



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:37 AM UTC

PDB ID : 1QU2 / pdb_00001qu2
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

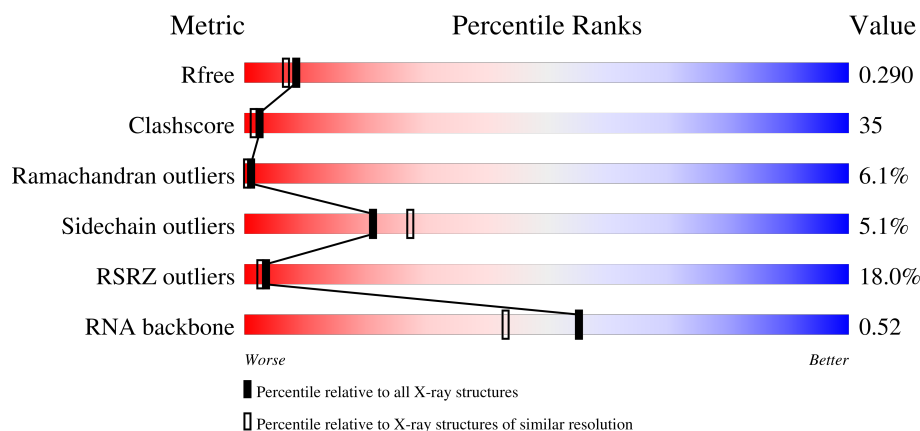
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	75	7% 36% 29% 24% 11%
2	A	917	19% 52% 38% 9%

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

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 (CCD ID: K) (formula: K).

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

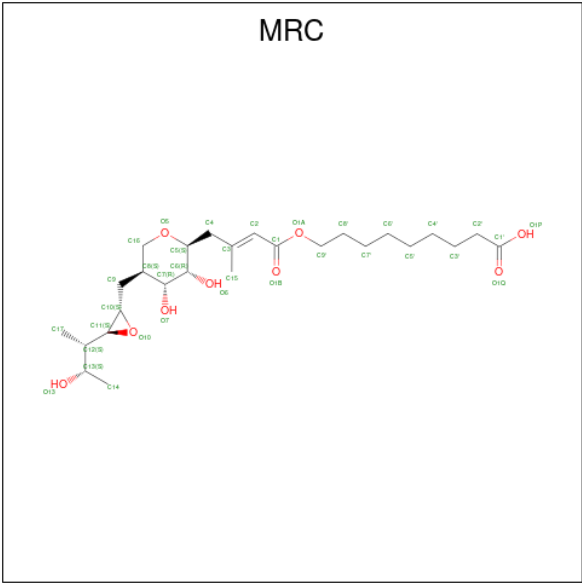
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is MUPIROCIN (CCD ID: MRC) (formula: C₂₆H₄₄O₉).



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

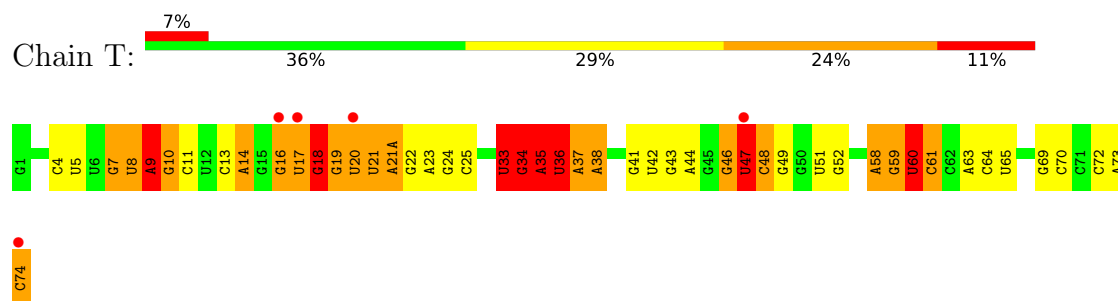
- Molecule 7 is water.

