



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:17 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 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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

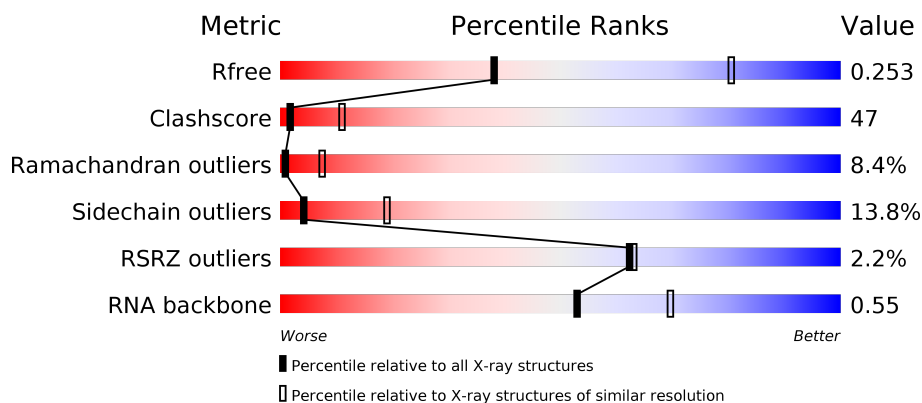
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)
RNA backbone	2435	1005 (3.90-2.82)

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. 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	A	393	<div> <div>12%</div> <div>33%</div> <div>52%</div> <div>14%</div> <div>.</div> </div>
2	B	77	<div> <div>26%</div> <div>62%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4810 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 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

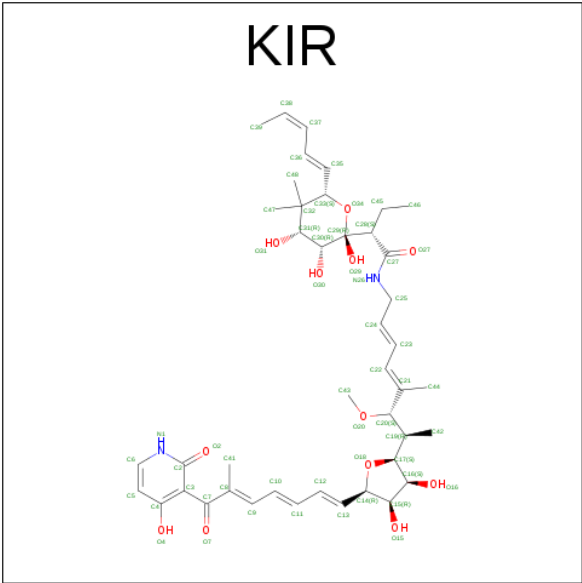
There is a discrepancy between the modelled and reference sequences:

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

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

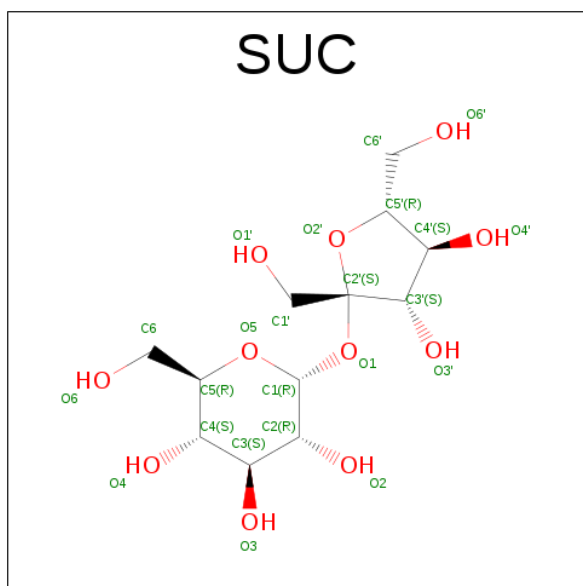
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	77	1662	754	295	537	76	0	0	0

