



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 05:04 PM EDT

PDB ID : 3OL8
Title : Poliovirus polymerase elongation complex with CTP-Mn
Authors : Gong, P.; Peersen, O.B.
Deposited on : 2010-08-25
Resolution : 2.75 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

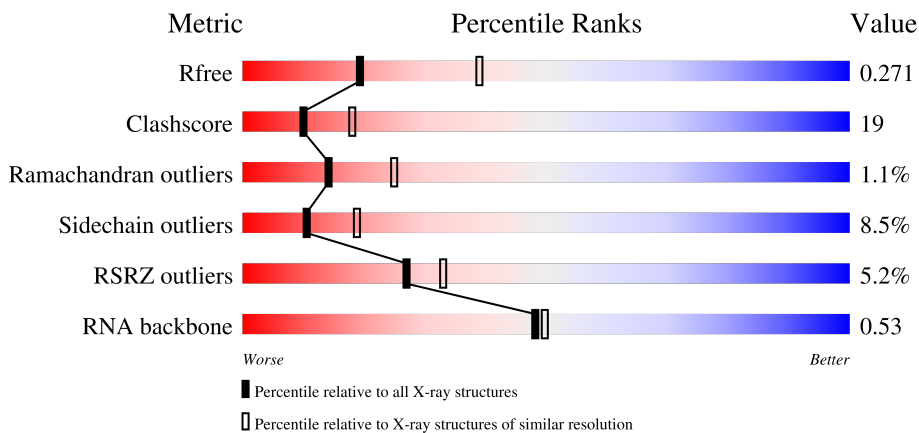
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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	471	
1	E	471	
1	I	471	
1	M	471	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	26	
2	F	26	
2	J	26	
2	N	26	
3	C	15	
3	G	15	
3	K	15	
3	O	15	
4	D	9	
4	H	9	
4	L	9	
4	P	9	

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
8	IPA	A	6011	-	-	X	X
8	IPA	E	6014	-	-	X	-
8	IPA	M	6019	-	-	X	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 18318 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 Polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	461	3697	2370	610	695	22	0	0	0
1	E	461	3697	2370	610	695	22	0	0	0
1	I	461	3697	2370	610	695	22	0	0	0
1	M	461	3697	2370	610	695	22	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	ASP	LEU	engineered mutation	UNP B3VQP5
A	462	GLY	-	expression tag	UNP B3VQP5
A	463	SER	-	expression tag	UNP B3VQP5
A	464	SER	-	expression tag	UNP B3VQP5
A	465	SER	-	expression tag	UNP B3VQP5
A	466	HIS	-	expression tag	UNP B3VQP5
A	467	HIS	-	expression tag	UNP B3VQP5
A	468	HIS	-	expression tag	UNP B3VQP5
A	469	HIS	-	expression tag	UNP B3VQP5
A	470	HIS	-	expression tag	UNP B3VQP5
A	471	HIS	-	expression tag	UNP B3VQP5
E	446	ASP	LEU	engineered mutation	UNP B3VQP5
E	462	GLY	-	expression tag	UNP B3VQP5
E	463	SER	-	expression tag	UNP B3VQP5
E	464	SER	-	expression tag	UNP B3VQP5
E	465	SER	-	expression tag	UNP B3VQP5
E	466	HIS	-	expression tag	UNP B3VQP5
E	467	HIS	-	expression tag	UNP B3VQP5
E	468	HIS	-	expression tag	UNP B3VQP5
E	469	HIS	-	expression tag	UNP B3VQP5
E	470	HIS	-	expression tag	UNP B3VQP5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	471	HIS	-	expression tag	UNP B3VQP5
I	446	ASP	LEU	engineered mutation	UNP B3VQP5
I	462	GLY	-	expression tag	UNP B3VQP5
I	463	SER	-	expression tag	UNP B3VQP5
I	464	SER	-	expression tag	UNP B3VQP5
I	465	SER	-	expression tag	UNP B3VQP5
I	466	HIS	-	expression tag	UNP B3VQP5
I	467	HIS	-	expression tag	UNP B3VQP5
I	468	HIS	-	expression tag	UNP B3VQP5
I	469	HIS	-	expression tag	UNP B3VQP5
I	470	HIS	-	expression tag	UNP B3VQP5
I	471	HIS	-	expression tag	UNP B3VQP5
M	446	ASP	LEU	engineered mutation	UNP B3VQP5
M	462	GLY	-	expression tag	UNP B3VQP5
M	463	SER	-	expression tag	UNP B3VQP5
M	464	SER	-	expression tag	UNP B3VQP5
M	465	SER	-	expression tag	UNP B3VQP5
M	466	HIS	-	expression tag	UNP B3VQP5
M	467	HIS	-	expression tag	UNP B3VQP5
M	468	HIS	-	expression tag	UNP B3VQP5
M	469	HIS	-	expression tag	UNP B3VQP5
M	470	HIS	-	expression tag	UNP B3VQP5
M	471	HIS	-	expression tag	UNP B3VQP5