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

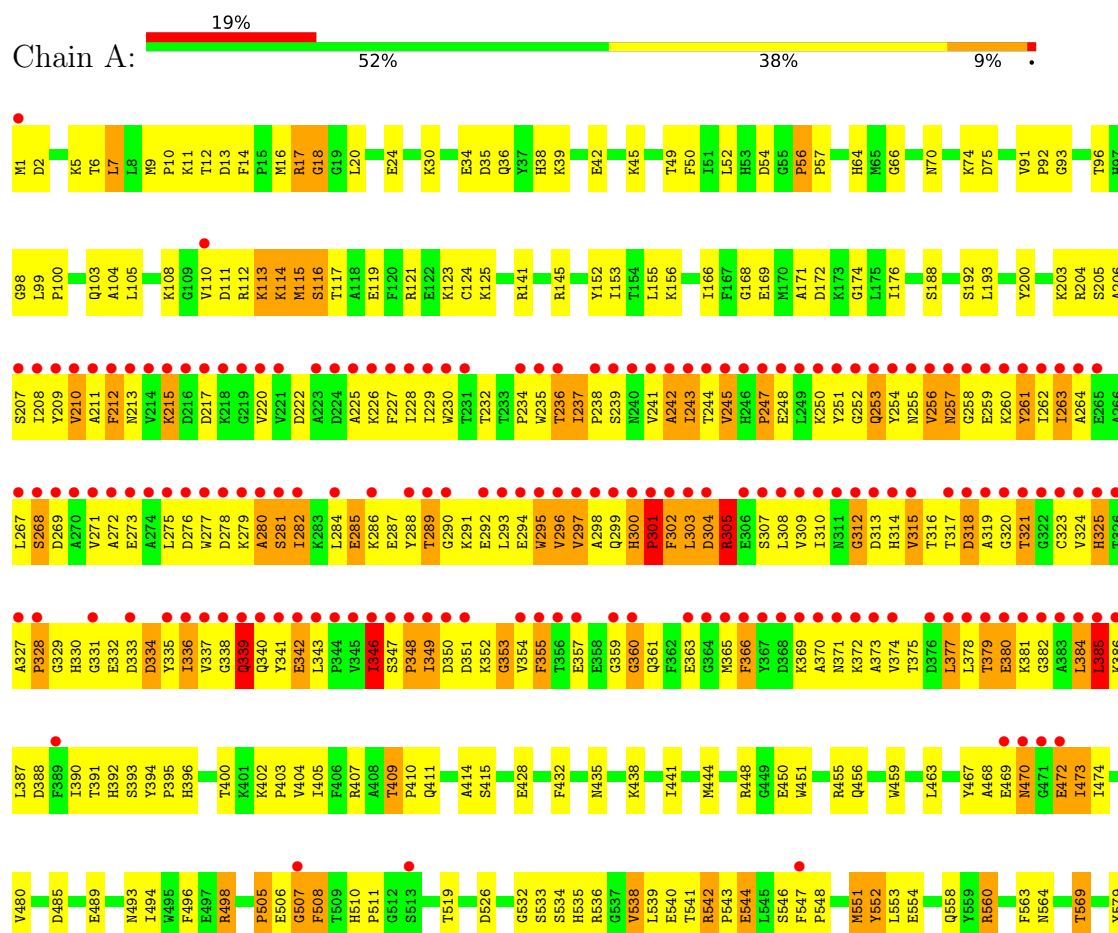
3 Residue-property plots

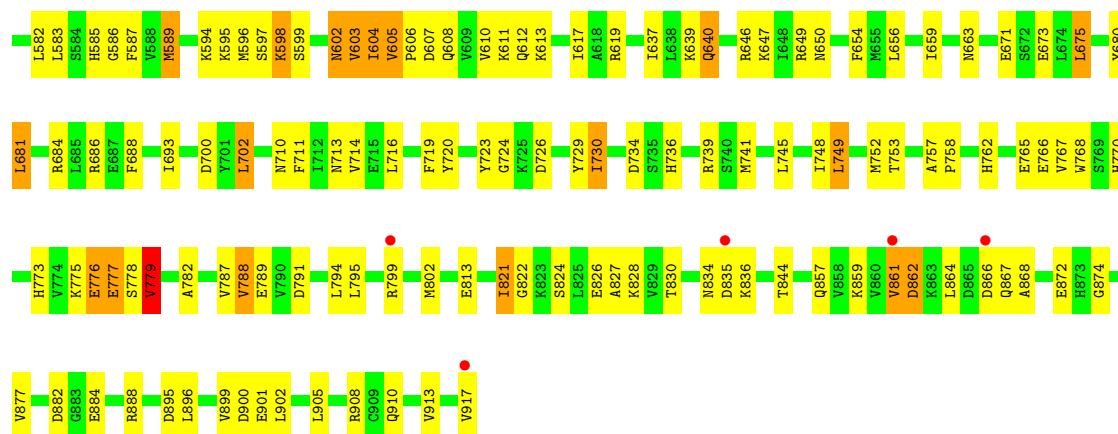
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ISOLEUCYL-TRNA



• Molecule 2: ISOLEUCYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.00Å 100.00Å 186.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	75.7 (10.00-2.20) 84.5 (10.00-2.20)	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 0.245 , 0.290	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)	0.41 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, MG, 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	0.36	0/1792	0.85	11/2794 (0.4%)
2	A	0.43	1/7586 (0.0%)	0.97	38/10282 (0.4%)
All	All	0.42	1/9378 (0.0%)	0.95	49/13076 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	589	MET	SD-CE	-6.26	1.64	1.79

