



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:38 AM GMT

PDB ID : 1OB2
Title : E. coli elongation factor EF-Tu complexed with the antibiotic kirromycin, a GTP analog, and Phe-tRNA
Authors : Kristensen, O.; Nissen, P.; Nyborg, J.
Deposited on : 2003-01-24
Resolution : 3.35 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

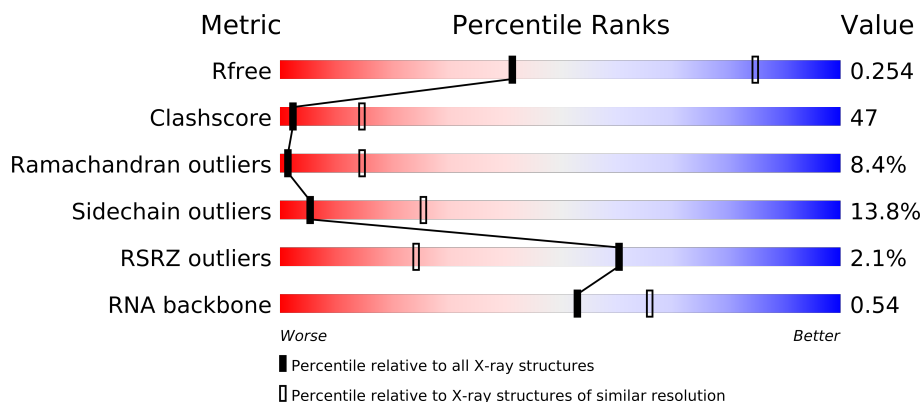
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

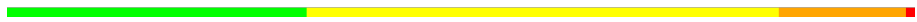
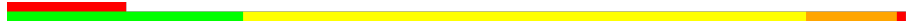
The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1141 (3.50-3.22)
Clashscore	79885	1030 (3.48-3.24)
Ramachandran outliers	78287	1008 (3.48-3.24)
Sidechain outliers	78261	1007 (3.48-3.24)
RSRZ outliers	66119	1141 (3.50-3.22)
RNA backbone	1838	1005 (4.00-2.72)

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

Mol	Chain	Length	Quality of chain
1	A	393	
2	B	77	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4810 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	393	3035	1918	523	581	13	0	0	0

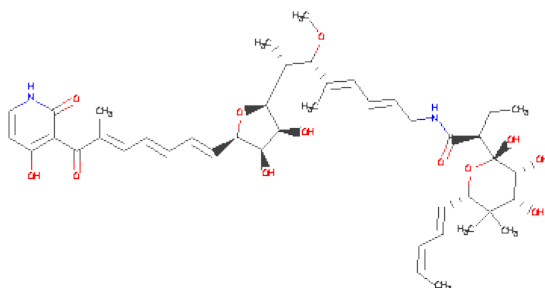
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	SER	CONFLICT	UNP P0CE48

- Molecule 2 is a RNA chain called TRANSFER-RNA, PHE.

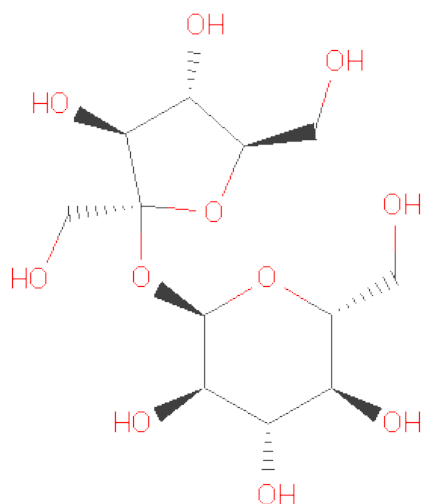
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	77	1662	754	295	537	76	0	0	0

- Molecule 3 is KIRROMYCIN (three-letter code: KIR) (formula: C₄₃H₆₀N₂O₁₂).



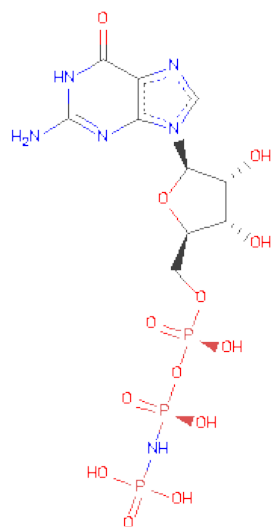
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			57	43	2	12		

- Molecule 4 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

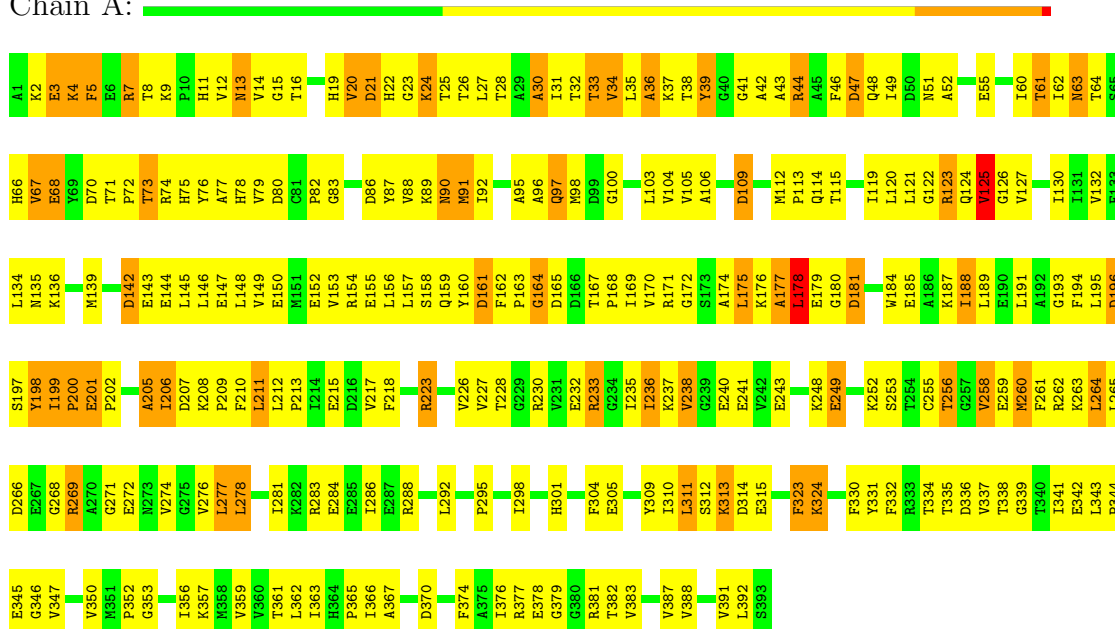
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

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

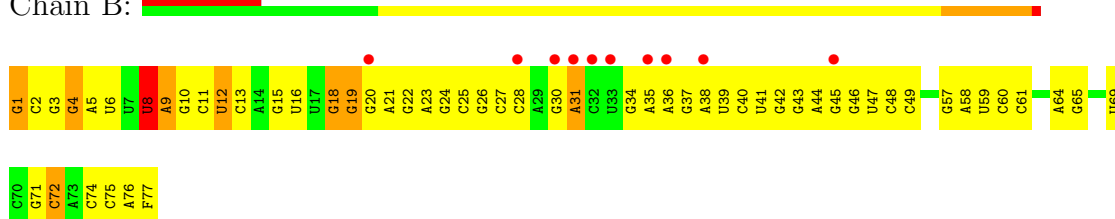
• Molecule 1: ELONGATION FACTOR TU

Chain A:



• Molecule 2: TRANSFER-RNA, PHE

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	196.41 Å 196.41 Å 196.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 3.35 47.64 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.64-3.35) 97.8 (47.64-3.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.33 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.265 0.212 , 0.254	Depositor DCC
R_{free} test set	963 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 18793 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4810	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, GNP, SUC, H2U, KIR, PHA, MG, YG, MAD, 2MG, 5MC, OMG, M2G, 7MG, PSU

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	A	0.49	0/3091	0.81	0/4182
2	B	0.58	1/1508 (0.1%)	0.72	0/2345
All	All	0.52	1/4599 (0.0%)	0.78	0/6527

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-7.00	1.52	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	22	G	Sidechain
2	B	8	U	Sidechain

5.2 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 hydrogens

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3035	0	3051	354	0
2	B	1662	0	867	70	0
3	A	57	0	58	3	0
4	A	23	0	22	1	0
5	A	32	0	13	4	0
6	A	1	0	0	0	0
All	All	4810	0	4011	413	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 47.