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	17	Total 341	C 150	N 56	O 118	P 17	0	0	0
2	F	17	Total 341	C 150	N 56	O 118	P 17	0	0	0
2	J	17	Total 341	C 150	N 56	O 118	P 17	0	0	0
2	N	17	Total 341	C 150	N 56	O 118	P 17	0	0	0

- Molecule 3 is a RNA chain called RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	0	0
			323	145	65	99	14			
3	G	15	Total	C	N	O	P	0	0	0
			323	145	65	99	14			
3	K	15	Total	C	N	O	P	0	0	0
			323	145	65	99	14			
3	O	15	Total	C	N	O	P	0	0	0
			323	145	65	99	14			

- Molecule 4 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	P	0	0	0
			68	30	15	20	3			
4	H	3	Total	C	N	O	P	0	0	0
			68	30	15	20	3			
4	L	4	Total	C	N	O	P	0	0	0
			91	40	20	27	4			
4	P	4	Total	C	N	O	P	0	0	0
			91	40	20	27	4			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		
5	I	1	Total	Zn	0	0
			1	1		
5	M	1	Total	Zn	0	0
			1	1		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

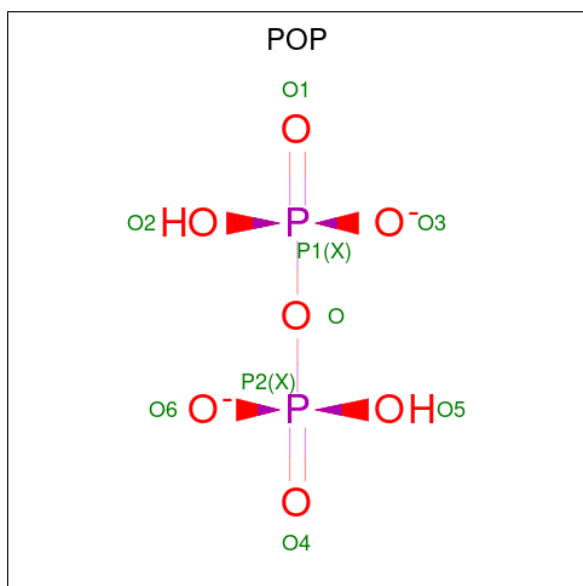
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mn	0	0
			2	2		
6	E	2	Total	Mn	0	0
			2	2		
6	I	2	Total	Mn	0	0
			2	2		

Continued on next page...

Continued from previous page...

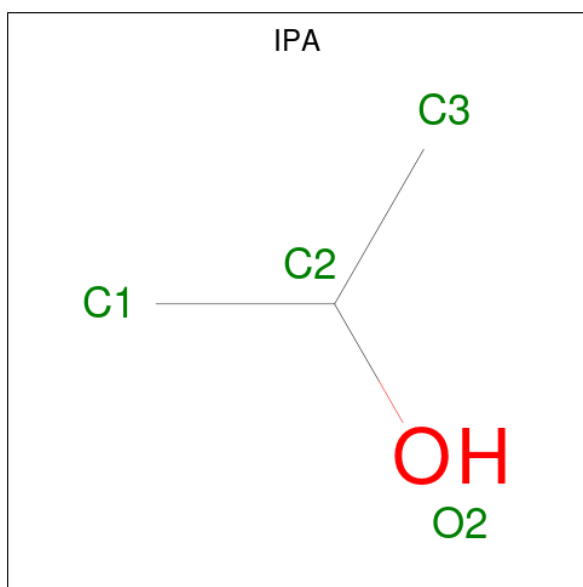
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	2	Total	Mn	0	0
			2	2		

- Molecule 7 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			9	7	2		
7	G	1	Total	O	P	0	0
			9	7	2		
7	I	1	Total	O	P	0	0
			9	7	2		
7	O	1	Total	O	P	0	0
			9	7	2		

- Molecule 8 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: $\text{C}_3\text{H}_8\text{O}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 3 1	0	0
8	A	1	Total C O 4 3 1	0	0
8	A	1	Total C O 4 3 1	0	0
8	A	1	Total C O 4 3 1	0	0
8	A	1	Total C O 4 3 1	0	0
8	E	1	Total C O 4 3 1	0	0
8	E	1	Total C O 4 3 1	0	0
8	M	1	Total C O 4 3 1	0	0
8	M	1	Total C O 4 3 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	E	1	Total C O 6 3 3	0	0
9	J	1	Total C O 6 3 3	0	0
9	N	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	106	Total O 106 106	0	0
10	B	12	Total O 12 12	0	0
10	C	7	Total O 7 7	0	0
10	E	111	Total O 111 111	0	0
10	F	13	Total O 13 13	0	0
10	G	8	Total O 8 8	0	0
10	I	76	Total O 76 76	0	0
10	J	14	Total O 14 14	0	0

Continued on next page...

