



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 08:32 PM JST

PDB ID : 9KDQ / pdb_00009kdq
EMDB ID : EMD-62284
Title : The structure of 3 ACTD bound to RNA polymerase II elongation complex with 4 CTG repeats.
Authors : Xu, J.; Zhao, W.; Zhu, L.
Deposited on : 2024-11-03
Resolution : 2.63 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

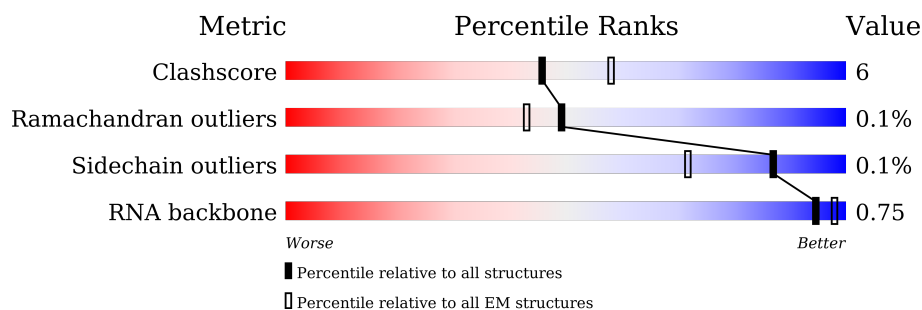
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY









The reported resolution of this entry is 2.63 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.









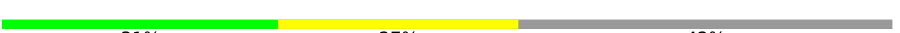



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1454	 84% 14% .
2	B	1224	 86% 11% .
3	C	268	 88% 11% .
4	D	221	 53% 22% 25%
5	E	215	 84% 15%
6	F	155	 50% 6% 44%
7	G	171	 71% 29%
8	H	146	 82% 14% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	122	 77% 18% 5%
10	J	70	 93% 6% .
11	K	120	 88% 8% .
12	L	70	 59% 6% 36%
13	N	52	 12% 25% 63%
14	P	12	 58% 17% 8% 17%
15	T	52	 31% 27% 42%
16	M	11	 9% 82% 9%
16	O	11	 9% 73% 18%
16	Q	11	 36% 55% 9%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 33324 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1426	Total	C	N	O	S	0	0
			11221	7070	1960	2129	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1190	Total	C	N	O	S	0	0
			9479	5989	1659	1775	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	166	Total	C	N	O	S	0	0
			1332	823	238	269	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	704	188	224	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 13 is a DNA chain called NTS(non-template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	19	Total	C	N	O	P	0	0
			389	186	66	118	19		

- Molecule 14 is a RNA chain called RNA (5'-R(*CP*CP*CP*UP*AP*AP*GP*AP*GP*UP

*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	10	Total	C	N	O	P	0	0
			214	96	40	68	10		

- Molecule 15 is a DNA chain called TS(template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	30	Total	C	N	O	P	0	0
			612	293	109	180	30		

- Molecule 16 is a protein called Actinomycin D.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	M	11	Total	C	N	O	0	0
			90	62	12	16		
16	O	11	Total	C	N	O	0	0
			90	62	12	16		
16	Q	11	Total	C	N	O	0	0
			90	62	12	16		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

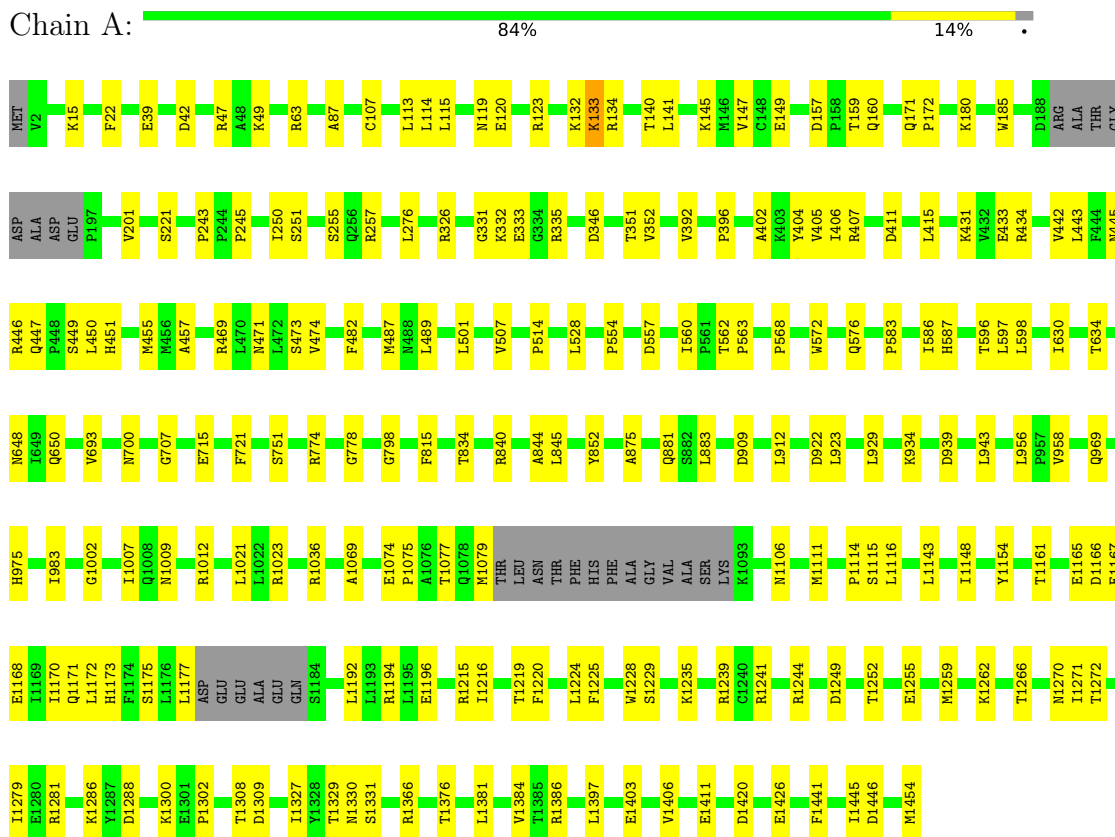
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