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	861	VAL	N-CA-C	13.03	123.02	111.81
1	T	7	G	C2'-C3'-O3'	-10.90	93.15	109.50
2	A	730	ILE	N-CA-C	10.09	120.49	111.81
1	T	9	A	C2'-C3'-O3'	-8.52	100.93	113.70
2	A	98	GLY	N-CA-C	8.14	119.68	111.95
2	A	56	PRO	N-CA-C	7.49	119.83	110.70
2	A	714	VAL	N-CA-C	7.13	117.23	110.74
2	A	599	SER	N-CA-C	-6.96	104.05	112.54
2	A	473	ILE	N-CA-C	6.93	123.75	109.34
2	A	300	HIS	CA-C-N	6.87	128.43	119.84
2	A	300	HIS	C-N-CA	6.87	128.43	119.84
2	A	867	GLN	N-CA-C	-6.73	104.23	113.18
2	A	675	LEU	N-CA-C	-6.47	101.38	110.50
2	A	14	PHE	CA-C-N	6.36	126.28	119.85
2	A	14	PHE	C-N-CA	6.36	126.28	119.85
2	A	377	LEU	N-CA-C	-6.31	104.03	111.03
2	A	560	ARG	N-CA-C	-6.28	105.77	113.50
2	A	777	GLU	N-CA-C	-6.26	99.06	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	684	ARG	N-CA-C	-6.23	104.60	111.82
1	T	36	U	C2'-C3'-O3'	-6.21	100.18	109.50
2	A	346	ILE	N-CA-C	6.20	118.91	109.12
2	A	435	ASN	N-CA-C	6.15	118.78	111.71
1	T	34	G	C2'-C3'-O3'	-6.11	100.34	109.50
1	T	47	U	C2'-C3'-O3'	6.11	118.66	109.50
2	A	542	ARG	CA-C-N	6.10	125.58	119.24
2	A	542	ARG	C-N-CA	6.10	125.58	119.24
1	T	33	U	C2'-C3'-O3'	-5.83	100.76	109.50
2	A	96	THR	N-CA-C	5.79	122.30	113.61
2	A	835	ASP	N-CA-C	-5.76	105.14	111.82
1	T	60	U	C2'-C3'-O3'	5.75	118.13	109.50
2	A	236	THR	N-CA-C	-5.66	106.97	112.97
2	A	779	VAL	CB-CA-C	-5.65	104.64	112.04
2	A	639	LYS	N-CA-C	-5.60	105.17	111.28
2	A	463	LEU	N-CA-C	-5.59	101.15	109.42
2	A	663	ASN	CA-C-N	5.56	125.66	119.32
2	A	663	ASN	C-N-CA	5.56	125.66	119.32
1	T	35	A	C2'-C3'-O3'	5.49	117.73	109.50
2	A	232	THR	N-CA-C	-5.47	106.45	113.02
2	A	552	TYR	N-CA-C	-5.43	100.54	109.40
2	A	773	HIS	N-CA-C	5.42	121.96	113.72
2	A	18	GLY	N-CA-C	5.40	118.77	112.50
1	T	21	U	C2'-C3'-O3'	-5.31	105.73	113.70
2	A	13	ASP	N-CA-C	-5.28	106.52	113.17
1	T	18	G	N9-C1'-C2'	5.27	119.90	112.00
2	A	385	LEU	N-CA-C	5.16	117.13	109.69
2	A	334	ASP	N-CA-C	-5.12	106.86	113.01
2	A	498	ARG	N-CA-C	5.11	118.34	110.42
1	T	7	G	N9-C1'-C2'	5.09	121.64	114.00
2	A	551	MET	N-CA-C	5.03	116.17	108.42

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	64	0
2	A	7407	0	7214	541	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	5	0
7	A	208	0	0	20	0
7	T	120	0	0	4	0
All	All	9386	0	8065	589	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 35.