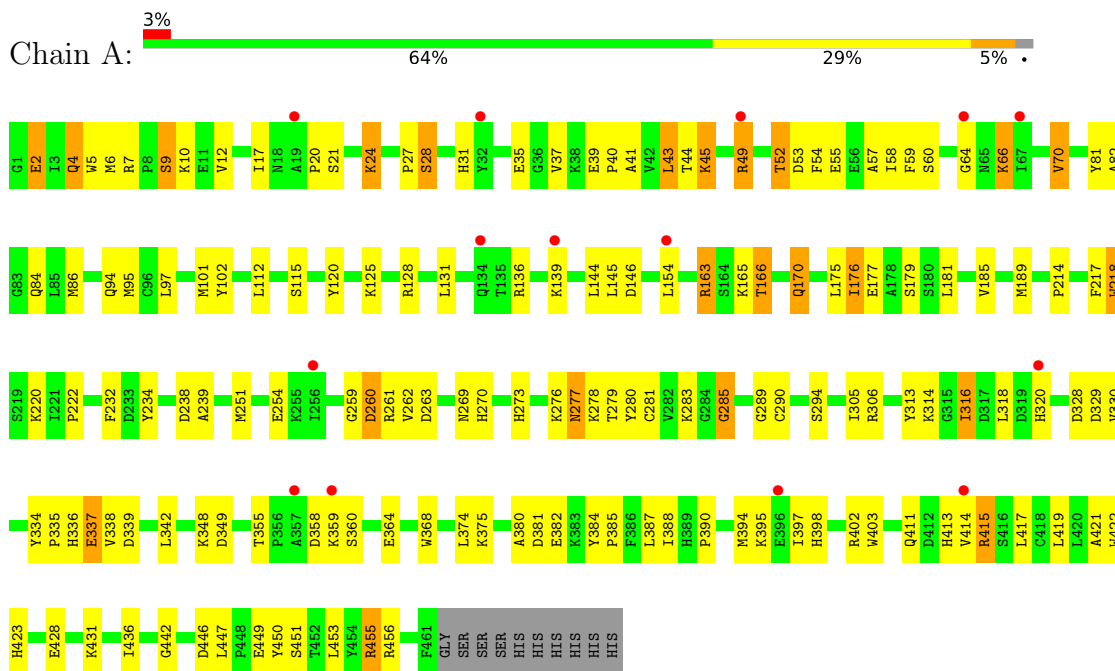
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	K	5	Total O 5 5	0	0
10	M	74	Total O 74 74	0	0
10	N	16	Total O 16 16	0	0
10	O	4	Total O 4 4	0	0
10	P	2	Total O 2 2	0	0