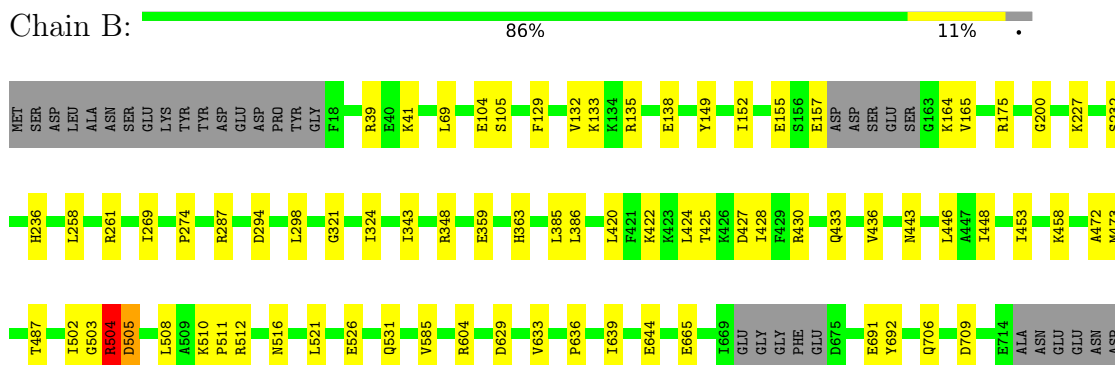
3 Residue-property plots

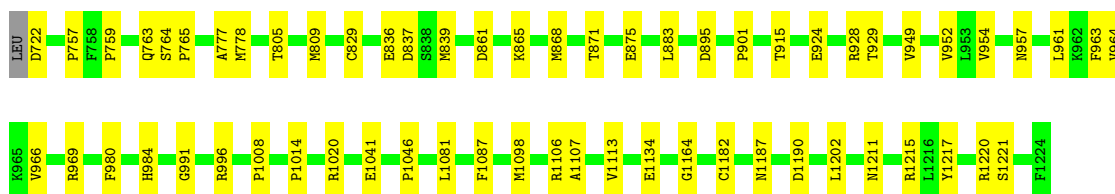
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



- Molecule 2: DNA-directed RNA polymerase II subunit RPB2





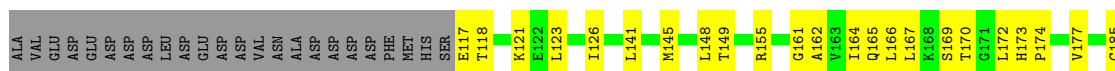
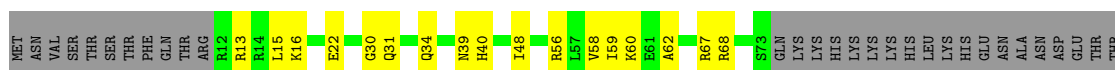
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 88% 11%



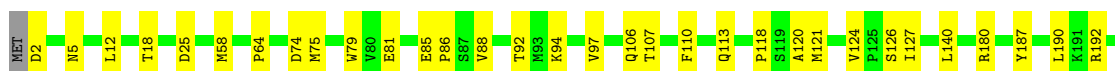
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 53% 22% 25%



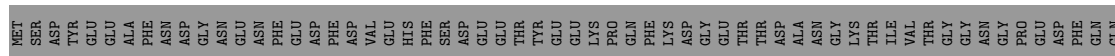
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 84% 15%



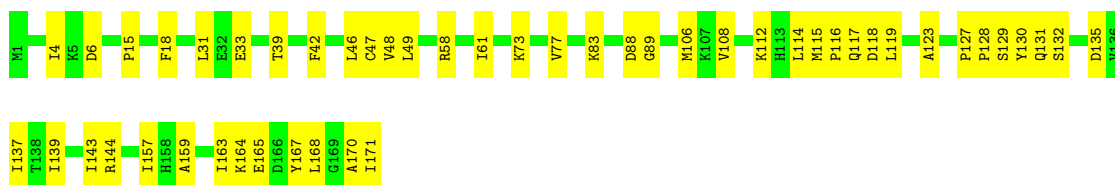
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 50% 6% 44%

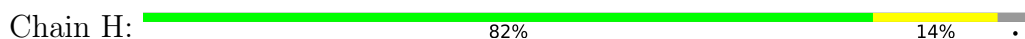


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

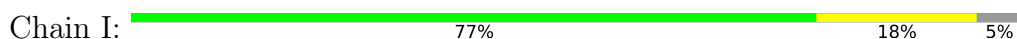
Chain G: 71% 29%



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



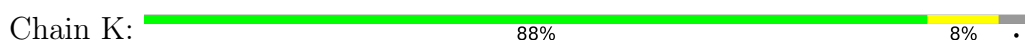
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



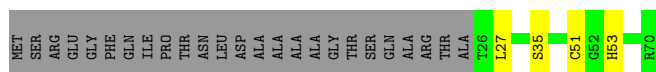
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



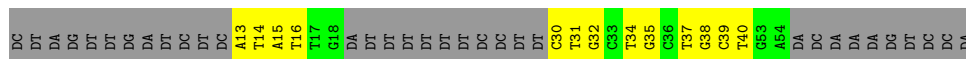
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



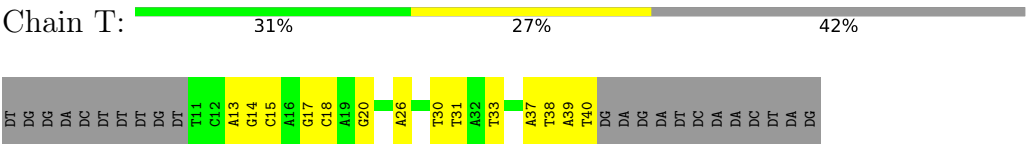
- Molecule 13: NTS(non-template strand)



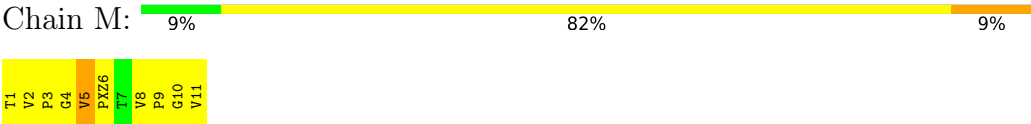
- Molecule 14: RNA (5'-R(*CP*CP*CP*UP*AP*AP*GP*AP*GP*UP*AP*C)-3')



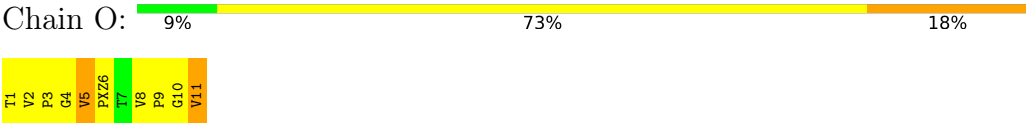
● Molecule 15: TS(template strand)



● Molecule 16: Actinomycin D



● Molecule 16: Actinomycin D



● Molecule 16: Actinomycin D



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78486	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MVA, PXZ, SAR, ZN, DVA

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	0.20	0/11422	0.36	1/15445 (0.0%)
2	B	0.25	0/9666	0.43	3/13037 (0.0%)
3	C	0.17	0/2124	0.33	0/2879
4	D	0.12	0/1340	0.35	0/1797
5	E	0.16	0/1788	0.31	0/2406
6	F	0.16	0/717	0.29	0/967
7	G	0.14	0/1367	0.35	0/1844
8	H	0.15	0/1139	0.30	0/1544
9	I	0.13	0/962	0.33	0/1295
10	J	0.18	0/578	0.31	0/775
11	K	0.16	0/942	0.29	0/1272
12	L	0.15	0/361	0.34	0/478
13	N	0.68	0/433	0.79	0/664
14	P	0.72	0/239	0.84	0/370
15	T	0.56	0/685	0.73	0/1054
16	M	1.32	0/26	0.97	0/30
16	O	0.27	0/26	0.40	0/30
16	Q	0.28	0/26	0.40	0/30
All	All	0.24	0/33841	0.40	4/45917 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	526	GLU	N-CA-CB	7.99	124.00	110.49
2	B	502	ILE	N-CA-C	-6.28	99.46	109.20
1	A	331	GLY	CA-C-O	-5.90	118.39	122.22
2	B	505	ASP	N-CA-C	-5.46	106.52	114.12

There are no chirality outliers.

