



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:33 PM UTC

PDB ID : 2FMT / pdb_00002fmt
Title : METHIONYL-TRNAFMET FORMYLTRANSFERASE COMPLEXED
WITH FORMYL-METHIONYL-TRNAFMET
Authors : Schmitt, E.; Mechulam, Y.; Blanquet, S.
Deposited on : 1998-07-29
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

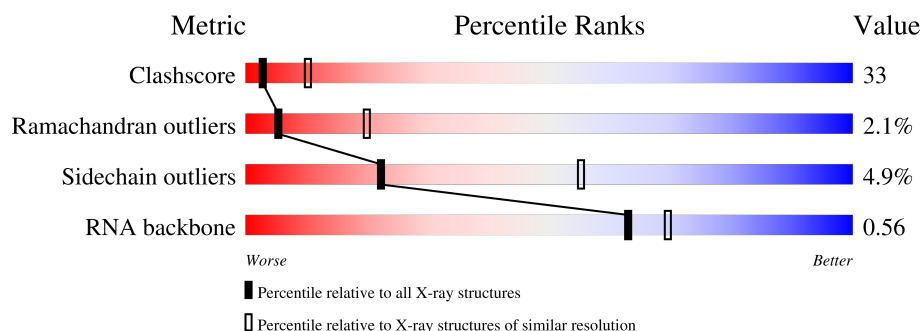
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	77	
1	D	77	
2	A	314	
2	B	314	

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
1	OMC	C	32	-	-	X	-
1	OMC	D	32	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8179 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 RNA chain called FORMYL-METHIONYL-TRNAFMET2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	77	Total	C	N	O	P	S	0	0	0
			1645	734	297	536	77	1			
1	D	77	Total	C	N	O	P	S	0	0	0
			1645	734	297	536	77	1			

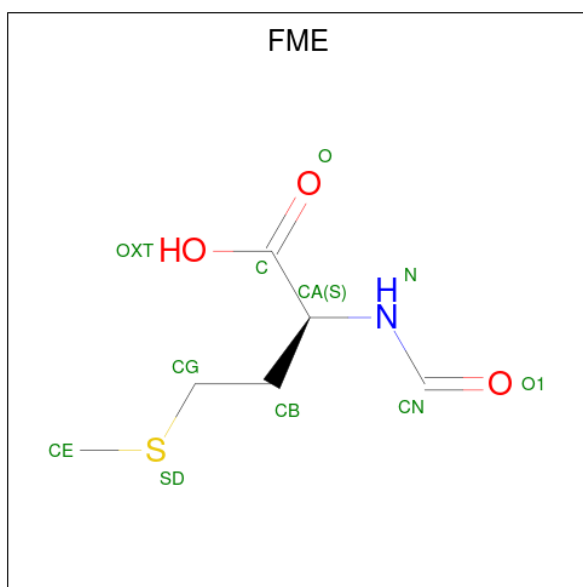
- Molecule 2 is a protein called METHIONYL-TRNA FMET FORMYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	314	Total	C	N	O	S	0	0	0
			2392	1517	414	450	11			
2	B	314	Total	C	N	O	S	0	0	0
			2392	1517	414	450	11			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
4	D	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 5 is water.

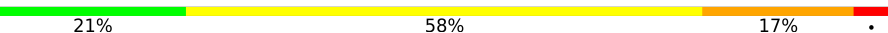
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	17	Total	O	0	0
			17	17		
5	D	13	Total	O	0	0
			13	13		
5	A	35	Total	O	0	0
			35	35		
5	B	18	Total	O	0	0
			18	18		

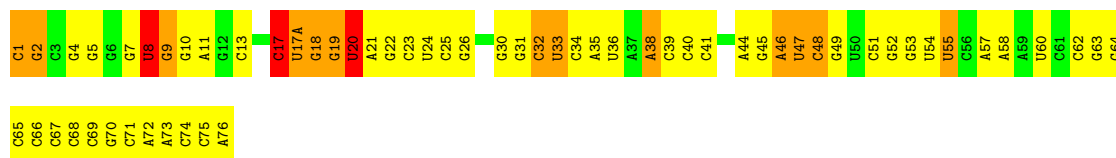
3 Residue-property plots

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. 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. 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.

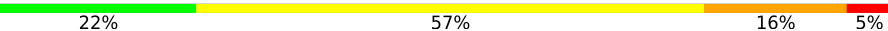
Note EDS was not executed.

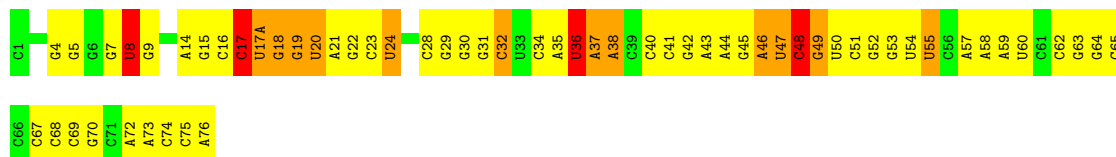
• Molecule 1: FORMYL-METHIONYL-TRNAFMET2

Chain C: 



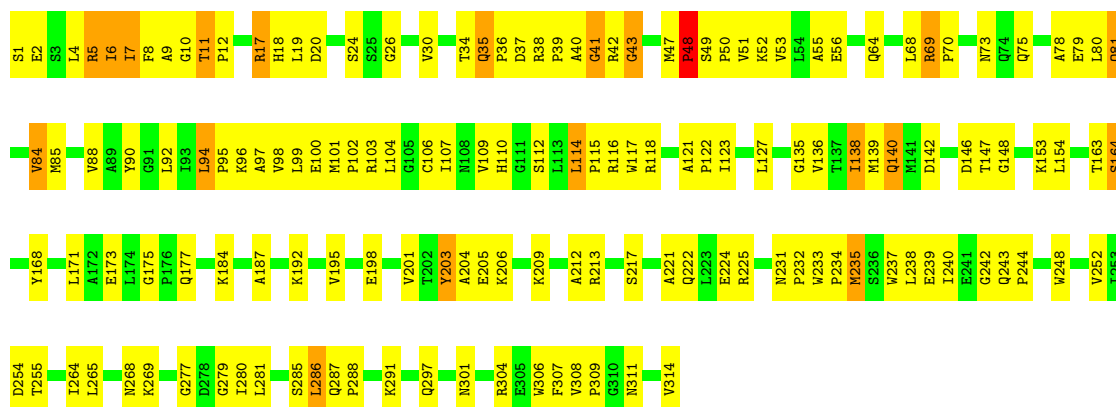
• Molecule 1: FORMYL-METHIONYL-TRNAFMET2

Chain D: 

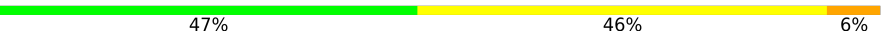


• Molecule 2: METHIONYL-TRNA FMET FORMYLTRANSFERASE

Chain A: 



• Molecule 2: METHIONYL-TRNA FMET FORMYLTRANSFERASE

Chain B: 

