



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:47 PM GMT

PDB ID : 3V11
Title : Structure of the ternary initiation complex AIF2:GDPNP:methionylate
dinitiator TRNA
Authors : Mechulam, Y.; Schmitt, E.
Deposited on : 2011-12-09
Resolution : 5.00 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>

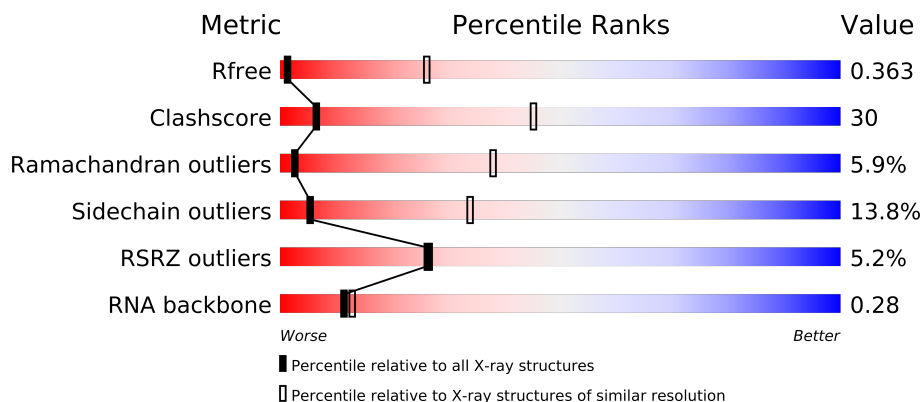
The following versions of software and data (see [references](#)) were used in the production of this report:

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

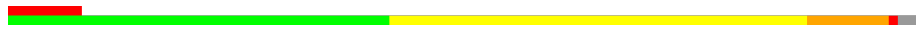
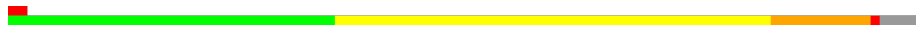


The reported resolution of this entry is 5.00 Å.

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	1052 (6.50-3.50)
Clashscore	79885	1327 (6.50-3.50)
Ramachandran outliers	78287	1242 (6.50-3.50)
Sidechain outliers	78261	1221 (6.50-3.50)
RSRZ outliers	66119	1051 (6.50-3.50)
RNA backbone	1838	1037 (7.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	414	
2	B	266	
3	C	138	
4	D	77	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6975 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 Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3131	2004	533	582	12			

- Molecule 2 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	254	Total	C	N	O	S	0	0	0
			2033	1301	346	384	2			

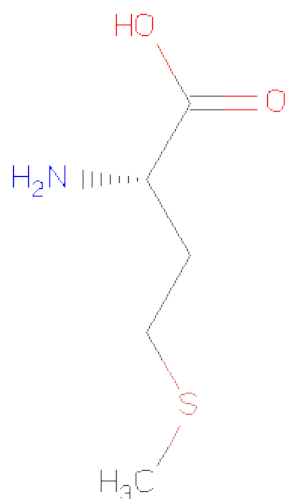
- Molecule 3 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	17	Total	C	N	O	S	0	0	0
			146	94	22	29	1			

- Molecule 4 is a RNA chain called Initiator tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	76	Total	C	N	O	P	S	0	0
			1624	725	294	528	76	1		

- Molecule 5 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).

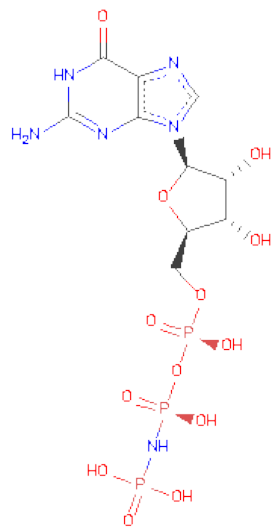


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

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

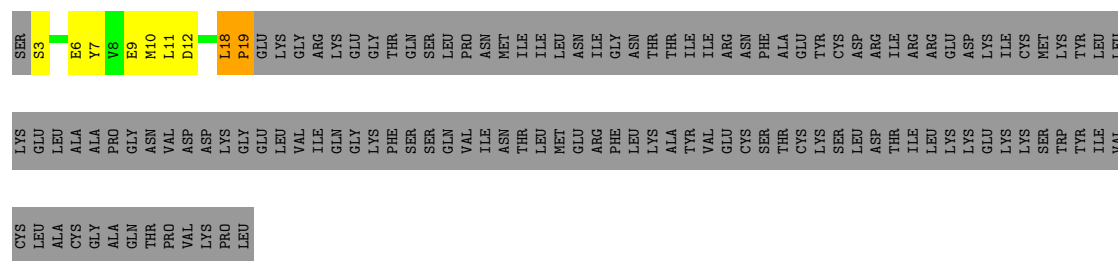
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

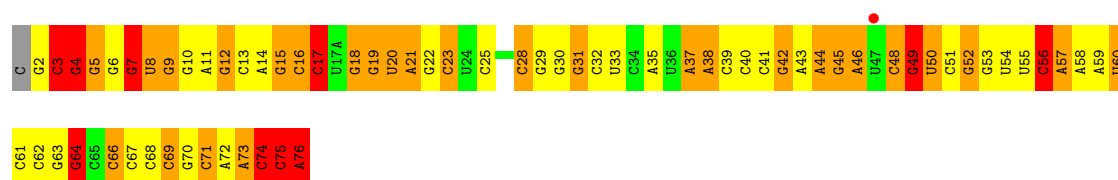


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

Chain C:



Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.00Å 133.00Å 167.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.43 – 5.00 47.43 – 5.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.43-5.00) 98.8 (47.43-5.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 5.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.262 , 0.344 0.289 , 0.363	Depositor DCC
R_{free} test set	355 reflections (4.67%)	DCC
Wilson B-factor (Å ²)	341.3	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 343.4	EDS
Estimated twinning fraction	0.071 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 7645 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6975	wwPDB-VP
Average B, all atoms (Å ²)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: 5MU, OMC, GNP, H2U, MG, 4SU, 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	0.51	0/3186	0.79	1/4313 (0.0%)
2	B	0.52	0/2058	0.76	1/2770 (0.0%)
3	C	0.65	0/148	1.10	2/197 (1.0%)
4	D	0.99	4/1702 (0.2%)	1.76	46/2653 (1.7%)
All	All	0.66	4/7094 (0.1%)	1.13	50/9933 (0.5%)

