



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:46 PM UTC

PDB ID : 3V11 / pdb_00003v11
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

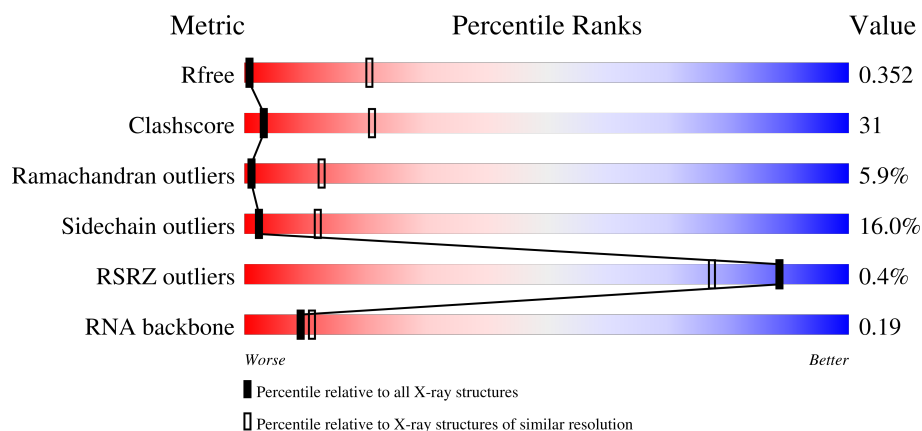
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)
RNA backbone	3983	1045 (6.76-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	414	38% 48% 11% ..
2	B	266	33% 48% 13% 5%
3	C	138	6% 5% 88%
4	D	77	12% 47% 38% ..

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
7	MET	D	101	-	-	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			

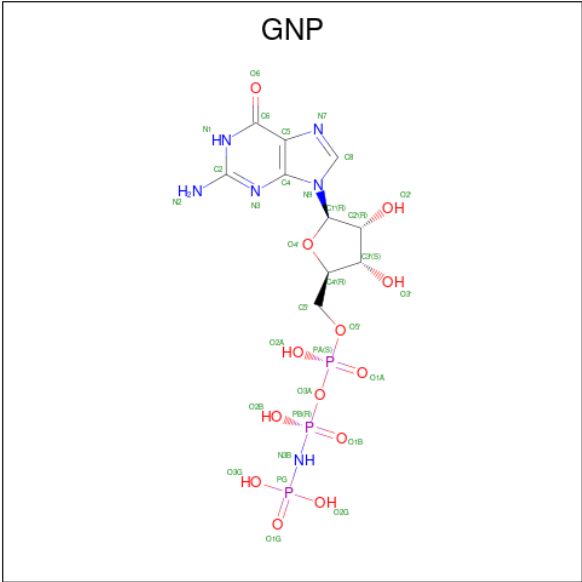
- Molecule 4 is a RNA chain called Initiator tRNA.

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

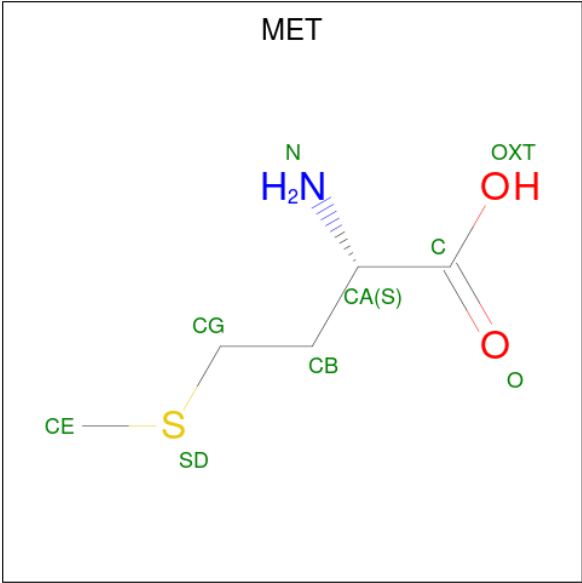
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

- Molecule 7 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).