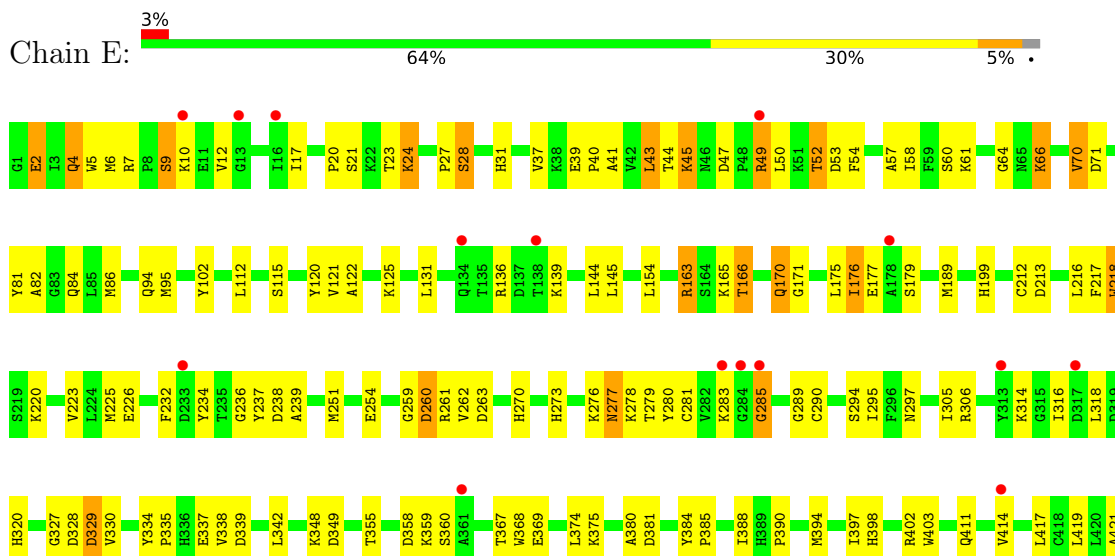
3 Residue-property plots i

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: Polymerase

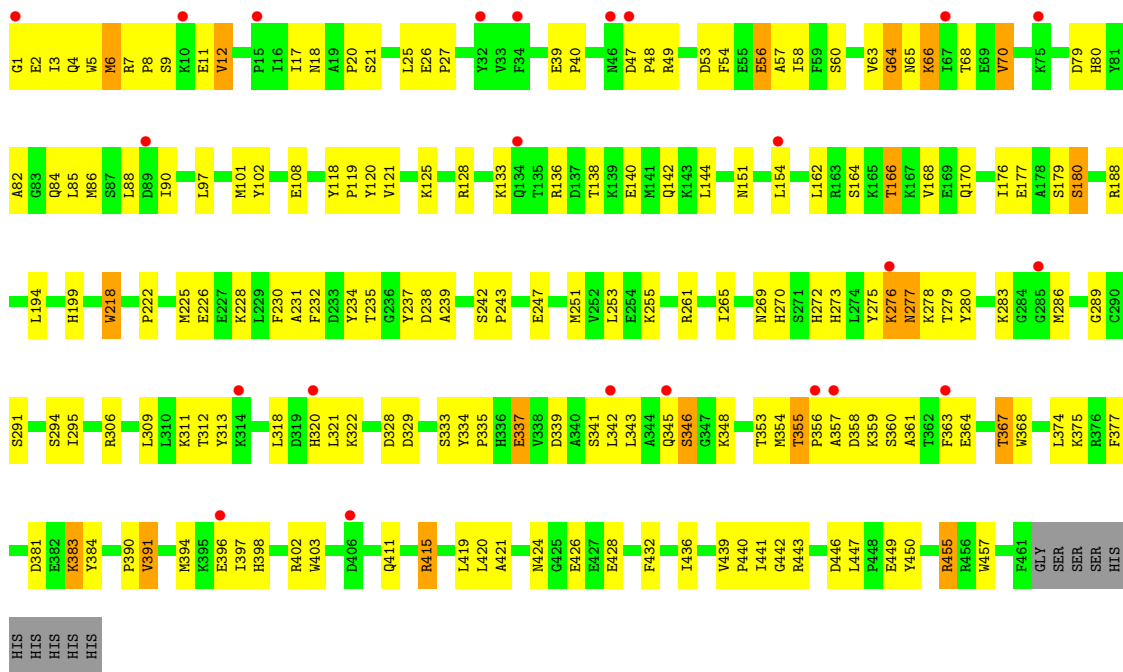


- Molecule 1: Polymerase

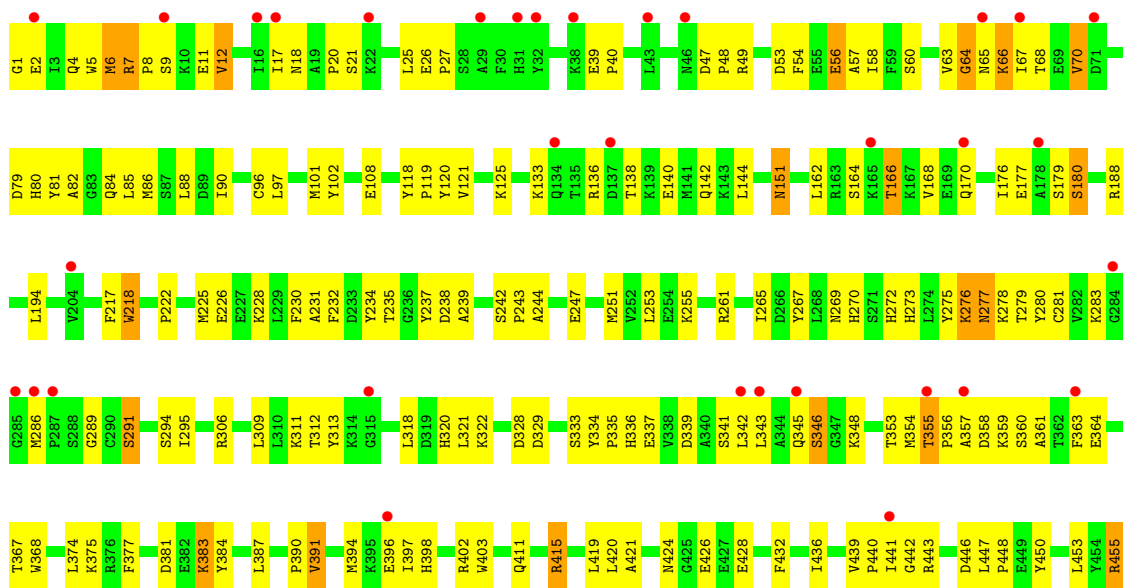


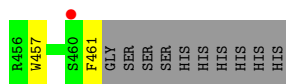


● Molecule 1: Polymerase

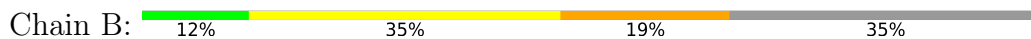


● Molecule 1: Polymerase

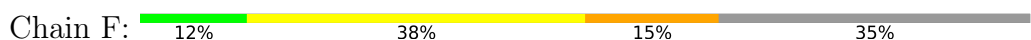




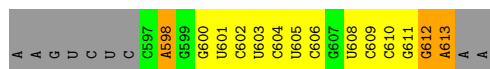
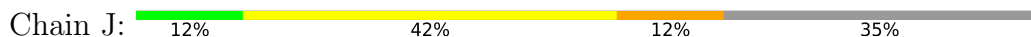
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')



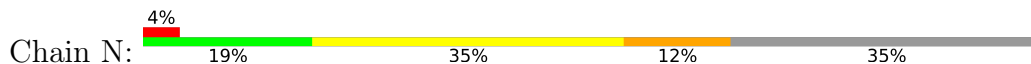
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')



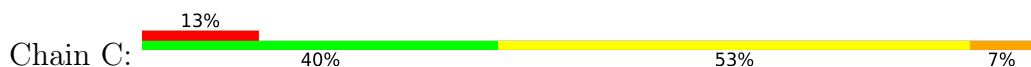
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

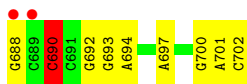


- Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*C)-3')



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

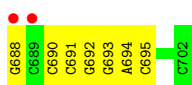




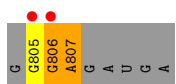
- Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*C)-3')



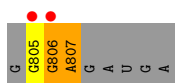
- Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*C)-3')



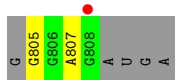
- Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



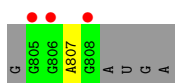
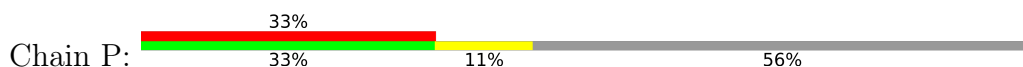
- Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



- Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



- Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.78Å 60.86Å 193.08Å 83.06° 83.04° 76.81°	Depositor
Resolution (Å)	44.16 – 2.75 44.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (44.16-2.75) 96.8 (44.16-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.224 , 0.277 0.213 , 0.271	Depositor DCC
R_{free} test set	5134 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtrriage
Anisotropy	0.337	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.63$, $\langle L^2 \rangle = 0.49$	Xtrriage
Estimated twinning fraction	0.398 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18318	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2443e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, ZN, MN, GOL, POP