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
1	A	0	1
2	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	76	A	N3-C4	16.59	1.44	1.34
4	D	76	A	C8-N7	12.46	1.40	1.31
4	D	76	A	C5-C4	6.94	1.43	1.38
4	D	76	A	C6-N1	5.21	1.39	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	76	A	C2-N3-C4	18.67	119.94	110.60
4	D	76	A	C8-N9-C4	18.01	113.00	105.80
4	D	76	A	N7-C8-N9	-15.89	105.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	76	A	N1-C2-N3	-15.02	121.79	129.30
4	D	56	C	C6-N1-C2	-13.76	114.80	120.30
4	D	76	A	N3-C4-N9	13.29	138.03	127.40
4	D	76	A	N3-C4-C5	-12.67	117.93	126.80
4	D	76	A	C5-N7-C8	10.02	108.91	103.90
4	D	75	C	C6-N1-C2	9.00	123.90	120.30
3	C	19	PRO	CA-N-CD	-8.58	99.49	111.50
4	D	3	C	C5-C6-N1	8.21	125.11	121.00
4	D	76	A	C5-C6-N6	-7.87	117.41	123.70
4	D	69	C	C6-N1-C2	-7.63	117.25	120.30
4	D	56	C	N3-C2-O2	-7.20	116.86	121.90
4	D	16	C	C4-C5-C6	7.16	120.98	117.40
4	D	57	A	C5-N7-C8	7.11	107.45	103.90
4	D	75	C	C2-N1-C1'	-6.98	111.12	118.80
4	D	23	C	C5-C6-N1	6.79	124.40	121.00
4	D	17	C	C2-N1-C1'	6.75	126.23	118.80
3	C	18	LEU	C-N-CD	6.71	142.50	128.40
4	D	76	A	C5-C6-N1	6.56	120.98	117.70
4	D	64	G	N9-C4-C5	-6.29	102.88	105.40
4	D	7	G	C4-C5-N7	6.28	113.31	110.80
4	D	57	A	C4-C5-N7	-6.12	107.64	110.70
4	D	4	G	N3-C4-N9	5.85	129.51	126.00
1	A	41	LEU	CA-CB-CG	5.82	128.68	115.30
4	D	66	C	C5-C6-N1	5.72	123.86	121.00
4	D	69	C	C5-C6-N1	5.65	123.83	121.00
4	D	7	G	C5-N7-C8	-5.63	101.49	104.30
4	D	42	G	N3-C2-N2	-5.57	116.00	119.90
4	D	56	C	C5-C6-N1	5.49	123.74	121.00
4	D	46	A	C8-N9-C4	-5.47	103.61	105.80
4	D	17	C	C6-N1-C2	-5.43	118.13	120.30
4	D	75	C	C5-C6-N1	-5.42	118.29	121.00
4	D	15	G	N3-C4-N9	-5.42	122.75	126.00
4	D	57	A	C4-C5-C6	5.37	119.68	117.00
4	D	74	C	C6-N1-C2	-5.36	118.15	120.30
4	D	66	C	C4-C5-C6	-5.36	114.72	117.40
4	D	66	C	C2-N1-C1'	5.36	124.69	118.80
4	D	23	C	C6-N1-C2	-5.33	118.17	120.30
4	D	38	A	C4-N9-C1'	5.30	135.84	126.30
4	D	64	G	C8-N9-C4	5.28	108.51	106.40
4	D	49	G	C4-N9-C1'	5.28	133.36	126.50
4	D	37	A	N1-C6-N6	5.22	121.73	118.60
4	D	66	C	N3-C4-C5	5.15	123.96	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	7	G	N9-C4-C5	-5.05	103.38	105.40
4	D	64	G	C4-C5-N7	5.04	112.82	110.80
2	B	214	LEU	CA-CB-CG	5.03	126.88	115.30
4	D	76	A	N1-C6-N6	5.02	121.61	118.60
4	D	76	A	C4-C5-N7	-5.01	108.19	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	SER	Peptide
2	B	212	GLU	Peptide

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	3131	0	3248	194	0
2	B	2033	0	2145	119	0
3	C	146	0	146	6	0
4	D	1624	0	830	97	0
5	D	8	0	8	5	0
6	A	1	0	0	0	0
7	A	32	0	13	2	0
All	All	6975	0	6390	393	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 30.