All (413) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:199:ILE:HB	1:A:200:PRO:HA	1.18	1.12
1:A:74:ARG:HE	1:A:199:ILE:HD11	1.14	1.05
1:A:199:ILE:HB	1:A:200:PRO:CA	1.86	1.05
1:A:74:ARG:HE	1:A:199:ILE:CD1	1.74	1.00
1:A:123:ARG:HG2	1:A:162:PHE:HE2	1.28	0.98
1:A:261:PHE:N	2:B:77:PHA:H	1.61	0.96
1:A:217:VAL:HG22	1:A:227:VAL:HG12	1.52	0.92
1:A:67:VAL:HG12	1:A:78:HIS:HB3	1.52	0.92
1:A:14:VAL:HG23	1:A:100:GLY:O	1.69	0.91
2:B:37:YG:H31	2:B:37:YG:H1'	1.54	0.90
1:A:22:HIS:HB2	1:A:106:ALA:HB2	1.56	0.87
1:A:237:LYS:O	1:A:240:GLU:HG3	1.74	0.87
1:A:13:ASN:HB3	1:A:77:ALA:HB3	1.55	0.86
1:A:215:GLU:HA	1:A:288:ARG:HG3	1.59	0.83
1:A:206:ILE:HD12	1:A:207:ASP:N	1.93	0.83
1:A:258:VAL:O	1:A:265:LEU:HB2	1.78	0.83
1:A:34:VAL:HG21	1:A:188:ILE:HG12	1.60	0.82
1:A:313:LYS:HD2	1:A:313:LYS:H	1.41	0.82
1:A:73:THR:O	1:A:74:ARG:HD3	1.80	0.82
1:A:208:LYS:HB3	1:A:209:PRO:HD2	1.62	0.81
1:A:74:ARG:NE	1:A:199:ILE:HD11	1.95	0.81
2:B:11:C:H2'	2:B:12:U:H5'	1.64	0.79
1:A:11:HIS:HE1	1:A:13:ASN:HD22	1.31	0.79
1:A:123:ARG:HD2	3:A:1394:KIR:H421	1.65	0.79
1:A:123:ARG:HG2	1:A:162:PHE:CE2	2.17	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:33:THR:HA	1:A:43:ALA:CB	2.14	0.78
1:A:82:PRO:HD2	1:A:91:MET:HB3	1.65	0.78
2:B:71:G:C3'	2:B:72:C:H5''	2.14	0.78
1:A:260:MET:SD	1:A:261:PHE:HD1	2.08	0.77
2:B:71:G:H3'	2:B:72:C:H5''	1.67	0.77
2:B:37:YG:H31	2:B:37:YG:C1'	2.15	0.77
2:B:9:A:O2'	2:B:10:2MG:N7	2.18	0.76
1:A:223:ARG:HD3	2:B:76:A:H62	1.49	0.76
1:A:33:THR:HA	1:A:43:ALA:HB2	1.68	0.76
1:A:199:ILE:CB	1:A:200:PRO:CA	2.64	0.75
1:A:34:VAL:HG11	1:A:188:ILE:HG21	1.68	0.75
1:A:7:ARG:H	1:A:7:ARG:CD	1.99	0.75
1:A:74:ARG:NE	1:A:199:ILE:CD1	2.49	0.75
1:A:7:ARG:HG3	1:A:269:ARG:HH22	1.52	0.72
1:A:103:LEU:CD2	1:A:119:ILE:HD11	2.19	0.72
1:A:9:LYS:HD2	1:A:74:ARG:N	2.04	0.72
1:A:95:ALA:HA	1:A:98:MET:HG3	1.70	0.72
1:A:20:VAL:HG12	1:A:21:ASP:H	1.55	0.72
1:A:261:PHE:O	1:A:263:LYS:HG3	1.88	0.71
1:A:211:LEU:HD12	1:A:212:LEU:N	2.05	0.71
1:A:164:GLY:N	1:A:167:THR:OG1	2.22	0.71
1:A:72:PRO:HG2	1:A:73:THR:HG22	1.70	0.71
2:B:3:G:H2'	2:B:4:G:H5''	1.73	0.71
2:B:12:U:H6	2:B:12:U:H5'	1.56	0.70
1:A:226:VAL:HG13	1:A:276:VAL:O	1.91	0.70
2:B:44:A:H2'	2:B:45:G:O4'	1.90	0.70
1:A:125:VAL:HG13	1:A:126:GLY:N	2.06	0.70
1:A:213:PRO:HB2	1:A:334:THR:HG23	1.74	0.70
1:A:205:ALA:O	1:A:206:ILE:HG13	1.91	0.70
1:A:269:ARG:N	1:A:269:ARG:HD3	2.07	0.69
1:A:135:ASN:HD21	1:A:174:ALA:H	1.39	0.69
1:A:170:VAL:HG21	1:A:191:LEU:HB2	1.73	0.69
1:A:34:VAL:HG11	1:A:188:ILE:CG2	2.23	0.69
1:A:14:VAL:HG22	1:A:15:GLY:H	1.57	0.69
2:B:74:C:O2'	2:B:75:C:H5'	1.93	0.69
1:A:142:ASP:O	1:A:144:GLU:N	2.25	0.69
1:A:14:VAL:HG22	1:A:15:GLY:N	2.08	0.69
1:A:38:THR:O	1:A:39:TYR:CD2	2.46	0.68
1:A:130:ILE:HG13	1:A:162:PHE:HE1	1.58	0.68
1:A:123:ARG:CG	1:A:162:PHE:HE2	2.04	0.68
1:A:7:ARG:CG	1:A:269:ARG:HH22	2.06	0.68
1:A:379:GLY:HA2	2:B:64:A:O4'	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:LEU:O	1:A:124:GLN:HG3	1.93	0.67
1:A:323:PHE:CD1	1:A:323:PHE:N	2.63	0.67
1:A:14:VAL:O	1:A:78:HIS:HA	1.96	0.66
2:B:18:G:H4'	2:B:19:G:OP1	1.94	0.66
1:A:227:VAL:HG11	1:A:286:ILE:HD13	1.76	0.66
1:A:28:THR:O	1:A:32:THR:HG23	1.96	0.66
2:B:3:G:C2'	2:B:4:G:H5''	2.26	0.65
1:A:19:HIS:HB3	1:A:22:HIS:CE1	2.30	0.65
1:A:19:HIS:CD2	1:A:114:GLN:HB2	2.30	0.65
2:B:58:MAD:HM12	2:B:61:C:H1'	1.77	0.65
1:A:11:HIS:CE1	1:A:13:ASN:HD22	2.15	0.65
2:B:30:G:H2'	2:B:31:A:H5''	1.77	0.64
1:A:24:LYS:H	1:A:104:VAL:HG11	1.61	0.64
2:B:30:G:H2'	2:B:31:A:C5'	2.27	0.64
1:A:24:LYS:HG3	1:A:104:VAL:CG1	2.27	0.64
1:A:16:THR:HG23	1:A:78:HIS:CE1	2.33	0.64
1:A:338:THR:O	1:A:363:ILE:HG23	1.99	0.63
1:A:149:VAL:HG23	1:A:150:GLU:N	2.14	0.63
1:A:19:HIS:HB3	1:A:22:HIS:NE2	2.14	0.63
1:A:212:LEU:HD23	1:A:212:LEU:C	2.19	0.63
1:A:256:THR:HG22	1:A:277:LEU:CG	2.29	0.63
1:A:261:PHE:H	2:B:77:PHA:H	0.80	0.62
1:A:149:VAL:HA	1:A:152:GLU:HG2	1.81	0.62
1:A:68:GLU:HB3	1:A:261:PHE:CE2	2.34	0.62
1:A:264:LEU:HD23	1:A:265:LEU:N	2.14	0.62
1:A:67:VAL:CG1	1:A:78:HIS:HB3	2.27	0.62
1:A:97:GLN:OE1	1:A:97:GLN:O	2.16	0.62
1:A:11:HIS:CD2	1:A:75:HIS:HD2	2.18	0.61
1:A:34:VAL:CG1	1:A:188:ILE:HG21	2.30	0.61
1:A:61:THR:HG22	1:A:82:PRO:HB3	1.81	0.61
1:A:103:LEU:HD21	1:A:119:ILE:HD11	1.83	0.61
1:A:256:THR:HG22	1:A:277:LEU:HD23	1.82	0.60
1:A:34:VAL:CB	1:A:188:ILE:HG21	2.30	0.60
1:A:160:TYR:O	1:A:161:ASP:HB2	2.00	0.60
1:A:44:ARG:CZ	1:A:44:ARG:HB3	2.30	0.60
1:A:74:ARG:HH21	1:A:199:ILE:HD12	1.67	0.60