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	0.46	0/3787	0.60	0/5122
1	E	0.47	0/3787	0.59	0/5122
1	I	0.46	0/3787	0.60	0/5122
1	M	0.45	0/3787	0.60	0/5122
2	B	0.83	2/378 (0.5%)	1.19	1/587 (0.2%)
2	F	0.81	2/378 (0.5%)	1.13	0/587
2	J	0.80	2/378 (0.5%)	1.06	0/587
2	N	0.82	2/378 (0.5%)	1.06	0/587
3	C	0.76	0/362	1.16	0/564
3	G	0.68	0/362	1.13	1/564 (0.2%)
3	K	0.70	0/362	1.08	0/564
3	O	0.68	0/362	1.03	0/564
4	D	0.36	0/76	0.63	0/117
4	H	0.33	0/76	0.61	0/117
4	L	0.38	0/102	0.69	0/158
4	P	0.36	0/102	0.68	0/158
All	All	0.52	8/18464 (0.0%)	0.72	2/25642 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	613	A	P-OP1	7.56	1.61	1.49
2	J	613	A	P-OP1	7.12	1.61	1.49
2	B	613	A	P-OP1	6.94	1.60	1.49
2	F	613	A	P-OP1	6.77	1.60	1.49
2	B	613	A	P-OP2	6.57	1.60	1.49
2	F	613	A	P-OP2	6.43	1.59	1.49
2	J	613	A	P-OP2	6.24	1.59	1.49
2	N	613	A	P-OP2	5.79	1.58	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	690	C	C5-C6-N1	5.51	123.76	121.00
2	B	602	C	C6-N1-C2	5.26	122.40	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3697	0	3658	121	0
1	E	3697	0	3658	122	0
1	I	3697	0	3658	151	0
1	M	3697	0	3658	167	0
2	B	341	0	172	23	0
2	F	341	0	172	17	0
2	J	341	0	172	15	0
2	N	341	0	172	13	0
3	C	323	0	167	12	0
3	G	323	0	167	14	0
3	K	323	0	167	3	0
3	O	323	0	167	5	0
4	D	68	0	34	6	0
4	H	68	0	34	4	0
4	L	91	0	45	1	0
4	P	91	0	45	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
5	M	1	0	0	0	0
6	A	2	0	0	0	0
6	E	2	0	0	0	0
6	I	2	0	0	0	0
6	M	2	0	0	0	0
7	A	9	0	0	0	0
7	G	9	0	0	1	0
7	I	9	0	0	1	0
7	O	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	20	0	40	12	0
8	E	8	0	16	14	0
8	M	8	0	16	6	0
9	A	6	0	8	0	0
9	E	6	0	8	0	0
9	J	6	0	8	0	0
9	N	6	0	8	0	0
10	A	106	0	0	7	0
10	B	12	0	0	1	0
10	C	7	0	0	2	0
10	E	111	0	0	9	0
10	F	13	0	0	0	0
10	G	8	0	0	1	0
10	I	76	0	0	6	0
10	J	14	0	0	0	0
10	K	5	0	0	0	0
10	M	74	0	0	5	0
10	N	16	0	0	1	0
10	O	4	0	0	0	0
10	P	2	0	0	0	0
All	All	18318	0	16250	647	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 19.