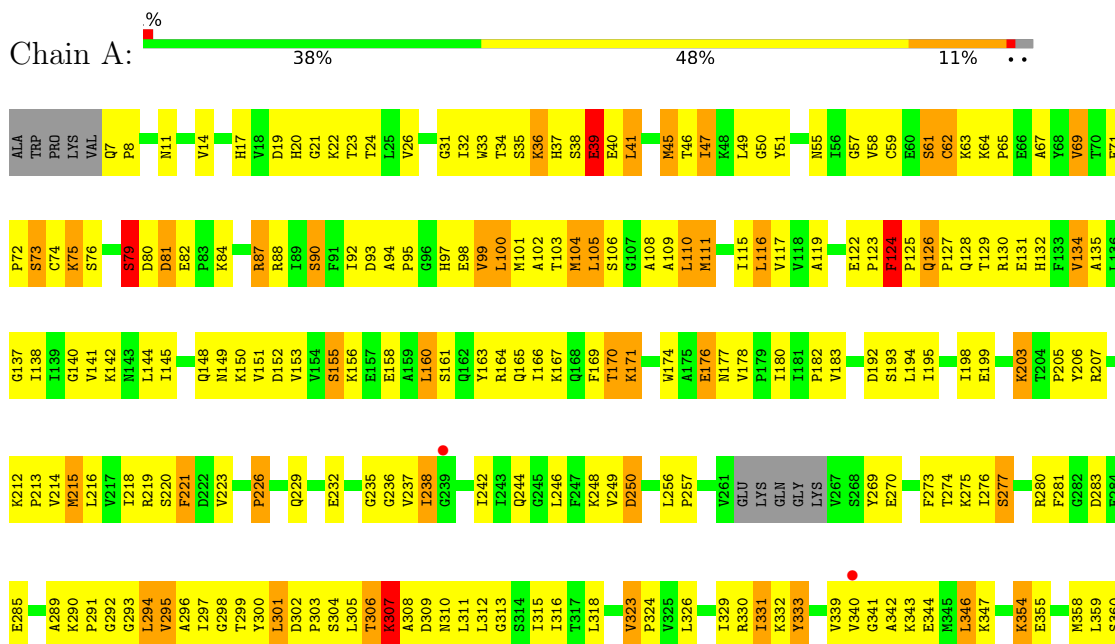


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

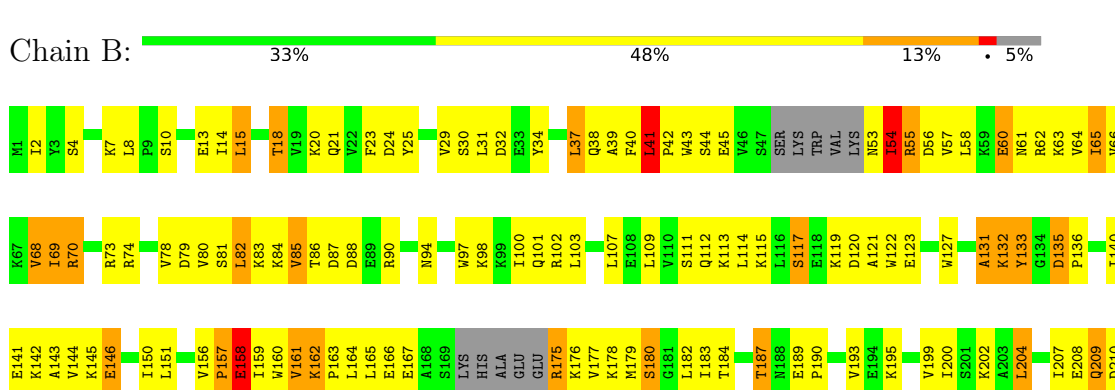
3 Residue-property plots [i](#)

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

- Molecule 1: Translation initiation factor 2 subunit gamma

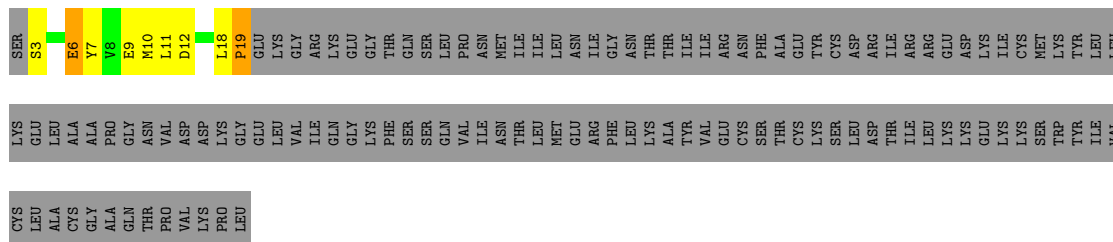


- Molecule 2: Translation initiation factor 2 subunit alpha

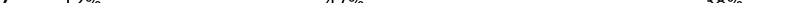


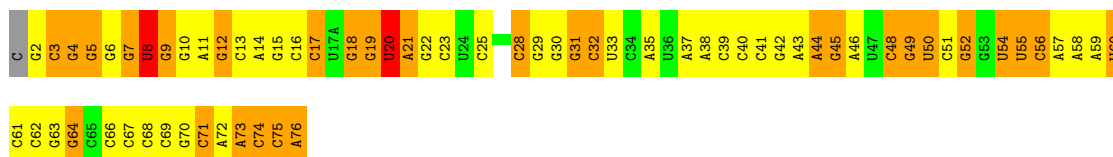
- Molecule 3: Translation initiation factor 2 subunit beta

Chain C: 6% 5% • 88%



- Molecule 4: Initiator tRNA

Chain D:  12% 47% 38% .



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 0.285 , 0.352	Depositor DCC
R_{free} test set	361 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	341.3	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 329.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.071 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	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.

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, PSU, H2U, MG, 5MU, 4SU, GNP

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	0.69	0/3186	1.20	27/4313 (0.6%)
2	B	0.70	0/2058	1.13	16/2770 (0.6%)
3	C	0.70	0/148	1.23	1/197 (0.5%)
4	D	0.53	0/1702	0.61	0/2653
All	All	0.66	0/7094	1.05	44/9933 (0.4%)