There are no planarity outliers.

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	11221	0	11292	139	0
2	B	9479	0	9478	92	0
3	C	2086	0	2045	20	0
4	D	1332	0	1353	40	0
5	E	1752	0	1776	18	0
6	F	705	0	731	7	0
7	G	1339	0	1357	36	0
8	H	1120	0	1086	14	0
9	I	944	0	899	13	0
10	J	569	0	585	3	0
11	K	924	0	934	9	0
12	L	359	0	381	3	0
13	N	389	0	218	31	0
14	P	214	0	109	3	0
15	T	612	0	340	25	0
16	M	90	0	84	12	0
16	O	90	0	84	12	0
16	Q	90	0	84	6	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	33324	0	32836	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 6.

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)
13:N:15:DA:C2'	13:N:16:DT:H71	1.58	1.31
13:N:32:DG:H2'	16:M:6:PXZ:N2	1.60	1.14
13:N:15:DA:H2''	13:N:16:DT:C7	1.77	1.12
13:N:15:DA:C2'	13:N:16:DT:C7	2.37	0.99
13:N:37:DT:H2''	13:N:38:DG:H5''	1.49	0.95
1:A:1386:ARG:NH1	16:M:5:MVA:O	2.02	0.91
13:N:15:DA:H2''	13:N:16:DT:H71	0.91	0.89
9:I:78:CYS:SG	9:I:106:CYS:HB3	2.14	0.87
1:A:250:ILE:CG2	2:B:1113:VAL:HG11	2.04	0.86
1:A:1386:ARG:HH22	16:M:5:MVA:HB	1.41	0.84
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.56	0.84
15:T:37:DA:H2''	15:T:38:DT:H71	1.58	0.84
1:A:597:LEU:HD21	8:H:103:LYS:HG2	1.59	0.83
13:N:32:DG:C2'	16:M:6:PXZ:N2	2.41	0.82
13:N:32:DG:H2''	16:M:1:THR:HG23	1.63	0.80
1:A:1166:ASP:OD2	1:A:1239:ARG:NH1	2.16	0.79
13:N:35:DG:N3	16:O:5:MVA:HN2	1.97	0.79
15:T:39:DA:H2''	15:T:40:DT:H71	1.64	0.79
13:N:15:DA:H2'	13:N:16:DT:H71	1.65	0.78
15:T:37:DA:C2'	15:T:38:DT:H71	2.13	0.77
1:A:469:ARG:NH2	2:B:991:GLY:O	2.17	0.77
1:A:250:ILE:HG21	2:B:1113:VAL:HG11	1.69	0.72
13:N:32:DG:H2'	16:M:6:PXZ:HN22	1.54	0.71
1:A:707:GLY:O	1:A:1281:ARG:NH1	2.24	0.71
1:A:455:MET:HE1	2:B:1134:GLU:HA	1.71	0.70
1:A:250:ILE:HG22	2:B:1113:VAL:HG11	1.73	0.69
1:A:1167:GLU:HA	1:A:1170:ILE:HG12	1.74	0.69
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.28	0.69
2:B:165:VAL:HB	2:B:448:ILE:HD13	1.75	0.68
1:A:1161:THR:HG22	1:A:1170:ILE:HD13	1.74	0.68
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.25	0.68
2:B:928:ARG:NH1	2:B:929:THR:O	2.26	0.67
1:A:1173:HIS:O	1:A:1177:LEU:N	2.21	0.67
4:D:155:ARG:NH1	4:D:220:LEU:O	2.28	0.67
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.28	0.67
1:A:180:LYS:HE3	1:A:201:VAL:HG11	1.77	0.66
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.28	0.66
15:T:39:DA:H2''	15:T:40:DT:C7	2.25	0.66
4:D:30:GLY:O	4:D:34:GLN:NE2	2.27	0.65
9:I:74:GLU:OE1	9:I:81:ARG:NH2	2.29	0.65
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.29	0.65
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.31	0.65
1:A:147:VAL:HG13	1:A:149:GLU:HG2	1.79	0.64
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.78	0.64
13:N:35:DG:H1'	16:O:1:THR:HG23	1.78	0.64
1:A:140:THR:HG23	1:A:141:LEU:HD12	1.79	0.64
1:A:157:ASP:OD1	1:A:160:GLN:NE2	2.30	0.64
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.31	0.63
1:A:473:SER:OG	1:A:650:GLN:NE2	2.32	0.63
1:A:1173:HIS:CE1	1:A:1229:SER:HA	2.34	0.63
10:J:48:ARG:NH1	10:J:49:MET:SD	2.72	0.62
1:A:840:ARG:NH1	1:A:1106:ASN:OD1	2.32	0.62
2:B:135:ARG:HD3	2:B:155:GLU:HG3	1.82	0.62
2:B:503:GLY:O	2:B:504:ARG:HB2	2.00	0.62
1:A:700:ASN:O	9:I:115:LYS:NZ	2.28	0.62
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.81	0.62
5:E:106:GLN:HG2	5:E:107:THR:HG23	1.81	0.62
1:A:1386:ARG:NE	1:A:1403:GLU:OE1	2.23	0.61
16:O:11:MVA:HG12	16:O:11:MVA:O	1.99	0.61
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.33	0.61
13:N:30:DC:H2'	13:N:31:DT:C6	2.36	0.61
1:A:451:HIS:HD2	1:A:1074:GLU:HG3	1.65	0.60
1:A:1386:ARG:NH2	16:M:5:MVA:HB	2.14	0.60
2:B:433:GLN:HA	2:B:436:VAL:HG12	1.81	0.60
1:A:251:SER:HB3	1:A:257:ARG:HA	1.83	0.60
16:Q:11:MVA:HG12	16:Q:11:MVA:O	1.99	0.60
1:A:834:THR:HB	1:A:1077:THR:HG22	1.83	0.60
13:N:37:DT:C2'	13:N:38:DG:H5''	2.30	0.60
4:D:48:ILE:HD11	7:G:4:ILE:HD11	1.84	0.60
15:T:14:DG:H2''	16:Q:6:PXZ:H7	1.84	0.59