All (647) 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:M:247:GLU:O	1:M:251:MET:HG3	1.64	0.97
1:I:247:GLU:O	1:I:251:MET:HG3	1.65	0.96
1:E:368:TRP:HB3	8:E:6029:IPA:H2	1.49	0.94
1:A:128:ARG:HG3	10:A:564:HOH:O	1.66	0.93
2:B:613:A:O5'	3:G:688:G:H5'	1.68	0.93
1:E:217:PHE:HB2	8:E:6014:IPA:H32	1.53	0.89
1:I:311:LYS:HD3	1:I:346:SER:HB3	1.55	0.88
1:M:311:LYS:HD3	1:M:346:SER:HB3	1.55	0.87
1:M:309:LEU:HD23	1:M:343:LEU:HD21	1.57	0.85
3:C:688:G:H5'	2:F:613:A:O5'	1.75	0.84
1:I:309:LEU:HD23	1:I:343:LEU:HD21	1.57	0.84
1:M:243:PRO:HB3	10:M:492:HOH:O	1.77	0.83
1:I:270:HIS:HD2	1:I:283:LYS:HG2	1.42	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:MET:HG2	1:E:280:TYR:HB3	1.60	0.82
1:M:377:PHE:HB2	1:M:391:VAL:HG22	1.61	0.82
2:B:598:A:H1'	4:D:805:G:N2	1.94	0.82
1:E:9:SER:HB3	1:E:277:ASN:O	1.79	0.82
1:E:254:GLU:HG3	1:E:262:VAL:HG11	1.61	0.82
1:A:9:SER:HB3	1:A:277:ASN:O	1.78	0.82
1:A:6:MET:HG2	1:A:280:TYR:HB3	1.60	0.82
1:M:7:ARG:HD2	1:M:12:VAL:HG23	1.63	0.80
1:M:270:HIS:HD2	1:M:283:LYS:HG2	1.44	0.80
1:A:254:GLU:HG3	1:A:262:VAL:HG11	1.63	0.80
1:I:7:ARG:HD2	1:I:12:VAL:HG23	1.64	0.79
1:A:9:SER:HB2	1:A:279:THR:OG1	1.83	0.79
1:A:270:HIS:HD2	1:A:283:LYS:HG2	1.47	0.79
1:E:270:HIS:HD2	1:E:283:LYS:HG2	1.47	0.78
1:M:12:VAL:HG12	1:M:12:VAL:O	1.83	0.78
1:E:212:CYS:HA	8:E:6014:IPA:H33	1.66	0.77
1:I:377:PHE:HB2	1:I:391:VAL:HG22	1.65	0.77
1:E:213:ASP:H	8:E:6014:IPA:H33	1.49	0.77
1:M:291:SER:HB2	10:N:299:HOH:O	1.86	0.76
1:A:27:PRO:HB3	1:A:31:HIS:ND1	2.00	0.76
1:I:253:LEU:CD1	1:I:265:ILE:HD11	2.15	0.76
1:I:12:VAL:HG12	1:I:12:VAL:O	1.86	0.76
1:M:49:ARG:HE	1:M:168:VAL:HG11	1.50	0.76
1:M:253:LEU:CD1	1:M:265:ILE:HD11	2.16	0.76
1:I:4:GLN:HG3	1:I:283:LYS:HE3	1.68	0.75
1:E:9:SER:HB2	1:E:279:THR:OG1	1.87	0.75
1:E:70:VAL:HG21	1:E:251:MET:CE	2.18	0.74
2:N:600:G:O2'	2:N:601:U:H5'	1.87	0.73
1:I:49:ARG:HE	1:I:168:VAL:HG11	1.51	0.72
2:J:600:G:O2'	2:J:601:U:H5'	1.89	0.72
1:A:70:VAL:HG21	1:A:251:MET:CE	2.20	0.72
1:M:1:GLY:HA2	1:M:65:ASN:OD1	1.88	0.72
1:A:115:SER:HB2	10:A:545:HOH:O	1.89	0.71
1:M:336:HIS:HB2	8:M:6019:IPA:H31	1.72	0.71
2:F:600:G:O2'	2:F:601:U:H5'	1.90	0.71
1:I:80:HIS:CE1	1:I:318:LEU:HB3	2.25	0.71
1:M:18:ASN:OD1	1:M:276:LYS:HG3	1.91	0.71
1:E:27:PRO:HB3	1:E:31:HIS:ND1	2.04	0.71
1:I:18:ASN:OD1	1:I:276:LYS:HG3	1.90	0.71
1:M:80:HIS:CE1	1:M:318:LEU:HB3	2.24	0.71
1:M:4:GLN:HG3	1:M:283:LYS:HE3	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ALA:HB2	1:A:163:ARG:HD3	1.73	0.71
1:I:7:ARG:HD2	1:I:12:VAL:CG2	2.21	0.70
1:I:1:GLY:HA2	1:I:65:ASN:OD1	1.91	0.70
1:M:232:PHE:HE1	1:M:354:MET:HE2	1.55	0.70
1:A:270:HIS:CD2	1:A:283:LYS:HG2	2.27	0.69
1:I:232:PHE:HE1	1:I:354:MET:HE2	1.56	0.69
1:I:20:PRO:HG3	2:J:598:A:C4	2.27	0.69
1:M:313:TYR:HD2	8:M:6019:IPA:H11	1.57	0.69
1:M:7:ARG:HD2	1:M:12:VAL:CG2	2.22	0.69
1:A:37:VAL:HG13	1:A:165:LYS:HD2	1.75	0.69
1:E:41:ALA:HB2	1:E:163:ARG:HD3	1.75	0.69
1:M:217:PHE:HD1	8:M:6018:IPA:H32	1.56	0.69
2:F:598:A:H3'	2:F:599:G:H5'	1.74	0.69
1:E:381:ASP:HB3	1:E:384:TYR:O	1.92	0.69
2:B:602:C:H2'	2:B:603:U:C6	2.28	0.68