All (393) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:LEU:HB3	5:D:101:MET:HG2	1.48	0.94
2:B:18:THR:HB	2:B:63:LYS:HG2	1.52	0.91
1:A:37:HIS:HB2	4:D:74:C:C4	2.08	0.88
2:B:240:SER:HA	2:B:243:LEU:HB3	1.55	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:62:CYS:SG	1:A:63:LYS:N	2.45	0.87
4:D:12:G:N2	4:D:23:C:O2	2.08	0.86
1:A:294:LEU:HB3	5:D:101:MET:CG	2.04	0.86
1:A:167:LYS:NZ	3:C:3:SER:O	2.07	0.86
4:D:29:G:H2'	4:D:30:G:C8	2.09	0.86
4:D:28:C:O2	4:D:42:G:N2	2.10	0.85
1:A:17:HIS:O	1:A:22:LYS:NZ	2.11	0.84
4:D:15:G:N1	4:D:48:C:O2	2.13	0.80
2:B:179:MET:HG3	2:B:239:ALA:HB1	1.62	0.79
1:A:390:SER:H	1:A:393:ILE:HD11	1.48	0.77
4:D:7:G:H1	4:D:66:C:H42	1.33	0.76
2:B:182:LEU:HD13	2:B:226:ARG:HD3	1.68	0.76
1:A:71:GLU:O	1:A:73:SER:N	2.19	0.76
1:A:55:ASN:OD1	1:A:88:ARG:NE	2.19	0.75
1:A:218:ILE:HD11	1:A:294:LEU:HD11	1.69	0.75
1:A:205:PRO:O	1:A:207:ARG:NH1	2.19	0.75
2:B:209:GLN:HA	2:B:212:GLU:HG3	1.70	0.74
4:D:29:G:H2'	4:D:30:G:H8	1.53	0.73
4:D:74:C:H4'	4:D:75:C:O5'	1.87	0.73
1:A:346:LEU:HD11	1:A:401:ILE:HD13	1.71	0.72
1:A:330:ARG:NH1	1:A:379:GLU:OE2	2.22	0.72
4:D:15:G:N7	4:D:16:C:H5	1.88	0.72
2:B:111:SER:HA	2:B:160:TRP:HZ3	1.54	0.72
4:D:15:G:N2	4:D:48:C:N3	2.36	0.71
1:A:280:ARG:O	5:D:101:MET:N	2.23	0.71
1:A:156:LYS:H	1:A:156:LYS:HD2	1.54	0.71
1:A:388:VAL:HG13	1:A:393:ILE:HG13	1.73	0.71
4:D:8:4SU:O2'	4:D:21:A:N1	2.17	0.71
1:A:306:THR:O	1:A:306:THR:OG1	2.07	0.70
2:B:220:TYR:OH	2:B:228:ARG:HD2	1.92	0.70
2:B:109:LEU:HD23	2:B:112:GLN:OE1	1.91	0.70
4:D:73:A:H2	4:D:74:C:H41	1.40	0.69
1:A:33:TRP:HE1	1:A:36:LYS:HD2	1.58	0.69
1:A:207:ARG:HE	1:A:291:PRO:HB2	1.58	0.69
4:D:8:4SU:S4	4:D:13:C:H3'	2.33	0.68
1:A:238:ILE:HG21	1:A:316:ILE:HD11	1.75	0.68
1:A:115:ILE:HG12	1:A:145:ILE:HB	1.76	0.68
4:D:63:G:H2'	4:D:64:G:H8	1.59	0.68
1:A:235:GLY:HA2	2:B:193:VAL:HG21	1.76	0.68
4:D:50:U:N3	4:D:64:G:O6	2.19	0.67
1:A:108:ALA:HA	1:A:111:MET:SD	2.34	0.67
4:D:63:G:H2'	4:D:64:G:C8	2.29	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:251:ILE:O	2:B:255:LYS:N	2.24	0.66
2:B:13:GLU:O	2:B:68:VAL:HG23	1.96	0.66
2:B:109:LEU:O	2:B:113:LYS:HG2	1.96	0.66
1:A:51:TYR:CE2	1:A:294:LEU:HB2	2.31	0.65
2:B:123:GLU:HA	2:B:127:TRP:CD1	2.31	0.65
1:A:11:ASN:OD1	1:A:293:GLY:N	2.29	0.65
4:D:18:G:H4'	4:D:60:U:O2	1.97	0.65
2:B:107:LEU:HB3	2:B:121:ALA:HB1	1.78	0.65
2:B:175:ARG:NH1	2:B:234:THR:O	2.29	0.65
2:B:131:ALA:O	2:B:133:TYR:N	2.30	0.64
2:B:97:TRP:HE1	4:D:56:C:N4	1.95	0.64
1:A:38:SER:O	1:A:40:GLU:N	2.28	0.64
1:A:23:THR:HG23	1:A:34:THR:HG23	1.80	0.64
1:A:20:HIS:O	1:A:149:ASN:ND2	2.28	0.63
2:B:83:LYS:O	2:B:85:VAL:N	2.30	0.63
3:C:7:TYR:O	3:C:10:MET:N	2.32	0.63
1:A:37:HIS:HB2	4:D:74:C:C5	2.34	0.63
1:A:35:SER:OG	1:A:37:HIS:HB3	1.98	0.63
2:B:217:ILE:HD13	2:B:246:ILE:HD11	1.80	0.62
4:D:8:4SU:O5'	4:D:8:4SU:H6	1.99	0.62
1:A:19:ASP:O	1:A:150:LYS:NZ	2.28	0.62
1:A:49:LEU:HD12	1:A:218:ILE:HD12	1.81	0.62
4:D:50:U:H2'	4:D:51:C:C6	2.35	0.62
1:A:393:ILE:HB	1:A:413:VAL:HB	1.81	0.62
1:A:226:PRO:O	4:D:2:G:H1'	2.00	0.62
4:D:9:G:N2	4:D:46:A:OP2	2.24	0.61
1:A:280:ARG:NH2	4:D:76:A:OP2	2.30	0.61
2:B:54:ILE:O	2:B:58:LEU:HB2	1.99	0.61
1:A:324:PRO:HD2	1:A:388:VAL:O	2.01	0.60
1:A:38:SER:C	1:A:40:GLU:H	2.03	0.60
1:A:294:LEU:HB3	5:D:101:MET:HG3	1.84	0.60
1:A:95:PRO:HG2	1:A:100:LEU:HD22	1.84	0.60
1:A:17:HIS:HB2	1:A:129:THR:OG1	2.02	0.60
2:B:69:ILE:HD11	2:B:81:SER:HB2	1.82	0.60
2:B:111:SER:O	2:B:115:LYS:N	2.35	0.59
1:A:155:SER:O	1:A:158:GLU:N	2.35	0.59
1:A:313:GLY:O	1:A:364:SER:HB3	2.02	0.59
2:B:163:PRO:O	2:B:167:GLU:HB2	2.03	0.59
1:A:358:MET:H	1:A:405:TRP:HZ3	1.50	0.59
2:B:114:LEU:HD12	2:B:160:TRP:CE3	2.37	0.58
1:A:37:HIS:N	1:A:41:LEU:HB2	2.18	0.58
1:A:37:HIS:HB2	4:D:74:C:N3	2.19	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:332:LYS:HG3	1:A:376:ASP:O	2.04	0.58
1:A:294:LEU:HD22	5:D:101:MET:SD	2.44	0.58
4:D:73:A:O2'	4:D:74:C:OP2	2.20	0.58
1:A:332:LYS:HB2	1:A:414:GLU:OE2	2.04	0.57
2:B:15:LEU:HD11	2:B:31:LEU:HD22	1.86	0.57
3:C:6:GLU:O	3:C:9:GLU:HB3	2.04	0.57
2:B:179:MET:HG3	2:B:239:ALA:CB	2.34	0.57
1:A:324:PRO:O	1:A:387:ALA:HA	2.04	0.57
4:D:17:C:OP1	4:D:60:U:O2'	2.20	0.57
2:B:90:ARG:O	2:B:94:ASN:HB2	2.05	0.56