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

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	N-CA-C	9.55	121.69	111.28
3	C	19	PRO	CA-N-CD	-8.94	99.49	112.00
1	A	333	TYR	N-CA-C	8.06	121.13	108.79
1	A	221	PHE	N-CA-C	7.73	121.50	109.52
1	A	124	PHE	CA-C-N	-7.72	110.19	119.84
1	A	124	PHE	C-N-CA	-7.72	110.19	119.84
2	B	224	ALA	CA-C-N	-7.68	110.24	119.84
2	B	224	ALA	C-N-CA	-7.68	110.24	119.84
2	B	41	LEU	CA-C-N	7.36	129.04	119.84
2	B	41	LEU	C-N-CA	7.36	129.04	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ALA	CA-C-N	-7.24	110.79	119.84
1	A	94	ALA	C-N-CA	-7.24	110.79	119.84
1	A	323	VAL	CA-C-N	7.23	127.49	119.90
1	A	323	VAL	C-N-CA	7.23	127.49	119.90
1	A	79	SER	N-CA-C	7.18	118.14	108.23
1	A	110	LEU	N-CA-C	-7.02	105.64	114.56
2	B	102	ARG	N-CA-C	-6.79	103.81	111.07
2	B	202	LYS	N-CA-C	-6.18	106.71	114.56
1	A	220	SER	CA-C-N	-6.06	113.07	122.59
1	A	220	SER	C-N-CA	-6.06	113.07	122.59
2	B	85	VAL	CB-CA-C	-5.85	103.12	111.31
1	A	126	GLN	CA-C-N	5.84	127.14	119.84
1	A	126	GLN	C-N-CA	5.84	127.14	119.84
1	A	331	ILE	CB-CA-C	-5.79	103.74	110.91
1	A	31	GLY	N-CA-C	-5.65	107.17	113.79
2	B	70	ARG	N-CA-C	5.61	118.05	108.90
1	A	270	GLU	CA-C-N	5.55	126.02	120.14
1	A	270	GLU	C-N-CA	5.55	126.02	120.14
1	A	410	TRP	N-CA-C	5.49	115.65	108.07
2	B	220	TYR	N-CA-C	5.43	117.33	109.07
1	A	304	SER	N-CA-C	-5.42	104.61	111.11
2	B	156	VAL	CA-C-N	5.39	126.58	119.84
2	B	156	VAL	C-N-CA	5.39	126.58	119.84
2	B	180	SER	N-CA-C	5.26	117.18	109.24
2	B	54	ILE	N-CA-C	5.20	120.16	109.34
1	A	397	ILE	N-CA-C	5.18	115.42	108.17
2	B	15	LEU	N-CA-C	5.15	116.12	108.60
2	B	135	ASP	CA-C-N	5.14	125.43	119.47
2	B	135	ASP	C-N-CA	5.14	125.43	119.47
1	A	82	GLU	CA-C-N	5.12	125.13	119.90
1	A	82	GLU	C-N-CA	5.12	125.13	119.90
1	A	343	LYS	N-CA-C	-5.08	105.25	111.75
1	A	238	ILE	N-CA-C	5.07	114.88	107.37
1	A	102	ALA	N-CA-C	5.07	118.24	111.75

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	209	0
2	B	2033	0	2145	120	0
3	C	146	0	146	5	0
4	D	1624	0	830	96	0
5	A	1	0	0	0	0
6	A	32	0	13	2	0
7	D	8	0	8	6	0
All	All	6975	0	6390	407	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 31.

