



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:47 PM GMT

PDB ID : 3V11  
Title : Structure of the ternary initiation complex AIF2:GDPNP:methionylated initiator tRNA  
Authors : Mechulam, Y.; Schmitt, E.  
Deposited on : 2011-12-09  
Resolution : 5.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

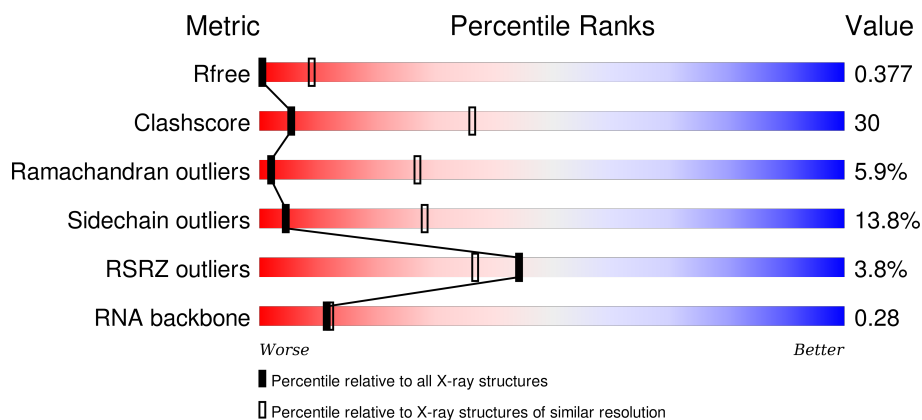
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1119 (6.22-3.60)
Clashscore	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)
RNA backbone	2183	1097 (7.04-2.80)

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  $\geq 3$ , 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	414	<div> <div>6%</div> <div>42%</div> <div>46%</div> <div>9%</div> <div>..</div> </div>
2	B	266	<div> <div>%</div> <div>36%</div> <div>48%</div> <div>11%</div> <div>5%</div> </div>
3	C	138	<div> <div>6%</div> <div>5%</div> <div>88%</div> </div>
4	D	77	<div> <div>%</div> <div>10%</div> <div>39%</div> <div>36%</div> <div>13%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	A	501	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6975 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 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			

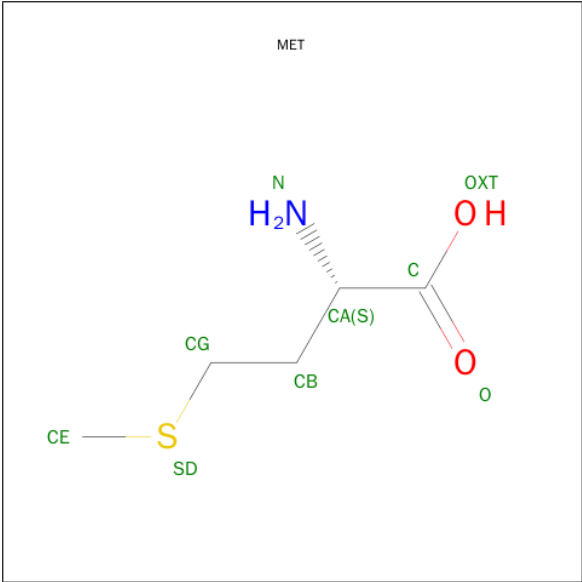
- Molecule 3 is a protein called Translation initiation factor 2 subunit beta.

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	0
			1624	725	294	528	76	1			

- Molecule 5 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).