M235	S1	G144	Q75
S236	E2	L145	
W237	S3	D146	A78
L238	L4	T147	E79
E239	R5	G148	L80
I240	I6		Q81
E241	I7	I158	A82
G242	F8		D83
Q243	A9	T163	V84
P244	G10	S164	M85
	T11		V86
V252	P12	Y168	V87
I253			
A256	R17	L171	Y90
	H13	A172	G91
A260		E173	L92
P261	L23	L174	I93
G262	S24	G175	L94
T263		P176	P95
I264	N28		K96
L265	V29	L179	A97
	V30		V98
I272	G31	L186	L99
Q273		A187	E100
V274	T34		M101
A275	Q35	A191	P102
T276	P36		R103
G277	D37	V195	L104
D278	R38	Q196	G105
	P39	D197	C106
G279	A40	E198	I107
I280	G41		N108
L281	R42	V201	V109
N282	G43	T202	H110
L284		Y203	G111
S285	M47	A204	S112
L286	P48	E205	L113
Q287	S49	K206	L114
P288	P50	L207	P115
A289	V51	S208	R116
	K52	K209	W117
S302	V53		R118
R303	L54	A212	G119
R304	A55	R213	A120
E305	E56	T214	A121
W306		D215	P122
F307	P61	W216	I123
V308	V62	S217	Q124
	F63	L218	R125
N311	Q64	S219	S126
R312	V66		L127
L313	S67	Q222	W128
V314	L68	L223	
	R69	E224	G135
	P70	R225	
	Q71		M139
E72		N231	Q140
N73		P232	M141
Q74		W233	D142
		P234	V143

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	201.71Å 68.06Å 86.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.00 – 2.80	Depositor
% Data completeness (in resolution range)	87.2 (19.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.247 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8179	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, FME, MG, PSU, H2U, OMC, 4SU

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	C	0.47	0/1725	0.67	2/2687 (0.1%)
1	D	0.47	1/1725 (0.1%)	0.69	4/2687 (0.1%)
2	A	0.65	0/2439	1.15	19/3317 (0.6%)
2	B	0.61	0/2439	1.14	19/3317 (0.6%)
All	All	0.57	1/8328 (0.0%)	0.96	44/12008 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	4SU	O3'-P	5.24	1.61	1.56

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	U	C2'-C3'-O3'	-8.24	101.33	113.70
2	A	94	LEU	CA-C-N	7.24	127.16	119.85
2	A	94	LEU	C-N-CA	7.24	127.16	119.85
2	B	201	VAL	N-CA-C	7.18	118.83	107.98
2	A	287	GLN	CA-C-N	7.09	127.35	119.90
2	A	287	GLN	C-N-CA	7.09	127.35	119.90
2	A	6	ILE	N-CA-C	6.81	117.64	108.11
2	B	163	THR	N-CA-C	-6.47	98.80	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	C	C2'-C3'-O3'	-6.44	104.04	113.70
1	D	17	C	C2'-C3'-O3'	-6.36	104.16	113.70
2	B	6	ILE	N-CA-C	6.30	116.93	108.11
2	A	40	ALA	N-CA-C	6.22	118.31	107.49
2	B	41	GLY	N-CA-C	6.15	127.77	113.18
2	B	203	TYR	N-CA-CB	-6.13	101.48	110.49
2	B	204	ALA	N-CA-C	6.04	119.36	110.30
2	A	41	GLY	N-CA-C	5.98	127.34	113.18
2	A	43	GLY	N-CA-C	-5.93	106.90	114.37
2	A	163	THR	N-CA-C	-5.92	99.73	109.80
2	B	94	LEU	CA-C-N	5.85	126.18	119.92
2	B	94	LEU	C-N-CA	5.85	126.18	119.92
2	B	43	GLY	N-CA-C	-5.82	107.35	114.92
2	B	164	SER	N-CA-C	-5.76	105.35	112.90
2	A	279	GLY	N-CA-C	-5.52	104.44	112.17
2	B	252	VAL	N-CA-C	5.51	115.88	108.17
2	A	173	GLU	N-CA-C	-5.45	105.44	112.68
1	D	48	C	C5'-C4'-C3'	5.44	123.35	115.20
2	A	7	ILE	N-CA-C	-5.35	100.71	108.36
2	B	198	GLU	N-CA-C	5.35	119.29	112.34
2	B	121	ALA	CA-C-N	5.31	126.47	119.84
2	B	121	ALA	C-N-CA	5.31	126.47	119.84
2	B	47	MET	CA-C-N	5.30	125.06	119.76
2	B	47	MET	C-N-CA	5.30	125.06	119.76
2	A	164	SER	N-CA-C	-5.29	106.67	113.23
2	A	136	VAL	N-CA-C	5.28	116.75	109.46
2	B	201	VAL	CB-CA-C	-5.28	105.53	111.23
1	C	1	C	C2'-C3'-O3'	-5.26	105.80	113.70
2	A	192	LYS	CA-C-N	5.25	125.18	119.78
2	A	192	LYS	C-N-CA	5.25	125.18	119.78
1	D	36	U	C4'-C3'-O3'	5.20	120.80	113.00
2	B	173	GLU	N-CA-C	-5.20	106.02	112.93
2	A	48	PRO	N-CA-C	-5.14	101.87	112.47
2	B	205	GLU	N-CA-C	5.07	117.39	110.55
2	A	84	VAL	CB-CA-C	-5.05	104.77	111.80
2	A	5	ARG	N-CA-C	-5.00	102.24	109.59

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	24	U	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1645	0	839	88	0
1	D	1645	0	839	76	0
2	A	2392	0	2442	146	0
2	B	2392	0	2442	190	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	10	0	10	1	0
4	D	10	0	10	1	0
5	A	35	0	0	0	0
5	B	18	0	0	0	0
5	C	17	0	0	0	0
5	D	13	0	0	0	0
All	All	8179	0	6582	479	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 33.