All (407) 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	7: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
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	7: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:205:PRO:O	1:A:207:ARG:NH1	2.19	0.75
1:A:218:ILE:HD11	1:A:294:LEU:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	7: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:109:LEU:HD23	2:B:112:GLN:OE1	1.91	0.70
2:B:220:TYR:OH	2:B:228:ARG:HD2	1.92	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
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
1:A:38:SER:C	1:A:40:GLU:H	2.03	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
1:A:38:SER:O	1:A:40:GLU:N	2.28	0.64
2:B:97:TRP:HE1	4:D:56:C:N4	1.95	0.64
2:B:131:ALA:O	2:B:133:TYR:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:106:SER:OG	1:A:363:SER:O	2.12	0.60
1:A:324:PRO:HD2	1:A:388:VAL:O	2.01	0.60
1:A:294:LEU:HB3	7:D:101:MET:HG3	1.84	0.60
2:B:43:TRP:C	2:B:45:GLU:H	2.09	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:389:TRP:CD1	1:A:390:SER:HG	2.21	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:219:ARG:CZ	7:D:101:MET:HE1	2.32	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:74:CYS:C	1:A:76:SER:H	2.09	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	7: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:ARG:O	2:B:94:ASN:HB2	2.05	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
4:D:6:G:H2'	4:D:7:G:C8	2.40	0.56
1:A:296:ALA:HB1	4:D:76:A:H1'	1.87	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
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:74:CYS:O	1:A:76:SER:N	2.39	0.55
1:A:194:LEU:O	1:A:198:ILE:HG23	2.06	0.55
1:A:8:PRO:HD2	1:A:281:PHE:CD2	2.42	0.55
2:B:199:VAL:HG12	2:B:253:ILE:HG22	1.87	0.55
4:D:49:G:C2	4:D:66:C:C2	2.95	0.55
1:A:215:MET:HG2	1:A:216:LEU:N	2.21	0.55
2:B:53:ASN:HB3	4:D:20:H2U:H62	1.89	0.55
1:A:274:THR:OG1	1:A:301:LEU:HD23	2.06	0.55
1:A:273:PHE:O	2:B:190:PRO:HA	2.07	0.55
4:D:52:G:N1	4:D:63:G:C6	2.75	0.55
1:A:221:PHE:CZ	4:D:73:A:H3'	2.41	0.55
1:A:249:VAL:HG12	1:A:250:ASP:OD2	2.06	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: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
1:A:101:MET:HE2	1:A:131:GLU:HG2	1.88	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:104:MET:HE2	1:A:104:MET:O	2.07	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:95:PRO:HG2	1:A:100:LEU:HB3	1.90	0.53
1:A:280:ARG:NH2	4:D:76:A:H2'	2.23	0.53
2:B:2:ILE:HG23	2:B:122:TRP:CH2	2.43	0.53
4:D:10:G:H2'	4:D:11:A:C8	2.43	0.53
4:D:54:5MU:H2'	4:D:55:PSU:O4'	2.09	0.53
2:B:86:THR:HG22	2:B:88:ASP:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:217:ILE:HG12	2:B:231:VAL:HG22	1.92	0.52
4:D:75:C:H5''	4:D:76:A:H5'	1.92	0.52
2:B:101:GLN:NE2	4:D:56:C:OP1	2.42	0.52
4:D:28:C:H2'	4:D:29:G:C8	2.44	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: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:38:SER:C	1:A:40:GLU:N	2.69	0.51
1:A:310:ASN:C	1:A:312:LEU:H	2.19	0.51
1:A:406:ARG:HG3	1:A:406:ARG:HH11	1.75	0.51
1:A:124:PHE:CE1	1:A:166:ILE:HG12	2.46	0.51
1:A:57:GLY:C	1:A:69:VAL:HG22	2.35	0.51
1:A:169:PHE:C	1:A:171:LYS:H	2.17	0.51
1:A:36:LYS:HE2	1:A:45:MET:HA	1.93	0.51
1:A:41:LEU:HD22	1:A:47:ILE:HB	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
1:A:97:HIS:CE1	1:A:99:VAL:HG23	2.46	0.50
1:A:373:VAL:HA	1:A:378:ILE:HG22	1.93	0.50
2:B:140:ILE:O	2:B:144:VAL:HG22	2.11	0.50
2:B:184:THR:HG23	2:B:225:PRO:HB2	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
1:A:167:LYS:HA	1:A:170:THR:HG22	1.93	0.50
2:B:187:THR:HG22	2:B:189:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:A:H2'	4:D:12:G:C8	2.47	0.50
4:D:21:A:N6	4:D:46:A:H2'	2.26	0.50
1:A:148:GLN:HB3	1:A:182:PRO:HA	1.93	0.50
1:A:135:ALA:HB2	1:A:407:MET:HE1	1.93	0.49
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:19:ASP:C	1:A:21:GLY:H	2.21	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
2:B:83:LYS:C	2:B:85:VAL:H	2.20	0.49
1:A:41:LEU:HD13	1:A:47:ILE:N	2.27	0.49
1:A:99:VAL:C	1:A:101:MET:H	2.20	0.49
1:A:32:ILE:HG22	1:A:33:TRP:O	2.12	0.49
1:A:152:ASP:OD2	1:A:153:VAL:HG13	2.13	0.49
1:A:160:LEU:O	1:A:164:ARG:HG2	2.11	0.49
1:A:274:THR:CG2	1:A:300:TYR:H	2.25	0.49
2:B:119:LYS:O	2:B:123:GLU:HB2	2.12	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
2:B:132:LYS:O	2:B:133:TYR:C	2.55	0.48
1:A:115:ILE:HD11	1:A:198:ILE:HG22	1.95	0.48
2:B:140:ILE:HA	2:B:143:ALA:HB3	1.94	0.48
4:D:15:G:C5	4:D:16:C:H5	2.31	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:23:THR:HG22	1:A:33:TRP:CZ3	2.48	0.48
1:A:36:LYS:NZ	6:A:502:GNP:O2A	2.46	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:215:MET:HB2	1:A:242:ILE:HA	1.96	0.48
4:D:28:C:H2'	4:D:29:G:H8	1.79	0.48
1:A:41:LEU:HD13	1:A:47:ILE:HB	1.95	0.48
1:A:45:MET:SD	1:A:45:MET:N	2.87	0.48
1:A:205:PRO:HB2	1:A:207:ARG:HH11	1.79	0.48
2:B:123:GLU:O	2:B:127:TRP:HB2	2.13	0.48
2:B:247:ILE:O	2:B:250:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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
1:A:137:GLY:HA3	1:A:174:TRP:CZ3	2.50	0.47
1:A:249:VAL:HG12	1:A:250:ASP:CG	2.40	0.47
1:A:269:TYR:CB	1:A:385:PRO:HG2	2.43	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
2:B:146:GLU:HB2	2:B:150:ILE:HD11	1.95	0.47
4:D:2:G:N1	4:D:3:C:C4	2.83	0.47
4:D:54:5MU:C4	4:D:55:PSU:C2	3.03	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:329:ILE:HD13	1:A:382:LEU:HD11	1.97	0.47
1:A:339:VAL:HG23	1:A:339:VAL:O	2.15	0.47
3:C:18:LEU:HB3	3:C:19:PRO:CD	2.45	0.46
4:D:22:G:H2'	4:D:23:C:C6	2.49	0.46
1:A:295:VAL:HG12	1:A:296:ALA:H	1.80	0.46
1:A:74:CYS:C	1:A:76:SER:N	2.73	0.46
2:B:41:LEU:HD12	2:B:80:VAL:O	2.16	0.46