All (589) 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
1:T:69:G:H5''	2:A:589:MET:HE2	1.45	0.95
2:A:716:LEU:HD11	2:A:748:ILE:HD11	1.49	0.94
2:A:211:ALA:HA	2:A:228:ILE:HA	1.47	0.94
2:A:380:GLU:HB3	2:A:385:LEU:H	1.29	0.94
2:A:336:ILE:HG13	2:A:337:VAL:H	1.30	0.93
2:A:239:SER:HB3	2:A:346:ILE:HG13	1.51	0.93
2:A:208:ILE:HG22	2:A:387:LEU:HA	1.50	0.92
2:A:213:ASN:HD22	2:A:215:LYS:HG3	1.34	0.92
1:T:73:A:H2'	1:T:74:C:H5'	1.50	0.90
2:A:264:ALA:HB3	2:A:267:LEU:HB2	1.50	0.90
1:T:69:G:H5''	2:A:589:MET:CE	2.02	0.89
1:T:13:C:H2'	1:T:14:A:H5''	1.56	0.88
2:A:534:SER:O	2:A:538:VAL:HG13	1.73	0.88
2:A:252:GLY:HA2	2:A:262:ILE:HG23	1.56	0.87
2:A:857:GLN:NE2	2:A:882:ASP:H	1.72	0.86
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:834:ASN:HB2	2:A:874:GLY:HA2	1.58	0.84
2:A:589:MET:HE3	2:A:594:LYS:C	2.03	0.84
2:A:857:GLN:HE22	2:A:882:ASP:H	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:872:GLU:CD	2:A:872:GLU:H	1.88	0.80
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:724:GLY:HA3	2:A:741:MET:HE1	1.64	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: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:444:MET:HE3	2:A:444:MET:O	1.87	0.75
2:A:209:TYR:C	2:A:385:LEU:HD13	2.12	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
1:T:69:G:C5'	2:A:589:MET:HE2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:58:A:H2'	1:T:60:U:OP2	1.90	0.72
2:A:711:PHE:CD2	2:A:752:MET:HE1	2.24	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
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: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:261:TYR:C	2:A:262:ILE:HD12	2.18	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:301:PRO:C	2:A:303:LEU:H	2.02	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:711:PHE:CE2	2:A:752:MET:HE1	2.30	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:260:LYS:HD2	2:A:286:LYS:HZ1	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:50:PHE:HZ	2:A:551:MET:HE3	1.61	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:688:PHE:CE2	2:A:752:MET:HE2	2.31	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
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
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:222:ASP:HB3	2:A:288:TYR:CD1	2.33	0.63
2:A:370:ALA:C	2:A:371:ASN:HD22	2.05	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
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: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:275:LEU:C	2:A:386:LYS:HE3	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:338:GLY:C	2:A:343:LEU:HD12	2.26	0.59
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:254:TYR:HD2	2:A:286:LYS:HZ2	1.50	0.59
2:A:52:LEU:C	2:A:52:LEU:HD23	2.27	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:2:ASP:HB3	2:A:5:LYS:HZ2	1.66	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:834:ASN:HD22	2:A:874:GLY:C	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:MET:HE3	2:A:901:GLU:HB3	1.87	0.57
2:A:766:GLU:O	2:A:770:HIS:HD2	1.86	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
2:A:236:THR:O	2:A:236:THR:HG22	2.04	0.56
2:A:209:TYR:CE2	2:A:321:THR:HG21	2.37	0.56
2:A:369:LYS:C	2:A:371:ASN:H	2.13	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:352:LYS:C	2:A:354:VAL:H	2.14	0.56
2:A:357:GLU:C	2:A:359:GLY:H	2.14	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:279:LYS:O	2:A:280:ALA:HB3	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:T:69:G:H5''	2:A:589:MET:HE1	1.87	0.54
1:T:58:A:O2'	1:T:59:G:O5'	2.21	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: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: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:276:ASP:HB3	2:A:386:LYS:HZ1	1.73	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:379:THR:HG23	2:A:380:GLU:CD	2.33	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:203:LYS:HG2	2:A:204:ARG:N	2.22	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:254:TYR:HD2	2:A:286:LYS:NZ	2.07	0.53
2:A:261:TYR:OH	2:A:384:LEU:HD12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:A:O2'	1:T:38:A:OP2	2.26	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
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:716:LEU:HD21	2:A:748:ILE:CD1	2.40	0.51
2:A:16:MET:HE2	2:A:650:ASN:ND2	2.26	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: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:352:LYS:HE3	2:A:354:VAL:CG1	2.41	0.51
2:A:872:GLU:CD	2:A:872:GLU:N	2.65	0.51
2:A:884:GLU:HB2	2:A:896:LEU:CD1	2.41	0.51
2:A:16:MET:HE2	2:A:650:ASN:HD21	1.75	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:375:THR:C	2:A:377:LEU:H	2.19	0.51
2:A:604:ILE:HA	7:A:2131:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:734:ASP:HA	2:A:739:ARG:HE	1.76	0.50
2:A:242:ALA:C	2:A:243:ILE:HD12	2.37	0.50
2:A:248:GLU:H	2:A:291:LYS:HB2	1.77	0.50
2:A:350:ASP:C	2:A:352:LYS:H	2.19	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: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:719:PHE:CZ	2:A:802:MET:HE1	2.46	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