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.84	0.59
4:D:167:LEU:O	4:D:170:THR:OG1	2.17	0.59
5:E:118:PRO:HA	5:E:121:MET:HB2	1.85	0.59
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.36	0.58
15:T:39:DA:C2'	15:T:40:DT:H71	2.33	0.58
15:T:37:DA:H2''	15:T:38:DT:C7	2.33	0.58
1:A:975:HIS:CD2	1:A:1036:ARG:HD2	2.38	0.58
2:B:487:THR:OG1	2:B:777:ALA:O	2.21	0.58
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.85	0.58
2:B:901:PRO:HA	2:B:949:VAL:HG13	1.86	0.58
13:N:15:DA:H2'	13:N:16:DT:C7	2.27	0.58
1:A:1329:THR:HG22	1:A:1331:SER:H	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:15:DA:H2''	13:N:16:DT:C5	2.38	0.57
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.37	0.57
8:H:86:ASP:O	8:H:87:ARG:NH1	2.37	0.57
13:N:35:DG:C2	16:O:5:MVA:HN2	2.40	0.57
3:C:245:VAL:HG13	11:K:102:LYS:HE2	1.87	0.57
2:B:954:VAL:HG12	2:B:964:VAL:HG12	1.87	0.57
7:G:88:ASP:OD1	7:G:89:GLY:N	2.38	0.56
1:A:1168:GLU:HA	1:A:1171:GLN:HG3	1.85	0.56
1:A:560:ILE:H	8:H:78:SER:HB2	1.70	0.56
8:H:32:THR:OG1	8:H:33:GLN:OE1	2.23	0.56
15:T:18:DC:C5'	16:O:6:PXZ:H8	2.36	0.56
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.87	0.55
5:E:121:MET:HE2	5:E:124:VAL:HG21	1.87	0.55
15:T:18:DC:H4'	16:O:3:PRO:HG3	1.88	0.55
15:T:39:DA:H2''	15:T:40:DT:C5	2.40	0.55
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.87	0.55
5:E:18:THR:OG1	5:E:140:LEU:O	2.22	0.55
2:B:41:LYS:NZ	2:B:692:TYR:OH	2.37	0.55
1:A:1165:GLU:OE2	1:A:1235:LYS:HD2	2.07	0.55
1:A:1286:LYS:HD2	1:A:1302:PRO:HB2	1.89	0.55
9:I:113:ASP:HB3	9:I:116:ASN:HB3	1.89	0.54
4:D:126:ILE:HD12	4:D:145:MET:HG3	1.89	0.54
7:G:143:ILE:HD11	7:G:163:ILE:HG21	1.89	0.54
1:A:402:ALA:HA	1:A:434:ARG:HA	1.88	0.54
10:J:68:LYS:H	12:L:35:SER:HB3	1.72	0.54
2:B:132:VAL:O	2:B:157:GLU:HB2	2.06	0.54
2:B:883:LEU:HD21	2:B:928:ARG:HD3	1.90	0.54
3:C:258:ILE:HG13	11:K:42:LEU:HD21	1.88	0.54
9:I:8:ARG:NH1	9:I:9:ASP:HB2	2.23	0.54
2:B:287:ARG:NH1	2:B:321:GLY:O	2.40	0.54
3:C:8:VAL:HG11	11:K:105:PHE:HA	1.90	0.54
1:A:335:ARG:HE	2:B:1202:LEU:HD23	1.72	0.54
1:A:1165:GLU:OE1	1:A:1194:ARG:NH2	2.41	0.54
1:A:1173:HIS:NE2	1:A:1228:TRP:O	2.37	0.54
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.89	0.54
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.90	0.54
4:D:174:PRO:HA	4:D:177:VAL:HG22	1.90	0.54
1:A:939:ASP:OD2	1:A:1023:ARG:NE	2.34	0.53
8:H:108:SER:OG	8:H:109:LYS:N	2.42	0.53
1:A:63:ARG:NE	1:A:63:ARG:O	2.40	0.53
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.90	0.53
1:A:42:ASP:OD2	1:A:47:ARG:NH1	2.41	0.53
2:B:722:ASP:OD1	2:B:722:ASP:N	2.42	0.53
1:A:1220:PHE:HD2	1:A:1224:LEU:HD22	1.73	0.53
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.90	0.53
5:E:79:TRP:NE1	5:E:81:GLU:OE1	2.38	0.53
9:I:22:ASN:HB2	9:I:24:ARG:HH11	1.74	0.53
8:H:36:CYS:HA	8:H:126:GLU:O	2.09	0.53
15:T:37:DA:C2'	15:T:38:DT:C7	2.86	0.53
2:B:129:PHE:HB3	2:B:164:LYS:HB2	1.91	0.52
2:B:424:LEU:O	2:B:428:ILE:HG12	2.08	0.52
15:T:15:DC:H5'	16:Q:6:PXZ:H8	1.91	0.52
5:E:12:LEU:HG	5:E:58:MET:HE1	1.90	0.52
2:B:1041:GLU:N	2:B:1041:GLU:OE1	2.40	0.52
2:B:924:GLU:O	2:B:928:ARG:HB3	2.09	0.52
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.91	0.52
14:P:3:C:H42	15:T:33:DT:H3	1.57	0.52
1:A:562:THR:O	1:A:576:GLN:NE2	2.38	0.52
15:T:37:DA:H2'	15:T:38:DT:H71	1.90	0.52
1:A:1252:THR:HA	1:A:1255:GLU:HG2	1.91	0.51
3:C:10:ILE:HA	3:C:20:PHE:HA	1.92	0.51
1:A:332:LYS:HG3	1:A:333:GLU:HG3	1.91	0.51
2:B:175:ARG:HG3	2:B:200:GLY:HA3	1.92	0.51
1:A:528:LEU:HD23	1:A:751:SER:HA	1.93	0.51
1:A:1143:LEU:HD12	1:A:1271:ILE:HD11	1.93	0.51
1:A:1215:ARG:NH2	1:A:1272:THR:O	2.44	0.51
1:A:596:THR:OG1	1:A:598:LEU:O	2.24	0.51
15:T:30:DT:H2'	15:T:31:DT:H71	1.92	0.51
7:G:116:PRO:HD2	7:G:119:LEU:HD23	1.92	0.51
1:A:250:ILE:HG21	2:B:1113:VAL:CG1	2.39	0.50
4:D:185:CYS:SG	4:D:186:ASP:N	2.83	0.50
4:D:39:ASN:HA	7:G:6:ASP:OD2	2.11	0.50
3:C:36:VAL:HG13	3:C:40:GLU:HB2	1.92	0.50