1:A:191:LEU:C	1:A:193:GLY:N	2.54	0.60
1:A:191:LEU:C	1:A:193:GLY:H	2.04	0.60
1:A:168:PRO:HB2	1:A:194:PHE:HD1	1.66	0.60
1:A:71:THR:CG2	1:A:74:ARG:H	2.15	0.60
2:B:18:G:H2'	2:B:57:G:H22	1.66	0.59
1:A:35:LEU:HD12	1:A:35:LEU:N	2.18	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:3:G:C3'	2:B:4:G:H5''	2.32	0.59
1:A:168:PRO:HB2	1:A:194:PHE:CD1	2.36	0.59
1:A:198:TYR:O	1:A:199:ILE:C	2.40	0.59
1:A:19:HIS:O	1:A:24:LYS:HE2	2.02	0.58
1:A:301:HIS:O	1:A:365:PRO:HA	2.04	0.58
1:A:21:ASP:O	1:A:21:ASP:CG	2.41	0.58
1:A:238:VAL:HG12	1:A:266:ASP:O	2.04	0.58
2:B:5:A:O2'	2:B:6:U:H5'	2.04	0.57
2:B:35:A:O2'	2:B:36:A:H5'	2.04	0.57
1:A:89:LYS:NZ	1:A:336:ASP:OD1	2.38	0.57
1:A:248:LYS:HG2	1:A:249:GLU:H	1.69	0.57
1:A:63:ASN:ND2	1:A:63:ASN:H	2.02	0.57
1:A:305:GLU:HG3	1:A:392:LEU:HD11	1.86	0.57
1:A:71:THR:HG22	1:A:74:ARG:O	2.04	0.57
1:A:5:PHE:HB2	1:A:263:LYS:HB2	1.87	0.57
1:A:264:LEU:C	1:A:264:LEU:HD23	2.24	0.57
1:A:20:VAL:O	1:A:22:HIS:N	2.38	0.57
1:A:170:VAL:HG12	1:A:171:ARG:N	2.20	0.56
1:A:312:SER:HA	1:A:352:PRO:HB2	1.87	0.56
1:A:196:ASP:N	1:A:196:ASP:OD2	2.38	0.56
1:A:24:LYS:NZ	1:A:83:GLY:HA3	2.20	0.56
1:A:209:PRO:HG2	1:A:233:ARG:NH2	2.19	0.56
1:A:35:LEU:C	1:A:37:LYS:H	2.09	0.56
1:A:63:ASN:HD22	1:A:63:ASN:H	1.53	0.56
1:A:63:ASN:HD22	1:A:63:ASN:N	2.04	0.56
1:A:92:ILE:CG1	1:A:121:LEU:HD13	2.35	0.56
1:A:243:GLU:HG3	1:A:295:PRO:HG3	1.87	0.56
1:A:272:GLU:O	1:A:274:VAL:HG13	2.05	0.56
1:A:260:MET:SD	1:A:261:PHE:CD1	2.94	0.56
1:A:341:ILE:CG2	1:A:342:GLU:N	2.69	0.56
1:A:241:GLU:CD	1:A:252:LYS:HE2	2.26	0.56
2:B:40:5MC:O2'	2:B:41:U:H5'	2.06	0.56
1:A:277:LEU:O	1:A:278:LEU:O	2.25	0.55
1:A:12:VAL:HG22	1:A:202:PRO:HG3	1.87	0.55
1:A:71:THR:OG1	1:A:72:PRO:HD2	2.07	0.55
1:A:32:THR:O	1:A:43:ALA:HB2	2.06	0.55
1:A:142:ASP:C	1:A:144:GLU:H	2.10	0.54
1:A:150:GLU:OE1	1:A:171:ARG:NE	2.33	0.54
1:A:185:GLU:O	1:A:189:LEU:HD12	2.07	0.54
1:A:178:LEU:O	1:A:178:LEU:HD23	2.07	0.54
1:A:205:ALA:C	1:A:206:ILE:HG13	2.28	0.54
1:A:172:GLY:HA2	1:A:184:TRP:CZ3	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:GLY:O	1:A:347:VAL:HG23	2.08	0.54
1:A:341:ILE:HG22	1:A:342:GLU:N	2.22	0.54
1:A:92:ILE:HG12	1:A:121:LEU:HD13	1.90	0.53
1:A:90:ASN:HD21	2:B:1:G:H4'	1.73	0.53
1:A:176:LYS:HE2	1:A:176:LYS:HA	1.91	0.53
1:A:34:VAL:HG21	1:A:188:ILE:HG21	1.91	0.53
2:B:11:C:C2'	2:B:12:U:H5'	2.35	0.53
1:A:269:ARG:HD3	1:A:269:ARG:H	1.74	0.53
1:A:236:ILE:H	1:A:236:ILE:HD12	1.73	0.52
1:A:36:ALA:HA	1:A:41:GLY:H	1.73	0.52
1:A:256:THR:HG22	1:A:277:LEU:CD2	2.40	0.52
1:A:87:TYR:O	1:A:90:ASN:N	2.42	0.52
1:A:122:GLY:O	1:A:123:ARG:C	2.48	0.52
1:A:136:LYS:HG2	5:A:1397:GNP:C6	2.40	0.52
1:A:24:LYS:N	1:A:104:VAL:HG11	2.25	0.52
1:A:5:PHE:HD1	1:A:263:LYS:HD2	1.75	0.52
1:A:142:ASP:C	1:A:144:GLU:N	2.62	0.52
1:A:334:THR:O	1:A:335:THR:HG23	2.10	0.51
1:A:88:VAL:HG23	1:A:89:LYS:N	2.25	0.51
1:A:200:PRO:O	1:A:201:GLU:O	2.28	0.51
1:A:123:ARG:HD2	3:A:1394:KIR:C42	2.39	0.51
1:A:256:THR:O	1:A:256:THR:CG2	2.59	0.51
1:A:13:ASN:CB	1:A:77:ALA:HB3	2.35	0.51
1:A:34:VAL:HG21	1:A:188:ILE:CG1	2.37	0.51
1:A:112:MET:HB3	1:A:113:PRO:HD2	1.93	0.51
1:A:130:ILE:HG13	1:A:162:PHE:CE1	2.42	0.51
2:B:18:G:O2'	2:B:57:G:N2	2.43	0.51
1:A:62:ILE:HG21	2:B:2:C:H4'	1.92	0.51
1:A:376:ILE:HG22	1:A:383:VAL:HB	1.92	0.51
2:B:11:C:H2'	2:B:12:U:C5'	2.37	0.51
2:B:39:PSU:H2'	2:B:40:5MC:C6	2.45	0.51
1:A:96:ALA:HB2	1:A:125:VAL:HG21	1.92	0.51
1:A:24:LYS:HZ3	1:A:83:GLY:HA3	1.76	0.50
1:A:188:ILE:HG22	1:A:189:LEU:N	2.25	0.50
1:A:14:VAL:CG2	1:A:15:GLY:H	2.23	0.50
1:A:62:ILE:HG23	1:A:87:TYR:CZ	2.46	0.50
2:B:15:G:H2'	2:B:16:H2U:H62	1.93	0.50
1:A:261:PHE:HA	2:B:77:PHA:O	2.11	0.50
1:A:232:GLU:HG2	1:A:233:ARG:HG3	1.93	0.50
2:B:12:U:H2'	2:B:13:C:O5'	2.11	0.50
1:A:164:GLY:O	1:A:167:THR:HB	2.11	0.50
1:A:194:PHE:CD2	1:A:194:PHE:N	2.80	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:ILE:CD1	1:A:367:ALA:HB1	2.42	0.50
1:A:210:PHE:CE1	1:A:236:ILE:HG13	2.47	0.50
1:A:235:ILE:HD13	1:A:237:LYS:HG3	1.94	0.50
2:B:11:C:C2'	2:B:12:U:C5'	2.90	0.50
1:A:235:ILE:C	1:A:235:ILE:HD12	2.31	0.50
1:A:35:LEU:HD12	1:A:35:LEU:H	1.77	0.50
1:A:177:ALA:O	1:A:179:GLU:N	2.44	0.50
1:A:377:ARG:HG2	1:A:382:THR:HG22	1.94	0.49
2:B:37:YG:O2'	2:B:38:A:H5'	2.12	0.49
2:B:37:YG:H31	2:B:37:YG:C2'	2.43	0.49
1:A:35:LEU:H	1:A:35:LEU:CD1	2.26	0.49
1:A:194:PHE:HD2	1:A:194:PHE:N	2.10	0.49
1:A:313:LYS:C	1:A:315:GLU:H	2.16	0.49
2:B:18:G:C2'	2:B:57:G:H22	2.25	0.49