All (479) 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:C:32:OMC:CM2	1:C:32:OMC:O2'	1.68	1.42
1:C:32:OMC:O2'	1:C:32:OMC:C2'	1.68	1.41
1:D:32:OMC:O2'	1:D:32:OMC:CM2	1.71	1.37
1:C:1:C:H3'	1:C:2:G:C5'	1.78	1.13
1:C:1:C:C3'	1:C:2:G:H5'	1.80	1.10
2:A:26:GLY:HA3	2:B:144:GLY:HA2	1.36	1.02
2:B:84:VAL:HG12	2:B:104:LEU:HB2	1.38	1.02
2:B:103:ARG:HG2	2:B:103:ARG:HH11	1.23	1.02
1:C:1:C:H3'	1:C:2:G:H5'	1.01	1.00
2:A:84:VAL:HG12	2:A:104:LEU:HB2	1.38	1.00
2:A:36:PRO:HA	2:A:64:GLN:HE21	1.31	0.96
2:A:139:MET:HE1	2:A:146:ASP:HA	1.46	0.96
2:B:68:LEU:O	2:B:95:PRO:HG2	1.67	0.93
2:B:69:ARG:HH21	2:B:95:PRO:HB3	1.34	0.93
2:B:17:ARG:HH11	2:B:17:ARG:HA	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:GLN:HE21	2:B:35:GLN:HA	1.35	0.92
1:D:47:U:H5'	1:D:48:C:OP2	1.71	0.91
1:C:17(A):U:H4'	1:C:18:G:OP1	1.70	0.88
2:B:36:PRO:HA	2:B:64:GLN:HE21	1.38	0.88
2:B:139:MET:HE1	2:B:146:ASP:HA	1.56	0.88
1:D:57:A:H2'	1:D:58:A:H5'	1.53	0.87
1:D:30:G:O2'	1:D:31:G:H5'	1.76	0.85
2:A:17:ARG:HA	2:A:17:ARG:HH11	1.40	0.84
2:A:68:LEU:O	2:A:95:PRO:HG2	1.77	0.83
2:A:110:HIS:ND1	2:A:114:LEU:HD21	1.94	0.82
1:D:57:A:C2'	1:D:58:A:H5'	2.09	0.82
2:B:121:ALA:O	2:B:125:ARG:HB2	1.81	0.80
2:B:110:HIS:ND1	2:B:114:LEU:HD21	1.98	0.78
1:C:39:C:O2'	1:C:40:C:H5'	1.83	0.78
2:B:17:ARG:HH11	2:B:17:ARG:CA	1.97	0.77
2:B:35:GLN:HE21	2:B:35:GLN:CA	1.98	0.76
2:B:125:ARG:NH2	2:B:207:LEU:HD23	2.00	0.76
1:C:57:A:H2'	1:C:58:A:H5'	1.68	0.75
2:B:215:ASP:OD2	2:B:217:SER:HB3	1.86	0.74
2:B:10:GLY:O	2:B:34:THR:HG22	1.87	0.74
2:A:36:PRO:HA	2:A:64:GLN:NE2	2.01	0.74
2:A:69:ARG:HH21	2:A:95:PRO:HB3	1.49	0.74
2:B:103:ARG:HG2	2:B:103:ARG:NH1	1.97	0.74
2:B:114:LEU:HB3	2:B:115:PRO:HA	1.70	0.73
2:B:11:THR:O	2:B:50:PRO:HD2	1.87	0.73
1:D:36:U:H2'	1:D:38:A:N7	2.03	0.73
2:A:285:SER:C	2:A:286:LEU:HD12	2.14	0.72
1:C:39:C:H2'	1:C:40:C:H6	1.53	0.72
1:D:17:C:H4'	1:D:17(A):U:OP2	1.88	0.72
1:D:16:C:OP2	1:D:17:C:N4	2.19	0.72
2:B:36:PRO:HG2	2:B:38:ARG:HE	1.54	0.72
1:D:64:G:O2'	1:D:65:C:H5'	1.90	0.71
2:B:117:TRP:CE3	2:B:204:ALA:HB2	2.25	0.71
1:C:7:G:H4'	1:C:8:4SU:OP2	1.89	0.71
2:A:213:ARG:HB2	2:A:237:TRP:CZ2	2.26	0.71
2:A:10:GLY:O	2:A:34:THR:HG22	1.91	0.71
2:B:239:GLU:OE2	2:B:242:GLY:HA2	1.91	0.70
2:B:69:ARG:NH2	2:B:95:PRO:HB3	2.07	0.70
1:C:57:A:C2'	1:C:58:A:H5'	2.22	0.70
2:A:114:LEU:HB3	2:A:115:PRO:HA	1.73	0.69
2:B:75:GLN:O	2:B:79:GLU:HB2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:5MU:H72	1:D:55:PSU:C2	2.29	0.68
1:C:1:C:H2'	1:C:1:C:O2	1.94	0.68
2:B:103:ARG:NH1	2:B:104:LEU:HG	2.08	0.68
2:B:123:ILE:HD12	2:B:168:TYR:CE1	2.29	0.67
2:B:36:PRO:HA	2:B:64:GLN:NE2	2.06	0.67
1:C:19:G:H4'	1:C:20:H2U:OP2	1.93	0.67
2:A:238:LEU:HD12	2:A:238:LEU:C	2.20	0.67
2:A:38:ARG:HB3	2:A:39:PRO:CD	2.26	0.66
2:A:69:ARG:N	2:A:70:PRO:CD	2.59	0.66
2:A:69:ARG:NH2	2:A:95:PRO:HB3	2.10	0.66
1:D:55:PSU:O2'	1:D:57:A:N7	2.28	0.66
2:B:7:ILE:HB	2:B:85:MET:HG3	1.76	0.65
2:A:240:ILE:O	2:A:243:GLN:HB3	1.97	0.65
2:A:286:LEU:HD12	2:A:286:LEU:N	2.12	0.65
2:B:38:ARG:HB3	2:B:39:PRO:HD2	1.77	0.65
1:D:76:A:H2	2:B:121:ALA:HB2	1.60	0.65
1:D:7:G:H4'	1:D:8:4SU:OP2	1.96	0.65
2:B:35:GLN:HA	2:B:35:GLN:NE2	2.06	0.65
2:B:36:PRO:O	2:B:38:ARG:HG3	1.97	0.65
1:D:22:G:O2'	1:D:23:C:H5'	1.97	0.64
2:B:69:ARG:N	2:B:70:PRO:CD	2.61	0.64
1:C:64:G:O2'	1:C:65:C:H5'	1.98	0.64
1:D:32:OMC:CM2	1:D:32:OMC:C2'	2.76	0.64
2:A:24:SER:O	2:B:145:LEU:HB2	1.96	0.64
1:C:17(A):U:C4'	1:C:18:G:OP1	2.45	0.63
1:C:10:G:O4'	2:B:311:ASN:ND2	2.31	0.63
1:C:38:A:O2'	1:C:39:C:H5'	1.98	0.63
2:A:121:ALA:O	2:A:204:ALA:HB1	1.99	0.63
1:C:30:G:O2'	1:C:31:G:H5'	1.98	0.63
1:C:69:C:H2'	1:C:70:G:H8	1.63	0.63
1:D:76:A:O2'	2:B:120:ALA:HB1	2.00	0.62
2:B:103:ARG:HH11	2:B:103:ARG:CG	2.04	0.62
1:C:32:OMC:CM2	1:C:32:OMC:H1'	2.29	0.62
2:B:11:THR:HB	2:B:12:PRO:HD3	1.81	0.62
2:B:216:TRP:O	2:B:277:GLY:N	2.33	0.62
1:D:31:G:H2'	1:D:32:OMC:O4'	1.98	0.62
1:D:72:A:O2'	1:D:73:A:H5'	1.99	0.62
2:A:36:PRO:O	2:A:38:ARG:HG3	2.00	0.62
2:A:38:ARG:HB3	2:A:39:PRO:HD2	1.80	0.62
2:B:35:GLN:HG3	2:B:36:PRO:HD2	1.81	0.62
2:B:3:SER:HB2	2:B:28:ASN:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:O	2:B:6:ILE:HG13	2.00	0.62
2:B:238:LEU:HD12	2:B:238:LEU:C	2.25	0.62
1:D:17(A):U:H4'	1:D:18:G:OP1	2.00	0.62
1:D:44:A:H2'	1:D:45:G:O4'	2.00	0.61
2:A:17:ARG:HH11	2:A:17:ARG:CA	2.10	0.61
1:C:55:PSU:O2'	1:C:57:A:N7	2.33	0.61
2:A:26:GLY:CA	2:B:144:GLY:HA2	2.22	0.61
2:B:285:SER:C	2:B:286:LEU:HD12	2.25	0.60
2:B:11:THR:HB	2:B:12:PRO:CD	2.31	0.60
2:A:140:GLN:O	2:A:148:GLY:HA3	2.02	0.60
2:A:114:LEU:N	2:A:114:LEU:HD23	2.15	0.60
2:B:115:PRO:O	2:B:118:ARG:HG3	2.00	0.60
2:A:118:ARG:HD3	2:A:201:VAL:HG13	1.83	0.60
1:C:17:C:H4'	1:C:17(A):U:OP2	2.02	0.60
2:A:84:VAL:CG1	2:A:104:LEU:HB2	2.23	0.59
2:A:69:ARG:H	2:A:70:PRO:HD3	1.66	0.59
2:A:135:GLY:HA2	2:A:171:LEU:CD2	2.33	0.59
2:B:282:ASN:ND2	2:B:284:LEU:HD21	2.17	0.59
1:C:39:C:H2'	1:C:40:C:C6	2.37	0.59
1:C:73:A:O2'	1:C:74:C:H5'	2.03	0.59
2:A:84:VAL:HG12	2:A:104:LEU:CB	2.25	0.58
1:D:35:A:H2'	1:D:36:U:C6	2.38	0.58
2:B:274:VAL:O	2:B:280:ILE:HG23	2.03	0.58