4:D:49:G:N2	4:D:66:C:H1'	2.30	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:183:ILE:O	2:B:226:ARG:HA	2.16	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:HB2	2:B:237:LYS:HE3	1.59	0.46
1:A:163:TYR:HE1	1:A:180:ILE:HB	1.81	0.46
1:A:213:PRO:HB2	1:A:318:LEU:HG	1.97	0.46
1:A:274:THR:HG22	1:A:275:LYS:N	2.30	0.46
1:A:59:CYS:SG	1:A:74:CYS:SG	3.13	0.46
4:D:3:C:H6	4:D:3:C:C5'	2.29	0.46
2:B:4:SER:HB2	2:B:34:TYR:HA	1.98	0.46
2:B:158:GLU:HA	2:B:161:VAL:HG23	1.98	0.46
1:A:155:SER:OG	1:A:158:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:235:ASN:HB3	2:B:238:GLU:CD	2.40	0.45
1:A:74:CYS:HB3	1:A:79:SER:O	2.16	0.45
1:A:37:HIS:CE1	4:D:74:C:O2'	2.69	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
4:D:30:G:H2'	4:D:31:G:O4'	2.16	0.45
4:D:72:A:C5	4:D:73:A:N7	2.84	0.45
2:B:182:LEU:HA	2:B:227:TYR:O	2.17	0.45
1:A:7:GLN:OE1	1:A:289:ALA:HA	2.17	0.45
1:A:37:HIS:H	1:A:41:LEU:HG	1.82	0.45
1:A:214:VAL:HB	1:A:244:GLN:HG2	1.97	0.45
2:B:240:SER:O	2:B:244:ASN:N	2.48	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
1:A:134:VAL:HG11	1:A:340:VAL:HG21	1.97	0.45
1:A:307:LYS:HB2	1:A:307:LYS:HE3	1.49	0.45
4:D:5:G:C6	4:D:6:G:C6	3.05	0.45
2:B:43:TRP:O	2:B:45:GLU:N	2.48	0.45
4:D:56:C:OP1	4:D:56:C:H6	2.00	0.45
4:D:72:A:C4	4:D:73:A:C8	3.05	0.45
1:A:331:ILE:O	1:A:377:GLU:HA	2.17	0.44
1:A:161:SER:O	1:A:165:GLN:HG3	2.17	0.44
4:D:22:G:H2'	4:D:23:C:H6	1.81	0.44
1:A:150:LYS:HG2	6: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
1:A:144:LEU:O	1:A:178:VAL:HG13	2.17	0.44
1:A:37:HIS:HB2	4:D:74:C:C2	2.53	0.44
1:A:41:LEU:HB3	1:A:45:MET:O	2.18	0.44
1:A:34:THR:C	1:A:36:LYS:H	2.25	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
1:A:17:HIS:HB2	1:A:129:THR:HG1	1.82	0.43
1:A:23:THR:OG1	1:A:93:ASP:OD1	2.35	0.43
2:B:157:PRO:C	2:B:159:ILE:H	2.22	0.43
4:D:70:G:C6	4:D:71:C:C5	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ILE:HG12	2:B:231:VAL:HA	1.99	0.43
2:B:250:LEU:HB3	2:B:261:ILE:HG21	2.01	0.43
4:D:75:C:H5'	4:D:76:A:C5'	2.48	0.43
1:A:273:PHE:O	1:A:274:THR:OG1	2.34	0.43
4:D:46:A:H8	4:D:46:A:H3'	1.82	0.43
1:A:256:LEU:HA	1:A:257:PRO:C	2.42	0.43
2:B:141:GLU:O	2:B:141:GLU:HG3	2.19	0.43
4:D:4:G:C3'	4:D:5:G:H5'	2.49	0.43
4:D:19:G:N2	4:D:57:A:H1'	2.34	0.43
2:B:21:GLN:HB3	2:B:23:PHE:CE1	2.54	0.43
2:B:151:LEU:HD13	2:B:161:VAL:HA	1.99	0.43
2:B:183:ILE:CG1	2:B:227:TYR:HB2	2.48	0.43
2:B:184:THR:HA	2:B:225:PRO:O	2.18	0.43
2:B:209:GLN:CA	2:B:212:GLU:HG3	2.44	0.43
4:D:70:G:H2'	4:D:70:G:N3	2.34	0.43
1:A:130:ARG:O	1:A:131:GLU:C	2.61	0.43
1:A:330:ARG:HB3	1:A:414:GLU:HB2	2.01	0.43
2:B:98:LYS:HE3	2:B:98:LYS:HB2	1.76	0.43
2:B:228:ARG:HD3	2:B:230:ASP:OD2	2.19	0.43
4:D:43:A:H2'	4:D:44:A:C8	2.54	0.43
4:D:73:A:N3	4:D:74:C:H5	2.17	0.43
1:A:354:LYS:HE3	1:A:354:LYS:HB2	1.63	0.43
2:B:7:LYS:HG3	2:B:8:LEU:N	2.34	0.43
2:B:45:GLU:HB3	2:B:81:SER:CB	2.49	0.43
2:B:142:LYS:HB3	2:B:150:ILE:HD13	2.01	0.43
4:D:10:G:H2'	4:D:11:A:H8	1.81	0.42
1:A:11:ASN:CG	1:A:293:GLY:H	2.24	0.42
1:A:37:HIS:C	1:A:39:GLU:N	2.76	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
2:B:183:ILE:HG12	2:B:227:TYR:HB2	2.00	0.42
1:A:33:TRP:HZ2	1:A:36:LYS:NZ	2.18	0.42
1:A:301:LEU:HD12	1:A:301:LEU:O	2.19	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
4:D:18:G:C4	4:D:58:A:C2	3.08	0.42
4:D:46:A:H3'	4:D:46:A:C8	2.54	0.42
4:D:72:A:H2'	4:D:73:A:H8	1.84	0.42
1:A:58:VAL:HG12	1:A:84:LYS:HG3	2.00	0.42
2:B:31:LEU:HG	2:B:37:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:C:H6	4:D:3:C:H5''	1.85	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
2:B:55:ARG:H	2:B:55:ARG:HG3	1.56	0.42
2:B:143:ALA:HA	2:B:150:ILE:HD12	2.00	0.42
1:A:51:TYR:CD2	1:A:294:LEU:HD13	2.54	0.42
1:A:108:ALA:C	1:A:110:LEU:H	2.27	0.42
1:A:160:LEU:O	1:A:163:TYR:HB3	2.19	0.42
1:A:366:THR:HG21	1:A:384:ARG:O	2.20	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:302:ASP:O	1:A:305:LEU:N	2.44	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
4:D:17:C:OP1	4:D:61:C:H5'	2.20	0.42
1:A:140:GLY:O	1:A:142:LYS:HG2	2.20	0.42
1:A:269:TYR:CE2	1:A:384:ARG:HG3	2.54	0.42
1:A:41:LEU:CD1	1:A:47:ILE:HB	2.50	0.41
4:D:9:G:H1'	4:D:45:G:H2'	2.01	0.41
4:D:67:C:H2'	4:D:68:C:C6	2.55	0.41
1:A:274:THR:HG23	2:B:190:PRO:O	2.19	0.41
1:A:358:MET:N	1:A:405:TRP:CZ3	2.87	0.41
2:B:177:VAL:HG21	2:B:236:PRO:HG3	2.02	0.41
1:A:19:ASP:C	1:A:21:GLY:N	2.77	0.41
4:D:52:G:C6	4:D:63:G:O6	2.73	0.41
4:D:75:C:OP1	4:D:76:A:H5'	2.20	0.41
1:A:236:GLY:O	1:A:299:THR:OG1	2.27	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
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
4:D:31:G:N2	4:D:39:C:C2	2.79	0.41
1:A:37:HIS:O	1:A:38:SER:C	2.64	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:132:HIS:O	1:A:135:ALA:N	2.54	0.41
1:A:163:TYR:CE1	1:A:180:ILE:HB	2.56	0.41
2:B:151:LEU:HD23	2:B:151:LEU:HA	1.91	0.41
1:A:37:HIS:O	1:A:39:GLU:N	2.54	0.40
1:A:95:PRO:CB	1:A:100:LEU:HD13	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ILE:HA	2:B:66:VAL:O	2.22	0.40
4:D:44:A:N6	4:D:45:G:N1	2.69	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
1:A:95:PRO:HG2	1:A:100:LEU:CB	2.51	0.40
1:A:206:TYR:C	1:A:207:ARG:HD3	2.46	0.40
2:B:62:ARG:HH21	4:D:19:G:C4'	2.35	0.40
2:B:151:LEU:HD12	2:B:161:VAL:HG13	2.03	0.40
4:D:15:G:O5'	4:D:15:G:H8	2.05	0.40
1:A:14:VAL:O	1:A:22:LYS:HD2	2.22	0.40
1:A:109:ALA:C	1:A:110:LEU:HD12	2.46	0.40
2:B:24:ASP:C	2:B:25:TYR:CD2	2.99	0.40
2:B:41:LEU:HA	2:B:42:PRO:HD3	1.67	0.40
2:B:87:ASP:OD2	2:B:87:ASP:N	2.54	0.40
4:D:8:4SU:H5'	4:D:9:G:P	2.61	0.40
1:A:34:THR:HG22	1:A:50:GLY:HA3	2.04	0.40
1:A:105:LEU:O	1:A:106:SER:C	2.64	0.40
1:A:149:ASN:HA	1:A:183:VAL:HG22	2.04	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%)	1	14
2	B	248/266 (93%)	183 (74%)	48 (19%)	17 (7%)	1	11
3	C	15/138 (11%)	9 (60%)	6 (40%)	0	100	100
All	All	663/818 (81%)	506 (76%)	118 (18%)	39 (6%)	1	13