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



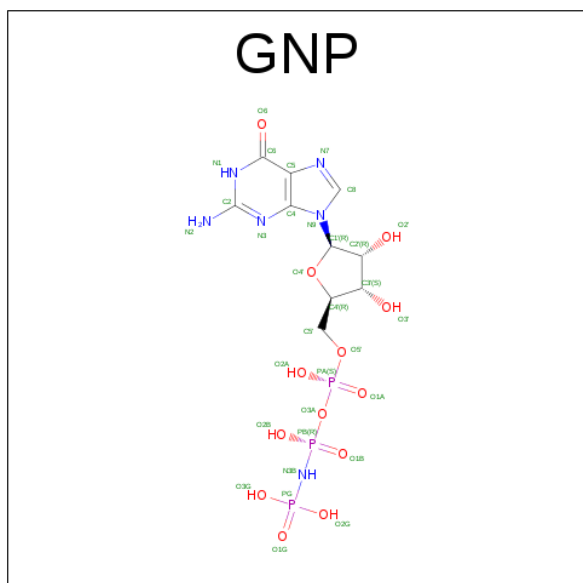
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			57	43	2	12		

- 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 PHOSPHOAMINOPHOSPHONIC ACID-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		

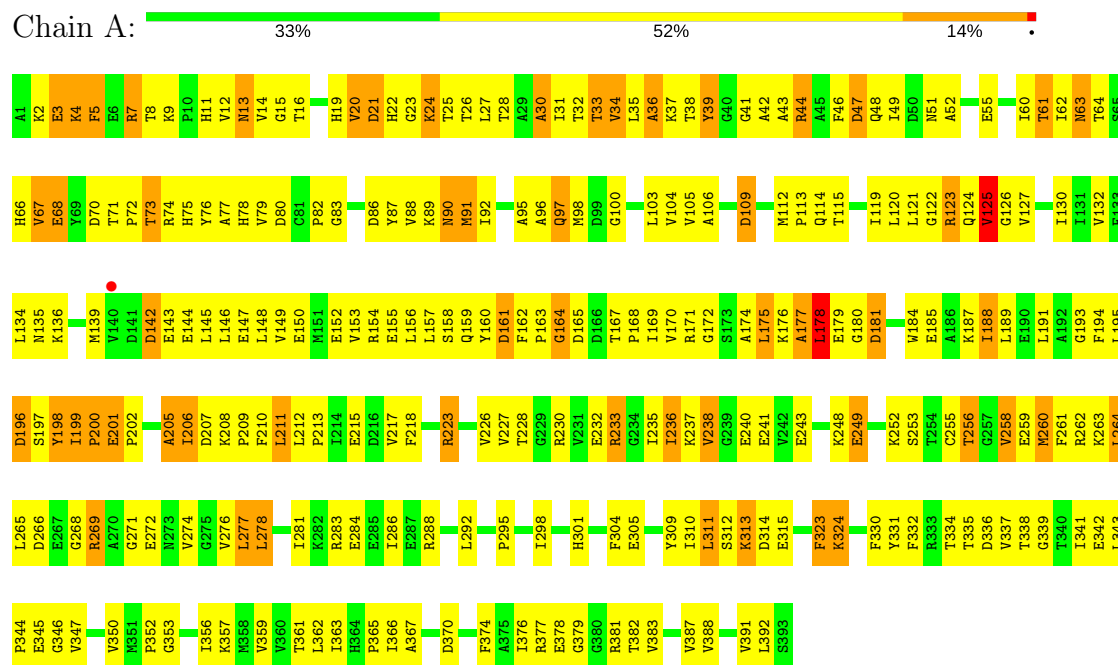
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

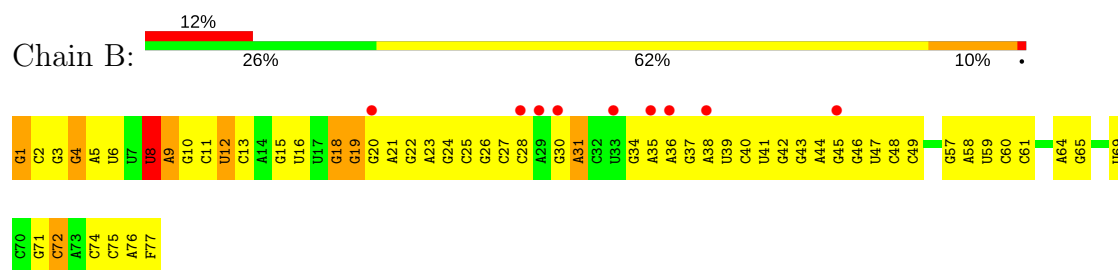
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ELONGATION FACTOR TU



• Molecule 2: TRANSFER-RNA, PHE



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 0.213 , 0.253	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 , 76.4	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	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.