4:D:6:G:H2'	4:D:7:G:C8	2.40	0.56
1:A:331:ILE:HG22	1:A:332:LYS:O	2.05	0.56
2:B:117:SER:OG	2:B:120:ASP:N	2.29	0.56
1:A:296:ALA:HB1	4:D:76:A:H1'	1.87	0.56
3:C:3:SER:O	3:C:3:SER:OG	2.20	0.56
1:A:55:ASN:HD21	1:A:88:ARG:HH21	1.53	0.56
1:A:33:TRP:NE1	1:A:36:LYS:HD2	2.20	0.56
2:B:43:TRP:C	2:B:45:GLU:H	2.09	0.56
1:A:125:PRO:HB2	1:A:130:ARG:HH11	1.70	0.56
4:D:35:A:O5'	4:D:35:A:H8	1.89	0.56
1:A:194:LEU:O	1:A:198:ILE:HG23	2.06	0.55
1:A:74:CYS:O	1:A:76:SER:N	2.39	0.55
1:A:8:PRO:HD2	1:A:281:PHE:CD2	2.42	0.55
4:D:49:G:C2	4:D:66:C:C2	2.95	0.55
2:B:199:VAL:HG12	2:B:253:ILE:HG22	1.87	0.55
2:B:53:ASN:HB3	4:D:20:H2U:H62	1.89	0.55
1:A:215:MET:HG2	1:A:216:LEU:N	2.21	0.55
1:A:274:THR:OG1	1:A:301:LEU:HD23	2.06	0.55
4:D:52:G:N1	4:D:63:G:C6	2.75	0.55
1:A:273:PHE:O	2:B:190:PRO:HA	2.07	0.55
1:A:221:PHE:CZ	4:D:73:A:H3'	2.41	0.55
2:B:64:VAL:HG12	2:B:65:ILE:H	1.72	0.55
2:B:204:LEU:HD23	2:B:207:ILE:HG21	1.89	0.55
1:A:249:VAL:HG12	1:A:250:ASP:OD2	2.06	0.55
1:A:296:ALA:O	1:A:297:ILE:HD13	2.07	0.54
2:B:221:THR:OG1	2:B:223:GLY:O	2.24	0.54
4:D:53:G:H3'	4:D:54:5MU:H71	1.89	0.54
2:B:252:LYS:O	2:B:256:GLU:N	2.41	0.54
2:B:111:SER:HA	2:B:160:TRP:CZ3	2.40	0.54
2:B:184:THR:O	2:B:261:ILE:HA	2.08	0.54
1:A:74:CYS:C	1:A:76:SER:H	2.09	0.54
4:D:3:C:H42	4:D:70:G:H1	1.56	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:180:SER:HB2	2:B:228:ARG:HD3	1.89	0.53
3:C:9:GLU:O	3:C:12:ASP:HB2	2.07	0.53
2:B:157:PRO:O	2:B:159:ILE:N	2.33	0.53
1:A:21:GLY:O	1:A:117:VAL:HG11	2.08	0.53
1:A:280:ARG:NH2	4:D:76:A:H2'	2.23	0.53
4:D:10:G:H2'	4:D:11:A:C8	2.43	0.53
1:A:95:PRO:HG2	1:A:100:LEU:HB3	1.90	0.53
4:D:54:5MU:H2'	4:D:55:PSU:O4'	2.09	0.53
2:B:2:ILE:HG23	2:B:122:TRP:CH2	2.43	0.53
4:D:2:G:C2	4:D:3:C:C5	2.97	0.53
4:D:14:A:N6	4:D:15:G:C2	2.77	0.53
4:D:62:C:H2'	4:D:63:G:C8	2.42	0.53
2:B:86:THR:HG22	2:B:88:ASP:H	1.74	0.53
1:A:177:ASN:O	1:A:177:ASN:ND2	2.42	0.53
1:A:87:ARG:NH1	1:A:199:GLU:OE2	2.42	0.53
1:A:277:SER:N	1:A:298:GLY:O	2.42	0.53
1:A:269:TYR:HB2	1:A:385:PRO:HG2	1.91	0.52
1:A:296:ALA:CB	4:D:76:A:H1'	2.39	0.52
2:B:247:ILE:HA	2:B:250:LEU:HD12	1.92	0.52
2:B:217:ILE:HG12	2:B:231:VAL:HG22	1.92	0.52
1:A:103:THR:O	1:A:106:SER:HB3	2.10	0.52
1:A:307:LYS:HG3	1:A:308:ALA:H	1.73	0.52
4:D:75:C:H5''	4:D:76:A:H5'	1.92	0.52
4:D:28:C:H2'	4:D:29:G:C8	2.44	0.52
2:B:101:GLN:NE2	4:D:56:C:OP1	2.42	0.52
1:A:24:THR:HA	1:A:33:TRP:HZ3	1.74	0.52
1:A:390:SER:N	1:A:393:ILE:HD11	2.21	0.52
1:A:236:GLY:O	1:A:299:THR:OG1	2.27	0.51
1:A:323:VAL:HG13	1:A:389:TRP:HA	1.92	0.51
1:A:37:HIS:CD2	4:D:74:C:C6	2.98	0.51
2:B:2:ILE:HB	2:B:32:ASP:O	2.10	0.51
1:A:355:GLU:OE2	1:A:399:ARG:NE	2.44	0.51
1:A:406:ARG:HH11	1:A:406:ARG:HG3	1.75	0.51
1:A:124:PHE:CE1	1:A:166:ILE:HG12	2.46	0.51
1:A:41:LEU:HD22	1:A:47:ILE:HB	1.93	0.51
1:A:36:LYS:HE2	1:A:45:MET:HA	1.93	0.51
2:B:254:GLY:HA3	2:B:261:ILE:HD12	1.93	0.51
4:D:18:G:C2	4:D:58:A:C5	2.98	0.51
4:D:30:G:N2	4:D:31:G:H1'	2.26	0.50
1:A:64:LYS:HG2	1:A:67:ALA:HB3	1.92	0.50
2:B:184:THR:HG23	2:B:225:PRO:HB2	1.93	0.50
1:A:97:HIS:CE1	1:A:99:VAL:HG23	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:140:ILE:O	2:B:144:VAL:HG22	2.11	0.50
1:A:373:VAL:HA	1:A:378:ILE:HG22	1.93	0.50
1:A:280:ARG:HH11	1:A:283:ASP:HA	1.76	0.50
2:B:178:LYS:HG3	2:B:232:VAL:HG12	1.93	0.50
4:D:11:A:H2'	4:D:12:G:C8	2.47	0.50
1:A:167:LYS:HA	1:A:170:THR:HG22	1.93	0.50
4:D:21:A:N6	4:D:46:A:H2'	2.26	0.50
2:B:187:THR:HG22	2:B:189:GLU:HG2	1.92	0.50
1:A:148:GLN:HB3	1:A:182:PRO:HA	1.93	0.50
1:A:358:MET:N	1:A:405:TRP:HZ3	2.10	0.49
4:D:71:C:H2'	4:D:72:A:H8	1.77	0.49
1:A:41:LEU:HD13	1:A:47:ILE:H	1.77	0.49
1:A:65:PRO:HB3	1:A:193:SER:HA	1.94	0.49
1:A:41:LEU:HD13	1:A:47:ILE:N	2.27	0.49
1:A:152:ASP:OD2	1:A:153:VAL:HG13	2.13	0.49
1:A:32:ILE:HG22	1:A:33:TRP:O	2.12	0.49
2:B:119:LYS:O	2:B:123:GLU:HB2	2.12	0.49
1:A:274:THR:CG2	1:A:300:TYR:H	2.25	0.49
1:A:160:LEU:O	1:A:164:ARG:HG2	2.11	0.49
1:A:124:PHE:O	1:A:126:GLN:N	2.45	0.49
2:B:162:LYS:HB2	2:B:162:LYS:NZ	2.28	0.49
1:A:303:PRO:HD3	2:B:193:VAL:HG22	1.95	0.49
2:B:161:VAL:O	2:B:165:LEU:HG	2.12	0.49
1:A:280:ARG:NH1	1:A:283:ASP:HA	2.28	0.48
2:B:45:GLU:O	2:B:82:LEU:HD12	2.12	0.48
1:A:115:ILE:HD11	1:A:198:ILE:HG22	1.95	0.48