1:A:447:GLN:HG3	15:T:26:DA:H2''	1.94	0.50
13:N:32:DG:H2'	16:M:6:PXZ:C2	2.34	0.50
2:B:133:LYS:HA	2:B:157:GLU:HB3	1.92	0.50
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.85	0.50
1:A:443:LEU:HD13	1:A:501:LEU:HD11	1.93	0.50
12:L:51:CYS:SG	12:L:53:HIS:HB2	2.51	0.50
5:E:25:ASP:OD2	5:E:187:TYR:OH	2.25	0.50
1:A:1454:MET:SD	1:A:1454:MET:N	2.84	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:ALA:HB2	7:G:49:LEU:HD13	1.94	0.50
1:A:883:LEU:HD13	1:A:943:LEU:HD13	1.94	0.49
7:G:127:PRO:HG2	7:G:139:ILE:HG12	1.92	0.49
7:G:39:THR:HG23	7:G:42:PHE:H	1.77	0.49
1:A:909:ASP:HB3	1:A:912:LEU:HG	1.94	0.49
4:D:67:ARG:HH21	4:D:68:ARG:NH1	2.09	0.49
4:D:126:ILE:HD13	4:D:149:THR:HG21	1.93	0.49
6:F:116:ASP:HB3	6:F:119:ARG:HG2	1.94	0.49
13:N:37:DT:H5'	16:O:9:PRO:HG2	1.95	0.49
4:D:166:LEU:O	4:D:170:THR:HG23	2.13	0.49
4:D:206:GLU:HA	4:D:209:ARG:HG2	1.95	0.49
11:K:114:LEU:H	11:K:114:LEU:HD23	1.78	0.49
1:A:929:LEU:HD11	1:A:983:ILE:HG21	1.95	0.49
2:B:706:GLN:HE21	2:B:709:ASP:HB3	1.77	0.49
10:J:48:ARG:O	10:J:52:THR:OG1	2.29	0.49
1:A:119:ASN:O	1:A:123:ARG:NH1	2.45	0.49
1:A:404:TYR:HB2	1:A:433:GLU:HB3	1.95	0.49
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.49
4:D:40:HIS:CE1	7:G:73:LYS:HB3	2.48	0.49
4:D:117:GLU:HA	4:D:121:LYS:HE3	1.94	0.49
5:E:126:SER:OG	5:E:127:ILE:N	2.45	0.49
15:T:17:DG:H8	15:T:17:DG:H5''	1.78	0.49
2:B:1081:LEU:O	3:C:189:THR:HG22	2.13	0.48
7:G:106:MET:HE3	7:G:157:ILE:HG23	1.94	0.48
15:T:18:DC:H5'	16:O:6:PXZ:H8	1.95	0.48
15:T:39:DA:H2''	15:T:40:DT:C6	2.46	0.48
2:B:420:LEU:HB3	2:B:453:ILE:HD13	1.94	0.48
2:B:636:PRO:HA	2:B:691:GLU:O	2.12	0.48
13:N:37:DT:H5'	16:O:9:PRO:CG	2.42	0.48
3:C:262:LEU:HD12	3:C:265:MET:HE2	1.95	0.48
1:A:568:PRO:HD2	8:H:46:LEU:HG	1.94	0.48
2:B:996:ARG:NH1	3:C:174:ALA:O	2.43	0.48
4:D:58:VAL:HG13	7:G:49:LEU:HD11	1.96	0.48
14:P:9:G:H4'	14:P:9:G:OP1	2.13	0.48
2:B:343:ILE:HB	2:B:348:ARG:HE	1.79	0.48
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.96	0.47
4:D:31:GLN:N	4:D:31:GLN:OE1	2.45	0.47
13:N:13:DA:H2''	13:N:14:DT:C5	2.49	0.47
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.96	0.47
2:B:957:ASN:OD1	2:B:961:LEU:N	2.44	0.47
1:A:1255:GLU:O	1:A:1259:MET:N	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.49	0.47
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.95	0.47
13:N:39:DC:H42	15:T:14:DG:H1	1.62	0.47
2:B:1217:TYR:CD1	4:D:13:ARG:HD3	2.50	0.47
1:A:1446:ASP:OD1	7:G:58:ARG:NH1	2.42	0.47
7:G:114:LEU:C	7:G:164:LYS:HG3	2.39	0.47
15:T:37:DA:H2''	15:T:38:DT:C6	2.50	0.47
7:G:112:LYS:HB3	7:G:130:TYR:OH	2.15	0.47
13:N:40:DT:H5'	16:Q:9:PRO:HG2	1.96	0.47
3:C:145:CYS:SG	3:C:146:LYS:N	2.87	0.47
1:A:120:GLU:HA	1:A:123:ARG:NH2	2.30	0.47
7:G:144:ARG:HH11	7:G:171:ILE:HG13	1.80	0.47
13:N:15:DA:C4	13:N:16:DT:C4	3.02	0.47
2:B:865:LYS:HG2	2:B:871:THR:HG22	1.96	0.46
2:B:875:GLU:OE2	2:B:915:THR:OG1	2.33	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.47	0.46
1:A:134:ARG:HD2	1:A:221:SER:O	2.15	0.46
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.95	0.46
1:A:447:GLN:O	1:A:449:SER:N	2.48	0.46
4:D:48:ILE:HG13	4:D:48:ILE:O	2.15	0.46
8:H:2:SER:HA	8:H:62:SER:HB3	1.98	0.46
2:B:510:LYS:HB3	2:B:510:LYS:HE3	1.56	0.46
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	1.96	0.46
1:A:1111:MET:HE3	1:A:1114:PRO:HA	1.97	0.46
2:B:138:GLU:N	2:B:138:GLU:OE1	2.49	0.46
1:A:159:THR:OG1	1:A:160:GLN:OE1	2.31	0.46
2:B:443:ASN:HB3	2:B:446:LEU:HD13	1.97	0.46
8:H:2:SER:N	8:H:61:SER:HG	2.13	0.46
11:K:53:ASP:OD1	11:K:54:ARG:N	2.47	0.46
1:A:132:LYS:HE3	1:A:1411:GLU:HG3	1.96	0.46
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.97	0.46
1:A:1420:ASP:OD1	1:A:1420:ASP:N	2.48	0.46
1:A:1281:ARG:NH2	1:A:1309:ASP:OD2	2.46	0.46
1:A:1154:TYR:OH	9:I:18:GLU:OE2	2.27	0.46
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.51	0.46
2:B:427:ASP:HA	2:B:430:ARG:HG2	1.98	0.46