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: OMC, GNP, SUC, H2U, KIR, PHA, MG, YG, 2MG, 5MC, 1MA, 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	1/1509 (0.1%)	0.72	0/2349
All	All	0.52	1/4600 (0.0%)	0.78	0/6531

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 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	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

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 47.

All (413) 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)
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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
1:A:223:ARG:HD3	2:B:76:A:H62	1.49	0.76
2:B:9:A:O2'	2:B:10:2MG:N7	2.18	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:20:VAL:HG12	1:A:21:ASP:H	1.55	0.72
1:A:95:ALA:HA	1:A:98:MET:HG3	1.70	0.72
1:A:211:LEU:HD12	1:A:212:LEU:N	2.05	0.71
1:A:261:PHE:O	1:A:263:LYS:HG3	1.88	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:205:ALA:O	1:A:206:ILE:HG13	1.91	0.70
1:A:213:PRO:HB2	1:A:334:THR:HG23	1.74	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:34:VAL:HG11	1:A:188:ILE:CG2	2.23	0.69
1:A:170:VAL:HG21	1:A:191:LEU:HB2	1.73	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:H	1.57	0.69
2:B:74:C:O2'	2:B:75:C:H5'	1.93	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLY:HA2	2:B:64:A:O4'	1.94	0.68
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:58:1MA: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:212:LEU:HD23	1:A:212:LEU:C	2.19	0.63
1:A:19:HIS:HB3	1:A:22:HIS:NE2	2.14	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:168:PRO:HB2	1:A:194:PHE:HD1	1.66	0.60
1:A:191:LEU:C	1:A:193:GLY:H	2.04	0.60
1:A:191:LEU:C	1:A:193:GLY:N	2.54	0.60
1:A:74:ARG:HH21	1:A:199:ILE:HD12	1.67	0.60
1:A:71:THR:CG2	1:A:74:ARG:H	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:G:H2'	2:B:57:G:H22	1.66	0.59
1:A:168:PRO:HB2	1:A:194:PHE:CD1	2.36	0.59
1:A:35:LEU:HD12	1:A:35:LEU:N	2.18	0.59
2:B:3:G:C3'	2:B:4:G:H5''	2.32	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
1:A:248:LYS:HG2	1:A:249:GLU:H	1.69	0.57
1:A:89:LYS:NZ	1:A:336:ASP:OD1	2.38	0.57
2:B:35:A:O2'	2:B:36:A:H5'	2.04	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: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:71:THR:HG22	1:A:74:ARG:O	2.04	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:209:PRO:HG2	1:A:233:ARG:NH2	2.19	0.56
1:A:243:GLU:HG3	1:A:295:PRO:HG3	1.87	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:24:LYS:NZ	1:A:83:GLY:HA3	2.20	0.56
1:A:92:ILE:CG1	1:A:121:LEU:HD13	2.35	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:178:LEU:O	1:A:178:LEU:HD23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:O	1:A:189:LEU:HD12	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
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:H	1:A:269:ARG:HD3	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:142:ASP:C	1:A:144:GLU:N	2.62	0.52
1:A:5:PHE:HD1	1:A:263:LYS:HD2	1.75	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:123:ARG:HD2	3:A:1394:KIR:C42	2.39	0.51
1:A:200:PRO:O	1:A:201:GLU:O	2.28	0.51
1:A:256:THR:O	1:A:256:THR:CG2	2.59	0.51
1:A:34:VAL:HG21	1:A:188:ILE:CG1	2.37	0.51
1:A:13:ASN:CB	1:A:77:ALA:HB3	2.35	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
1:A:376:ILE:HG22	1:A:383:VAL:HB	1.92	0.51
1:A:62:ILE:HG21	2:B:2:C:H4'	1.92	0.51
