0.46
2:A:686:ARG:HD3	2:A:788:VAL:CG2	2.45	0.46
1:T:58:A:H4'	1:T:59:G:OP1	2.15	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: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
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

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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
1:T:60:U:O2'	1:T:61:C:OP1	2.30	0.46
2:A:250:LYS:HB3	2:A:290:GLY:H	1.80	0.46
2:A:284:LEU:HD12	2:A:285:GLU:N	2.31	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
2:A:141:ARG:CG	2:A:610:VAL:HG11	2.46	0.45
2:A:237:ILE:N	2:A:238:PRO:CD	2.79	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
1:T:4:C:O2'	1:T:5:U:H5'	2.16	0.45
2:A:734:ASP:HA	2:A:739:ARG:NE	2.31	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:75:ASP:OD2	2:A:619:ARG:NH2	2.36	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:724:GLY:HA3	2:A:741:MET:CE	2.47	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:HD12	2:A:262:ILE:N	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:HD12	2:A:659:ILE:C	2.37	0.44
1:T:8:U:H6	1:T:8:U:O5'	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:243:ILE:HB	2:A:310:ILE:HD11	1.98	0.44
2:A:200:TYR:HB3	2:A:393:SER:OG	2.18	0.43
2:A:276:ASP:HB3	2:A:386:LYS:NZ	2.33	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:371:ASN:O	2:A:373:ALA:N	2.51	0.43
1:T:37:A:O2'	1:T:38:A:P	2.77	0.43
2:A:168:GLY:HA3	2:A:480:VAL:HG11	2.00	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:17:ARG:CB	2:A:17:ARG:NH1	2.80	0.43
2:A:284:LEU:HD12	2:A:284:LEU:C	2.38	0.43
2:A:560:ARG:O	2:A:560:ARG:HG3	2.18	0.43
2:A:17:ARG:HH11	2:A:17:ARG:HB2	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:O	2:A:287:GLU:HG3	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: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
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:56:PRO:HA	2:A:57:PRO:HD2	2.00	0.42
2:A:264:ALA:HB3	2:A:267:LEU:CB	2.36	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:64:HIS:CD2	2:A:66:GLY:H	2.33	0.41
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:H	2:A:342:GLU:CD	2.24	0.41
1:T:24:G:H2'	1:T:25:C:O4'	2.20	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
2:A:2:ASP:HB3	2:A:5:LYS:HZ2	1.85	0.41
2:A:99:LEU:HB3	2:A:100:PRO:HD3	2.01	0.41
2:A:868:ALA:HB2	2:A:877:VAL:HG22	2.01	0.41
1:T:21(A):A:N6	1:T:46:G:H2'	2.35	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
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:HD22	2:A:602:ASN:N	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
1:T:63:A:H2'	1:T:64:C:H6	1.77	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
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:188:SER:HB3	2:A:400:THR:HG21	2.01	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: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: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: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
1:T:58:A:O2'	1:T:60:U:C5	2.70	0.40
2:A:247:PRO:CD	2:A:313:ASP:H	2.35	0.40
2:A:872:GLU:CD	2:A:872:GLU:N	2.65	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
1:T:11:C:O2	2:A:640:GLN:NE2	2.55	0.40
2:A:250:LYS:HE3	2:A:289:THR:HG23	2.03	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	A	915/917 (100%)	763 (83%)	96 (10%)	56 (6%)	1 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 (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	A	806/806 (100%)	769 (95%)	37 (5%)	27 34

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

Sometimes 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 (i)

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

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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

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 (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)

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	-	35,36,36	2.29	10 (28%)	40,48,48	2.05	7 (17%)