2:A:296:VAL:O	2:A:297:VAL:C	2.55	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:243:ILE:HD12	2:A:243:ILE:N	2.27	0.49
2:A:659:ILE:HD12	2:A:659:ILE:C	2.37	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:54:ASP:OD2	2:A:74:LYS:NZ	2.46	0.48
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:365:MET:HE2	2:A:370:ALA:CB	2.43	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:C	2:A:303:LEU:N	2.71	0.48
2:A:301:PRO:HA	2:A:304:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:589:MET:CE	2:A:594:LYS:C	2.82	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:284:LEU:HD12	2:A:284:LEU:C	2.38	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:290:GLY:O	2:A:291:LYS:C	2.57	0.47
2:A:318:ASP:CG	2:A:319:ALA:H	2.21	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: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
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:235:TRP:H	2:A:235:TRP:CD1	2.33	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
1:T:34:G:O2'	2:A:9:MET:HE1	2.15	0.47
2:A:39:LYS:HA	2:A:42:GLU:HG2	1.96	0.47
2:A:111:ASP:O	2:A:115:MET:HE3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:247:PRO:O	2:A:248:GLU:HB3	2.15	0.47
2:A:275:LEU:C	2:A:277:TRP:H	2.23	0.47
2:A:1:MET:HB3	2:A:902:LEU:HD23	1.97	0.47
2:A:302:PHE:CD1	2:A:302:PHE:C	2.93	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:380:GLU:C	2:A:382:GLY:H	2.22	0.47
2:A:296:VAL:O	2:A:296:VAL:HG12	2.14	0.46
2:A:298:ALA:N	2:A:307:SER:HB3	2.30	0.46
2:A:506:GLU:O	2:A:506:GLU:HG3	2.14	0.46
2:A: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:370:ALA:C	2:A:374:VAL:HB	2.40	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:342:GLU:H	2:A:342:GLU:CD	2.24	0.46
2:A:380:GLU:HB3	2:A:385:LEU:HB2	1.97	0.46
2:A:538:VAL:HG22	2:A:539:LEU:N	2.29	0.46
2:A:554:GLU:OE1	6:A:1993:MRC:O7	2.28	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:281:SER:O	2:A:282:ILE:C	2.59	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
2:A:267:LEU:O	2:A:268:SER:C	2.59	0.46
2:A:327:ALA:C	2:A:329:GLY:H	2.23	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:589:MET:HE1	2:A:595:LYS:N	2.31	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:248:GLU:N	2:A:291:LYS:HB2	2.32	0.45
2:A:237:ILE:C	2:A:239:SER:H	2.25	0.45
2:A:280:ALA:O	2:A:282:ILE:N	2.50	0.45
2:A:432:PHE:CE2	2:A:582:LEU:HD23	2.51	0.45
2:A:172:ASP:C	2:A:174:GLY:H	2.24	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:444:MET:HE3	2:A:444:MET:C	2.40	0.45
1:T:4:C:O2'	1:T:5:U:H5'	2.16	0.45
2:A:365:MET:CE	2:A:374:VAL:HG21	2.47	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:791:ASP:C	2:A:791:ASP:OD1	2.59	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:369:LYS:C	2:A:371:ASN:N	2.74	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:350:ASP:CG	2:A:351:ASP:H	2.25	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
1:T:58:A:HO2'	1:T:59:G:P	2.41	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
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:350:ASP:C	2:A:352:LYS:N	2.72	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:280:ALA:O	2:A:281:SER:C	2.61	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:255:ASN:C	2:A:260:LYS:HG2	2.42	0.43
2:A:269:ASP:O	2:A:273:GLU:HB2	2.17	0.43
2:A:352:LYS:C	2:A:354:VAL:N	2.75	0.43
2:A:371:ASN:O	2:A:373:ALA:N	2.51	0.43
2:A:375:THR:C	2:A:377:LEU:N	2.75	0.43
1:T:37:A:O2'	1:T:38:A:P	2.77	0.43
2:A:152:TYR:C	2:A:153:ILE:HG13	2.43	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:560:ARG:O	2:A:560:ARG:HG3	2.18	0.43
2:A:596:MET:HE2	6:A:1993:MRC:H8'2	2.00	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:257:ASN:CG	2:A:258:GLY:H	2.26	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:506:GLU:O	2:A:507:GLY:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:241:VAL:HG11	2:A:328:PRO:HD2	2.01	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
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: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:254:TYR:HB3	2:A:286:LYS:HZ2	1.85	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:169:GLU:CD	2:A:536:ARG:HH22	2.27	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: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
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:99:LEU:HB3	2:A:100:PRO:HD3	2.01	0.41
2:A:357:GLU:C	2:A:359:GLY:N	2.79	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:365:MET:HE1	2:A:374:VAL:HG21	2.01	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
2:A:602:ASN:HD22	2:A:602:ASN:C	2.29	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: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: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:237:ILE:HA	2:A:237:ILE:HD12	1.94	0.40
2:A:745:LEU:C	2:A:748:ILE:HG22	2.46	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: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:293:LEU:C	2:A:296:VAL:HG23	2.46	0.40
2:A:318:ASP:C	2:A:320:GLY:N	2.79	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
2:A:280:ALA:C	2:A:282:ILE:N	2.79	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 ⓘ