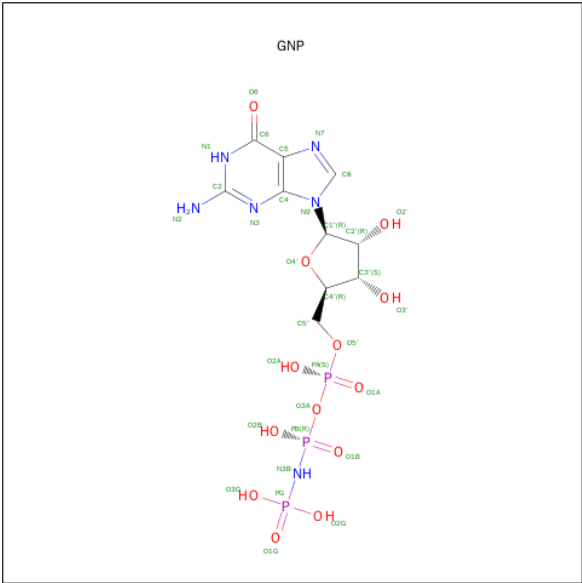


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	D	1	8	5	1	1	1	0	0

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

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

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

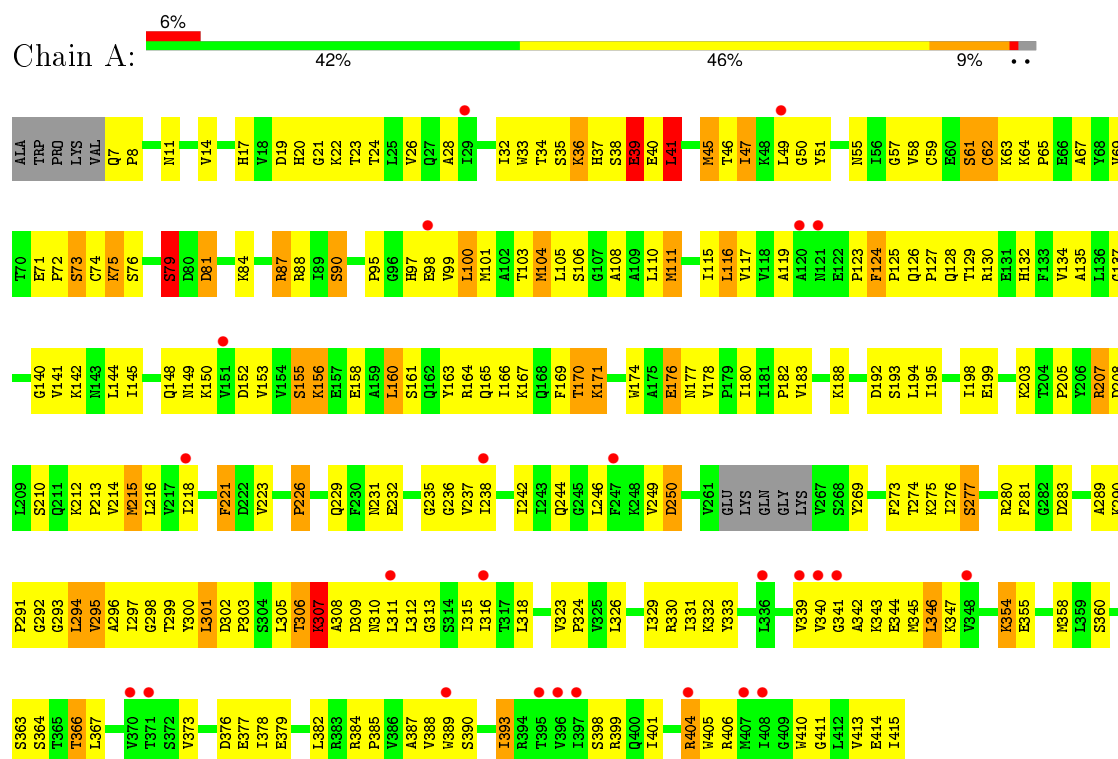


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

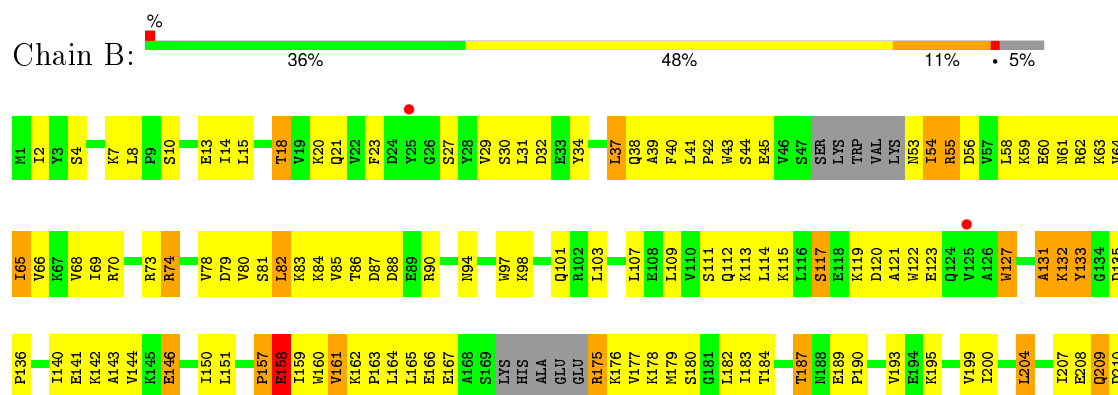
### 3 Residue-property plots

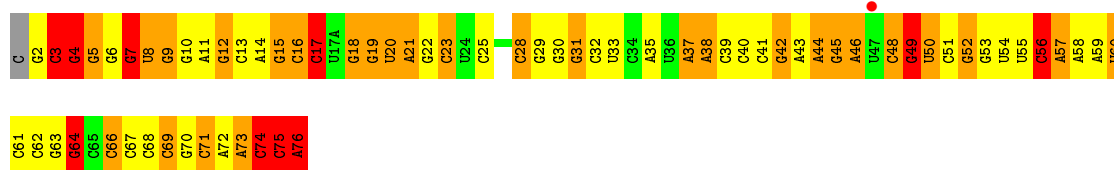
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Translation initiation factor 2 subunit gamma



- Molecule 2: Translation initiation factor 2 subunit alpha







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 5.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.262 , 0.344 0.308 , 0.377	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	341.3	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 390.5	EDS
Estimated twinning fraction	0.071 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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

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 30.

All (393) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:SER:HA	2:B:243:LEU:HB3	1.55	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	2	29
2	B	248/266 (93%)	183 (74%)	48 (19%)	17 (7%)	1	23
3	C	15/138 (11%)	9 (60%)	6 (40%)	0	100	100
All	All	663/818 (81%)	506 (76%)	118 (18%)	39 (6%)	2	27

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
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	25
2	B	227/239 (95%)	199 (88%)	28 (12%)	6	32
3	C	17/125 (14%)	16 (94%)	1 (6%)	24	63
All	All	592/720 (82%)	511 (86%)	81 (14%)	4	28

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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

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Mol	Chain	Res	Type
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
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 [i](#)