1:C:54:5MU:H72	1:C:55:PSU:C2	2.38	0.58
2:B:140:GLN:O	2:B:148:GLY:HA3	2.03	0.58
2:B:243:GLN:HE21	2:B:289:ALA:HB3	1.68	0.57
1:D:32:OMC:CM2	1:D:32:OMC:H1'	2.34	0.57
1:C:72:A:N1	2:A:42:ARG:N	2.52	0.57
2:B:118:ARG:HH21	2:B:147:THR:HA	1.69	0.57
2:A:115:PRO:O	2:A:118:ARG:HG3	2.05	0.57
1:C:53:G:O2'	1:C:54:5MU:H5''	2.04	0.57
1:D:51:C:H2'	1:D:52:G:C8	2.40	0.57
2:B:123:ILE:HD12	2:B:168:TYR:CZ	2.39	0.57
1:C:75:C:O2'	1:C:76:A:H5'	2.04	0.57
2:B:234:PRO:O	2:B:235:MET:HB2	2.04	0.57
1:D:69:C:H2'	1:D:70:G:H8	1.69	0.57
2:A:139:MET:CE	2:A:146:ASP:HA	2.29	0.57
1:D:32:OMC:H1'	1:D:32:OMC:HM23	1.85	0.57
1:C:32:OMC:H1'	1:C:32:OMC:HM23	1.85	0.56
4:C:585:FME:CN	2:A:90:TYR:H	2.18	0.56
2:B:12:PRO:HA	2:B:50:PRO:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:OMC:O2	1:C:32:OMC:HM22	2.05	0.56
2:A:35:GLN:HE21	2:A:35:GLN:CA	2.17	0.56
2:B:3:SER:HB2	2:B:28:ASN:CB	2.34	0.56
2:A:11:THR:HB	2:A:12:PRO:HD3	1.86	0.56
1:C:18:G:O4'	1:C:18:G:OP2	2.23	0.56
2:A:164:SER:HB2	2:A:231:ASN:O	2.06	0.56
2:A:41:GLY:O	2:A:42:ARG:HB3	2.05	0.56
1:C:40:C:H2'	1:C:41:C:H6	1.71	0.56
1:D:40:C:H2'	1:D:41:C:H6	1.70	0.56
2:A:127:LEU:HD12	2:A:127:LEU:O	2.06	0.55
1:D:73:A:O2'	1:D:74:C:H5'	2.06	0.55
2:B:37:ASP:O	2:B:38:ARG:CG	2.54	0.55
2:B:103:ARG:HH12	2:B:104:LEU:HD21	1.71	0.55
2:B:70:PRO:HB2	2:B:73:ASN:HD22	1.72	0.55
2:B:216:TRP:NE1	2:B:314:VAL:O	2.35	0.55
1:C:55:PSU:H2'	1:C:57:A:OP2	2.06	0.55
2:B:117:TRP:HE3	2:B:204:ALA:HB2	1.69	0.55
2:B:238:LEU:CD1	2:B:240:ILE:HG12	2.36	0.55
1:C:19:G:H3'	1:C:20:H2U:H5''	1.87	0.55
1:D:32:OMC:HM22	1:D:32:OMC:O2	2.07	0.55
2:A:118:ARG:CD	2:A:201:VAL:HG13	2.37	0.54
2:B:97:ALA:O	2:B:101:MET:HG3	2.07	0.54
2:A:36:PRO:HG2	2:A:38:ARG:HE	1.72	0.54
2:A:118:ARG:HH21	2:A:147:THR:HA	1.72	0.54
2:B:127:LEU:HD13	2:B:158:ILE:HG21	1.89	0.54
1:D:55:PSU:H2'	1:D:57:A:OP2	2.07	0.54
2:A:135:GLY:HA2	2:A:171:LEU:HD22	1.90	0.54
2:B:5:ARG:HB3	2:B:30:VAL:HG11	1.90	0.54
1:C:2:G:O6	2:A:42:ARG:HA	2.06	0.54
2:A:69:ARG:N	2:A:70:PRO:HD3	2.22	0.54
2:A:123:ILE:HD12	2:A:168:TYR:CZ	2.42	0.54
2:B:223:LEU:HD12	2:B:276:THR:HG21	1.90	0.54
2:A:239:GLU:HA	2:A:243:GLN:O	2.08	0.54
2:B:303:ARG:HD2	2:B:306:TRP:CE2	2.43	0.54
1:C:1:C:C3'	1:C:2:G:C5'	2.60	0.54
1:C:76:A:N1	2:A:206:LYS:HB2	2.23	0.54
2:B:37:ASP:H	2:B:64:GLN:HE22	1.55	0.54
1:D:17(A):U:H5''	1:D:18:G:OP2	2.06	0.53
1:C:22:G:O2'	1:C:23:C:H5'	2.07	0.53
2:A:217:SER:O	2:A:277:GLY:HA3	2.08	0.53
2:B:118:ARG:HD3	2:B:201:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:C:O2'	1:D:68:C:H5'	2.09	0.53
2:A:11:THR:HB	2:A:12:PRO:CD	2.39	0.53
2:A:90:TYR:OH	2:A:92:LEU:HD12	2.08	0.53
2:A:123:ILE:HD12	2:A:168:TYR:CE1	2.44	0.53
1:C:4:G:H2'	1:C:5:G:H8	1.74	0.53
2:B:69:ARG:H	2:B:70:PRO:HD3	1.73	0.53
1:C:46:A:O2'	1:C:47:U:P	2.67	0.52
1:D:36:U:H2'	1:D:38:A:C8	2.44	0.52
2:A:55:ALA:O	2:A:56:GLU:C	2.52	0.52
2:A:234:PRO:O	2:A:235:MET:HB2	2.09	0.52
2:B:239:GLU:HA	2:B:243:GLN:O	2.10	0.52
2:B:128:TRP:O	2:B:225:ARG:HD2	2.10	0.52
2:A:37:ASP:H	2:A:64:GLN:HE22	1.57	0.52
2:A:49:SER:O	2:A:53:VAL:HG23	2.09	0.52
1:D:40:C:H2'	1:D:41:C:C6	2.45	0.52
2:A:97:ALA:O	2:A:101:MET:HG3	2.10	0.52
2:B:94:LEU:HD12	2:B:141:MET:CE	2.39	0.52
1:C:32:OMC:CM2	1:C:32:OMC:C2'	2.88	0.52
2:A:35:GLN:HG3	2:A:36:PRO:HD2	1.91	0.52
2:B:80:LEU:O	2:B:81:GLN:C	2.52	0.52
2:A:24:SER:HB2	2:B:203:TYR:OH	2.10	0.52
2:B:69:ARG:N	2:B:70:PRO:HD3	2.25	0.51
2:B:90:TYR:OH	2:B:92:LEU:HD12	2.10	0.51
1:C:31:G:C2'	1:C:32:OMC:H5''	2.40	0.51
1:C:33:U:O2	1:C:35:A:C8	2.64	0.51
1:C:67:C:H2'	1:C:68:C:H6	1.75	0.51
2:A:114:LEU:HA	2:A:116:ARG:N	2.24	0.51
2:B:112:SER:HB3	2:B:122:PRO:CB	2.40	0.51
2:B:276:THR:OG1	2:B:278:ASP:O	2.28	0.51
1:C:25:C:C2	1:C:26:G:C8	2.98	0.51
2:A:103:ARG:HG2	2:A:103:ARG:HH11	1.75	0.51
2:B:31:GLY:HA2	2:B:61:PRO:HG2	1.93	0.51
2:B:114:LEU:HD23	2:B:114:LEU:N	2.24	0.51
1:C:58:A:O2'	1:C:60:U:OP2	2.27	0.51
1:C:69:C:O2'	1:C:70:G:H5'	2.10	0.51
2:A:308:VAL:HG23	2:A:311:ASN:OD1	2.10	0.51
1:D:28:C:O2'	1:D:29:G:H5'	2.11	0.51
1:D:76:A:C2	2:B:121:ALA:HB2	2.44	0.51
2:B:78:ALA:HB2	2:B:101:MET:SD	2.51	0.51
2:B:186:LEU:HD23	2:B:191:ALA:HB2	1.93	0.51
2:B:282:ASN:HD21	2:B:284:LEU:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:G:O2'	1:D:43:A:H5'	2.11	0.50
2:A:224:GLU:HG3	2:A:252:VAL:HG23	1.92	0.50
1:D:49:G:O2'	1:D:50:U:H5'	2.11	0.50
2:B:103:ARG:HH12	2:B:104:LEU:CG	2.25	0.50
1:D:62:C:H2'	1:D:63:G:H8	1.76	0.50
2:A:265:LEU:HD12	2:A:280:ILE:HD13	1.94	0.50
1:D:67:C:H2'	1:D:68:C:H6	1.76	0.50
1:D:57:A:O2'	1:D:58:A:H5'	2.11	0.50
2:B:68:LEU:HD12	2:B:94:LEU:HD23	1.94	0.50
2:B:240:ILE:HD11	2:B:313:LEU:HD22	1.93	0.50
2:B:103:ARG:NH1	2:B:104:LEU:CG	2.75	0.50
1:D:31:G:O2'	1:D:32:OMC:H5''	2.11	0.49
2:B:286:LEU:HD12	2:B:286:LEU:N	2.27	0.49
1:D:30:G:C2'	1:D:31:G:H5'	2.43	0.49
2:A:4:LEU:HD11	2:A:187:ALA:HB2	1.93	0.49
2:A:238:LEU:CD1	2:A:240:ILE:HG12	2.42	0.49
1:C:46:A:O2'	1:C:47:U:OP1	2.27	0.49
2:B:18:HIS:CE1	2:B:176:PRO:HD3	2.48	0.49
2:B:103:ARG:HH12	2:B:104:LEU:CD2	2.25	0.49
2:B:139:MET:CE	2:B:146:ASP:HA	2.36	0.49
2:A:1:SER:HB2	2:B:96:LYS:NZ	2.27	0.49
2:A:240:ILE:HG21	2:A:306:TRP:CD2	2.48	0.49