2:B:18:G:O2'	2:B:57:G:N2	2.43	0.51
2:B:11:C:H2'	2:B:12:U:C5'	2.37	0.51
1:A:96:ALA:HB2	1:A:125:VAL:HG21	1.92	0.51
2:B:39:PSU:H2'	2:B:40:5MC:C6	2.45	0.51
1:A:188:ILE:HG22	1:A:189:LEU:N	2.25	0.50
1:A:24:LYS:HZ3	1:A:83:GLY:HA3	1.76	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:164:GLY:O	1:A:167:THR:HB	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PHE:CD2	1:A:194:PHE:N	2.80	0.50
1:A:232:GLU:HG2	1:A:233:ARG:HG3	1.93	0.50
1:A:298:ILE:CD1	1:A:367:ALA:HB1	2.42	0.50
2:B:12:U:H2'	2:B:13:C:O5'	2.11	0.50
1:A:261:PHE:HA	2:B:77:PHA:O	2.11	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
1:A:194:PHE:HD2	1:A:194:PHE:N	2.10	0.49
1:A:35:LEU:H	1:A:35:LEU:CD1	2.26	0.49
2:B:37:YG:H31	2:B:37:YG:C2'	2.43	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:O	1:A:298:ILE:HG23	2.11	0.49
1:A:175:LEU:HD12	1:A:176:LYS:H	1.77	0.49
1:A:16:THR:HG23	1:A:78:HIS:NE2	2.28	0.49
1:A:153:VAL:O	1:A:156:LEU:HB3	2.14	0.48
1:A:205:ALA:O	1:A:207:ASP:N	2.39	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:30:G:H2'	2:B:31:A:H5'	1.95	0.48
2:B:71:G:C2'	2:B:72:C:H5''	2.44	0.48
1:A:205:ALA:CB	1:A:233:ARG:HB3	2.43	0.48
1:A:71:THR:HG21	1:A:196:ASP:OD1	2.14	0.48
1:A:125:VAL:CG1	1:A:126:GLY:N	2.76	0.48
1:A:37:LYS:C	1:A:39:TYR:H	2.16	0.48
1:A:51:ASN:N	1:A:51:ASN:OD1	2.47	0.48
2:B:24:G:H2'	2:B:25:C:C6	2.49	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
1:A:277:LEU:HD22	2:B:76:A:H61	1.79	0.47
2:B:12:U:C2'	2:B:13:C:O5'	2.62	0.47
1:A:23:GLY:O	1:A:24:LYS:C	2.52	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:24:LYS:HG3	1:A:104:VAL:HG11	1.94	0.47
1:A:311:LEU:H	1:A:311:LEU:HD23	1.79	0.47
2:B:1:G:O2'	2:B:2:C:H5'	2.15	0.47
2:B:39:PSU:O2'	2:B:40:5MC:H5'	2.15	0.47
1:A:66:HIS:HB2	2:B:77:PHA:CE2	2.44	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:235:ILE:O	1:A:235:ILE:HD12	2.15	0.47
1:A:24:LYS:HB2	1:A:24:LYS:HE3	1.73	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
1:A:168:PRO:CB	1:A:194:PHE:HD1	2.28	0.47
1:A:31:ILE:O	1:A:35:LEU:HD13	2.15	0.47
2:B:34:OMG:HM22	2:B:35:A:O4'	2.15	0.47
1:A:337:VAL:HG11	1:A:366:ILE:HD12	1.97	0.46
1:A:377:ARG:HE	1:A:382:THR:CG2	2.29	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
1:A:26:THR:HG23	5:A:1397:GNP:O1A	2.15	0.46
1:A:2:LYS:O	1:A:3:GLU:O	2.32	0.46
2:B:26:M2G:HM23	2:B:27:C:H1'	1.97	0.46
2:B:74:C:C2'	2:B:75:C:H5'	2.45	0.46
1:A:114:GLN:HA	1:A:114:GLN:OE1	2.15	0.46
1:A:377:ARG:HE	1:A:382:THR:HG23	1.80	0.46
1:A:236:ILE:HD11	1:A:268:GLY:HA3	1.97	0.46
1:A:26:THR:HG22	1:A:46:PHE:CD1	2.50	0.46
1:A:12:VAL:O	1:A:76:TYR:HA	2.15	0.46
1:A:148:LEU:HD23	1:A:148:LEU:C	2.36	0.46
1:A:323:PHE:HD1	1:A:323:PHE:N	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:19:HIS:CD2	1:A:112:MET:HB2	2.51	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
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
1:A:243:GLU:OE1	1:A:295:PRO:HA	2.16	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: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:9:LYS:HD3	1:A:72:PRO:O	2.16	0.45
1:A:156:LEU:O	1:A:157:LEU:C	2.55	0.45
1:A:227:VAL:HG11	1:A:286:ILE:CD1	2.45	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:260:MET:O	1:A:261:PHE:HB2	2.16	0.44
1:A:331:TYR:CE2	1:A:377:ARG:HB2	2.51	0.44
2:B:23:A:H2'	2:B:24:G:C8	2.52	0.44
1:A:11:HIS:CE1	1:A:13:ASN:ND2	2.84	0.44
1:A:71:THR:HG23	1:A:73:THR:H	1.82	0.44
1:A:34:VAL:CG2	1:A:188:ILE:HG21	2.48	0.44