1:A:33:TRP:HZ2	1:A:36:LYS:HZ2	1.61	0.48
4:D:15:G:C5	4:D:16:C:H5	2.31	0.48
2:B:140:ILE:HA	2:B:143:ALA:HB3	1.94	0.48
4:D:73:A:O2'	4:D:74:C:P	2.70	0.48
1:A:116:LEU:HD21	1:A:129:THR:HG23	1.95	0.48
1:A:17:HIS:CE1	1:A:128:GLN:H	2.31	0.48
1:A:110:LEU:CD2	1:A:218:ILE:HD13	2.44	0.48
1:A:150:LYS:O	1:A:153:VAL:HG22	2.12	0.48
1:A:23:THR:HG22	1:A:33:TRP:CZ3	2.48	0.48
4:D:28:C:H2'	4:D:29:G:H8	1.79	0.48
1:A:215:MET:HB2	1:A:242:ILE:HA	1.96	0.48
1:A:41:LEU:HD13	1:A:47:ILE:HB	1.95	0.48
1:A:45:MET:N	1:A:45:MET:SD	2.87	0.48
1:A:205:PRO:HB2	1:A:207:ARG:HH11	1.79	0.48
2:B:247:ILE:O	2:B:250:LEU:HB2	2.13	0.48
2:B:123:GLU:O	2:B:127:TRP:HB2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:ILE:HA	1:A:198:ILE:HG12	1.96	0.47
1:A:388:VAL:CG1	1:A:393:ILE:HG13	2.42	0.47
2:B:10:SER:O	2:B:13:GLU:HB2	2.15	0.47
1:A:307:LYS:HD2	2:B:224:ALA:HB3	1.96	0.47
2:B:7:LYS:HG3	2:B:8:LEU:H	1.79	0.47
1:A:332:LYS:O	1:A:411:GLY:HA3	2.15	0.47
4:D:58:A:C6	4:D:61:C:C2	3.02	0.47
1:A:281:PHE:CZ	1:A:295:VAL:HG22	2.50	0.47
4:D:8:4SU:H5'	4:D:9:G:OP2	2.15	0.47
4:D:2:G:N1	4:D:3:C:C4	2.83	0.47
1:A:280:ARG:CZ	4:D:76:A:H2'	2.45	0.47
2:B:64:VAL:HG12	2:B:65:ILE:N	2.30	0.47
4:D:54:5MU:C4	4:D:55:PSU:C2	3.03	0.47
1:A:269:TYR:CB	1:A:385:PRO:HG2	2.43	0.47
1:A:106:SER:OG	1:A:363:SER:O	2.12	0.47
2:B:146:GLU:HB2	2:B:150:ILE:HD11	1.95	0.47
1:A:137:GLY:HA3	1:A:174:TRP:CZ3	2.50	0.47
2:B:8:LEU:CD1	2:B:73:ARG:HA	2.45	0.47
1:A:221:PHE:O	1:A:237:VAL:HB	2.14	0.47
1:A:339:VAL:HG23	1:A:339:VAL:O	2.15	0.47
1:A:329:ILE:HD13	1:A:382:LEU:HD11	1.97	0.47
4:D:22:G:H2'	4:D:23:C:C6	2.49	0.46
2:B:21:GLN:O	2:B:27:SER:OG	2.18	0.46
3:C:18:LEU:HB3	3:C:19:PRO:CD	2.45	0.46
1:A:295:VAL:HG12	1:A:296:ALA:H	1.80	0.46
4:D:49:G:N2	4:D:66:C:H1'	2.30	0.46
2:B:41:LEU:HD12	2:B:80:VAL:O	2.16	0.46
1:A:310:ASN:C	1:A:312:LEU:H	2.19	0.46
2:B:183:ILE:O	2:B:226:ARG:HA	2.16	0.46
1:A:145:ILE:HD12	1:A:198:ILE:HG22	1.98	0.46
1:A:269:TYR:CZ	1:A:384:ARG:HG3	2.51	0.46
2:B:219:ILE:HG23	2:B:229:VAL:HG12	1.98	0.46
1:A:22:LYS:O	1:A:26:VAL:HG23	2.15	0.46
2:B:237:LYS:HE3	2:B:237:LYS:HB2	1.59	0.46
1:A:163:TYR:HE1	1:A:180:ILE:HB	1.81	0.46
1:A:57:GLY:C	1:A:69:VAL:HG22	2.35	0.46
1:A:169:PHE:C	1:A:171:LYS:H	2.17	0.46
1:A:274:THR:HG22	1:A:275:LYS:N	2.30	0.46
1:A:213:PRO:HB2	1:A:318:LEU:HG	1.97	0.46
4:D:3:C:C5'	4:D:3:C:H6	2.29	0.46
1:A:59:CYS:SG	1:A:74:CYS:SG	3.13	0.46
2:B:158:GLU:HA	2:B:161:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:4:SER:HB2	2:B:34:TYR:HA	1.98	0.46
1:A:155:SER:OG	1:A:158:GLU:HG3	2.16	0.46
2:B:204:LEU:CD2	2:B:207:ILE:HG21	2.46	0.46
1:A:333:TYR:CD2	1:A:376:ASP:HA	2.51	0.45
1:A:74:CYS:HB3	1:A:79:SER:O	2.16	0.45
4:D:72:A:C5	4:D:73:A:N7	2.84	0.45
1:A:37:HIS:CE1	4:D:74:C:O2'	2.69	0.45
4:D:30:G:H2'	4:D:31:G:O4'	2.16	0.45
1:A:57:GLY:O	1:A:69:VAL:HG22	2.16	0.45
2:B:176:LYS:HE3	2:B:215:LEU:HG	1.97	0.45
2:B:182:LEU:HA	2:B:227:TYR:O	2.17	0.45
1:A:37:HIS:H	1:A:41:LEU:HG	1.82	0.45
2:B:240:SER:O	2:B:244:ASN:N	2.48	0.45
1:A:214:VAL:HB	1:A:244:GLN:HG2	1.97	0.45
1:A:7:GLN:OE1	1:A:289:ALA:HA	2.17	0.45
2:B:162:LYS:HB2	2:B:163:PRO:HD3	1.98	0.45
2:B:200:ILE:O	2:B:204:LEU:HB2	2.17	0.45
4:D:5:G:C6	4:D:6:G:C6	3.05	0.45
1:A:307:LYS:HE3	1:A:307:LYS:HB2	1.49	0.45
1:A:134:VAL:HG11	1:A:340:VAL:HG21	1.97	0.45
1:A:19:ASP:C	1:A:21:GLY:H	2.21	0.45
2:B:83:LYS:C	2:B:85:VAL:H	2.20	0.45
4:D:72:A:C4	4:D:73:A:C8	3.05	0.45
4:D:56:C:OP1	4:D:56:C:H6	2.00	0.45
2:B:43:TRP:O	2:B:45:GLU:N	2.48	0.45
1:A:331:ILE:O	1:A:377:GLU:HA	2.17	0.44
1:A:99:VAL:C	1:A:101:MET:H	2.20	0.44
1:A:208:ASP:OD2	1:A:210:SER:OG	2.28	0.44
4:D:22:G:H2'	4:D:23:C:H6	1.81	0.44
1:A:161:SER:O	1:A:165:GLN:HG3	2.17	0.44
1:A:150:LYS:HG2	7:A:502:GNP:C6	2.47	0.44
4:D:69:C:H6	4:D:69:C:O5'	2.00	0.44
1:A:358:MET:HA	1:A:367:LEU:HD23	2.00	0.44
2:B:60:GLU:O	2:B:61:ASN:ND2	2.51	0.44
1:A:20:HIS:CG	1:A:119:ALA:HB2	2.53	0.44
1:A:342:ALA:HB3	1:A:344:GLU:O	2.18	0.44
2:B:132:LYS:O	2:B:133:TYR:C	2.55	0.44
1:A:144:LEU:O	1:A:178:VAL:HG13	2.17	0.44
1:A:41:LEU:HB3	1:A:45:MET:O	2.18	0.44
1:A:37:HIS:HB2	4:D:74:C:C2	2.53	0.44
1:A:38:SER:C	1:A:40:GLU:N	2.69	0.44
2:B:195:LYS:HD2	2:B:257:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:85:VAL:HG21	2:B:90:ARG:HH21	1.83	0.43