2:B:114:LEU:HA	2:B:116:ARG:N	2.27	0.49
2:B:231:ASN:C	2:B:231:ASN:OD1	2.54	0.49
1:C:72:A:O2'	1:C:73:A:H5'	2.12	0.49
2:A:11:THR:H	2:A:12:PRO:HD2	1.76	0.49
1:C:25:C:H1'	2:A:301:ASN:ND2	2.27	0.49
1:D:31:G:C2'	1:D:32:OMC:H5''	2.43	0.49
2:B:265:LEU:HD12	2:B:280:ILE:HD13	1.95	0.49
1:C:53:G:C2	1:C:62:C:C2	3.01	0.48
1:D:41:C:O2'	1:D:42:G:H5'	2.13	0.48
1:D:62:C:H2'	1:D:63:G:C8	2.48	0.48
2:A:9:ALA:HB2	2:A:85:MET:HE2	1.95	0.48
2:B:218:LEU:O	2:B:276:THR:HB	2.12	0.48
2:B:308:VAL:HG23	2:B:311:ASN:OD1	2.13	0.48
2:A:308:VAL:HG23	2:A:311:ASN:CG	2.38	0.48
1:D:68:C:H2'	1:D:69:C:C6	2.49	0.48
2:B:263:THR:HA	2:B:312:ARG:HA	1.96	0.48
1:D:54:5MU:H72	1:D:55:PSU:N1	2.29	0.48
2:B:5:ARG:HD3	2:B:81:GLN:O	2.14	0.48
2:B:212:ALA:HB2	2:B:234:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:235:MET:HE2	2:A:248:TRP:CE2	2.49	0.48
2:B:55:ALA:O	2:B:56:GLU:C	2.56	0.48
1:C:19:G:H3'	1:C:20:H2U:O4'	2.14	0.48
2:A:203:TYR:N	2:A:203:TYR:CD1	2.82	0.48
1:C:23:C:H2'	1:C:24:U:H6	1.78	0.48
2:B:209:LYS:O	2:B:212:ALA:HB3	2.13	0.48
1:D:50:U:H2'	1:D:51:C:C6	2.49	0.48
2:B:30:VAL:O	2:B:61:PRO:CG	2.62	0.48
1:C:53:G:N2	1:C:62:C:C2	2.82	0.47
2:A:233:TRP:CD1	2:A:234:PRO:HA	2.48	0.47
1:D:36:U:H4'	1:D:37:A:OP1	2.14	0.47
2:B:84:VAL:CG1	2:B:104:LEU:HD12	2.44	0.47
2:B:4:LEU:HD11	2:B:187:ALA:HB2	1.95	0.47
2:B:308:VAL:HG23	2:B:311:ASN:CG	2.39	0.47
1:C:35:A:O2'	1:C:36:U:H5'	2.14	0.47
1:D:7:G:C4'	1:D:8:4SU:OP2	2.62	0.47
2:A:233:TRP:CG	2:A:234:PRO:HA	2.50	0.47
2:B:37:ASP:O	2:B:38:ARG:HG3	2.14	0.47
2:B:219:SER:O	2:B:223:LEU:HG	2.14	0.47
1:C:30:G:C2'	1:C:31:G:H5'	2.44	0.47
1:C:40:C:H2'	1:C:41:C:C6	2.48	0.47
2:A:118:ARG:HH21	2:A:147:THR:HG22	1.80	0.47
2:A:78:ALA:HB2	2:A:101:MET:SD	2.55	0.47
2:A:221:ALA:O	2:A:225:ARG:HG3	2.13	0.47
2:B:94:LEU:HD12	2:B:141:MET:HE1	1.97	0.47
2:B:135:GLY:HA2	2:B:171:LEU:HD21	1.97	0.47
1:C:4:G:H2'	1:C:5:G:C8	2.50	0.47
1:C:24:U:O2'	2:A:304:ARG:NH2	2.47	0.47
1:D:46:A:O2'	1:D:47:U:OP1	2.31	0.47
2:B:216:TRP:CZ3	2:B:274:VAL:HG11	2.50	0.47
1:C:10:G:C1'	2:B:311:ASN:ND2	2.78	0.47
1:C:13:C:OP1	2:A:291:LYS:HE3	2.14	0.47
1:D:69:C:O2'	1:D:70:G:H5'	2.15	0.47
2:A:80:LEU:O	2:A:81:GLN:C	2.58	0.47
2:A:286:LEU:N	2:A:286:LEU:CD1	2.77	0.47
1:C:46:A:HO2'	1:C:47:U:P	2.36	0.46
2:A:35:GLN:HA	2:A:35:GLN:NE2	2.30	0.46
2:B:240:ILE:O	2:B:241:GLU:HB2	2.15	0.46
1:D:46:A:O2'	1:D:47:U:P	2.73	0.46
2:A:90:TYR:CZ	2:A:92:LEU:HD12	2.51	0.46
2:B:112:SER:N	2:B:135:GLY:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:C:H2'	1:D:69:C:H6	1.80	0.46
2:B:5:ARG:NH1	2:B:80:LEU:O	2.49	0.46
2:B:84:VAL:HG12	2:B:104:LEU:CB	2.26	0.46
2:B:234:PRO:O	2:B:235:MET:CB	2.62	0.46
2:B:135:GLY:HA2	2:B:171:LEU:CD2	2.45	0.46
2:B:63:PHE:O	2:B:65:PRO:HD2	2.16	0.46
2:A:2:GLU:HG3	2:A:2:GLU:O	2.15	0.46
2:A:238:LEU:HD12	2:A:238:LEU:O	2.15	0.46
2:B:95:PRO:O	2:B:99:LEU:HD13	2.14	0.46
2:B:112:SER:HB3	2:B:122:PRO:HB3	1.96	0.46
2:A:314:VAL:OXT	2:A:314:VAL:HG12	2.16	0.46
2:B:74:GLN:OE1	2:B:97:ALA:HB3	2.16	0.46
2:B:112:SER:HB2	2:B:117:TRP:HB2	1.98	0.46
2:A:8:PHE:CD2	2:A:19:LEU:HD13	2.51	0.46
2:A:239:GLU:OE2	2:A:242:GLY:HA2	2.16	0.46
2:A:153:LYS:O	2:A:154:LEU:HD23	2.15	0.46
2:B:36:PRO:O	2:B:37:ASP:C	2.59	0.46
2:A:212:ALA:HB2	2:A:234:PRO:CG	2.46	0.45
2:A:308:VAL:CG2	2:A:311:ASN:CG	2.89	0.45
2:B:69:ARG:HE	2:B:69:ARG:HA	1.81	0.45
1:C:70:G:N7	2:A:42:ARG:NH2	2.63	0.45
2:A:103:ARG:HG2	2:A:103:ARG:NH1	2.32	0.45
2:A:138:ILE:HD12	2:A:138:ILE:N	2.31	0.45
2:A:8:PHE:CG	2:A:19:LEU:HD13	2.52	0.45
1:D:72:A:H2'	1:D:73:A:O4'	2.16	0.45
1:C:1:C:O2	1:C:1:C:C2'	2.64	0.45
1:D:58:A:O2'	1:D:60:U:OP2	2.33	0.45
2:A:198:GLU:OE1	2:A:198:GLU:HA	2.16	0.45
2:B:233:TRP:CG	2:B:234:PRO:HA	2.52	0.45
2:A:18:HIS:NE2	2:A:109:VAL:HG11	2.32	0.45
2:B:87:VAL:O	2:B:108:ASN:HA	2.17	0.45
1:C:71:C:OP1	2:A:209:LYS:NZ	2.50	0.45
2:B:222:GLN:HA	2:B:225:ARG:NH1	2.32	0.45
2:B:288:PRO:O	2:B:289:ALA:C	2.60	0.45
2:A:19:LEU:O	2:A:20:ASP:C	2.60	0.45
2:A:75:GLN:HG3	2:A:79:GLU:HG2	1.98	0.45
2:B:118:ARG:CD	2:B:201:VAL:HG13	2.46	0.45
1:C:63:G:O2'	1:C:64:G:H5'	2.16	0.44
1:C:10:G:C2	1:C:11:A:C8	3.05	0.44
1:D:35:A:H2'	1:D:36:U:H6	1.82	0.44
2:A:7:ILE:HB	2:A:85:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:84:VAL:CG1	2:A:104:LEU:HD12	2.47	0.44
2:B:263:THR:N	2:B:312:ARG:HG3	2.33	0.44
1:D:47:U:C5'	1:D:48:C:OP2	2.55	0.44
2:A:68:LEU:HD12	2:A:94:LEU:HD23	1.99	0.44
1:C:31:G:O2'	1:C:32:OMC:H5''	2.18	0.44
2:A:4:LEU:O	2:A:6:ILE:HG13	2.17	0.44
2:A:35:GLN:CA	2:A:35:GLN:NE2	2.80	0.44
2:A:114:LEU:HA	2:A:115:PRO:C	2.42	0.44
2:B:253:ILE:HD12	2:B:273:GLN:HG2	1.99	0.44
2:B:303:ARG:O	2:B:306:TRP:HB2	2.17	0.44
1:D:49:G:H1	1:D:65:C:H42	1.64	0.44
1:D:54:5MU:H72	1:D:55:PSU:O2	2.17	0.44
2:A:135:GLY:HA2	2:A:171:LEU:HD21	2.00	0.44
2:B:233:TRP:CD1	2:B:234:PRO:HA	2.52	0.44
2:B:262:GLY:C	2:B:312:ARG:HG3	2.42	0.44
2:A:69:ARG:H	2:A:70:PRO:CD	2.24	0.44
2:A:94:LEU:HB2	2:A:99:LEU:HD11	2.00	0.44
2:A:96:LYS:O	2:A:100:GLU:HG3	2.17	0.44
2:A:238:LEU:C	2:A:238:LEU:CD1	2.90	0.44
2:B:10:GLY:C	2:B:51:VAL:HG21	2.42	0.44
2:A:35:GLN:HE21	2:A:35:GLN:HA	1.82	0.44