1:A:5:PHE:HB2	1:A:263:LYS:CB	2.47	0.44
1:A:256:THR:O	1:A:256:THR:HG23	2.17	0.44
1:A:387:VAL:HG22	1:A:388:VAL:N	2.32	0.44
1:A:259:GLU:OE1	2:B:76:A:C8	2.70	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:132:VAL:HG11	1:A:153:VAL:HG11	1.99	0.44
1:A:188:ILE:HG22	1:A:189:LEU:HD12	1.99	0.44
1:A:146:LEU:O	1:A:149:VAL:HG22	2.17	0.44
1:A:76:TYR:OH	1:A:195:LEU:O	2.33	0.44
1:A:64:THR:HA	1:A:80:ASP:O	2.18	0.44
1:A:134:LEU:HD23	1:A:169:ILE:HG21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLU:OE1	1:A:252:LYS:HE2	2.17	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
1:A:256:THR:HG22	1:A:277:LEU:CB	2.48	0.43
1:A:13:ASN:ND2	1:A:271:GLY:O	2.50	0.43
1:A:288:ARG:HE	1:A:335:THR:CG2	2.31	0.43
2:B:40:5MC:H2'	2:B:41:U:H6	1.83	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: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:46:PHE:O	1:A:49:ILE:N	2.51	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:177:ALA:O	1:A:180:GLY:N	2.51	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:33:THR:HG23	1:A:43:ALA:HB1	1.99	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: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:123:ARG:NH2	1:A:123:ARG:HG2	2.34	0.43
1:A:184:TRP:O	1:A:185:GLU:C	2.57	0.43
2:B:38:A:H2'	2:B:39:PSU:O4'	2.18	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:38:THR:CB	1:A:189:LEU:HD21	2.49	0.42
1:A:263:LYS:HE3	4:A:1396:SUC:O4'	2.19	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:120:LEU:HD11	1:A:124:GLN:NE2	2.34	0.42
1:A:71:THR:HG23	1:A:74:ARG:H	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:G:H2'	2:B:58:1MA: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:154:ARG:O	1:A:155:GLU:C	2.58	0.42
1:A:172:GLY:HA2	1:A:184:TRP:HZ3	1.83	0.42
1:A:180:GLY:O	1:A:181:ASP:C	2.57	0.42
1:A:324:LYS:HD2	1:A:343:LEU:H	1.85	0.42
1:A:7:ARG:H	1:A:7:ARG:HD3	1.79	0.42
1:A:109:ASP:N	1:A:109:ASP:OD1	2.53	0.42
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: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: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
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:46:PHE:O	1:A:48:GLN:N	2.53	0.41
2:B:8:U:C2	2:B:15:G:O6	2.73	0.41
1:A:103:LEU:HD22	1:A:119:ILE:HD11	2.02	0.41
1:A:35:LEU:C	1:A:37:LYS:N	2.74	0.41
1:A:15:GLY:N	1:A:98:MET:CE	2.83	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:30:G:C2'	2:B:31:A:C5'	2.96	0.41
2:B:36:A:H2'	2:B:37:YG:O4'	2.20	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:105:VAL:O	1:A:134:LEU:HA	2.20	0.41
1:A:170:VAL:CG1	1:A:171:ARG:N	2.83	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:212:LEU:C	1:A:212:LEU:CD2	2.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:ARG:NH1	1:A:169:ILE:HD12	2.36	0.40
1:A:189:LEU:C	1:A:191:LEU:H	2.24	0.40
1:A:200:PRO:HG2	1:A:200:PRO:O	2.21	0.40
1:A:378:GLU:HB3	1:A:383:VAL:HG21	2.03	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:165:ASP:C	1:A:167:THR:H	2.24	0.40
1:A:34:VAL:CG2	1:A:188:ILE:HG12	2.42	0.40
1:A:201:GLU:HA	1:A:202:PRO:HD3	1.91	0.40
2:B:18:G:C2'	2:B:57:G:N2	2.84	0.40
1:A:206:ILE:HD12	1:A:206:ILE:C	2.41	0.40
1:A:336:ASP:N	1:A:336:ASP:OD2	2.54	0.40
2:B:11:C:O2'	2:B:12:U:H5''	2.21	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
1:A:71:THR:CG2	1:A:74:ARG:N	2.83	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
1	A	391/393 (100%)	294 (75%)	64 (16%)	33 (8%)	1 7