4:D:70:G:C6	4:D:71:C:C5	3.07	0.43
4:D:75:C:H5''	4:D:76:A:C5'	2.48	0.43
2:B:250:LEU:HB3	2:B:261:ILE:HG21	2.01	0.43
2:B:217:ILE:HG12	2:B:231:VAL:HA	1.99	0.43
4:D:46:A:H8	4:D:46:A:H3'	1.82	0.43
4:D:4:G:C3'	4:D:5:G:H5'	2.49	0.43
2:B:141:GLU:O	2:B:141:GLU:HG3	2.19	0.43
4:D:19:G:N2	4:D:57:A:H1'	2.34	0.43
4:D:70:G:H2'	4:D:70:G:N3	2.34	0.43
2:B:183:ILE:CG1	2:B:227:TYR:HB2	2.48	0.43
2:B:209:GLN:CA	2:B:212:GLU:HG3	2.44	0.43
2:B:184:THR:HA	2:B:225:PRO:O	2.18	0.43
2:B:151:LEU:HD13	2:B:161:VAL:HA	1.99	0.43
2:B:21:GLN:HB3	2:B:23:PHE:CE1	2.54	0.43
4:D:73:A:N3	4:D:74:C:H5	2.17	0.43
1:A:330:ARG:HB3	1:A:414:GLU:HB2	2.01	0.43
4:D:43:A:H2'	4:D:44:A:C8	2.54	0.43
2:B:228:ARG:HD3	2:B:230:ASP:OD2	2.19	0.43
2:B:98:LYS:HB2	2:B:98:LYS:HE3	1.76	0.43
2:B:45:GLU:HB3	2:B:81:SER:CB	2.49	0.43
2:B:7:LYS:HG3	2:B:8:LEU:N	2.34	0.43
1:A:354:LYS:HB2	1:A:354:LYS:HE3	1.63	0.43
2:B:142:LYS:HB3	2:B:150:ILE:HD13	2.01	0.43
1:A:36:LYS:NZ	7:A:502:GNP:O2A	2.46	0.42
4:D:10:G:H2'	4:D:11:A:H8	1.81	0.42
2:B:183:ILE:HG12	2:B:227:TYR:HB2	2.00	0.42
1:A:203:LYS:O	1:A:205:PRO:HD3	2.19	0.42
1:A:404:ARG:HD3	1:A:406:ARG:NH2	2.34	0.42
2:B:161:VAL:O	2:B:164:LEU:HB2	2.19	0.42
1:A:33:TRP:HZ2	1:A:36:LYS:NZ	2.18	0.42
2:B:240:SER:HB2	2:B:244:ASN:OD1	2.19	0.42
4:D:40:C:H2'	4:D:41:C:C6	2.53	0.42
1:A:301:LEU:O	1:A:301:LEU:HD12	2.19	0.42
4:D:72:A:H2'	4:D:73:A:H8	1.84	0.42
4:D:46:A:C8	4:D:46:A:H3'	2.54	0.42
4:D:18:G:C4	4:D:58:A:C2	3.08	0.42
4:D:3:C:H5''	4:D:3:C:H6	1.85	0.42
2:B:31:LEU:HG	2:B:37:LEU:O	2.19	0.42
1:A:58:VAL:HG12	1:A:84:LYS:HG3	2.00	0.42
2:B:20:LYS:HG2	2:B:21:GLN:HG3	2.02	0.42
1:A:37:HIS:H	1:A:41:LEU:CG	2.33	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:VAL:HG12	1:A:250:ASP:CG	2.40	0.42
2:B:143:ALA:HA	2:B:150:ILE:HD12	2.00	0.42
2:B:55:ARG:HG3	2:B:55:ARG:H	1.56	0.42
1:A:51:TYR:CD2	1:A:294:LEU:HD13	2.54	0.42
2:B:247:ILE:O	2:B:251:ILE:HG13	2.19	0.42
4:D:58:A:N6	4:D:61:C:O2	2.53	0.42
1:A:366:THR:HG21	1:A:384:ARG:O	2.20	0.42
1:A:160:LEU:O	1:A:163:TYR:HB3	2.19	0.42
4:D:17:C:OP1	4:D:61:C:H5'	2.20	0.42
1:A:384:ARG:HA	1:A:385:PRO:HD3	1.91	0.42
2:B:40:PHE:O	2:B:79:ASP:HA	2.19	0.42
1:A:302:ASP:O	1:A:305:LEU:N	2.44	0.42
1:A:28:ALA:HA	1:A:188:LYS:HZ2	1.85	0.42
1:A:269:TYR:CE2	1:A:384:ARG:HG3	2.54	0.42
1:A:140:GLY:O	1:A:142:LYS:HG2	2.20	0.42
1:A:41:LEU:CD1	1:A:47:ILE:HB	2.50	0.41
4:D:67:C:H2'	4:D:68:C:C6	2.55	0.41
4:D:9:G:H1'	4:D:45:G:H2'	2.01	0.41
1:A:358:MET:N	1:A:405:TRP:CZ3	2.87	0.41
1:A:274:THR:HG23	2:B:190:PRO:O	2.19	0.41
2:B:177:VAL:HG21	2:B:236:PRO:HG3	2.02	0.41
1:A:74:CYS:C	1:A:76:SER:N	2.73	0.41
2:B:235:ASN:HB3	2:B:238:GLU:CD	2.40	0.41
4:D:75:C:OP1	4:D:76:A:H5'	2.20	0.41
4:D:52:G:C6	4:D:63:G:O6	2.73	0.41
1:A:333:TYR:HB2	1:A:410:TRP:O	2.21	0.41
2:B:114:LEU:HD21	2:B:163:PRO:CG	2.50	0.41
4:D:31:G:N2	4:D:39:C:C2	2.79	0.41
1:A:203:LYS:HE3	1:A:203:LYS:HB3	1.73	0.41
2:B:136:PRO:O	2:B:140:ILE:HG13	2.20	0.41
1:A:59:CYS:HA	1:A:74:CYS:SG	2.61	0.41
2:B:29:VAL:O	2:B:38:GLN:HA	2.20	0.41
2:B:39:ALA:HB1	2:B:78:VAL:O	2.21	0.41
1:A:163:TYR:CE1	1:A:180:ILE:HB	2.56	0.41
2:B:151:LEU:HA	2:B:151:LEU:HD23	1.91	0.41
1:A:132:HIS:O	1:A:135:ALA:N	2.54	0.41
1:A:37:HIS:O	1:A:39:GLU:N	2.54	0.40
4:D:44:A:N6	4:D:45:G:N1	2.69	0.40
1:A:95:PRO:CB	1:A:100:LEU:HD13	2.52	0.40
2:B:14:ILE:HA	2:B:66:VAL:O	2.22	0.40
1:A:20:HIS:O	1:A:150:LYS:HE3	2.22	0.40
1:A:51:TYR:OH	1:A:90:SER:HB2	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:15:G:O5'	4:D:15:G:H8	2.05	0.40
1:A:95:PRO:HG2	1:A:100:LEU:CB	2.51	0.40
2:B:151:LEU:HD12	2:B:161:VAL:HG13	2.03	0.40
2:B:62:ARG:HH21	4:D:19:G:C4'	2.35	0.40
1:A:14:VAL:O	1:A:22:LYS:HD2	2.22	0.40
4:D:8:4SU:H5'	4:D:9:G:P	2.61	0.40
2:B:41:LEU:HA	2:B:42:PRO:HD3	1.67	0.40
2:B:87:ASP:N	2:B:87:ASP:OD2	2.54	0.40
1:A:149:ASN:HA	1:A:183:VAL:HG22	2.04	0.40
1:A:34:THR:HG22	1:A:50:GLY:HA3	2.04	0.40
1:A:104:MET:HE1	1:A:108:ALA:HB2	2.03	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	400/414 (97%)	314 (78%)	64 (16%)	22 (6%)	3	40
2	B	248/266 (93%)	183 (74%)	48 (19%)	17 (7%)	2	33
3	C	15/138 (11%)	9 (60%)	6 (40%)	0	100	100
All	All	663/818 (81%)	506 (76%)	118 (18%)	39 (6%)	2	38