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%)	289 (83%)	59 (17%)	2	11
2	B	227/239 (95%)	194 (86%)	33 (14%)	3	14
3	C	17/125 (14%)	15 (88%)	2 (12%)	5	19
All	All	592/720 (82%)	498 (84%)	94 (16%)	2	12

All (94) 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	69	VAL
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	92	ILE
1	A	99	VAL
1	A	100	LEU
1	A	104	MET
1	A	105	LEU
1	A	111	MET
1	A	116	LEU
1	A	122	GLU
1	A	134	VAL
1	A	138	ILE
1	A	151	VAL
1	A	155	SER

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Mol	Chain	Res	Type
1	A	160	LEU
1	A	171	LYS
1	A	176	GLU
1	A	192	ASP
1	A	203	LYS
1	A	212	LYS
1	A	215	MET
1	A	223	VAL
1	A	229	GLN
1	A	232	GLU
1	A	246	LEU
1	A	248	LYS
1	A	277	SER
1	A	285	GLU
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	346	LEU
1	A	347	LYS
1	A	354	LYS
1	A	359	LEU
1	A	360	SER
1	A	366	THR
1	A	398	SER
1	A	401	ILE
1	A	404	ARG
1	A	408	ILE
1	A	415	ILE
2	B	18	THR
2	B	30	SER
2	B	41	LEU
2	B	54	ILE
2	B	55	ARG
2	B	56	ASP
2	B	57	VAL
2	B	60	GLU
2	B	65	ILE

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Mol	Chain	Res	Type
2	B	68	VAL
2	B	69	ILE
2	B	70	ARG
2	B	82	LEU
2	B	100	ILE
2	B	103	LEU
2	B	117	SER
2	B	135	ASP
2	B	145	LYS
2	B	158	GLU
2	B	162	LYS
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
2	B	230	ASP
2	B	256	GLU
2	B	257	GLU
2	B	263	VAL
3	C	6	GLU
3	C	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) 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
2	B	249	ASN

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
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	PSU	D	55	4	18,21,22	1.22	1 (5%)	21,30,33	1.39	3 (14%)
4	OMC	D	32	4	19,22,23	1.89	3 (15%)	25,31,34	1.05	1 (4%)
4	5MU	D	54	4	19,22,23	2.32	6 (31%)	27,32,35	1.47	4 (14%)
4	H2U	D	20	4	18,21,22	1.32	2 (11%)	19,30,33	2.80	5 (26%)
4	4SU	D	8	4	18,21,22	2.26	5 (27%)	25,30,33	1.84	4 (16%)

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	PSU	D	55	4	-	0/7/25/26	0/2/2/2
4	OMC	D	32	4	-	2/9/27/28	0/2/2/2
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
4	H2U	D	20	4	-	3/7/38/39	0/2/2/2
4	4SU	D	8	4	-	2/7/25/26	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	54	5MU	C6-N1	6.88	1.49	1.38
4	D	8	4SU	C4-N3	5.42	1.43	1.37
4	D	8	4SU	C5-C4	5.10	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	32	OMC	C2-N3	4.57	1.45	1.36
4	D	32	OMC	C4-N4	4.54	1.44	1.33
4	D	32	OMC	C5-C4	4.11	1.52	1.42
4	D	55	PSU	C6-C5	4.06	1.39	1.35
4	D	54	5MU	C2-N3	3.94	1.44	1.38
4	D	20	H2U	C2-N1	3.72	1.40	1.35
4	D	54	5MU	C2-N1	3.41	1.43	1.38
4	D	8	4SU	C6-N1	3.40	1.46	1.38
4	D	8	4SU	C2-N1	3.38	1.43	1.38
4	D	54	5MU	C4-C5	3.27	1.50	1.44
4	D	20	H2U	C6-C5	3.08	1.59	1.52
4	D	54	5MU	C6-C5	3.01	1.39	1.34
4	D	8	4SU	C2-N3	2.67	1.42	1.38
4	D	54	5MU	C4-N3	2.25	1.43	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	H2U	O2-C2-N1	8.39	133.19	123.10
4	D	20	H2U	O2-C2-N3	-6.62	109.28	121.49
4	D	8	4SU	C5-C4-S4	-6.00	117.45	124.31
4	D	54	5MU	O4-C4-C5	-4.60	119.66	124.92
4	D	8	4SU	S4-C4-N3	3.95	124.34	120.20
4	D	8	4SU	C5-C4-N3	3.72	118.21	114.75
4	D	20	H2U	O4-C4-N3	3.33	125.44	120.30
4	D	54	5MU	C5-C4-N3	3.31	118.20	115.32
4	D	55	PSU	C4-N3-C2	-3.30	121.83	126.37
4	D	54	5MU	C5-C6-N1	-2.95	120.11	123.31
4	D	55	PSU	O2-C2-N1	-2.90	119.79	122.79
4	D	20	H2U	C5-C6-N1	2.58	119.31	111.52
4	D	8	4SU	C4-N3-C2	-2.44	124.98	127.31
4	D	20	H2U	O4-C4-C5	-2.40	117.29	122.20
4	D	54	5MU	C4-N3-C2	-2.32	124.29	127.34
4	D	55	PSU	O4-C4-N3	-2.21	115.96	120.11
4	D	32	OMC	C5-C6-N1	-2.09	118.45	121.84