1:A:19:HIS:HA	1:A:114:GLN:HB2	1.94	0.49
1:A:211:LEU:C	1:A:211:LEU:HD12	2.33	0.49
1:A:298:ILE:HG23	1:A:298:ILE:O	2.11	0.49
1:A:16:THR:HG23	1:A:78:HIS:NE2	2.28	0.49
1:A:175:LEU:HD12	1:A:176:LYS:H	1.77	0.49
1:A:205:ALA:O	1:A:207:ASP:N	2.39	0.48
1:A:153:VAL:O	1:A:156:LEU:HB3	2.14	0.48
1:A:269:ARG:CD	1:A:269:ARG:H	2.26	0.48
1:A:253:SER:HB2	1:A:281:ILE:HD11	1.94	0.48
1:A:311:LEU:HD23	1:A:311:LEU:N	2.28	0.48
2:B:71:G:C2'	2:B:72:C:H5''	2.44	0.48
2:B:30:G:H2'	2:B:31:A:H5'	1.95	0.48
1:A:71:THR:HG21	1:A:196:ASP:OD1	2.14	0.48
1:A:205:ALA:CB	1:A:233:ARG:HB3	2.43	0.48
1:A:37:LYS:C	1:A:39:TYR:H	2.16	0.48
1:A:125:VAL:CG1	1:A:126:GLY:N	2.76	0.48
2:B:24:G:H2'	2:B:25:C:C6	2.49	0.48
1:A:51:ASN:N	1:A:51:ASN:OD1	2.47	0.48
1:A:112:MET:HB3	1:A:113:PRO:CD	2.44	0.48
1:A:356:ILE:HD12	1:A:357:LYS:H	1.77	0.48
2:B:12:U:C2'	2:B:13:C:O5'	2.62	0.47
1:A:277:LEU:HD22	2:B:76:A:H61	1.79	0.47
1:A:23:GLY:O	1:A:24:LYS:C	2.52	0.47
1:A:309:TYR:HE2	1:A:353:GLY:O	1.98	0.47
1:A:191:LEU:O	1:A:193:GLY:N	2.47	0.47
1:A:19:HIS:CD2	1:A:114:GLN:H	2.33	0.47
1:A:298:ILE:HD13	1:A:367:ALA:HB1	1.96	0.47
1:A:66:HIS:HB2	2:B:77:PHA:CE2	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:39:PSU:O2'	2:B:40:5MC:H5'	2.15	0.47
1:A:24:LYS:HG3	1:A:104:VAL:HG11	1.94	0.47
2:B:1:G:O2'	2:B:2:C:H5'	2.15	0.47
1:A:134:LEU:HD23	1:A:169:ILE:CG2	2.44	0.47
1:A:132:VAL:HB	1:A:169:ILE:HG12	1.97	0.47
1:A:311:LEU:H	1:A:311:LEU:HD23	1.79	0.47
2:B:30:G:C2'	2:B:31:A:H5''	2.42	0.47
1:A:14:VAL:CG2	1:A:15:GLY:N	2.76	0.47
1:A:24:LYS:HB2	1:A:24:LYS:HE3	1.73	0.47
1:A:235:ILE:O	1:A:235:ILE:HD12	2.15	0.47
1:A:256:THR:HG22	1:A:277:LEU:HB3	1.97	0.47
1:A:130:ILE:CD1	1:A:162:PHE:CE1	2.98	0.47
1:A:25:THR:HG22	1:A:25:THR:O	2.15	0.47
2:B:34:OMG:HM22	2:B:35:A:O4'	2.15	0.47
1:A:31:ILE:O	1:A:35:LEU:HD13	2.15	0.47
1:A:168:PRO:CB	1:A:194:PHE:HD1	2.28	0.47
1:A:377:ARG:HE	1:A:382:THR:CG2	2.29	0.46
1:A:337:VAL:HG11	1:A:366:ILE:HD12	1.97	0.46
1:A:26:THR:HG23	5:A:1397:GNP:O1A	2.15	0.46
1:A:189:LEU:O	1:A:193:GLY:N	2.47	0.46
1:A:256:THR:HG22	1:A:277:LEU:HG	1.97	0.46
2:B:74:C:C2'	2:B:75:C:H5'	2.45	0.46
2:B:26:M2G:HM23	2:B:27:C:H1'	1.97	0.46
1:A:2:LYS:O	1:A:3:GLU:O	2.32	0.46
1:A:377:ARG:HE	1:A:382:THR:HG23	1.80	0.46
1:A:114:GLN:HA	1:A:114:GLN:OE1	2.15	0.46
1:A:26:THR:HG22	1:A:46:PHE:CD1	2.50	0.46
1:A:236:ILE:HD11	1:A:268:GLY:HA3	1.97	0.46
1:A:12:VAL:O	1:A:76:TYR:HA	2.15	0.46
1:A:323:PHE:HD1	1:A:323:PHE:N	2.13	0.46
1:A:148:LEU:HD23	1:A:148:LEU:C	2.36	0.46
1:A:76:TYR:CE2	1:A:195:LEU:HB3	2.50	0.46
1:A:103:LEU:O	1:A:103:LEU:HG	2.15	0.46
1:A:164:GLY:CA	1:A:167:THR:OG1	2.64	0.46
1:A:7:ARG:H	1:A:7:ARG:HD2	1.77	0.46
2:B:59:U:C4	2:B:60:C:N4	2.84	0.46
1:A:19:HIS:CD2	1:A:112:MET:HB2	2.51	0.45
1:A:106:ALA:HB1	1:A:136:LYS:HD2	1.97	0.45
1:A:157:LEU:O	1:A:159:GLN:N	2.49	0.45
1:A:339:GLY:HA2	1:A:362:LEU:HA	1.98	0.45
1:A:52:ALA:HB3	1:A:55:GLU:HG3	1.98	0.45
1:A:146:LEU:HA	1:A:149:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:ALA:O	1:A:178:LEU:C	2.55	0.45
1:A:304:PHE:HE2	1:A:362:LEU:HD11	1.81	0.45
2:B:39:PSU:H2'	2:B:40:5MC:H6	1.81	0.45
2:B:9:A:H2'	2:B:11:C:H41	1.82	0.45
1:A:243:GLU:OE1	1:A:295:PRO:HA	2.16	0.45
1:A:9:LYS:HD3	1:A:72:PRO:O	2.16	0.45
1:A:19:HIS:HD2	1:A:114:GLN:N	2.14	0.45
1:A:3:GLU:HB3	1:A:4:LYS:H	1.58	0.45
1:A:227:VAL:HG11	1:A:286:ILE:CD1	2.45	0.45
1:A:156:LEU:O	1:A:157:LEU:C	2.55	0.45
1:A:24:LYS:HE3	5:A:1397:GNP:PB	2.57	0.45
1:A:19:HIS:CD2	1:A:112:MET:CB	3.00	0.45
1:A:38:THR:HB	1:A:189:LEU:HD21	1.98	0.45
1:A:276:VAL:HG12	1:A:277:LEU:N	2.31	0.45
1:A:284:GLU:HG2	1:A:284:GLU:O	2.16	0.45
1:A:331:TYR:CE2	1:A:377:ARG:HB2	2.51	0.44
1:A:260:MET:O	1:A:261:PHE:HB2	2.16	0.44
2:B:23:A:H2'	2:B:24:G:C8	2.52	0.44
1:A:71:THR:HG23	1:A:73:THR:H	1.82	0.44
1:A:11:HIS:CE1	1:A:13:ASN:ND2	2.84	0.44
1:A:5:PHE:HB2	1:A:263:LYS:CB	2.47	0.44
1:A:34:VAL:CG2	1:A:188:ILE:HG21	2.48	0.44
1:A:256:THR:O	1:A:256:THR:HG23	2.17	0.44
1:A:259:GLU:OE1	2:B:76:A:C8	2.70	0.44
1:A:387:VAL:HG22	1:A:388:VAL:N	2.32	0.44
1:A:149:VAL:CG2	1:A:150:GLU:N	2.78	0.44
1:A:176:LYS:HB3	1:A:184:TRP:CD1	2.53	0.44
1:A:25:THR:HG23	1:A:80:ASP:OD2	2.18	0.44
1:A:238:VAL:HA	1:A:255:CYS:SG	2.58	0.44
1:A:188:ILE:HG22	1:A:189:LEU:HD12	1.99	0.44
1:A:132:VAL:HG11	1:A:153:VAL:HG11	1.99	0.44
1:A:76:TYR:OH	1:A:195:LEU:O	2.33	0.44
1:A:146:LEU:O	1:A:149:VAL:HG22	2.17	0.44
1:A:64:THR:HA	1:A:80:ASP:O	2.18	0.44