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	-	3/3/11/12	13/32/54/54	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1993	MRC	C11-C10	-6.82	1.36	1.46
6	A	1993	MRC	C8-C7	5.78	1.60	1.53
6	A	1993	MRC	C9-C8	4.02	1.61	1.53
6	A	1993	MRC	C16-C8	3.38	1.56	1.51
6	A	1993	MRC	O1A-C1	3.35	1.42	1.34
6	A	1993	MRC	C2-C1	-3.17	1.39	1.46
6	A	1993	MRC	C2-C3	3.02	1.39	1.33
6	A	1993	MRC	C9-C10	2.53	1.57	1.52
6	A	1993	MRC	C6-C5	2.01	1.57	1.53
6	A	1993	MRC	O1P-C1'	-2.01	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1993	MRC	C9-C8-C7	5.54	121.20	113.32
6	A	1993	MRC	C11-C12-C13	5.08	121.96	111.11
6	A	1993	MRC	C11-O10-C10	-4.91	57.46	60.59
6	A	1993	MRC	O1A-C1-C2	4.37	119.58	110.60
6	A	1993	MRC	C17-C12-C11	3.96	118.50	111.40
6	A	1993	MRC	C9'-O1A-C1	-3.55	110.30	116.58
6	A	1993	MRC	O1A-C1-O1B	-2.34	117.78	122.93

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1993	MRC	C6
6	A	1993	MRC	C7
6	A	1993	MRC	C12

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1993	MRC	C2-C1-O1A-C9'
6	A	1993	MRC	O10-C11-C12-C13
6	A	1993	MRC	C11-C12-C13-C14
6	A	1993	MRC	C11-C12-C13-O13
6	A	1993	MRC	O1B-C1-O1A-C9'
6	A	1993	MRC	C5'-C6'-C7'-C8'
6	A	1993	MRC	C6'-C7'-C8'-C9'
6	A	1993	MRC	C1'-C2'-C3'-C4'
6	A	1993	MRC	C4'-C5'-C6'-C7'
6	A	1993	MRC	C2'-C3'-C4'-C5'
6	A	1993	MRC	O1P-C1'-C2'-C3'
6	A	1993	MRC	O1Q-C1'-C2'-C3'
6	A	1993	MRC	C11-C10-C9-C8

There are no ring outliers.

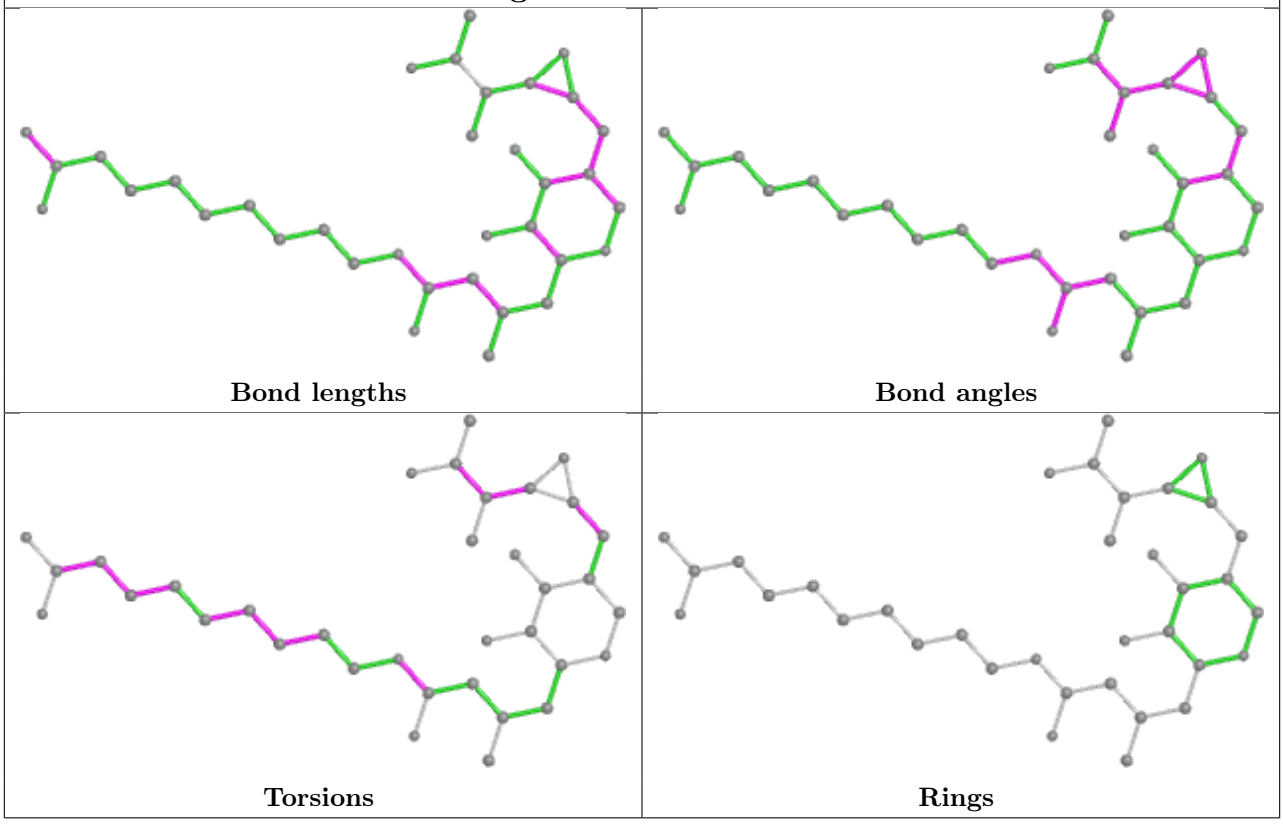
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1993	MRC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MRC A 1993