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%)	765 (95%)	41 (5%)	21	27

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	7	LEU
2	A	17	ARG
2	A	20	LEU
2	A	210	VAL
2	A	212	PHE

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Mol	Chain	Res	Type
2	A	237	ILE
2	A	295	TRP
2	A	301	PRO
2	A	305	ARG
2	A	325	HIS
2	A	339	GLN
2	A	346	ILE
2	A	355	PHE
2	A	366	PHE
2	A	380	GLU
2	A	385	LEU
2	A	404	VAL
2	A	409	THR
2	A	485	ASP
2	A	489	GLU
2	A	526	ASP
2	A	538	VAL
2	A	544	GLU
2	A	546	SER
2	A	569	THR
2	A	602	ASN
2	A	605	VAL
2	A	640	GLN
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	788	VAL
2	A	821	ILE
2	A	844	THR
2	A	866	ASP
2	A	895	ASP
2	A	917	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	26	GLN
2	A	36	GLN

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Mol	Chain	Res	Type
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	314	HIS
2	A	339	GLN
2	A	392	HIS
2	A	396	HIS
2	A	411	GLN
2	A	421	GLN
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	718	ASN
2	A	732	GLN
2	A	736	HIS
2	A	742	GLN
2	A	770	HIS
2	A	809	ASN
2	A	850	HIS
2	A	857	GLN
2	A	891	ASN

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
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 oligosaccharides 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	-	36,36,36	2.16	10 (27%)	43,48,48	2.22	8 (18%)

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	-6.89	1.36	1.46
6	A	1993	MRC	C9-C8	4.04	1.61	1.53
6	A	1993	MRC	O1A-C1	3.51	1.42	1.34
6	A	1993	MRC	C16-C8	3.35	1.56	1.51
6	A	1993	MRC	C2-C1	-3.21	1.39	1.46
6	A	1993	MRC	C2-C3	3.16	1.39	1.33
6	A	1993	MRC	C12-C13	2.86	1.58	1.53
6	A	1993	MRC	C8-C7	2.61	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1993	MRC	C9-C10	2.45	1.57	1.52
6	A	1993	MRC	O1P-C1'	-2.07	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1993	MRC	C17-C12-C13	6.16	118.92	111.67
6	A	1993	MRC	C9-C8-C7	5.54	121.20	113.32
6	A	1993	MRC	C11-C12-C13	5.29	121.96	111.11
6	A	1993	MRC	C11-O10-C10	-5.02	57.46	60.62
6	A	1993	MRC	O1A-C1-C2	4.51	119.58	110.67
6	A	1993	MRC	C17-C12-C11	4.03	118.50	111.40
6	A	1993	MRC	C9'-O1A-C1	-3.44	110.30	116.42
6	A	1993	MRC	O1A-C1-O1B	-2.46	117.78	122.96

All (3) chirality outliers are listed below:

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

All (13) torsion outliers are listed below:

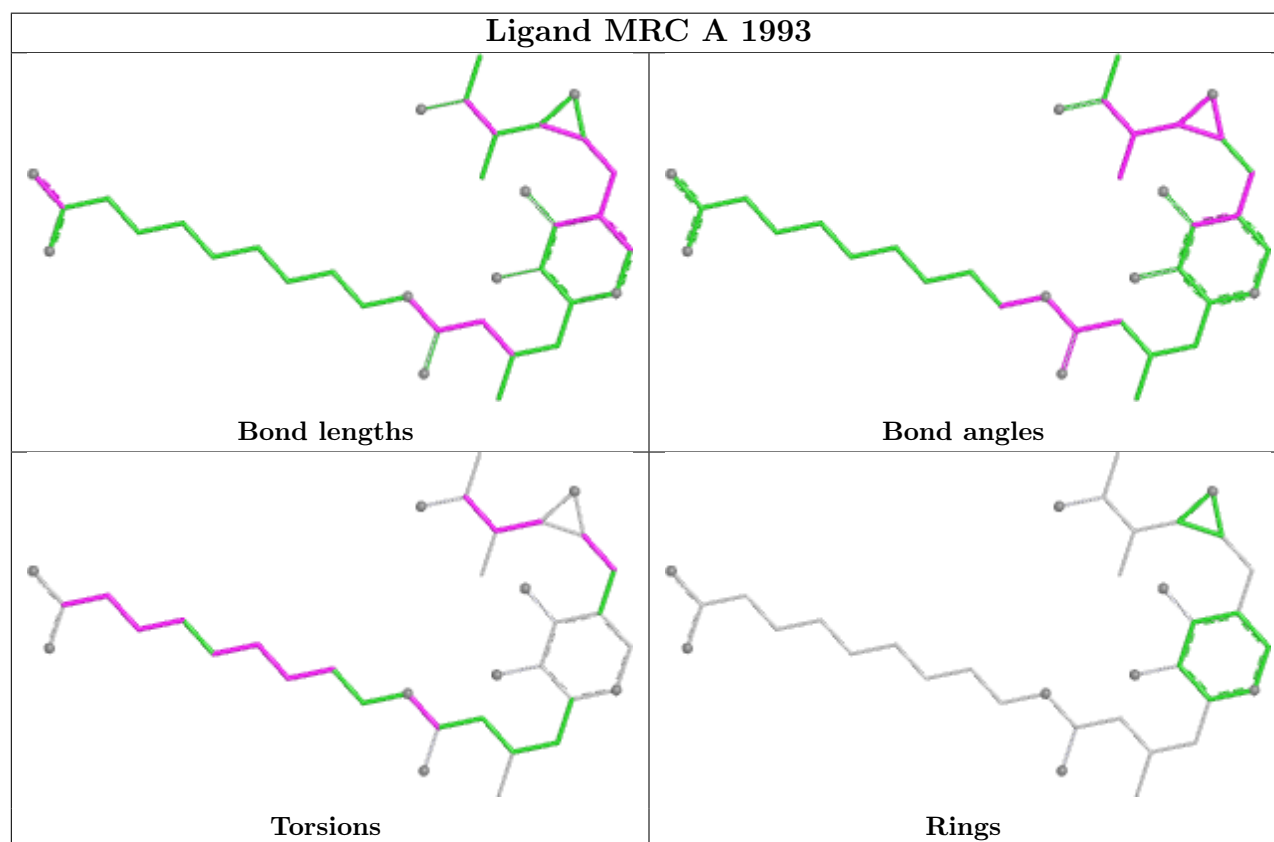
Mol	Chain	Res	Type	Atoms
6	A	1993	MRC	C2-C1-O1A-C9'
6	A	1993	MRC	O10-C11-C12-C13
6	A	1993	MRC	C11-C12-C13-C14
6	A	1993	MRC	C11-C12-C13-O13
6	A	1993	MRC	O1B-C1-O1A-C9'
6	A	1993	MRC	C5'-C6'-C7'-C8'
6	A	1993	MRC	C6'-C7'-C8'-C9'
6	A	1993	MRC	C1'-C2'-C3'-C4'
6	A	1993	MRC	C4'-C5'-C6'-C7'
6	A	1993	MRC	C2'-C3'-C4'-C5'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