1:A:241:GLU:OE1	1:A:252:LYS:HE2	2.17	0.44
1:A:134:LEU:HD23	1:A:169:ILE:HG21	1.98	0.44
1:A:79:VAL:O	1:A:79:VAL:HG13	2.18	0.44
1:A:189:LEU:C	1:A:191:LEU:N	2.70	0.43
1:A:305:GLU:CG	1:A:392:LEU:HD11	2.48	0.43
3:A:1394:KIR:H473	3:A:1394:KIR:O30	2.18	0.43
2:B:40:5MC:H2'	2:B:41:U:H6	1.83	0.43
1:A:13:ASN:ND2	1:A:271:GLY:O	2.50	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:ARG:HE	1:A:335:THR:CG2	2.31	0.43
1:A:256:THR:HG22	1:A:277:LEU:CB	2.48	0.43
1:A:163:PRO:O	1:A:165:ASP:N	2.51	0.43
1:A:62:ILE:HG23	1:A:87:TYR:CE2	2.53	0.43
1:A:46:PHE:O	1:A:49:ILE:N	2.51	0.43
1:A:11:HIS:HE1	1:A:13:ASN:ND2	2.08	0.43
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.83	0.43
1:A:114:GLN:CA	1:A:114:GLN:OE1	2.65	0.43
1:A:218:PHE:HE1	1:A:228:THR:HG21	1.83	0.43
1:A:74:ARG:NH2	1:A:199:ILE:HD12	2.30	0.43
2:B:18:G:O2'	2:B:19:G:P	2.76	0.43
1:A:177:ALA:O	1:A:180:GLY:N	2.51	0.43
1:A:33:THR:HG23	1:A:43:ALA:HB1	1.99	0.43
1:A:71:THR:HG23	1:A:72:PRO:N	2.34	0.43
1:A:379:GLY:HA2	2:B:64:A:C4'	2.48	0.43
1:A:157:LEU:C	1:A:159:GLN:H	2.22	0.43
1:A:332:PHE:CE2	1:A:374:PHE:HB3	2.53	0.43
1:A:123:ARG:NH2	1:A:123:ARG:HG2	2.34	0.43
2:B:38:A:H2'	2:B:39:PSU:O4'	2.18	0.43
1:A:184:TRP:O	1:A:185:GLU:C	2.57	0.43
1:A:124:GLN:OE1	1:A:382:THR:HG21	2.19	0.42
2:B:64:A:C6	2:B:65:G:N7	2.87	0.42
1:A:277:LEU:O	1:A:278:LEU:C	2.57	0.42
1:A:27:LEU:O	1:A:30:ALA:HB3	2.20	0.42
1:A:97:GLN:HA	1:A:230:ARG:HH11	1.85	0.42
2:B:8:U:H5'	2:B:49:5MC:OP2	2.19	0.42
2:B:44:A:O2'	2:B:45:G:H5'	2.19	0.42
1:A:263:LYS:HE3	4:A:1396:SUC:O4'	2.19	0.42
1:A:38:THR:CB	1:A:189:LEU:HD21	2.49	0.42
1:A:276:VAL:HG12	1:A:278:LEU:HD22	2.01	0.42
1:A:3:GLU:O	1:A:4:LYS:HG2	2.20	0.42
2:B:28:C:H42	2:B:42:G:H1	1.67	0.42
1:A:71:THR:HG23	1:A:74:ARG:H	1.82	0.42
1:A:120:LEU:HD11	1:A:124:GLN:NE2	2.34	0.42
2:B:57:G:H2'	2:B:58:MAD:H5'	2.02	0.42
1:A:146:LEU:O	1:A:147:GLU:C	2.57	0.42
1:A:149:VAL:HG23	1:A:150:GLU:H	1.83	0.42
1:A:172:GLY:HA2	1:A:184:TRP:HZ3	1.83	0.42
1:A:7:ARG:H	1:A:7:ARG:HD3	1.79	0.42
1:A:180:GLY:O	1:A:181:ASP:C	2.57	0.42
1:A:154:ARG:O	1:A:155:GLU:C	2.58	0.42
1:A:324:LYS:HD2	1:A:343:LEU:H	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:24:LYS:HE3	5:A:1397:GNP:O1B	2.20	0.42
1:A:33:THR:CG2	1:A:43:ALA:HB1	2.50	0.42
2:B:71:G:H2'	2:B:72:C:H5''	2.02	0.42
1:A:109:ASP:N	1:A:109:ASP:OD1	2.53	0.42
1:A:184:TRP:O	1:A:187:LYS:N	2.52	0.42
1:A:278:LEU:HD22	1:A:278:LEU:N	2.34	0.42
1:A:87:TYR:O	1:A:88:VAL:C	2.57	0.42
1:A:46:PHE:O	1:A:48:GLN:N	2.53	0.41
1:A:146:LEU:HG	1:A:146:LEU:H	1.64	0.41
1:A:149:VAL:O	1:A:152:GLU:HG2	2.20	0.41
2:B:8:U:C2	2:B:15:G:O6	2.73	0.41
1:A:304:PHE:HE2	1:A:362:LEU:CD1	2.33	0.41
1:A:324:LYS:CD	1:A:343:LEU:H	2.33	0.41
1:A:344:PRO:O	1:A:345:GLU:C	2.58	0.41
1:A:15:GLY:N	1:A:98:MET:CE	2.83	0.41
1:A:35:LEU:C	1:A:37:LYS:N	2.74	0.41
1:A:103:LEU:HD22	1:A:119:ILE:HD11	2.02	0.41
1:A:213:PRO:HB2	1:A:334:THR:CG2	2.47	0.41
1:A:278:LEU:HD11	1:A:292:LEU:HD11	2.02	0.41
1:A:123:ARG:HG2	1:A:123:ARG:HH21	1.85	0.41
2:B:36:A:H2'	2:B:37:YG:O4'	2.20	0.41
2:B:30:G:C2'	2:B:31:A:C5'	2.96	0.41
1:A:11:HIS:HA	1:A:75:HIS:HB3	2.03	0.41
1:A:187:LYS:HD3	1:A:187:LYS:HA	1.94	0.41
1:A:35:LEU:N	1:A:35:LEU:CD1	2.80	0.41
1:A:370:ASP:OD1	1:A:391:VAL:HG23	2.21	0.41
1:A:170:VAL:CG1	1:A:171:ARG:N	2.83	0.41
1:A:105:VAL:O	1:A:134:LEU:HA	2.20	0.41
1:A:19:HIS:ND1	1:A:20:VAL:N	2.68	0.41
1:A:134:LEU:HD13	1:A:134:LEU:HA	1.87	0.41
1:A:209:PRO:O	1:A:233:ARG:CD	2.69	0.41
1:A:277:LEU:HD22	2:B:76:A:N6	2.36	0.41
1:A:212:LEU:C	1:A:212:LEU:CD2	2.89	0.41
1:A:200:PRO:HG2	1:A:200:PRO:O	2.21	0.40
1:A:22:HIS:CB	1:A:106:ALA:HB2	2.38	0.40
1:A:19:HIS:HB2	1:A:115:THR:OG1	2.20	0.40
1:A:189:LEU:C	1:A:191:LEU:H	2.24	0.40
1:A:378:GLU:HB3	1:A:383:VAL:HG21	2.03	0.40
1:A:154:ARG:NH1	1:A:169:ILE:HD12	2.36	0.40
1:A:122:GLY:O	1:A:124:GLN:N	2.54	0.40
1:A:330:PHE:O	1:A:336:ASP:HA	2.21	0.40
1:A:201:GLU:HA	1:A:202:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:34:VAL:CG2	1:A:188:ILE:HG12	2.42	0.40
1:A:165:ASP:C	1:A:167:THR:H	2.24	0.40
2:B:18:G:C2'	2:B:57:G:N2	2.84	0.40
1:A:206:ILE:C	1:A:206:ILE:HD12	2.41	0.40
2:B:11:C:O2'	2:B:12:U:H5''	2.21	0.40
1:A:336:ASP:N	1:A:336:ASP:OD2	2.54	0.40
1:A:71:THR:CG2	1:A:74:ARG:N	2.83	0.40
1:A:175:LEU:HD12	1:A:176:LYS:N	2.37	0.40
1:A:269:ARG:N	1:A:269:ARG:CD	2.75	0.40
1:A:310:ILE:HG13	1:A:350:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	391/393 (100%)	294 (75%)	64 (16%)	33 (8%)	1 14