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^{th} 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%)	0.45	9 (12%) 4 3	18, 32, 72, 99	2 (2%)
2	A	917/917 (100%)	1.04	191 (20%) 1 1	10, 29, 99, 100	0
All	All	992/992 (100%)	0.99	200 (20%) 1 1	10, 30, 99, 100	2 (0%)

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	288	TYR	16.6
2	A	219	GLY	16.2
2	A	289	THR	15.8
2	A	315	VAL	13.3
2	A	280	ALA	13.1
2	A	214	VAL	12.6
2	A	337	VAL	12.1
2	A	241	VAL	11.0
2	A	254	TYR	10.8
2	A	225	ALA	10.5
2	A	262	ILE	10.0
2	A	283	LYS	9.9
1	T	74	C	9.2
2	A	290	GLY	9.1
2	A	324	VAL	9.0
2	A	267	LEU	9.0
2	A	317	THR	8.8
2	A	383	ALA	8.4
2	A	284	LEU	8.3
2	A	245	VAL	8.3
2	A	298	ALA	8.2
2	A	314	HIS	8.1
2	A	268	SER	7.8
2	A	345	VAL	7.6

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Mol	Chain	Res	Type	RSRZ
2	A	379	THR	7.5
2	A	248	GLU	7.4
2	A	215	LYS	7.4
2	A	917	VAL	7.3
2	A	366	PHE	7.2
2	A	221	VAL	7.1
2	A	242	ALA	6.9
2	A	270	ALA	6.9
2	A	227	PHE	6.5
2	A	223	ALA	6.5
2	A	281	SER	6.5
2	A	276	ASP	6.4
2	A	319	ALA	6.4
2	A	269	ASP	6.3
2	A	307	SER	6.3
2	A	285	GLU	6.1
2	A	228	ILE	6.1
2	A	282	ILE	6.0
2	A	213	ASN	5.8
2	A	286	LYS	5.8
2	A	302	PHE	5.8
2	A	217	ASP	5.7
2	A	292	GLU	5.6
2	A	293	LEU	5.6
2	A	220	VAL	5.6
2	A	304	ASP	5.6
2	A	222	ASP	5.6
2	A	252	GLY	5.5
2	A	339	GLN	5.5
2	A	327	ALA	5.5
2	A	311	ASN	5.4
2	A	263	ILE	5.3
2	A	513	SER	5.3
2	A	251	TYR	5.3
2	A	318	ASP	5.2
2	A	303	LEU	5.2
2	A	247	PRO	5.2
2	A	249	LEU	5.1
2	A	323	CYS	5.1
2	A	372	LYS	5.1
2	A	384	LEU	5.0
2	A	250	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
2	A	210	VAL	4.9
2	A	373	ALA	4.9
2	A	347	SER	4.9
2	A	340	GLN	4.8
2	A	335	TYR	4.8
2	A	265	GLU	4.8
2	A	216	ASP	4.7
2	A	226	LYS	4.7
2	A	211	ALA	4.7
2	A	1	MET	4.7
2	A	346	ILE	4.7
1	T	17	U	4.6
2	A	309	VAL	4.6
2	A	357	GLU	4.6
2	A	255	ASN	4.5
2	A	274	ALA	4.5
2	A	374	VAL	4.5
2	A	243	ILE	4.4