2:B:11:THR:H	2:B:12:PRO:HD2	1.82	0.44
2:A:212:ALA:HB2	2:A:234:PRO:HG2	1.99	0.44
2:A:231:ASN:OD1	2:A:231:ASN:C	2.61	0.44
1:C:23:C:H2'	1:C:24:U:C6	2.53	0.44
1:D:32:OMC:CM2	1:D:32:OMC:C1'	2.95	0.44
2:A:2:GLU:O	2:A:2:GLU:CG	2.65	0.44
1:C:32:OMC:O2'	1:C:32:OMC:C1'	2.57	0.43
1:C:69:C:H2'	1:C:70:G:C8	2.49	0.43
1:D:34:C:O2'	1:D:35:A:H5'	2.18	0.43
2:A:107:ILE:HA	2:A:139:MET:O	2.18	0.43
2:A:110:HIS:HE1	2:A:117:TRP:O	2.00	0.43
1:C:73:A:H2'	1:C:74:C:O4'	2.18	0.43
1:C:44:A:H2'	1:C:45:G:O4'	2.18	0.43
1:D:36:U:H5''	1:D:37:A:OP1	2.18	0.43
2:A:11:THR:O	2:A:50:PRO:HD2	2.18	0.43
2:A:94:LEU:HA	2:A:95:PRO:HD3	1.77	0.43
2:B:85:MET:HB3	2:B:106:CYS:SG	2.57	0.43
2:B:66:VAL:O	2:B:66:VAL:HG12	2.19	0.43
2:B:117:TRP:CE3	2:B:117:TRP:HA	2.53	0.43
1:C:7:G:C4'	1:C:8:4SU:OP2	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:SER:HB2	2:B:231:ASN:O	2.19	0.43
1:D:46:A:HO2'	1:D:47:U:P	2.42	0.43
2:A:177:GLN:NE2	2:B:201:VAL:O	2.52	0.43
2:B:52:LYS:O	2:B:55:ALA:N	2.52	0.43
2:B:110:HIS:HE1	2:B:117:TRP:O	2.02	0.43
1:D:19:G:C4	1:D:57:A:C2	3.07	0.43
2:B:198:GLU:HA	2:B:198:GLU:OE1	2.19	0.43
1:C:66:C:O2'	1:C:67:C:H5'	2.19	0.43
2:B:70:PRO:HB2	2:B:73:ASN:ND2	2.33	0.43
1:D:14:A:O2'	1:D:15:G:H5'	2.19	0.42
2:A:88:VAL:HG22	2:A:109:VAL:HG23	2.00	0.42
2:A:47:MET:C	2:A:48:PRO:O	2.59	0.42
2:A:112:SER:HB3	2:A:122:PRO:CB	2.48	0.42
2:A:123:ILE:HG21	2:A:168:TYR:CD1	2.54	0.42
2:B:94:LEU:HA	2:B:95:PRO:HD3	1.78	0.42
2:B:198:GLU:HA	2:B:201:VAL:HG23	2.01	0.42
1:C:32:OMC:H2'	1:C:33:U:H6	1.84	0.42
1:D:36:U:H2'	1:D:38:A:C5	2.54	0.42
2:A:281:LEU:HA	2:A:281:LEU:HD12	1.81	0.42
2:B:63:PHE:C	2:B:65:PRO:HD2	2.44	0.42
2:B:96:LYS:O	2:B:100:GLU:HG3	2.20	0.42
2:B:9:ALA:HB2	2:B:85:MET:HE2	2.00	0.42
2:B:52:LYS:O	2:B:53:VAL:C	2.63	0.42
2:B:262:GLY:C	2:B:313:LEU:H	2.26	0.42
2:B:262:GLY:O	2:B:313:LEU:N	2.47	0.42
1:D:44:A:N6	1:D:45:G:N1	2.67	0.42
4:D:586:FME:CN	2:B:90:TYR:H	2.33	0.42
2:B:47:MET:HA	2:B:48:PRO:HD3	1.86	0.42
2:B:115:PRO:O	2:B:118:ARG:CG	2.65	0.42
2:B:238:LEU:C	2:B:238:LEU:CD1	2.91	0.42
1:C:57:A:O2'	1:C:58:A:H5'	2.19	0.42
2:A:254:ASP:C	2:A:255:THR:HG23	2.45	0.42
2:B:101:MET:HB2	2:B:102:PRO:HD3	2.00	0.42
2:B:212:ALA:HB3	2:B:237:TRP:HE1	1.84	0.42
2:B:240:ILE:HG21	2:B:306:TRP:CD2	2.55	0.42
1:D:4:G:H2'	1:D:5:G:C8	2.55	0.42
1:D:36:U:C4'	1:D:37:A:OP1	2.68	0.42
1:D:69:C:O2'	1:D:70:G:C5'	2.68	0.42
2:B:71:GLN:O	2:B:72:GLU:C	2.63	0.42
1:C:68:C:H2'	1:C:69:C:C6	2.55	0.42
2:B:23:LEU:O	2:B:24:SER:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:C:H2'	1:C:17(A):U:C5	2.55	0.41
2:A:5:ARG:HB3	2:A:30:VAL:HG11	2.02	0.41
2:A:5:ARG:NH1	2:A:80:LEU:O	2.53	0.41
2:A:10:GLY:C	2:A:51:VAL:HG21	2.45	0.41
2:A:288:PRO:O	2:A:291:LYS:HB2	2.20	0.41
2:B:260:ALA:HA	2:B:261:PRO:HD3	1.89	0.41
2:A:52:LYS:O	2:A:55:ALA:N	2.53	0.41
2:A:70:PRO:HB2	2:A:73:ASN:HD22	1.85	0.41
1:C:48:C:H6	1:C:48:C:OP2	2.02	0.41
2:A:98:VAL:O	2:A:102:PRO:HD3	2.20	0.41
2:B:147:THR:C	2:B:196:GLN:NE2	2.78	0.41
2:A:198:GLU:HA	2:A:201:VAL:HG23	2.03	0.41
2:A:264:ILE:CD1	2:A:307:PHE:HA	2.51	0.41
2:B:38:ARG:HB3	2:B:39:PRO:CD	2.46	0.41
2:B:273:GLN:HB3	2:B:280:ILE:HG21	2.02	0.41
2:B:308:VAL:CG2	2:B:311:ASN:CG	2.93	0.41
2:B:314:VAL:OXT	2:B:314:VAL:HG12	2.20	0.41
2:A:84:VAL:HG13	2:A:104:LEU:HD12	2.02	0.41
2:B:5:ARG:HG3	2:B:83:ASP:OD2	2.21	0.41
1:C:19:G:H3'	1:C:20:H2U:C5'	2.49	0.41
1:D:53:G:N2	1:D:62:C:C2	2.88	0.41
2:B:99:LEU:HD21	2:B:142:ASP:O	2.21	0.41
2:B:176:PRO:O	2:B:179:LEU:HB3	2.21	0.41
1:C:67:C:O2'	1:C:68:C:H5'	2.20	0.41
2:B:30:VAL:O	2:B:61:PRO:HG2	2.21	0.41
1:C:34:C:H2'	1:C:35:A:O4'	2.20	0.41
1:D:57:A:C2'	1:D:58:A:C5'	2.91	0.41
2:A:244:PRO:O	2:A:244:PRO:HG2	2.20	0.41
1:C:2:G:N7	2:A:43:GLY:CA	2.84	0.41
2:B:114:LEU:HB3	2:B:115:PRO:CA	2.47	0.41
2:B:198:GLU:OE1	2:B:201:VAL:HG21	2.20	0.41
2:B:244:PRO:HG2	2:B:244:PRO:O	2.21	0.41
2:B:281:LEU:HD12	2:B:281:LEU:HA	1.91	0.41
1:C:36:U:H2'	1:C:38:A:N7	2.36	0.41
2:A:269:LYS:HE3	2:A:297:GLN:HE22	1.86	0.41
2:B:212:ALA:O	2:B:213:ARG:C	2.64	0.41
1:D:4:G:H2'	1:D:5:G:H8	1.86	0.40
2:A:114:LEU:HD23	2:A:114:LEU:H	1.82	0.40
2:B:30:VAL:O	2:B:61:PRO:HG3	2.21	0.40
2:B:90:TYR:CZ	2:B:92:LEU:HD12	2.56	0.40
2:B:114:LEU:HA	2:B:115:PRO:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:4SU:H5'	1:C:9:G:OP2	2.22	0.40
1:C:31:G:H2'	1:C:32:OMC:O4'	2.22	0.40
2:A:308:VAL:HA	2:A:309:PRO:HD3	1.94	0.40
2:B:238:LEU:HD12	2:B:238:LEU:O	2.20	0.40
2:B:94:LEU:HB2	2:B:99:LEU:HD11	2.03	0.40
2:B:212:ALA:HB2	2:B:234:PRO:CG	2.50	0.40
1:D:24:U:O2'	2:B:304:ARG:NH2	2.55	0.40
2:A:85:MET:HB3	2:A:106:CYS:SG	2.61	0.40
2:B:112:SER:HB3	2:B:122:PRO:HB2	2.03	0.40
2:B:272:ILE:HD13	2:B:307:PHE:CG	2.57	0.40
1:C:51:C:H2'	1:C:52:G:O4'	2.21	0.40
1:D:75:C:O2'	1:D:76:A:H5'	2.22	0.40
2:B:87:VAL:HG21	2:B:94:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	312/314 (99%)	262 (84%)	45 (14%)	5 (2%)	7	27
2	B	312/314 (99%)	264 (85%)	40 (13%)	8 (3%)	4	15
All	All	624/628 (99%)	526 (84%)	85 (14%)	13 (2%)	5	20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	256	ALA
2	B	175	GLY
2	A	11	THR
2	B	42	ARG
2	A	235	MET