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	21	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
-----	-------	----------	-----------	----------	-------------

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	325/325 (100%)	280 (86%)	45 (14%)	4 19

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	75/77 (97%)	15 (20%)	0

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	46	7MG
2	B	47	U
2	B	48	C
2	B	69	U
2	B	72	C

There are no RNA pucker outliers to report.

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	19,26,27	1.06	2 (10%)	20,38,41	2.65	5 (25%)
2	H2U	B	16	2	17,21,22	0.61	0	21,30,33	0.69	0
2	H2U	B	17	2	17,21,22	0.49	0	21,30,33	0.71	0
2	M2G	B	26	2	20,27,28	1.17	3 (15%)	21,40,43	2.69	4 (19%)
2	OMC	B	32	2	15,22,23	0.73	0	19,31,34	0.70	0
2	OMG	B	34	2	18,26,27	1.10	1 (5%)	22,38,41	2.50	5 (22%)
2	YG	B	37	2	29,42,43	1.64	4 (13%)	29,62,65	2.18	10 (34%)
2	PSU	B	39	2	16,21,22	1.19	2 (12%)	20,30,33	6.04	4 (20%)
2	5MC	B	40	2	15,22,23	0.79	1 (6%)	17,32,35	0.51	0
2	7MG	B	46	2	20,26,27	1.68	3 (15%)	22,39,42	2.23	2 (9%)
2	5MC	B	49	2	15,22,23	0.92	1 (6%)	17,32,35	0.60	0
2	PSU	B	55	2	16,21,22	1.23	2 (12%)	20,30,33	6.06	4 (20%)
2	1MA	B	58	2	16,25,26	0.98	1 (6%)	13,37,40	1.37	1 (7%)
2	PHA	B	77	2	11,11,11	0.55	0	12,13,13	0.57	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	-	0/5/27/28	0/3/3/3
2	H2U	B	16	2	-	0/7/38/39	0/2/2/2
2	H2U	B	17	2	-	0/7/38/39	0/2/2/2
2	M2G	B	26	2	-	0/7/29/30	0/3/3/3
2	OMC	B	32	2	-	0/5/27/28	0/2/2/2
2	OMG	B	34	2	-	0/5/27/28	0/3/3/3
2	YG	B	37	2	-	2/20/42/43	0/4/4/4
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
2	5MC	B	40	2	-	0/3/25/26	0/2/2/2
2	7MG	B	46	2	-	0/7/37/38	0/3/3/3
2	5MC	B	49	2	-	0/3/25/26	0/2/2/2
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2
2	1MA	B	58	2	-	0/3/25/26	0/3/3/3
2	PHA	B	77	2	-	0/4/6/6	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	YG	O23-C21	-6.01	1.25	1.34
2	B	46	7MG	C8-N9	-5.16	1.37	1.45
2	B	55	PSU	C6-C5	-3.18	1.34	1.38
2	B	37	YG	O18-C16	-3.02	1.25	1.33