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	20	H2U	C4'-C5'-O5'-P
4	D	20	H2U	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
4	D	20	H2U	O4'-C1'-N1-C6
4	D	8	4SU	O4'-C4'-C5'-O5'
4	D	32	OMC	O4'-C4'-C5'-O5'
4	D	32	OMC	C3'-C4'-C5'-O5'
4	D	8	4SU	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	MET	D	101	4	6,7,8	1.17	1 (16%)	2,7,9	1.19	0
6	GNP	A	502	5	34,34,34	2.20	7 (20%)	47,54,54	1.07	4 (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
7	MET	D	101	4	-	2/5/6/8	-
6	GNP	A	502	5	-	6/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	502	GNP	PA-O3A	-7.70	1.51	1.59
6	A	502	GNP	PB-O3A	-7.51	1.49	1.59
6	A	502	GNP	PB-O2B	-3.68	1.47	1.56
7	D	101	MET	CB-CA	-2.57	1.49	1.53
6	A	502	GNP	PG-O3G	-2.44	1.50	1.56
6	A	502	GNP	PG-N3B	-2.28	1.57	1.63
6	A	502	GNP	PG-O2G	-2.23	1.50	1.56
6	A	502	GNP	PB-N3B	-2.17	1.57	1.63

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	502	GNP	O3G-PG-O1G	-3.61	104.41	113.45
6	A	502	GNP	O2B-PB-O1B	2.73	115.73	109.87
6	A	502	GNP	C3'-C2'-C1'	2.47	106.13	101.46
6	A	502	GNP	O2G-PG-O3G	2.11	113.26	107.59

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	GNP	PG-N3B-PB-O1B
6	A	502	GNP	PG-N3B-PB-O3A
6	A	502	GNP	C5'-O5'-PA-O3A
7	D	101	MET	N-CA-CB-CG
7	D	101	MET	C-CA-CB-CG
6	A	502	GNP	O4'-C4'-C5'-O5'
6	A	502	GNP	C3'-C4'-C5'-O5'
6	A	502	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 8 short contacts:

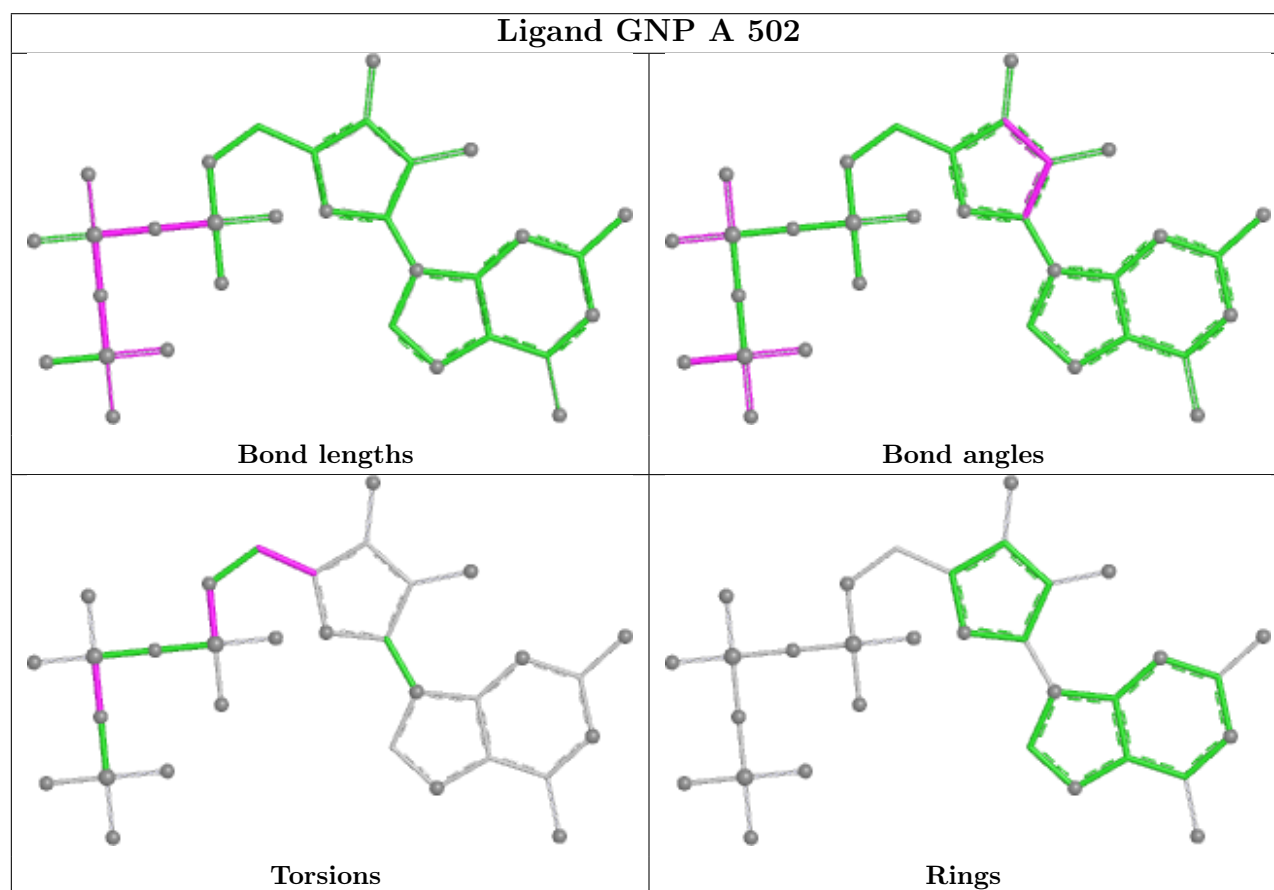
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	101	MET	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	GNP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.82	3 (0%) 84 71	300, 300, 300, 300	0
2	B	254/266 (95%)	-0.96	0 100 100	300, 300, 300, 300	0
3	C	17/138 (12%)	-1.16	0 100 100	300, 300, 300, 300	0
4	D	71/77 (92%)	-1.00	0 100 100	300, 300, 300, 300	0
All	All	746/895 (83%)	-0.89	3 (0%) 88 77	300, 300, 300, 300	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	VAL	3.0
1	A	239	GLY	3.0
1	A	407	MET	2.9