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	75	LYS
1	A	124	PHE
1	A	176	GLU
1	A	307	LYS
1	A	309	ASP
2	B	74	ARG
2	B	84	LYS

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Mol	Chain	Res	Type
2	B	132	LYS
2	B	158	GLU
2	B	239	ALA
2	B	251	ILE
1	A	36	LYS
1	A	170	THR
2	B	44	SER
2	B	133	TYR
2	B	146	GLU
2	B	210	ASP
1	A	72	PRO
1	A	81	ASP
1	A	98	GLU
1	A	250	ASP
2	B	212	GLU
2	B	225	PRO
2	B	250	LEU
1	A	61	SER
1	A	127	PRO
2	B	131	ALA
1	A	123	PRO
1	A	311	LEU
2	B	157	PRO
2	B	37	LEU
2	B	161	VAL
1	A	276	ILE
1	A	141	VAL
1	A	292	GLY
1	A	226	PRO
1	A	341	GLY
1	A	393	ILE

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	348/356 (98%)	296 (85%)	52 (15%)	4 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	227/239 (95%)	199 (88%)	28 (12%)	7	40
3	C	17/125 (14%)	16 (94%)	1 (6%)	28	74
All	All	592/720 (82%)	511 (86%)	81 (14%)	5	34

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	LEU
1	A	45	MET
1	A	46	THR
1	A	47	ILE
1	A	61	SER
1	A	62	CYS
1	A	73	SER
1	A	75	LYS
1	A	79	SER
1	A	81	ASP
1	A	87	ARG
1	A	90	SER
1	A	100	LEU
1	A	104	MET
1	A	105	LEU
1	A	111	MET
1	A	116	LEU
1	A	155	SER
1	A	156	LYS
1	A	160	LEU
1	A	171	LYS
1	A	176	GLU
1	A	192	ASP
1	A	207	ARG
1	A	212	LYS
1	A	215	MET
1	A	221	PHE
1	A	223	VAL
1	A	229	GLN
1	A	231	ASN
1	A	232	GLU
1	A	246	LEU
1	A	277	SER

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Mol	Chain	Res	Type
1	A	290	LYS
1	A	294	LEU
1	A	295	VAL
1	A	301	LEU
1	A	306	THR
1	A	307	LYS
1	A	315	ILE
1	A	326	LEU
1	A	343	LYS
1	A	345	MET
1	A	346	LEU
1	A	347	LYS
1	A	354	LYS
1	A	360	SER
1	A	366	THR
1	A	398	SER
1	A	404	ARG
1	A	415	ILE
2	B	18	THR
2	B	30	SER
2	B	54	ILE
2	B	55	ARG
2	B	56	ASP
2	B	59	LYS
2	B	65	ILE
2	B	70	ARG
2	B	74	ARG
2	B	82	LEU
2	B	103	LEU
2	B	117	SER
2	B	127	TRP
2	B	135	ASP
2	B	158	GLU
2	B	166	GLU
2	B	175	ARG
2	B	187	THR
2	B	204	LEU
2	B	208	GLU
2	B	209	GLN
2	B	214	LEU
2	B	215	LEU
2	B	222	ILE

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Mol	Chain	Res	Type
2	B	230	ASP
2	B	255	LYS
2	B	256	GLU
2	B	257	GLU
3	C	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	177	ASN
1	A	400	GLN
2	B	61	ASN
2	B	245	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	75/77 (97%)	34 (45%)	2 (2%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	3	C
4	D	4	G
4	D	5	G
4	D	7	G
4	D	8	4SU
4	D	9	G
4	D	12	G
4	D	17	C
4	D	18	G
4	D	19	G
4	D	20	H2U
4	D	21	A
4	D	25	C
4	D	28	C
4	D	31	G
4	D	32	OMC
4	D	33	U

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Mol	Chain	Res	Type
4	D	37	A
4	D	38	A
4	D	44	A
4	D	45	G
4	D	48	C
4	D	49	G
4	D	50	U
4	D	52	G
4	D	56	C
4	D	59	A
4	D	60	U
4	D	64	G
4	D	71	C
4	D	73	A
4	D	74	C
4	D	75	C
4	D	76	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	73	A
4	D	74	C

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

5 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	$\# Z > 2$
4	H2U	D	20	4	19,21,22	1.63	3 (15%)	27,30,33	3.10	8 (29%)
4	OMC	D	32	4	20,22,23	2.41	6 (30%)	25,31,34	1.78	4 (16%)
4	5MU	D	54	4	20,22,23	2.39	6 (30%)	25,32,35	1.09	2 (8%)
4	PSU	D	55	4	19,21,22	1.18	2 (10%)	23,30,33	1.71	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	4SU	D	8	4	19,21,22	2.83	6 (31%)	23,30,33	16.49	2 (8%)