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	17,21,22	1.50	2 (11%)	23,30,33	3.38	7 (30%)
4	OMC	D	32	4	13,22,23	2.13	3 (23%)	20,31,34	1.22	1 (5%)
4	5MU	D	54	4	12,22,23	3.27	2 (16%)	14,32,35	3.35	3 (21%)
4	PSU	D	55	4	13,21,22	1.12	1 (7%)	18,30,33	4.90	7 (38%)
4	4SU	D	8	4	11,21,22	3.27	2 (18%)	13,30,33	1.62	1 (7%)

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	-	0/7/38/39	0/2/2/2
4	OMC	D	32	4	-	0/5/27/28	0/2/2/2
4	5MU	D	54	4	-	0/3/25/26	0/2/2/2
4	PSU	D	55	4	-	0/7/25/26	0/2/2/2
4	4SU	D	8	4	-	0/3/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	55	PSU	C4-N3	2.94	1.38	1.33
4	D	32	OMC	C4-N4	3.31	1.44	1.35
4	D	20	H2U	C2-N1	3.35	1.40	1.35
4	D	20	H2U	C6-C5	4.41	1.59	1.52
4	D	32	OMC	C6-N1	4.43	1.42	1.35
4	D	32	OMC	C5-C4	5.02	1.52	1.40
4	D	54	5MU	C4-N3	5.37	1.43	1.33
4	D	8	4SU	C6-N1	7.38	1.46	1.35
4	D	8	4SU	C5-C4	7.83	1.48	1.38
4	D	54	5MU	C6-N1	9.85	1.49	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	55	PSU	N1-C2-N3	-17.83	116.96	128.33
4	D	20	H2U	O2-C2-N3	-6.24	109.28	121.48
4	D	54	5MU	C5-C4-N3	-6.23	118.20	125.14
4	D	8	4SU	C5-C4-N3	-5.53	118.21	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	55	PSU	C5-C1'-C2'	-3.82	108.73	115.52
4	D	55	PSU	C5-C6-N1	-2.53	120.82	124.39
4	D	20	H2U	O4-C4-C5	-2.25	117.29	122.34
4	D	55	PSU	O2'-C2'-C1'	-2.19	107.00	111.83
4	D	54	5MU	C5M-C5-C6	2.04	122.73	118.62
4	D	55	PSU	O4'-C1'-C2'	2.20	106.97	104.73
4	D	20	H2U	O4-C4-N3	3.19	125.44	120.45
4	D	32	OMC	C2-N3-C4	3.60	120.69	115.61
4	D	55	PSU	C6-N1-C2	4.53	122.75	115.47
4	D	20	H2U	C1'-N1-C2	5.75	126.22	118.27
4	D	20	H2U	C4-N3-C2	6.52	131.17	125.79
4	D	20	H2U	O2-C2-N1	7.56	133.19	123.30
4	D	55	PSU	C4-N3-C2	7.61	121.83	115.25
4	D	20	H2U	C5-C6-N1	7.95	119.31	110.70
4	D	54	5MU	C4-N3-C2	10.46	124.29	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	20	H2U	1	0
4	D	54	5MU	3	0
4	D	55	PSU	2	0
4	D	8	4SU	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	28,34,34	2.09	9 (32%)	33,54,54	2.38	7 (21%)
5	MET	D	101	4	6,7,8	1.79	1 (16%)	4,7,9	2.15	2 (50%)