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	21	ASP
1	A	24	LYS
1	A	127	VAL
1	A	143	GLU
1	A	199	ILE
1	A	201	GLU
1	A	278	LEU
1	A	158	SER
1	A	161	ASP
1	A	206	ILE
1	A	5	PHE
1	A	39	TYR

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Mol	Chain	Res	Type
1	A	42	ALA
1	A	61	THR
1	A	178	LEU
1	A	264	LEU
1	A	47	ASP
1	A	142	ASP
1	A	177	ALA
1	A	181	ASP
1	A	205	ALA
1	A	258	VAL
1	A	262	ARG
1	A	30	ALA
1	A	60	ILE
1	A	314	ASP
1	A	4	LYS
1	A	8	THR
1	A	36	ALA
1	A	164	GLY
1	A	34	VAL
1	A	125	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
1	A	325/325 (100%)	280 (86%)	45 (14%)	5 25

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	13	ASN
1	A	20	VAL
1	A	33	THR
1	A	44	ARG
1	A	47	ASP
1	A	63	ASN
1	A	67	VAL

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Mol	Chain	Res	Type
1	A	68	GLU
1	A	70	ASP
1	A	73	THR
1	A	86	ASP
1	A	90	ASN
1	A	91	MET
1	A	97	GLN
1	A	109	ASP
1	A	123	ARG
1	A	125	VAL
1	A	139	MET
1	A	145	LEU
1	A	175	LEU
1	A	178	LEU
1	A	188	ILE
1	A	196	ASP
1	A	197	SER
1	A	198	TYR
1	A	200	PRO
1	A	211	LEU
1	A	223	ARG
1	A	233	ARG
1	A	236	ILE
1	A	238	VAL
1	A	249	GLU
1	A	256	THR
1	A	260	MET
1	A	269	ARG
1	A	277	LEU
1	A	283	ARG
1	A	311	LEU
1	A	313	LYS
1	A	323	PHE
1	A	324	LYS
1	A	359	VAL
1	A	361	THR
1	A	381	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS