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
4	H2U	D	20	4	-	0/8/38/39	0/2/2/2
4	OMC	D	32	4	-	0/8/27/28	0/2/2/2
4	5MU	D	54	4	-	0/6/25/26	0/2/2/2
4	PSU	D	55	4	-	0/8/25/26	0/2/2/2
4	4SU	D	8	4	-	0/6/25/26	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8	4SU	C6-N1	6.38	1.46	1.35
4	D	54	5MU	C6-N1	6.16	1.49	1.34
4	D	8	4SU	C5-C4	5.95	1.48	1.38
4	D	32	OMC	C2-N1	5.42	1.44	1.38
4	D	54	5MU	C2-N1	4.96	1.43	1.38
4	D	8	4SU	C2-N1	4.91	1.43	1.38
4	D	32	OMC	C5-C4	4.91	1.52	1.40
4	D	8	4SU	P-OP1	4.68	1.52	1.46
4	D	32	OMC	P-OP1	4.54	1.51	1.46
4	D	20	H2U	C6-C5	4.43	1.59	1.52
4	D	8	4SU	C4-N3	3.92	1.43	1.35
4	D	54	5MU	C2-N3	3.85	1.44	1.37
4	D	32	OMC	C6-N1	3.82	1.42	1.35
4	D	32	OMC	C2-N3	3.73	1.45	1.35
4	D	20	H2U	P-OP1	3.66	1.50	1.46
4	D	55	PSU	C6-N1	3.57	1.35	1.32
4	D	54	5MU	C4-N3	3.49	1.43	1.37
4	D	54	5MU	C4-C5	3.32	1.50	1.42
4	D	20	H2U	C2-N1	3.28	1.40	1.35
4	D	32	OMC	C4-N4	3.14	1.44	1.35
4	D	54	5MU	P-OP1	3.08	1.50	1.46
4	D	8	4SU	C2-N3	2.72	1.42	1.37
4	D	55	PSU	P-OP1	2.37	1.49	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	8	4SU	C4-N3-C2	78.98	124.98	121.60
4	D	20	H2U	C5-C6-N1	7.68	119.31	110.71
4	D	20	H2U	O2-C2-N1	7.52	133.19	123.25
4	D	32	OMC	C6-C5-C4	6.20	120.04	117.47
4	D	20	H2U	C4-N3-C2	6.18	131.17	125.83
4	D	20	H2U	O2-C2-N3	-6.06	109.28	121.42
4	D	55	PSU	O4'-C1'-C5	5.90	116.88	109.55
4	D	20	H2U	C1'-N1-C2	5.74	126.22	118.16
4	D	55	PSU	C5-C1'-C2'	-3.90	108.73	115.61
4	D	32	OMC	C2-N3-C4	3.54	120.69	115.57
4	D	54	5MU	C5M-C5-C4	-3.18	117.80	121.04
4	D	20	H2U	O4-C4-N3	3.15	125.44	120.44
4	D	20	H2U	C6-N1-C1'	-3.02	113.30	119.30
4	D	32	OMC	C6-N1-C2	2.54	122.81	117.73
4	D	32	OMC	C5-C6-N1	-2.44	118.45	121.21
4	D	8	4SU	C6-N1-C2	2.31	122.72	119.51
4	D	54	5MU	C2-N1-C1'	2.17	119.57	118.21
4	D	55	PSU	O2'-C2'-C1'	-2.15	107.00	111.93
4	D	20	H2U	O4-C4-C5	-2.08	117.29	122.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
7	GNP	A	502	6	34,34,34	2.58	7 (20%)	50,54,54	5.88	9 (18%)
5	MET	D	101	4	7,7,8	6.77	2 (28%)	5,7,9	1.93	2 (40%)

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
7	GNP	A	502	6	-	0/18/38/38	0/1/3/3
5	MET	D	101	4	-	0/4/6/8	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	101	MET	O-C	17.18	1.23	1.11
7	A	502	GNP	PG-N3B	-7.92	1.57	1.64
7	A	502	GNP	PB-N3B	-7.59	1.57	1.64
7	A	502	GNP	PB-O3A	-6.66	1.49	1.59
7	A	502	GNP	PA-O3A	-4.80	1.51	1.59
5	D	101	MET	CB-CA	-4.63	1.49	1.53
7	A	502	GNP	PB-O2B	-2.79	1.47	1.55
7	A	502	GNP	PG-O1G	2.19	1.48	1.46
7	A	502	GNP	C8-N7	-2.01	1.30	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	502	GNP	C6-C5-N7	-38.60	128.94	134.14
7	A	502	GNP	PB-N3B-PG	-11.64	110.48	130.07
7	A	502	GNP	O3G-PG-O1G	-3.58	104.41	113.60
5	D	101	MET	CB-CA-N	3.34	120.44	110.67
7	A	502	GNP	C3'-C2'-C1'	3.34	106.13	100.91
7	A	502	GNP	PA-O3A-PB	-3.29	120.56	131.81
7	A	502	GNP	C6-N1-C2	3.00	124.76	119.51
7	A	502	GNP	O2B-PB-O1B	2.53	115.73	109.89
7	A	502	GNP	C8-N9-C4	-2.38	105.09	106.90
5	D	101	MET	CE-SD-CG	2.32	108.90	100.27
7	A	502	GNP	C2-N3-C4	-2.20	112.00	115.09

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	404/414 (97%)	0.28	32 (7%) 13 18	300, 300, 300, 300	0
2	B	254/266 (95%)	-0.02	6 (2%) 56 46	300, 300, 300, 300	0
3	C	17/138 (12%)	-0.14	0 100 100	300, 300, 300, 300	0
4	D	76/77 (98%)	-0.47	1 (1%) 74 61	300, 300, 300, 300	0
All	All	751/895 (83%)	0.09	39 (5%) 26 26	300, 300, 300, 300	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	ALA	5.2
1	A	396	VAL	4.6
1	A	98	GLU	4.4
1	A	29	ILE	4.2
1	A	311	LEU	4.1
1	A	404	ARG	3.9
1	A	395	THR	3.8
1	A	407	MET	3.6
1	A	341	GLY	3.5
1	A	218	ILE	3.4
1	A	339	VAL	3.4
2	B	25	TYR	3.4
1	A	346	LEU	3.3
1	A	121	ASN	3.3
2	B	125	VAL	3.3
1	A	238	ILE	3.2
1	A	397	ILE	3.2
4	D	47	U	3.2
1	A	336	LEU	3.2
1	A	340	VAL	3.0
1	A	49	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	348	VAL	2.9
1	A	408	ILE	2.9
1	A	247	PHE	2.9
2	B	116	LEU	2.8
1	A	151	VAL	2.8
1	A	316	ILE	2.6
1	A	97	HIS	2.5
1	A	389	TRP	2.4
1	A	233	LEU	2.4
1	A	371	THR	2.4
1	A	342	ALA	2.3
1	A	370	VAL	2.3
2	B	129	LEU	2.3
1	A	217	VAL	2.3
2	B	15	LEU	2.1
1	A	246	LEU	2.0
2	B	126	ALA	2.0
1	A	122	GLU	2.0

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
4	4SU	D	8	20/21	0.14	-	300,300,300,300	0
4	OMC	D	32	21/22	0.14	-	300,300,300,300	0
4	PSU	D	55	20/21	0.14	-	300,300,300,300	0
4	H2U	D	20	20/21	0.19	-	300,300,300,300	0
4	5MU	D	54	21/22	0.14	-	300,300,300,300	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(Å ²)	Q<0.9
5	MET	D	101	8/9	0.12	-	300,300,300,300	0
7	GNP	A	502	32/32	0.20	-	300,300,300,300	0
6	MG	A	501	1/1	0.19	-	300,300,300,300	0

6.5 Other polymers

There are no such residues in this entry.