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	-	0/12/38/38	0/3/3/3
5	MET	D	101	4	-	0/4/6/8	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	502	GNP	PB-O3A	-7.49	1.49	1.59
5	D	101	MET	CB-CA	-4.21	1.49	1.53
7	A	502	GNP	PB-O2B	-3.47	1.47	1.56
7	A	502	GNP	PG-O3G	-2.28	1.50	1.56
7	A	502	GNP	PG-N3B	-2.24	1.57	1.63
7	A	502	GNP	PB-N3B	-2.13	1.57	1.63
7	A	502	GNP	PG-O2G	-2.08	1.50	1.56
7	A	502	GNP	C8-N7	-2.07	1.30	1.34
7	A	502	GNP	PG-O1G	2.41	1.48	1.46
7	A	502	GNP	C6-N1	3.58	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	502	GNP	C5-C6-N1	-8.74	111.64	123.59
7	A	502	GNP	PA-O3A-PB	-3.61	120.56	132.67
7	A	502	GNP	O3G-PG-O1G	-3.42	104.41	113.49
7	A	502	GNP	N3-C2-N1	-2.15	124.17	127.44
5	D	101	MET	CE-SD-CG	2.50	108.90	100.37
7	A	502	GNP	O3A-PA-O5'	2.53	109.66	102.94
7	A	502	GNP	O2B-PB-O1B	2.74	115.73	110.00
5	D	101	MET	CB-CA-N	3.49	120.44	110.52
7	A	502	GNP	C6-N1-C2	6.35	124.76	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	502	GNP	2	0
5	D	101	MET	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/414 (97%)	-0.19	25 (6%) 24 19	300, 300, 300, 300	0
2	B	254/266 (95%)	-0.48	2 (0%) 87 82	300, 300, 300, 300	0
3	C	17/138 (12%)	-0.58	0 100 100	300, 300, 300, 300	0
4	D	71/77 (92%)	-0.23	1 (1%) 78 70	300, 300, 300, 300	0
All	All	746/895 (83%)	-0.30	28 (3%) 44 37	300, 300, 300, 300	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	ALA	4.7
1	A	396	VAL	4.4
1	A	98	GLU	3.7
1	A	121	ASN	3.6
1	A	395	THR	3.6
1	A	29	ILE	3.5
1	A	404	ARG	3.2
1	A	341	GLY	3.1
1	A	311	LEU	3.1
2	B	125	VAL	2.9
1	A	218	ILE	2.9
1	A	339	VAL	2.8
4	D	47	U	2.7
1	A	397	ILE	2.5
1	A	238	ILE	2.5
1	A	340	VAL	2.5
1	A	151	VAL	2.4
1	A	348	VAL	2.4
1	A	407	MET	2.4
1	A	336	LEU	2.3
1	A	247	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	25	TYR	2.3
1	A	371	THR	2.3
1	A	389	TRP	2.1
1	A	370	VAL	2.1
1	A	49	LEU	2.1
1	A	408	ILE	2.1
1	A	316	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	4SU	D	8	20/21	0.79	0.14	-	300,300,300,300	0
4	OMC	D	32	21/22	0.89	0.13	-	300,300,300,300	0
4	PSU	D	55	20/21	0.81	0.15	-	300,300,300,300	0
4	H2U	D	20	20/21	0.75	0.20	-	300,300,300,300	0
4	5MU	D	54	21/22	0.71	0.14	-	300,300,300,300	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	MG	A	501	1/1	0.98	0.19	2.39	300,300,300,300	0
7	GNP	A	502	32/32	0.90	0.20	-0.11	300,300,300,300	0
5	MET	D	101	8/9	0.70	0.13	-0.64	300,300,300,300	0

## 6.5 Other polymers

There are no such residues in this entry.