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Mol	Chain	Res	Type
2	B	11	THR
2	B	81	GLN
2	B	198	GLU
2	B	235	MET
2	B	302	SER
2	A	48	PRO
2	A	81	GLN
2	A	175	GLY

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	
2	A	257/257 (100%)	242 (94%)	15 (6%)	18	49
2	B	257/257 (100%)	247 (96%)	10 (4%)	28	64
All	All	514/514 (100%)	489 (95%)	25 (5%)	22	55

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	ARG
2	A	35	GLN
2	A	69	ARG
2	A	114	LEU
2	A	138	ILE
2	A	140	GLN
2	A	142	ASP
2	A	184	LYS
2	A	195	VAL
2	A	203	TYR
2	A	205	GLU
2	A	222	GLN
2	A	232	PRO
2	A	268	ASN
2	A	286	LEU

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Mol	Chain	Res	Type
2	B	17	ARG
2	B	35	GLN
2	B	79	GLU
2	B	103	ARG
2	B	114	LEU
2	B	140	GLN
2	B	142	ASP
2	B	195	VAL
2	B	222	GLN
2	B	238	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	35	GLN
2	A	64	GLN
2	A	73	ASN
2	A	177	GLN
2	A	222	GLN
2	A	243	GLN
2	A	282	ASN
2	A	297	GLN
2	A	301	ASN
2	B	27	HIS
2	B	35	GLN
2	B	73	ASN
2	B	185	GLN
2	B	196	GLN
2	B	222	GLN
2	B	243	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	76/77 (98%)	14 (18%)	3 (3%)
1	D	76/77 (98%)	14 (18%)	4 (5%)
All	All	152/154 (98%)	28 (18%)	7 (4%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	G
1	C	8	4SU
1	C	9	G
1	C	17	C
1	C	17(A)	U
1	C	18	G
1	C	19	G
1	C	20	H2U
1	C	21	A
1	C	33	U
1	C	38	A
1	C	47	U
1	C	48	C
1	C	49	G
1	D	8	4SU
1	D	9	G
1	D	17	C
1	D	17(A)	U
1	D	18	G
1	D	19	G
1	D	20	H2U
1	D	21	A
1	D	37	A
1	D	38	A
1	D	47	U
1	D	48	C
1	D	49	G
1	D	59	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	17	C
1	C	17(A)	U
1	C	46	A
1	D	17	C
1	D	17(A)	U
1	D	36	U
1	D	46	A