2	A	275	LEU	4.4
2	A	361	GLN	4.3
2	A	218	LYS	4.2
2	A	354	VAL	4.2
2	A	299	GLN	4.2
2	A	336	ILE	4.2
2	A	257	ASN	4.1
2	A	866	ASP	4.1
2	A	208	ILE	4.1
2	A	358	GLU	4.1
2	A	321	THR	4.1
2	A	355	PHE	4.1
2	A	506	GLU	4.0
2	A	328	PRO	4.0
2	A	387	LEU	3.9
2	A	547	PHE	3.9
2	A	224	ASP	3.9
2	A	350	ASP	3.9
2	A	338	GLY	3.9
2	A	363	GLU	3.9
2	A	305	ARG	3.9
2	A	306	GLU	3.8
2	A	246	HIS	3.8
2	A	390	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	A	295	TRP	3.8
2	A	370	ALA	3.8
2	A	234	PRO	3.8
2	A	360	GLY	3.8
1	T	16	G	3.7
2	A	382	GLY	3.7
2	A	229	ILE	3.7
2	A	343	LEU	3.6
2	A	861	VAL	3.6
2	A	240	ASN	3.6
2	A	271	VAL	3.5
2	A	308	LEU	3.5
2	A	356	THR	3.5
2	A	266	ALA	3.5
2	A	333	ASP	3.5
2	A	261	TYR	3.4
2	A	341	TYR	3.4
2	A	353	GLY	3.4
2	A	204	ARG	3.4
2	A	326	THR	3.4
2	A	300	HIS	3.4
2	A	313	ASP	3.3
2	A	367	TYR	3.3
2	A	256	VAL	3.3
2	A	259	GLU	3.3
2	A	389	PHE	3.3
2	A	244	THR	3.3
2	A	381	LYS	3.3
2	A	369	LYS	3.2
2	A	253	GLN	3.2
2	A	469	GLU	3.2
2	A	368	ASP	3.1
2	A	209	TYR	3.1
2	A	231	THR	3.1
1	T	47	U	3.1
2	A	385	LEU	3.0
2	A	365	MET	3.0
2	A	349	ILE	3.0
2	A	301	PRO	3.0
2	A	235	TRP	3.0
2	A	316	THR	3.0
2	A	322	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	212	PHE	2.9
2	A	294	GLU	2.9
2	A	470	ASN	2.9
2	A	310	ILE	2.9
2	A	278	ASP	2.9
2	A	296	VAL	2.9
2	A	352	LYS	2.8
2	A	273	GLU	2.8
2	A	665	ASP	2.8
2	A	348	PRO	2.8
2	A	471	GLY	2.8
2	A	342	GLU	2.7
2	A	287	GLU	2.7
2	A	277	TRP	2.6
2	A	378	LEU	2.6
1	T	73	A	2.6
2	A	835	ASP	2.6
2	A	377	LEU	2.6
1	T	1	G	2.6
2	A	380	GLU	2.6
2	A	331	GLY	2.6
2	A	312	GLY	2.6
2	A	264	ALA	2.5
2	A	239	SER	2.5
2	A	332	GLU	2.5
2	A	45	LYS	2.5
1	T	46	G	2.5
2	A	238	PRO	2.4
2	A	375	THR	2.4
2	A	507	GLY	2.4
2	A	272	ALA	2.4
2	A	236	THR	2.4
2	A	472	GLU	2.4
2	A	325	HIS	2.3
2	A	260	LYS	2.3
2	A	167	PHE	2.3
2	A	258	GLY	2.3
2	A	406	PHE	2.3
2	A	775	LYS	2.3
1	T	45	G	2.2
2	A	362	PHE	2.2
2	A	164	ILE	2.2