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.97	0.46
1:A:852:TYR:OH	6:F:89:GLU:OE2	2.29	0.46
1:A:1454:MET:HE1	6:F:108:PHE:HB3	1.98	0.46
2:B:510:LYS:N	2:B:511:PRO:HD2	2.30	0.46
2:B:895:ASP:HB2	12:L:27:LEU:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:ILE:HD11	11:K:112:GLN:CG	2.46	0.46
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.97	0.46
15:T:20:DG:H2'	16:M:6:PXZ:C8	2.46	0.45
4:D:118:THR:HG23	4:D:121:LYS:H	1.80	0.45
4:D:123:LEU:HA	4:D:126:ILE:HG12	1.98	0.45
13:N:31:DT:H2'	13:N:32:DG:C8	2.51	0.45
5:E:64:PRO:HB3	5:E:75:MET:SD	2.57	0.45
2:B:287:ARG:NH1	2:B:324:ILE:O	2.50	0.45
4:D:166:LEU:HD21	4:D:210:ILE:HB	1.99	0.45
3:C:6:PRO:O	11:K:104:ASN:ND2	2.46	0.45
1:A:881:GLN:NE2	1:A:958:VAL:O	2.44	0.45
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.99	0.45
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.98	0.45
5:E:88:VAL:HG21	5:E:110:PHE:HE2	1.80	0.45
2:B:138:GLU:OE1	2:B:152:ILE:HB	2.17	0.45
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.99	0.45
4:D:141:LEU:HA	7:G:46:LEU:HD12	1.99	0.45
1:A:1177:LEU:HD21	1:A:1225:PHE:HZ	1.82	0.44
2:B:133:LYS:HA	2:B:157:GLU:CB	2.47	0.44
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.99	0.44
2:B:1215:ARG:NH2	4:D:15:LEU:HD22	2.32	0.44
7:G:144:ARG:HH21	7:G:167:TYR:C	2.25	0.44
1:A:407:ARG:HH21	1:A:411:ASP:HB3	1.82	0.44
13:N:38:DG:H2''	13:N:39:DC:O5'	2.17	0.44
4:D:202:ILE:HG23	4:D:207:LEU:HB2	1.98	0.44
1:A:514:PRO:HB3	1:A:875:ALA:HB3	1.99	0.44
2:B:274:PRO:HG2	2:B:359:GLU:HB3	2.00	0.44
13:N:13:DA:H2''	13:N:14:DT:H71	1.99	0.44
1:A:113:LEU:HD23	1:A:115:LEU:H	1.83	0.44
16:Q:8:DVA:HA	16:Q:9:PRO:HA	1.91	0.44
1:A:250:ILE:CG2	2:B:1113:VAL:CG1	2.88	0.44
1:A:396:PRO:HD3	1:A:415:LEU:HB3	1.99	0.44
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.00	0.44
2:B:1221:SER:HB3	4:D:13:ARG:CZ	2.47	0.44
4:D:22:GLU:OE1	7:G:83:LYS:N	2.50	0.44
1:A:1216:ILE:HA	1:A:1219:THR:HG22	1.99	0.44
13:N:13:DA:H2''	13:N:14:DT:C7	2.48	0.44
2:B:1182:CYS:HB3	2:B:1187:ASN:OD1	2.18	0.44
15:T:13:DA:H4'	15:T:14:DG:OP2	2.18	0.44
5:E:94:LYS:HA	5:E:97:VAL:HG12	1.99	0.43
1:A:442:VAL:HG21	1:A:489:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:THR:OG1	2:B:809:MET:SD	2.73	0.43
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.18	0.43
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.53	0.43
1:A:1075:PRO:O	1:A:1079:MET:HG3	2.19	0.43
3:C:89:GLU:HG2	3:C:90:ASP:H	1.83	0.43
13:N:38:DG:H2''	16:Q:6:PXZ:N2	2.33	0.43
1:A:587:HIS:CE1	1:A:969:GLN:HG3	2.53	0.43
1:A:1148:ILE:N	1:A:1196:GLU:O	2.51	0.43
1:A:1115:SER:OG	1:A:1330:ASN:OD1	2.32	0.43
1:A:1266:THR:O	1:A:1270:ASN:HB3	2.19	0.43
15:T:39:DA:C2'	15:T:40:DT:C7	2.94	0.43
16:O:2:DVA:HA	16:O:3:PRO:HA	1.80	0.43
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.01	0.43
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	2.01	0.43
4:D:15:LEU:O	4:D:16:LYS:HG2	2.18	0.43
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.54	0.43
4:D:60:LYS:NZ	4:D:126:ILE:HG22	2.34	0.43
7:G:31:LEU:C	7:G:33:GLU:H	2.27	0.43
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.58	0.43
14:P:3:C:H2'	14:P:4:U:C6	2.54	0.43
1:A:39:GLU:OE1	1:A:49:LYS:NZ	2.49	0.43
2:B:644:GLU:OE1	2:B:644:GLU:N	2.45	0.43
2:B:952:VAL:HG12	2:B:966:VAL:HG22	2.01	0.43
4:D:161:GLY:HA2	4:D:164:ILE:HG22	2.01	0.43
1:A:922:ASP:OD1	1:A:923:LEU:N	2.52	0.43
2:B:232:SER:O	2:B:261:ARG:NH1	2.45	0.43
5:E:2:ASP:HB2	5:E:5:ASN:HB3	2.01	0.43
16:M:2:DVA:HA	16:M:3:PRO:HA	1.68	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HB3	1.84	0.42
2:B:868:MET:N	2:B:868:MET:SD	2.93	0.42
4:D:59:ILE:HD11	7:G:77:VAL:HG21	2.01	0.42
2:B:104:GLU:HG3	2:B:105:SER:H	1.84	0.42
5:E:74:ASP:OD1	5:E:74:ASP:N	2.49	0.42
1:A:630:ILE:O	1:A:634:THR:HG22	2.20	0.42
1:A:1161:THR:H	1:A:1170:ILE:HD13	1.83	0.42
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.59	0.42
1:A:557:ASP:OD1	1:A:557:ASP:N	2.50	0.42