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	5MU	D	54	21/22	0.96	0.04	300,300,300,300	0
4	OMC	D	32	21/22	0.97	0.03	300,300,300,300	0
4	4SU	D	8	20/21	0.98	0.04	300,300,300,300	0
4	H2U	D	20	20/21	0.98	0.06	300,300,300,300	0
4	PSU	D	55	20/21	0.98	0.03	300,300,300,300	0

6.3 Carbohydrates [i](#)

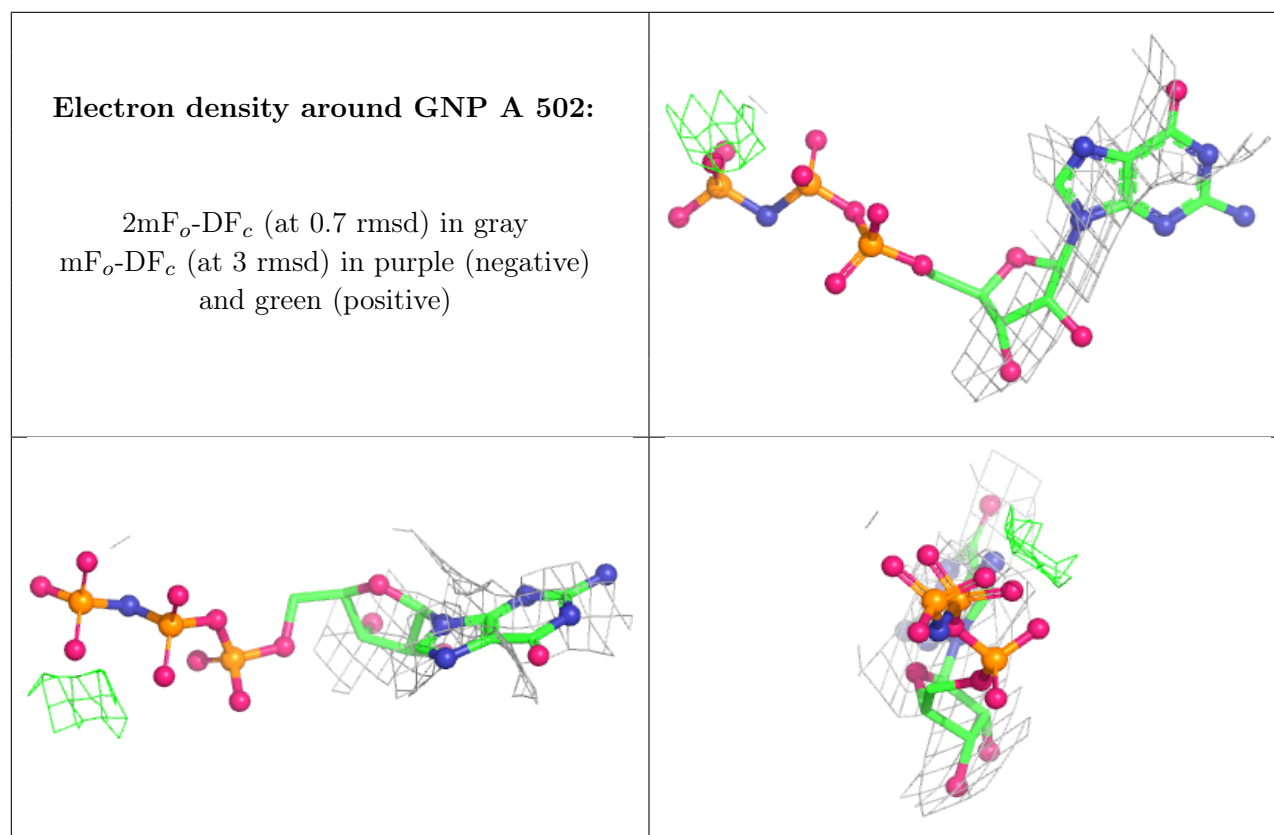
There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MET	D	101	8/9	0.98	0.06	300,300,300,300	0
6	GNP	A	502	32/32	0.99	0.03	300,300,300,300	0
5	MG	A	501	1/1	1.00	0.02	300,300,300,300	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.