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1993	MRC	5	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 than 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.



5.7 Other polymers [i](#)

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%)	0.04	5 (6%) 24 21	11, 31, 72, 99	2 (2%)
2	A	917/917 (100%)	0.60	174 (18%) 3 2	10, 29, 99, 100	0
All	All	992/992 (100%)	0.56	179 (18%) 3 2	10, 30, 99, 100	2 (0%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	280	ALA	8.7
2	A	383	ALA	8.4
2	A	219	GLY	8.1
2	A	288	TYR	6.9
2	A	304	ASP	6.5
2	A	225	ALA	6.4
2	A	254	TYR	6.2
2	A	327	ALA	6.2
2	A	917	VAL	6.1
2	A	324	VAL	6.0
2	A	315	VAL	5.9
2	A	298	ALA	5.9
2	A	241	VAL	5.8
2	A	290	GLY	5.6
2	A	336	ILE	5.5
2	A	245	VAL	5.4
2	A	213	ASN	5.3
2	A	211	ALA	5.3
2	A	323	CYS	5.2
2	A	513	SER	5.2
2	A	243	ILE	5.2
2	A	242	ALA	5.2
2	A	370	ALA	5.1
2	A	252	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
2	A	223	ALA	5.0
2	A	340	GLN	4.9
2	A	360	GLY	4.9
2	A	289	THR	4.9
2	A	214	VAL	4.8
2	A	373	ALA	4.8
2	A	247	PRO	4.8
2	A	338	GLY	4.7
2	A	366	PHE	4.7
2	A	309	VAL	4.6
2	A	379	THR	4.6
2	A	239	SER	4.6
2	A	236	THR	4.6
2	A	224	ASP	4.5
2	A	301	PRO	4.4
2	A	274	ALA	4.4
1	T	74	C	4.4
2	A	377	LEU	4.4
2	A	256	VAL	4.3
2	A	335	TYR	4.3
2	A	326	THR	4.3
2	A	216	ASP	4.2
2	A	384	LEU	4.2
2	A	319	ALA	4.2
2	A	385	LEU	4.1
2	A	258	GLY	4.1
2	A	221	VAL	4.1
2	A	339	GLN	4.1
2	A	253	GLN	4.0
2	A	276	ASP	3.9
2	A	374	VAL	3.9
2	A	226	LYS	3.9
2	A	234	PRO	3.8
2	A	355	PHE	3.8
2	A	331	GLY	3.8
2	A	356	THR	3.7
2	A	228	ILE	3.7
2	A	269	ASP	3.7
2	A	311	ASN	3.7
2	A	368	ASP	3.7
2	A	299	GLN	3.7
2	A	240	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	281	SER	3.7
2	A	268	SER	3.6
2	A	275	LEU	3.6
1	T	17	U	3.6
2	A	341	TYR	3.6
2	A	310	ILE	3.6
2	A	861	VAL	3.6
2	A	261	TYR	3.5
2	A	302	PHE	3.5
2	A	547	PHE	3.5
2	A	372	LYS	3.5
2	A	251	TYR	3.5
2	A	382	GLY	3.5
2	A	471	GLY	3.5
2	A	267	LEU	3.5
2	A	262	ILE	3.5
2	A	263	ILE	3.5
2	A	343	LEU	3.5
2	A	337	VAL	3.4
2	A	264	ALA	3.4
2	A	230	TRP	3.4
2	A	270	ALA	3.4
2	A	307	SER	3.4
2	A	272	ALA	3.3
2	A	231	THR	3.3
2	A	345	VAL	3.2
2	A	363	GLU	3.2
2	A	249	LEU	3.2
2	A	303	LEU	3.2
2	A	348	PRO	3.2
2	A	371	ASN	3.2
2	A	346	ILE	3.2
2	A	248	GLU	3.1
2	A	364	GLY	3.1
2	A	282	ILE	3.1
2	A	321	THR	3.1
2	A	220	VAL	3.1
2	A	354	VAL	3.1
2	A	209	TYR	3.1
2	A	255	ASN	3.1
2	A	328	PRO	3.1
2	A	381	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	359	GLY	3.1
2	A	250	LYS	3.1
2	A	367	TYR	3.0
2	A	300	HIS	3.0
2	A	306	GLU	3.0
2	A	229	ILE	3.0
2	A	257	ASN	3.0
1	T	20	U	3.0
2	A	317	THR	3.0
2	A	212	PHE	2.9
2	A	217	ASP	2.9
2	A	210	VAL	2.9
2	A	235	TRP	2.9
2	A	271	VAL	2.9
2	A	277	TRP	2.9
2	A	378	LEU	2.8
2	A	470	ASN	2.8
2	A	284	LEU	2.8
2	A	308	LEU	2.8
2	A	296	VAL	2.8
2	A	246	HIS	2.8
2	A	347	SER	2.8
2	A	469	GLU	2.8
2	A	369	LYS	2.8
2	A	318	ASP	2.7
2	A	380	GLU	2.7
2	A	312	GLY	2.7
2	A	286	LYS	2.7
2	A	295	TRP	2.7
2	A	866	ASP	2.7
2	A	260	LYS	2.7
2	A	297	VAL	2.7
2	A	215	LYS	2.7
2	A	325	HIS	2.6
2	A	342	GLU	2.6
2	A	351	ASP	2.6
2	A	293	LEU	2.6
2	A	227	PHE	2.6
2	A	350	ASP	2.6
2	A	244	THR	2.6
2	A	357	GLU	2.6
2	A	238	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	320	GLY	2.6
2	A	279	LYS	2.6
2	A	265	GLU	2.5
1	T	47	U	2.5
2	A	207	SER	2.5
2	A	208	ILE	2.4
2	A	314	HIS	2.4
2	A	376	ASP	2.4
1	T	16	G	2.4
2	A	389	PHE	2.4
2	A	292	GLU	2.4
2	A	333	ASP	2.4
2	A	322	GLY	2.3
2	A	259	GLU	2.3
2	A	799	ARG	2.3
2	A	278	ASP	2.3
2	A	313	ASP	2.3
2	A	472	GLU	2.3
2	A	273	GLU	2.3
2	A	349	ILE	2.3
2	A	110	VAL	2.2
2	A	1	MET	2.1
2	A	218	LYS	2.1
2	A	507	GLY	2.1
2	A	294	GLU	2.1
2	A	835	ASP	2.1
2	A	386	LYS	2.0
2	A	344	PRO	2.0
2	A	365	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