1:A:975:HIS:HD2	1:A:1036:ARG:HD2	1.83	0.42
4:D:205:ASP:OD1	4:D:206:GLU:N	2.52	0.42
1:A:450:LEU:HD13	1:A:1077:THR:HG21	2.01	0.42
1:A:583:PRO:HG2	1:A:586:ILE:HG13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.85	0.42
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.84	0.42
2:B:1217:TYR:CG	4:D:13:ARG:HD3	2.54	0.42
4:D:210:ILE:O	4:D:214:LEU:HD23	2.20	0.42
7:G:119:LEU:HD12	7:G:131:GLN:C	2.44	0.42
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.19	0.42
2:B:472:ALA:O	2:B:473:MET:HB2	2.19	0.42
2:B:829:CYS:SG	2:B:1014:PRO:HD2	2.60	0.42
8:H:40:LEU:HD13	8:H:123:MET:HG3	2.01	0.42
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.55	0.42
1:A:445:ASN:OD1	1:A:446:ARG:N	2.53	0.41
1:A:1192:LEU:HD12	1:A:1241:ARG:CZ	2.50	0.41
1:A:1262:LYS:O	1:A:1266:THR:HG22	2.19	0.41
1:A:114:LEU:HD23	1:A:145:LYS:HG3	2.02	0.41
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	2.01	0.41
4:D:172:LEU:HG	4:D:173:HIS:H	1.85	0.41
5:E:190:LEU:HD11	5:E:196:VAL:HG13	2.02	0.41
6:F:133:VAL:HG12	6:F:147:SER:HA	2.01	0.41
13:N:13:DA:C2'	13:N:14:DT:H71	2.50	0.41
16:O:8:DVA:HA	16:O:9:PRO:HA	1.91	0.41
1:A:405:VAL:HG23	1:A:415:LEU:HD21	2.02	0.41
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.55	0.41
4:D:166:LEU:O	4:D:169:SER:OG	2.27	0.41
8:H:7:ASP:OD1	8:H:7:ASP:N	2.52	0.41
9:I:15:TYR:OH	9:I:17:ARG:NH2	2.53	0.41
13:N:34:DT:H1'	16:O:5:MVA:HN3	2.02	0.41
9:I:58:VAL:HA	9:I:62:ILE:HD12	2.01	0.41
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.03	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.55	0.41
1:A:346:ASP:HB3	2:B:1107:ALA:O	2.21	0.41
2:B:69:LEU:HD11	2:B:425:THR:O	2.19	0.41
4:D:56:ARG:HB2	4:D:148:LEU:HD22	2.03	0.41
7:G:117:GLN:HG2	7:G:118:ASP:N	2.36	0.41
15:T:37:DA:H2''	15:T:38:DT:C5	2.56	0.41
2:B:422:LYS:O	2:B:425:THR:HG22	2.20	0.41
16:M:8:DVA:HA	16:M:9:PRO:HA	1.85	0.41
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.55	0.41
2:B:512:ARG:NH1	2:B:531:GLN:O	2.51	0.41
7:G:132:SER:OG	7:G:135:ASP:OD1	2.38	0.41
11:K:77:THR:OG1	11:K:81:TYR:O	2.33	0.41
1:A:1376:THR:HG22	1:A:1381:LEU:HD23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:PRO:HD2	1:A:648:ASN:OD1	2.20	0.41
1:A:1288:ASP:OD2	1:A:1300:LYS:HB3	2.21	0.41
1:A:1386:ARG:HH12	16:M:5:MVA:HB	1.86	0.41
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.02	0.41
4:D:40:HIS:NE2	7:G:73:LYS:HB3	2.36	0.41
5:E:85:GLU:OE2	5:E:92:THR:HG21	2.21	0.41
5:E:120:ALA:O	5:E:124:VAL:HG23	2.21	0.41
7:G:123:ALA:HA	7:G:128:PRO:HB3	2.02	0.41
7:G:143:ILE:HD11	7:G:163:ILE:HD13	2.02	0.41
2:B:39:ARG:NH2	2:B:665:GLU:HB2	2.36	0.41
2:B:298:LEU:HD12	9:I:6:PHE:CZ	2.56	0.41
2:B:458:LYS:HE2	2:B:458:LYS:HB3	1.91	0.41
7:G:112:LYS:HA	7:G:115:MET:HE2	2.03	0.41
8:H:34:ASP:OD1	8:H:34:ASP:N	2.54	0.41
2:B:861:ASP:O	2:B:963:PHE:HB2	2.21	0.40
7:G:144:ARG:HH12	7:G:170:ALA:C	2.29	0.40
7:G:165:GLU:O	7:G:168:LEU:HB2	2.20	0.40
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.86	0.40
1:A:351:THR:OG1	1:A:352:VAL:N	2.54	0.40
1:A:457:ALA:O	1:A:507:VAL:HG23	2.21	0.40
1:A:1244:ARG:NH2	1:A:1249:ASP:OD2	2.54	0.40
4:D:162:ALA:O	4:D:165:GLN:HG3	2.22	0.40
8:H:40:LEU:HG	8:H:42:ILE:HG13	2.03	0.40
1:A:15:LYS:HB3	2:B:1220:ARG:HE	1.87	0.40
2:B:778:MET:HE1	2:B:1098:MET:HE2	2.02	0.40
4:D:59:ILE:HD11	7:G:77:VAL:HG11	2.02	0.40
7:G:47:CYS:SG	7:G:48:VAL:N	2.94	0.40
7:G:129:SER:HB3	7:G:137:ILE:O	2.20	0.40
9:I:70:ARG:HD3	9:I:84:VAL:HG12	2.03	0.40
1:A:133:LYS:HE3	1:A:133:LYS:HB2	1.96	0.40
1:A:471:ASN:O	1:A:474:VAL:HG12	2.22	0.40
1:A:1172:LEU:O	1:A:1175:SER:OG	2.35	0.40
2:B:138:GLU:O	2:B:149:TYR:HA	2.21	0.40
2:B:629:ASP:OD1	2:B:629:ASP:N	2.54	0.40
2:B:764:SER:OG	2:B:765:PRO:HD3	2.21	0.40
7:G:167:TYR:O	7:G:168:LEU:HD22	2.22	0.40
1:A:934:LYS:HE3	1:A:934:LYS:HB3	1.91	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 PDB entries followed by that with respect to all EM entries.