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Mol	Chain	Res	Type
1	A	19	HIS
1	A	63	ASN
1	A	75	HIS
1	A	90	ASN
1	A	135	ASN
1	A	329	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	74/77 (96%)	15 (20%)	1 (1%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	G
2	B	8	U
2	B	9	A
2	B	12	U
2	B	18	G
2	B	19	G
2	B	20	G
2	B	21	A
2	B	31	A
2	B	43	G
2	B	46	7MG
2	B	47	U
2	B	48	C
2	B	69	U
2	B	72	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	18	G

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2MG	B	10	2	24,26,27	0.81	2 (8%)	32,38,41	5.13	4 (12%)
2	H2U	B	16	2	19,21,22	0.90	1 (5%)	27,30,33	0.80	0
2	H2U	B	17	2	19,21,22	0.78	1 (5%)	27,30,33	0.91	2 (7%)
2	M2G	B	26	2	25,27,28	0.89	2 (8%)	34,40,43	5.18	3 (8%)
2	OMC	B	32	2	20,22,23	0.96	2 (10%)	25,31,34	0.94	1 (4%)
2	OMG	B	34	2	24,26,27	0.83	0	32,38,41	5.02	3 (9%)
2	YG	B	37	2	40,42,43	1.92	9 (22%)	50,62,65	10.57	14 (28%)
2	PSU	B	39	2	19,21,22	1.61	3 (15%)	23,30,33	0.92	1 (4%)
2	5MC	B	40	2	20,22,23	0.98	3 (15%)	26,32,35	1.29	2 (7%)
2	7MG	B	46	2	24,26,27	2.49	2 (8%)	34,39,42	1.90	5 (14%)
2	5MC	B	49	2	20,22,23	1.06	2 (10%)	26,32,35	1.26	2 (7%)
2	PSU	B	55	2	19,21,22	1.71	3 (15%)	23,30,33	1.08	2 (8%)
2	MAD	B	58	2	23,25,26	0.99	1 (4%)	32,37,40	1.00	1 (3%)
2	PHA	B	77	2	11,11,11	0.61	0	13,13,13	0.60	0