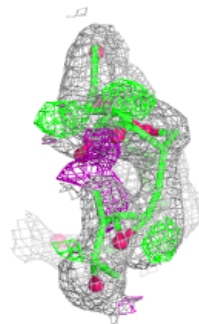
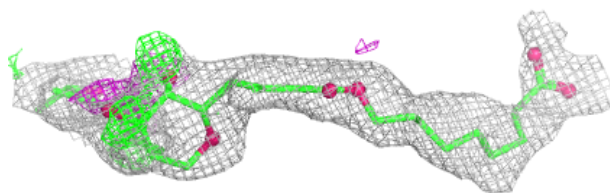
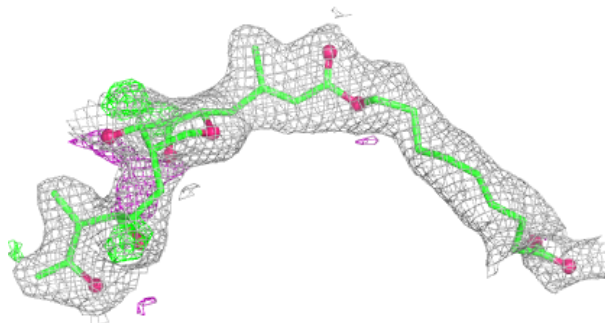
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	T	1206	1/1	0.39	0.19	37,37,37,37	0
4	MG	T	1205	1/1	0.62	0.12	29,29,29,29	0
4	MG	T	1202	1/1	0.69	0.09	54,54,54,54	0
4	MG	T	1210	1/1	0.69	0.19	36,36,36,36	0
4	MG	T	1203	1/1	0.75	0.15	37,37,37,37	0
4	MG	T	1209	1/1	0.77	0.06	45,45,45,45	0
4	MG	T	1204	1/1	0.82	0.09	30,30,30,30	0
4	MG	T	1208	1/1	0.85	0.18	33,33,33,33	0
6	MRC	A	1993	35/35	0.85	0.12	14,29,54,55	0
4	MG	T	1207	1/1	0.91	0.07	37,37,37,37	0
4	MG	T	1201	1/1	0.92	0.12	37,37,37,37	0
3	K	T	301	1/1	0.97	0.10	26,26,26,26	0
5	ZN	A	1992	1/1	0.98	0.04	26,26,26,26	0
5	ZN	A	1001	1/1	0.98	0.03	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.