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

10 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$
1	5MU	D	54	1	19,22,23	0.26	0	27,32,35	0.33	0
1	5MU	C	54	1	19,22,23	0.22	0	27,32,35	0.33	0
1	H2U	C	20	1	18,21,22	0.81	1 (5%)	19,30,33	0.75	0
1	OMC	D	32	1	19,22,23	2.29	2 (10%)	25,31,34	0.71	0
1	4SU	D	8	1	18,21,22	5.76	1 (5%)	25,30,33	0.30	0
1	PSU	C	55	1	18,21,22	1.75	1 (5%)	21,30,33	0.81	1 (4%)
1	OMC	C	32	1	19,22,23	3.03	2 (10%)	25,31,34	0.82	1 (4%)
1	H2U	D	20	1	18,21,22	1.12	1 (5%)	19,30,33	0.70	0
1	4SU	C	8	1	18,21,22	5.41	1 (5%)	25,30,33	0.43	0
1	PSU	D	55	1	18,21,22	1.79	1 (5%)	21,30,33	0.78	1 (4%)

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
1	5MU	D	54	1	-	0/7/25/26	0/2/2/2
1	5MU	C	54	1	-	0/7/25/26	0/2/2/2
1	H2U	C	20	1	-	3/7/38/39	0/2/2/2
1	OMC	D	32	1	-	1/9/27/28	0/2/2/2
1	4SU	D	8	1	-	0/7/25/26	0/2/2/2
1	PSU	C	55	1	-	1/7/25/26	0/2/2/2
1	OMC	C	32	1	-	1/9/27/28	0/2/2/2
1	H2U	D	20	1	-	5/7/38/39	0/2/2/2
1	4SU	C	8	1	-	0/7/25/26	0/2/2/2
1	PSU	D	55	1	-	1/7/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	4SU	C4-S4	-24.40	1.25	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	4SU	C4-S4	-22.87	1.27	1.68
1	C	32	OMC	O2'-C2'	10.59	1.68	1.42
1	D	32	OMC	O2'-CM2	8.39	1.71	1.42
1	C	32	OMC	O2'-CM2	7.62	1.68	1.42
1	D	55	PSU	C6-N1	-7.20	1.24	1.36
1	C	55	PSU	C6-N1	-7.08	1.24	1.36
1	D	32	OMC	O2'-C2'	4.95	1.54	1.42
1	D	20	H2U	C2-N1	3.97	1.41	1.35
1	C	20	H2U	C2-N1	2.36	1.38	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	PSU	C5-C6-N1	2.38	125.45	122.14
1	C	55	PSU	C5-C6-N1	2.36	125.42	122.14
1	C	32	OMC	O3'-C3'-C4'	-2.21	104.73	111.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	20	H2U	C3'-C4'-C5'-O5'
1	C	32	OMC	C1'-C2'-O2'-CM2
1	D	20	H2U	O4'-C1'-N1-C6
1	D	20	H2U	C2'-C1'-N1-C2
1	D	20	H2U	C2'-C1'-N1-C6
1	D	32	OMC	C1'-C2'-O2'-CM2
1	C	20	H2U	O4'-C4'-C5'-O5'
1	D	55	PSU	O4'-C1'-C5-C4
1	C	55	PSU	O4'-C1'-C5-C6
1	C	20	H2U	C4'-C5'-O5'-P
1	D	20	H2U	O4'-C1'-N1-C2
1	D	20	H2U	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	54	5MU	3	0
1	C	54	5MU	2	0
1	C	20	H2U	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	32	OMC	9	0
1	D	8	4SU	2	0
1	C	55	PSU	3	0
1	C	32	OMC	11	0
1	C	8	4SU	3	0
1	D	55	PSU	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are 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
4	FME	C	585	1	8,9,10	1.45	2 (25%)	8,9,11	1.61	2 (25%)
4	FME	D	586	1	8,9,10	0.95	0	8,9,11	2.02	3 (37%)

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	FME	C	585	1	-	5/7/9/11	-
4	FME	D	586	1	-	2/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	585	FME	CN-N	2.91	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	585	FME	O-C	2.09	1.27	1.20

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	586	FME	C-CA-N	3.44	116.14	109.50
4	D	586	FME	O-C-CA	-3.08	116.84	124.77
4	D	586	FME	CB-CA-N	-2.83	105.36	110.52
4	C	585	FME	O-C-CA	-2.70	117.82	124.77
4	C	585	FME	C-CA-N	2.42	114.16	109.50

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	585	FME	O1-CN-N-CA
4	C	585	FME	N-CA-CB-CG
4	C	585	FME	C-CA-CB-CG
4	C	585	FME	O-C-CA-CB
4	D	586	FME	O1-CN-N-CA
4	C	585	FME	CB-CG-SD-CE
4	D	586	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	585	FME	1	0
4	D	586	FME	1	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.