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
2	2MG	B	10	2	-	0/10/27/28	0/1/3/3
2	H2U	B	16	2	-	0/8/38/39	0/2/2/2
2	H2U	B	17	2	-	0/8/38/39	0/2/2/2
2	M2G	B	26	2	-	0/12/29/30	0/1/3/3
2	OMC	B	32	2	-	0/8/27/28	0/2/2/2
2	OMG	B	34	2	-	0/10/27/28	0/1/3/3
2	YG	B	37	2	-	2/25/42/43	0/1/4/4
2	PSU	B	39	2	-	0/8/25/26	0/2/2/2
2	5MC	B	40	2	-	0/6/25/26	0/2/2/2
2	7MG	B	46	2	-	1/8/37/38	0/1/3/3
2	5MC	B	49	2	-	0/6/25/26	0/2/2/2
2	PSU	B	55	2	-	0/8/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAD	B	58	2	-	0/8/25/26	0/1/3/3
2	PHA	B	77	2	-	0/5/6/6	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46	7MG	C8-N9	-10.45	1.37	1.46
2	B	55	PSU	C6-N1	6.32	1.38	1.32
2	B	37	YG	O23-C21	-5.94	1.25	1.34
2	B	39	PSU	C6-N1	5.88	1.37	1.32
2	B	46	7MG	C8-N7	-5.48	1.30	1.45
2	B	37	YG	C12-C11	5.37	1.47	1.36
2	B	37	YG	C2-N3	-4.51	1.32	1.38
2	B	37	YG	C12-N1	-3.05	1.37	1.39
2	B	49	5MC	C2-N1	2.97	1.41	1.38
2	B	37	YG	O18-C16	-2.86	1.25	1.33
2	B	58	MAD	P-OP2	2.79	1.49	1.46
2	B	32	OMC	C2-N1	2.77	1.41	1.38
2	B	37	YG	C15-N20	2.57	1.51	1.45
2	B	55	PSU	C6-C5	-2.52	1.34	1.38
2	B	16	H2U	P-OP1	2.52	1.49	1.46
2	B	39	PSU	C6-C5	-2.38	1.34	1.38
2	B	40	5MC	C2-N1	2.32	1.40	1.38
2	B	39	PSU	P-OP1	2.30	1.49	1.46
2	B	37	YG	C10-C11	-2.27	1.45	1.50
2	B	55	PSU	P-OP1	2.26	1.49	1.46
2	B	37	YG	C2-N1	-2.22	1.36	1.39
2	B	40	5MC	P-OP1	2.17	1.49	1.46
2	B	49	5MC	C6-C5	-2.11	1.34	1.40
2	B	32	OMC	P-OP1	2.11	1.49	1.46
2	B	17	H2U	C1'-N1	2.09	1.49	1.45
2	B	40	5MC	C6-C5	-2.09	1.34	1.40
2	B	26	M2G	P-OP1	2.07	1.49	1.46
2	B	26	M2G	C2-N2	2.06	1.37	1.34
2	B	37	YG	P-OP1	2.03	1.49	1.46
2	B	10	2MG	C8-N7	-2.01	1.30	1.34
2	B	10	2MG	P-OP1	2.00	1.49	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	YG	C6-C5-N7	-73.60	130.32	134.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	M2G	C6-C5-N7	-28.96	130.24	134.14
2	B	10	2MG	C6-C5-N7	-28.41	130.31	134.14
2	B	34	OMG	C6-C5-N7	-27.73	130.41	134.14
2	B	26	M2G	C6-N1-C2	7.12	125.30	120.28
2	B	46	7MG	N7-C8-N9	7.02	112.36	103.08
2	B	40	5MC	C2-N3-C4	5.11	120.04	115.41
2	B	37	YG	C13-C12-C11	-5.09	123.87	131.05
2	B	49	5MC	C2-N3-C4	4.95	119.89	115.41
2	B	46	7MG	C2-N3-C4	-4.05	111.84	117.61
2	B	37	YG	C13-C12-N1	4.03	130.50	123.31
2	B	37	YG	O23-C21-N20	4.01	118.44	110.72
2	B	37	YG	O23-C21-O22	-3.96	119.55	124.64
2	B	37	YG	O18-C16-C15	3.63	121.52	111.59
2	B	58	MAD	C2-N3-C4	-3.35	110.51	116.23
2	B	37	YG	C11-C12-N1	-3.31	102.96	104.24
2	B	46	7MG	C6-N1-C2	3.24	125.17	119.51
2	B	34	OMG	C6-N1-C2	3.23	125.17	119.51
2	B	37	YG	C13-C14-C15	3.22	117.73	112.52
2	B	46	7MG	CM7-N7-C8	3.16	127.07	119.23
2	B	40	5MC	C6-N1-C2	3.16	120.17	118.62
2	B	46	7MG	C4-C5-N7	3.06	110.35	106.82
2	B	32	OMC	C2-N3-C4	3.05	119.99	115.57
2	B	10	2MG	C6-N1-C2	3.00	125.05	119.87
2	B	49	5MC	C6-N1-C2	2.88	120.04	118.62
2	B	37	YG	C14-C15-C16	-2.77	101.62	110.38
2	B	37	YG	C11-N2-C2	-2.66	103.94	107.23
2	B	55	PSU	O4'-C1'-C5	2.60	112.79	109.55
2	B	37	YG	C14-C13-C12	-2.42	105.96	112.95
2	B	37	YG	O18-C16-O17	-2.42	118.87	123.79
2	B	37	YG	C5-C6-N1	-2.42	111.42	117.68
2	B	10	2MG	CM2-N2-C2	-2.37	119.89	123.73
2	B	10	2MG	C2-N3-C4	-2.33	111.89	115.03
2	B	39	PSU	C5-C4-N3	-2.33	114.62	118.86
2	B	17	H2U	C2'-C1'-N1	2.22	119.68	114.59
2	B	34	OMG	C2-N3-C4	-2.19	112.02	115.09
2	B	17	H2U	C1'-N1-C2	2.16	121.20	118.16
2	B	26	M2G	C2-N3-C4	-2.11	112.16	115.14
2	B	55	PSU	C5-C4-N3	-2.10	115.04	118.86
2	B	37	YG	C3-N3-C4	2.07	125.80	121.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	37	YG	C24-O23-C21-N20
2	B	37	YG	C24-O23-C21-O22
2	B	46	7MG	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
3	KIR	A	1394	-	59,59,59	3.44	17 (28%)	82,84,84	1.71	17 (20%)
4	SUC	A	1396	-	24,24,24	0.87	1 (4%)	36,36,36	0.61	0
5	GNP	A	1397	6	34,34,34	1.81	9 (26%)	50,54,54	4.81	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KIR	A	1394	-	-	0/53/98/98	0/3/3/3
4	SUC	A	1396	-	-	0/12/51/51	0/2/2/2
5	GNP	A	1397	6	-	0/18/38/38	0/1/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1394	KIR	O18-C17	-14.41	1.21	1.44
3	A	1394	KIR	O34-C33	-13.59	1.25	1.44
3	A	1394	KIR	O30-C30	-11.99	1.16	1.42
3	A	1394	KIR	C45-C28	4.89	1.60	1.54
5	A	1397	GNP	PG-O1G	4.61	1.51	1.46
3	A	1394	KIR	C22-C21	3.91	1.37	1.34
3	A	1394	KIR	C27-N26	3.90	1.42	1.33
5	A	1397	GNP	PG-N3B	3.76	1.67	1.64
5	A	1397	GNP	C6-N1	3.51	1.43	1.37
3	A	1394	KIR	C19-C20	3.41	1.59	1.53
5	A	1397	GNP	PB-O1B	3.20	1.50	1.46
3	A	1394	KIR	C19-C17	3.11	1.61	1.54
3	A	1394	KIR	O29-C29	3.04	1.46	1.40
3	A	1394	KIR	C37-C38	2.97	1.37	1.32
5	A	1397	GNP	PG-O2G	-2.86	1.46	1.55
3	A	1394	KIR	C29-C28	2.85	1.62	1.55
5	A	1397	GNP	C2-N3	2.79	1.37	1.33
3	A	1394	KIR	C42-C19	2.63	1.59	1.53
3	A	1394	KIR	C6-C5	2.57	1.44	1.37
4	A	1396	SUC	O5-C1	2.53	1.48	1.41
3	A	1394	KIR	C5-C4	2.36	1.44	1.39
5	A	1397	GNP	C8-N7	-2.34	1.30	1.34
3	A	1394	KIR	C9-C8	2.23	1.40	1.34
3	A	1394	KIR	C8-C7	2.16	1.53	1.47
3	A	1394	KIR	C6-N1	2.13	1.37	1.33
5	A	1397	GNP	PB-N3B	2.11	1.66	1.64
5	A	1397	GNP	C2-N1	2.07	1.40	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1397	GNP	C6-C5-N7	-32.43	129.77	134.14
3	A	1394	KIR	C45-C28-C27	6.38	112.75	108.10
3	A	1394	KIR	C3-C2-N1	5.24	119.81	115.40
5	A	1397	GNP	O1G-PG-N3B	-4.76	104.63	111.83
3	A	1394	KIR	O29-C29-O34	-4.05	103.63	110.22
5	A	1397	GNP	O3G-PG-O2G	3.85	118.70	107.66
3	A	1394	KIR	C29-C30-C31	-3.24	106.37	110.65
3	A	1394	KIR	C11-C10-C9	-3.23	116.21	123.36
3	A	1394	KIR	O34-C33-C32	3.14	114.89	112.04
5	A	1397	GNP	O4'-C1'-N9	3.13	111.35	108.44
5	A	1397	GNP	O2G-PG-O1G	-2.81	106.38	113.60
3	A	1394	KIR	O34-C29-C28	2.80	112.24	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1397	GNP	O3G-PG-O1G	-2.77	106.49	113.60
5	A	1397	GNP	C6-N1-C2	2.76	124.33	119.51
3	A	1394	KIR	C44-C21-C20	2.74	120.25	115.58
3	A	1394	KIR	C23-C22-C21	-2.74	124.13	127.61
3	A	1394	KIR	O20-C20-C21	-2.64	107.26	111.07
3	A	1394	KIR	C16-C15-C14	-2.41	98.84	101.77
3	A	1394	KIR	O4-C4-C3	-2.37	119.33	121.72
3	A	1394	KIR	C22-C23-C24	-2.33	119.28	124.26
3	A	1394	KIR	C48-C32-C47	-2.32	103.78	107.70
3	A	1394	KIR	C20-C21-C22	-2.29	117.04	118.92
3	A	1394	KIR	O18-C17-C16	2.27	108.96	104.12
3	A	1394	KIR	C29-O34-C33	2.21	119.88	115.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/393 (100%)	-0.24	0 100 100	2, 25, 64, 90	0
2	B	77/77 (100%)	0.55	10 (12%) 4 2	8, 39, 184, 199	0
All	All	470/470 (100%)	-0.11	10 (2%) 60 24	2, 27, 80, 199	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	U	4.8
2	B	36	A	4.1
2	B	35	A	3.4
2	B	38	A	3.0
2	B	32	OMC	2.9
2	B	20	G	2.5
2	B	28	C	2.5
2	B	30	G	2.4
2	B	45	G	2.3
2	B	31	A	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	H2U	B	17	20/21	0.25	8.80	57,69,86,87	0
2	MAD	B	58	23/24	0.23	2.43	13,22,33,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	YG	B	37	39/40	0.73	1.84	194,198,199,199	0
2	OMC	B	32	21/22	0.63	1.34	174,188,190,195	0
2	7MG	B	46	24/25	0.29	1.11	41,51,60,68	0
2	M2G	B	26	25/26	0.34	0.35	55,68,72,81	0
2	2MG	B	10	24/25	0.24	0.18	20,40,49,65	0
2	PHA	B	77	11/11	0.19	0.00	1,14,23,23	0
2	PSU	B	55	20/21	0.20	-0.10	17,35,43,49	0
2	5MC	B	49	21/22	0.17	-0.65	0,16,22,34	0
2	H2U	B	16	20/21	0.20	-0.88	52,59,63,67	0
2	OMG	B	34	24/25	0.48	-1.04	176,182,190,193	0
2	PSU	B	39	20/21	0.31	-3.25	142,149,168,170	0
2	5MC	B	40	21/22	0.23	-4.50	140,149,159,159	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	KIR	A	1394	57/57	0.27	1.76	7,21,40,48	0
5	GNP	A	1397	32/32	0.19	-0.28	26,36,47,50	0
6	MG	A	1398	1/1	0.17	-0.46	7,7,7,7	0
4	SUC	A	1396	23/23	0.17	-0.47	34,45,50,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.