2	B	39	PSU	C6-C5	-2.99	1.34	1.38
2	B	46	7MG	C8-N7	-2.97	1.30	1.43
2	B	37	YG	C10-C11	-2.51	1.45	1.50
2	B	49	5MC	C6-C5	-2.17	1.34	1.40
2	B	10	2MG	C8-N7	-2.15	1.30	1.34
2	B	40	5MC	C6-C5	-2.14	1.34	1.40
2	B	26	M2G	C8-N7	-2.06	1.30	1.34
2	B	26	M2G	C2-N1	2.04	1.38	1.34
2	B	55	PSU	C4-N3	2.50	1.37	1.33
2	B	37	YG	C15-N20	2.65	1.51	1.45
2	B	58	1MA	C6-N6	2.72	1.33	1.27
2	B	39	PSU	C4-N3	2.91	1.38	1.33
2	B	10	2MG	C6-N1	3.24	1.38	1.33
2	B	46	7MG	C6-N1	3.39	1.39	1.33
2	B	26	M2G	C6-N1	3.71	1.39	1.33
2	B	34	OMG	C6-N1	3.72	1.39	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	PSU	N1-C2-N3	-18.86	114.84	128.40
2	B	39	PSU	N1-C2-N3	-18.65	114.99	128.40
2	B	39	PSU	C5-C4-N3	-13.18	114.62	125.43
2	B	55	PSU	C5-C4-N3	-12.67	115.04	125.43
2	B	34	OMG	C5-C6-N1	-8.38	111.55	123.48
2	B	26	M2G	C5-C6-N1	-8.32	111.64	123.48
2	B	10	2MG	C5-C6-N1	-8.31	111.65	123.48
2	B	46	7MG	C5-C6-N1	-7.65	111.36	123.37
2	B	37	YG	C13-C12-C11	-3.90	123.87	130.66
2	B	58	1MA	C2-N3-C4	-3.84	110.51	116.41
2	B	37	YG	O23-C21-O22	-3.69	119.55	124.60
2	B	10	2MG	CM2-N2-C2	-3.08	119.89	123.63
2	B	37	YG	C14-C15-C16	-2.93	101.62	110.29
2	B	10	2MG	C2-N3-C4	-2.83	111.89	115.11
2	B	37	YG	C14-C13-C12	-2.76	105.96	113.01
2	B	34	OMG	C2-N3-C4	-2.69	112.02	115.16
2	B	26	M2G	C2-N3-C4	-2.59	112.16	115.11
2	B	37	YG	O18-C16-O17	-2.46	118.87	123.82
2	B	34	OMG	N3-C2-N1	-2.43	123.91	127.46
2	B	34	OMG	C6-C5-C4	-2.05	118.81	120.84
2	B	37	YG	C13-C14-C15	2.24	117.73	113.18
2	B	26	M2G	N3-C2-N2	2.75	119.99	117.15
2	B	37	YG	C3-N3-C2	2.76	122.25	118.31
2	B	10	2MG	N2-C2-N3	3.45	120.31	116.95
2	B	55	PSU	C6-N1-C2	3.50	120.96	115.36
2	B	39	PSU	C6-N1-C2	3.58	121.09	115.36
2	B	37	YG	O18-C16-C15	3.78	121.52	111.54
2	B	37	YG	O23-C21-N20	3.98	118.44	110.82
2	B	37	YG	C3-N3-C4	5.26	125.80	118.31
2	B	10	2MG	C6-N1-C2	5.51	125.05	115.18
2	B	34	OMG	C6-N1-C2	6.33	125.17	116.06
2	B	46	7MG	C6-N1-C2	6.34	125.17	116.06
2	B	26	M2G	C6-N1-C2	7.66	125.30	116.18
2	B	39	PSU	C4-N3-C2	13.57	127.03	115.16
2	B	55	PSU	C4-N3-C2	13.76	127.19	115.16