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

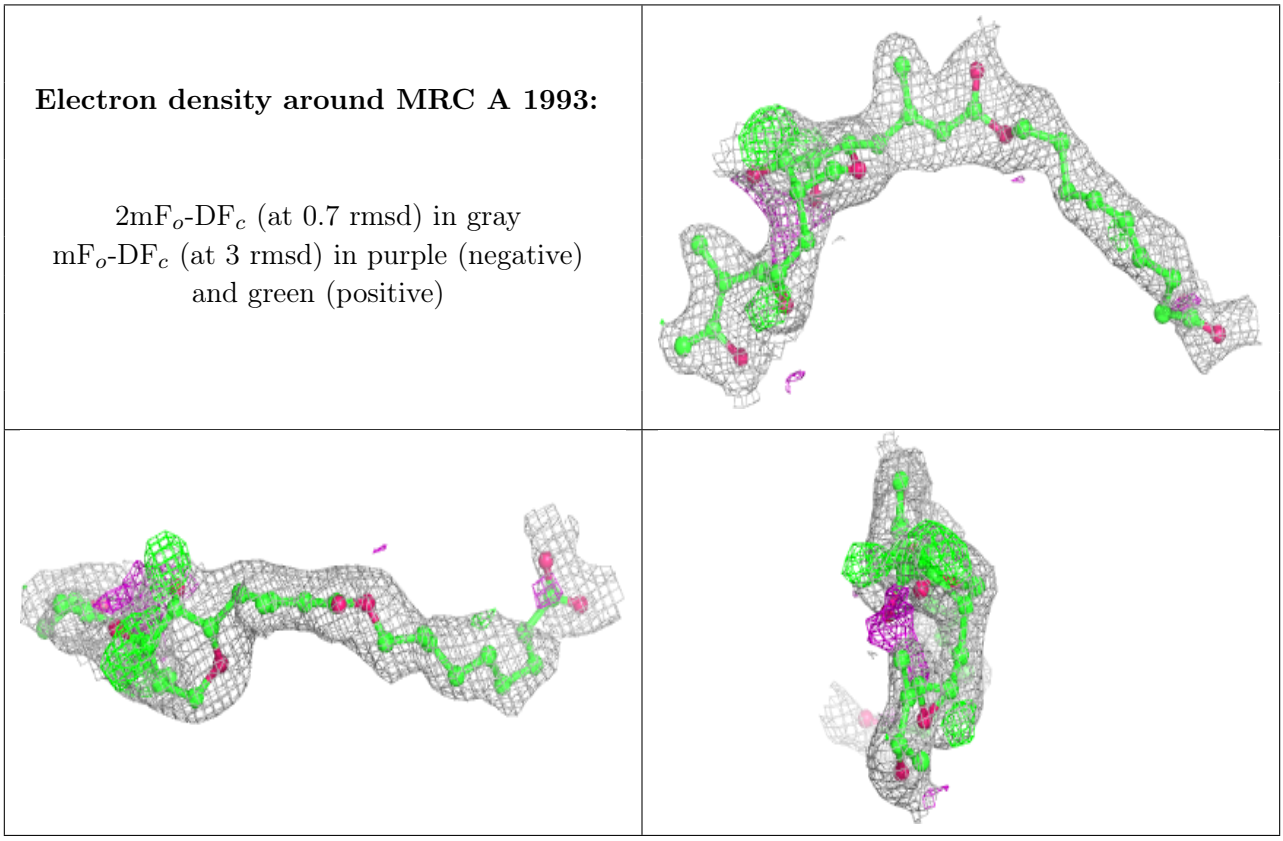
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	MG	T	1202	1/1	0.57	0.18	54,54,54,54	0
4	MG	T	1206	1/1	0.64	0.29	37,37,37,37	0
4	MG	T	1205	1/1	0.71	0.17	29,29,29,29	0
4	MG	T	1203	1/1	0.80	0.21	37,37,37,37	0
6	MRC	A	1993	35/35	0.81	0.21	14,29,54,55	0
4	MG	T	1210	1/1	0.83	0.17	36,36,36,36	0
4	MG	T	1201	1/1	0.86	0.07	37,37,37,37	0
4	MG	T	1204	1/1	0.87	0.16	30,30,30,30	0
4	MG	T	1209	1/1	0.88	0.19	45,45,45,45	0
4	MG	T	1208	1/1	0.93	0.43	33,33,33,33	0
4	MG	T	1207	1/1	0.96	0.14	37,37,37,37	0
3	K	T	301	1/1	0.97	0.05	26,26,26,26	0
5	ZN	A	1992	1/1	0.99	0.04	26,26,26,26	0
5	ZN	A	1001	1/1	0.99	0.04	26,26,26,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MRC A 1993:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.