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	1418/1454 (98%)	1388 (98%)	29 (2%)	1 (0%)	48	64
2	B	1182/1224 (97%)	1141 (96%)	40 (3%)	1 (0%)	48	64
3	C	263/268 (98%)	257 (98%)	6 (2%)	0	100	100
4	D	162/221 (73%)	158 (98%)	4 (2%)	0	100	100
5	E	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
6	F	85/155 (55%)	83 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
8	H	136/146 (93%)	135 (99%)	1 (1%)	0	100	100
9	I	114/122 (93%)	108 (95%)	6 (5%)	0	100	100
10	J	67/70 (96%)	67 (100%)	0	0	100	100
11	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
16	M	2/11 (18%)	2 (100%)	0	0	100	100
16	O	2/11 (18%)	2 (100%)	0	0	100	100
16	Q	2/11 (18%)	2 (100%)	0	0	100	100
All	All	3970/4269 (93%)	3865 (97%)	103 (3%)	2 (0%)	49	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	504	ARG
1	A	255	SER

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 PDB entries followed by that with respect to all EM

entries.

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	1248/1269 (98%)	1247 (100%)	1 (0%)	88	95
2	B	1032/1061 (97%)	1029 (100%)	3 (0%)	86	93
3	C	233/236 (99%)	233 (100%)	0	100	100
4	D	148/200 (74%)	148 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
16	M	4/4 (100%)	4 (100%)	0	100	100
16	O	4/4 (100%)	4 (100%)	0	100	100
16	Q	4/4 (100%)	4 (100%)	0	100	100
All	All	3534/3732 (95%)	3530 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LYS
2	B	504	ARG
2	B	505	ASP
2	B	508	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	118	HIS
1	A	169	ASN
1	A	171	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	447	GLN
1	A	451	HIS
1	A	479	ASN
1	A	587	HIS
1	A	650	GLN
1	A	659	HIS
1	A	767	GLN
1	A	877	HIS
1	A	975	HIS
1	A	1078	GLN
1	A	1130	GLN
1	A	1265	ASN
1	A	1390	ASN
2	B	115	GLN
2	B	357	GLN
2	B	366	GLN
2	B	383	ASN
2	B	513	GLN
2	B	518	HIS
2	B	706	GLN
2	B	733	HIS
2	B	835	GLN
2	B	1141	HIS
3	C	73	GLN
5	E	153	HIS
7	G	24	GLN
7	G	57	GLN
7	G	122	ASN
8	H	35	GLN
8	H	133	ASN
9	I	90	GLN
10	J	53	HIS
11	K	110	ASN
11	K	112	GLN
12	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/12 (75%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	9	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

18 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$
16	MVA	M	5	16	6,7,8	6.47	2 (33%)	7,8,10	2.45	3 (42%)
16	SAR	O	4	16	4,4,5	1.11	0	1,3,5	2.69	1 (100%)
16	MVA	Q	11	16	6,7,8	1.10	1 (16%)	7,8,10	2.07	3 (42%)
16	SAR	M	4	16	4,4,5	1.07	0	1,3,5	4.03	1 (100%)
16	SAR	Q	10	16	4,4,5	1.05	0	1,3,5	2.69	1 (100%)
16	SAR	Q	4	16	4,4,5	1.12	0	1,3,5	2.70	1 (100%)
16	MVA	M	11	16	6,7,8	5.12	2 (33%)	7,8,10	1.77	2 (28%)
16	MVA	Q	5	16	6,7,8	0.79	0	7,8,10	1.31	2 (28%)
16	SAR	O	10	16	4,4,5	1.07	0	1,3,5	2.69	1 (100%)
16	SAR	M	10	16	4,4,5	0.99	0	1,3,5	4.41	1 (100%)
16	MVA	O	11	16	6,7,8	1.08	1 (16%)	7,8,10	2.06	3 (42%)
16	MVA	O	5	16	6,7,8	0.80	0	7,8,10	1.31	2 (28%)

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
16	MVA	M	5	16	-	3/6/8/10	-
16	SAR	O	4	16	-	1/1/2/3	-
16	MVA	Q	11	16	-	5/6/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SAR	M	4	16	-	1/1/2/3	-
16	SAR	Q	10	16	-	1/1/2/3	-
16	SAR	Q	4	16	-	1/1/2/3	-
16	MVA	M	11	16	-	3/6/8/10	-
16	MVA	Q	5	16	-	6/6/8/10	-
16	SAR	O	10	16	-	1/1/2/3	-
16	SAR	M	10	16	-	1/1/2/3	-
16	MVA	O	11	16	-	5/6/8/10	-
16	MVA	O	5	16	-	6/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	5	MVA	CA-N	-13.40	1.23	1.47
16	M	11	MVA	CA-N	-10.98	1.27	1.47
16	M	5	MVA	CN-N	-8.41	1.24	1.46
16	M	11	MVA	CN-N	-5.91	1.31	1.46
16	Q	11	MVA	O-C	2.61	1.30	1.19
16	O	11	MVA	O-C	2.57	1.30	1.19

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	10	SAR	O-C-CA	-4.41	112.64	125.42
16	Q	11	MVA	O-C-CA	-4.29	112.88	124.83
16	O	11	MVA	O-C-CA	-4.23	113.04	124.83
16	M	5	MVA	O-C-CA	-4.19	113.15	124.83
16	M	4	SAR	O-C-CA	-4.03	113.76	125.42
16	M	5	MVA	CB-CA-N	3.57	115.82	111.17
16	M	11	MVA	CB-CA-N	2.77	114.78	111.17
16	Q	4	SAR	O-C-CA	-2.70	117.61	125.42
16	Q	10	SAR	O-C-CA	-2.69	117.63	125.42
16	O	10	SAR	O-C-CA	-2.69	117.64	125.42
16	O	4	SAR	O-C-CA	-2.69	117.65	125.42
16	Q	5	MVA	CB-CA-N	-2.48	107.94	111.17
16	O	5	MVA	CB-CA-N	-2.47	107.96	111.17
16	M	11	MVA	CB-CA-C	-2.42	110.01	113.04
16	O	11	MVA	C-CA-N	2.32	118.64	110.88
16	M	5	MVA	C-CA-N	2.29	118.54	110.88
16	Q	11	MVA	C-CA-N	2.27	118.48	110.88
16	O	11	MVA	CB-CA-C	-2.14	110.36	113.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	11	MVA	CB-CA-C	-2.14	110.36	113.04
16	O	5	MVA	CG1-CB-CA	2.05	114.34	111.21
16	Q	5	MVA	CG1-CB-CA	2.04	114.33	111.21

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	M	4	SAR	C-CA-N-CN
16	O	4	SAR	C-CA-N-CN
16	Q	4	SAR	C-CA-N-CN
16	M	5	MVA	CB-CA-N-CN
16	M	5	MVA	N-CA-CB-CG1
16	M	5	MVA	N-CA-CB-CG2
16	O	5	MVA	N-CA-CB-CG1
16	O	5	MVA	N-CA-CB-CG2
16	O	5	MVA	C-CA-CB-CG1
16	O	5	MVA	C-CA-CB-CG2
16	Q	5	MVA	N-CA-CB-CG1
16	Q	5	MVA	N-CA-CB-CG2
16	Q	5	MVA	C-CA-CB-CG1
16	Q	5	MVA	C-CA-CB-CG2
16	O	10	SAR	C-CA-N-CN
16	Q	10	SAR	C-CA-N-CN
16	M	11	MVA	N-CA-CB-CG1
16	M	11	MVA	N-CA-CB-CG2
16	O	11	MVA	CB-CA-N-CN
16	O	11	MVA	N-CA-CB-CG1
16	O	11	MVA	N-CA-CB-CG2
16	O	11	MVA	C-CA-CB-CG1
16	O	11	MVA	C-CA-CB-CG2
16	Q	11	MVA	CB-CA-N-CN
16	Q	11	MVA	N-CA-CB-CG1
16	Q	11	MVA	N-CA-CB-CG2
16	Q	11	MVA	C-CA-CB-CG1
16	Q	11	MVA	C-CA-CB-CG2
16	O	5	MVA	CB-CA-N-CN
16	Q	5	MVA	CB-CA-N-CN
16	M	11	MVA	CB-CA-N-CN
16	O	5	MVA	O-C-CA-CB
16	Q	5	MVA	O-C-CA-CB
16	M	10	SAR	C-CA-N-CN

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	5	MVA	4	0
16	Q	11	MVA	1	0
16	O	11	MVA	1	0
16	O	5	MVA	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.