There are no chirality outliers.

All (2) 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

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	10	2MG	1	0
2	B	16	H2U	1	0
2	B	26	M2G	1	0
2	B	34	OMG	1	0
2	B	37	YG	5	0
2	B	39	PSU	4	0
2	B	40	5MC	5	0
2	B	49	5MC	1	0
2	B	58	1MA	2	0
2	B	77	PHA	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	53,59,59	3.19	14 (26%)	57,84,84	1.60	13 (22%)
4	SUC	A	1396	-	24,24,24	0.91	1 (4%)	36,36,36	0.62	0
5	GNP	A	1397	6	27,34,34	2.76	8 (29%)	26,54,54	1.81	5 (19%)

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	-	-	0/54/98/98	0/3/3/3
4	SUC	A	1396	-	-	0/12/51/51	0/2/2/2
5	GNP	A	1397	6	-	0/16/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1394	KIR	O18-C17	-15.55	1.21	1.44
3	A	1394	KIR	O30-C30	-12.66	1.16	1.42
5	A	1397	GNP	C4-N9	-7.64	1.37	1.47
5	A	1397	GNP	C5-C6	-5.50	1.43	1.53
5	A	1397	GNP	PG-O2G	-3.61	1.46	1.56
5	A	1397	GNP	C8-N9	-2.83	1.38	1.46
5	A	1397	GNP	PG-O3G	-2.54	1.49	1.56
3	A	1394	KIR	C16-C17	2.01	1.57	1.53
3	A	1394	KIR	C8-C7	2.18	1.53	1.48
3	A	1394	KIR	C37-C38	2.43	1.37	1.32
3	A	1394	KIR	C5-C4	2.47	1.44	1.39
4	A	1396	SUC	O5-C1	2.61	1.48	1.41
3	A	1394	KIR	C5-C6	2.61	1.44	1.38
3	A	1394	KIR	C42-C19	2.62	1.59	1.53
3	A	1394	KIR	C19-C17	2.63	1.61	1.54
3	A	1394	KIR	C2-N1	3.00	1.38	1.33
3	A	1394	KIR	O29-C29	3.21	1.46	1.40
3	A	1394	KIR	C22-C21	3.46	1.37	1.33
5	A	1397	GNP	PB-O1B	3.52	1.50	1.46
3	A	1394	KIR	C27-N26	4.10	1.42	1.33
3	A	1394	KIR	C45-C28	4.77	1.60	1.54
5	A	1397	GNP	PG-O1G	5.06	1.51	1.46
5	A	1397	GNP	C6-N1	5.99	1.43	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1397	GNP	O1G-PG-N3B	-4.79	104.63	111.79
3	A	1394	KIR	O29-C29-O34	-3.89	103.63	110.22
3	A	1394	KIR	C11-C10-C9	-3.40	116.21	123.46
3	A	1394	KIR	C29-C30-C31	-3.24	106.37	110.70
3	A	1394	KIR	C5-C6-N1	-2.82	120.67	123.92
5	A	1397	GNP	O2G-PG-O1G	-2.77	106.38	113.41
5	A	1397	GNP	O3G-PG-O1G	-2.72	106.49	113.41
3	A	1394	KIR	C48-C32-C47	-2.57	103.78	107.72
3	A	1394	KIR	C16-C15-C14	-2.54	98.84	101.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1394	KIR	O4-C4-C3	-2.27	119.33	121.83
3	A	1394	KIR	C14-C13-C12	-2.03	121.37	125.61
3	A	1394	KIR	O18-C17-C16	2.40	108.96	104.24
3	A	1394	KIR	C44-C21-C20	2.70	120.25	115.69
3	A	1394	KIR	C6-N1-C2	2.76	122.87	116.60
3	A	1394	KIR	C45-C28-C27	2.99	112.75	108.67
3	A	1394	KIR	O34-C33-C32	3.16	114.89	112.18
5	A	1397	GNP	O6-C6-C5	3.74	126.85	119.69
5	A	1397	GNP	O3G-PG-O2G	3.93	118.70	107.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1394	KIR	3	0
4	A	1396	SUC	1	0
5	A	1397	GNP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.30	1 (0%) 93 95	2, 25, 64, 90	0
2	B	63/77 (81%)	0.66	9 (14%) 3 3	8, 36, 170, 199	0
All	All	456/470 (97%)	-0.16	10 (2%) 62 63	2, 26, 77, 199	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	U	5.6
2	B	36	A	4.1
2	B	35	A	3.6
2	B	38	A	3.3
2	B	20	G	3.3
2	B	28	C	2.9
2	B	45	G	2.5
2	B	30	G	2.5
1	A	140	VAL	2.3
2	B	29	A	2.3

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	2MG	B	10	24/25	0.95	0.26	-	20,40,49,65	0
2	5MC	B	40	21/22	0.82	0.20	-	140,149,159,159	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	OMG	B	34	24/25	0.46	0.53	-	176,182,190,193	0
2	OMC	B	32	21/22	0.56	0.58	-	174,188,190,195	0
2	H2U	B	16	20/21	0.95	0.21	-	52,59,63,67	0
2	5MC	B	49	21/22	0.98	0.19	-	0,16,22,34	0
2	PHA	B	77	11/11	0.97	0.19	-	1,14,23,23	0
2	PSU	B	39	20/21	0.71	0.30	-	142,149,168,170	0
2	7MG	B	46	24/25	0.95	0.30	-	41,51,60,68	0
2	1MA	B	58	23/24	0.97	0.24	-	13,22,33,41	0
2	YG	B	37	39/40	0.58	0.74	-	194,198,199,199	0
2	M2G	B	26	25/26	0.94	0.32	-	55,68,72,81	0
2	PSU	B	55	20/21	0.97	0.21	-	17,35,43,49	0
2	H2U	B	17	20/21	0.94	0.23	-	57,69,86,87	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	KIR	A	1394	57/57	0.93	0.29	1.58	7,21,40,48	0
5	GNP	A	1397	32/32	0.94	0.21	-0.14	26,36,47,50	0
4	SUC	A	1396	23/23	0.94	0.17	-0.51	34,45,50,51	0
6	MG	A	1398	1/1	0.95	0.17	-0.52	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.