2:B:600:G:O2'	2:B:601:U:H5'	1.92	0.68
1:A:337:GLU:HB2	10:A:571:HOH:O	1.93	0.68
1:E:37:VAL:HG13	1:E:165:LYS:HD2	1.76	0.68
1:I:415:ARG:HH11	1:I:415:ARG:HG2	1.58	0.68
3:C:694:A:N7	10:C:243:HOH:O	2.26	0.68
1:I:253:LEU:HD12	1:I:265:ILE:CD1	2.24	0.68
1:M:311:LYS:O	1:M:311:LYS:HG2	1.93	0.68
2:N:609:C:C4	2:N:610:C:C5	2.82	0.68
1:A:381:ASP:HB3	1:A:384:TYR:O	1.94	0.68
1:M:232:PHE:CE1	1:M:354:MET:HE2	2.29	0.68
1:M:7:ARG:HH11	1:M:11:GLU:HG2	1.58	0.67
2:B:598:A:H3'	2:B:599:G:H5'	1.75	0.67
1:E:374:LEU:O	1:E:375:LYS:HB2	1.94	0.67
1:E:380:ALA:HA	1:E:388:ILE:HD13	1.78	0.66
2:J:609:C:C4	2:J:610:C:C5	2.84	0.66
1:E:270:HIS:CD2	1:E:283:LYS:HG2	2.27	0.66
1:I:311:LYS:HG2	1:I:311:LYS:O	1.95	0.66
1:E:213:ASP:H	8:E:6014:IPA:C3	2.08	0.66
2:F:602:C:H2'	2:F:603:U:C6	2.30	0.66
1:M:235:THR:HG22	1:M:353:THR:HB	1.78	0.66
1:E:57:ALA:O	1:E:60:SER:HB3	1.96	0.66
1:M:96:CYS:HB3	10:M:536:HOH:O	1.94	0.66
1:A:374:LEU:O	1:A:375:LYS:HB2	1.94	0.65
1:E:199:HIS:NE2	10:E:497:HOH:O	2.28	0.65
1:M:20:PRO:HG3	2:N:598:A:C4	2.30	0.65
1:A:380:ALA:HA	1:A:388:ILE:HD13	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:232:PHE:CE1	1:I:354:MET:HE2	2.32	0.65
1:A:336:HIS:HB2	8:A:6011:IPA:H11	1.78	0.65
1:A:388:ILE:HD12	8:A:6030:IPA:H32	1.78	0.65
1:M:253:LEU:HD12	1:M:265:ILE:CD1	2.26	0.65
1:M:419:LEU:HD11	2:N:606:C:H4'	1.77	0.64
10:E:560:HOH:O	3:G:697:A:H2	1.80	0.64
1:I:140:GLU:O	1:I:144:LEU:HG	1.97	0.64
1:E:212:CYS:CA	8:E:6014:IPA:H33	2.28	0.64
1:I:7:ARG:HH11	1:I:11:GLU:HG2	1.60	0.64
1:E:213:ASP:N	8:E:6014:IPA:H33	2.13	0.63
1:A:20:PRO:HG3	2:B:598:A:C4	2.34	0.63
1:A:57:ALA:O	1:A:60:SER:HB3	1.98	0.63
1:I:419:LEU:HD11	2:J:606:C:H4'	1.79	0.63
1:M:49:ARG:HH21	1:M:168:VAL:HG13	1.62	0.63
3:C:688:G:H8	3:C:688:G:HO5'	1.45	0.63
1:E:306:ARG:HG2	1:E:318:LEU:HD13	1.79	0.63
1:I:235:THR:HG22	1:I:353:THR:HB	1.80	0.63
1:A:259:GLY:O	1:A:262:VAL:HG22	1.98	0.63
1:E:21:SER:HB2	1:E:44:THR:HG21	1.81	0.63
1:I:309:LEU:HD12	1:I:321:LEU:HD22	1.81	0.63
1:I:397:ILE:HD13	1:I:421:ALA:HB2	1.80	0.63
1:E:20:PRO:HG3	2:F:598:A:C4	2.33	0.62
1:M:238:ASP:OD1	1:M:239:ALA:N	2.33	0.62
1:M:270:HIS:NE2	1:M:281:CYS:SG	2.73	0.62
1:E:70:VAL:HG21	1:E:251:MET:HE3	1.81	0.62
1:E:71:ASP:HB3	10:E:482:HOH:O	1.99	0.62
1:M:397:ILE:HD13	1:M:421:ALA:HB2	1.82	0.62
1:A:21:SER:HB2	1:A:44:THR:HG21	1.80	0.61
1:E:47:ASP:OD1	1:E:49:ARG:HD3	1.99	0.61
1:I:49:ARG:HH21	1:I:168:VAL:HG13	1.64	0.61
1:I:356:PRO:HG2	1:I:361:ALA:H	1.66	0.61
1:E:289:GLY:HA2	2:F:600:G:N3	2.16	0.61
1:I:118:TYR:CD1	1:I:119:PRO:HA	2.36	0.61
1:E:259:GLY:O	1:E:262:VAL:HG22	2.00	0.61
1:I:199:HIS:NE2	10:I:493:HOH:O	2.31	0.61
1:I:367:THR:HB	10:I:515:HOH:O	2.00	0.61
2:B:598:A:H1'	4:D:805:G:C2	2.36	0.61
1:M:277:ASN:ND2	1:M:278:LYS:HG2	2.15	0.61
1:I:334:TYR:CG	1:I:335:PRO:HD2	2.35	0.60
1:M:356:PRO:HG2	1:M:361:ALA:H	1.66	0.60
1:E:234:TYR:CD1	1:E:328:ASP:HB2	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ARG:HD3	2:B:606:C:O2'	2.01	0.60
1:M:56:GLU:HG2	10:M:522:HOH:O	2.00	0.60
1:M:140:GLU:O	1:M:144:LEU:HG	2.00	0.60
1:M:309:LEU:HD12	1:M:321:LEU:HD22	1.83	0.60
1:M:234:TYR:CD1	1:M:328:ASP:HB2	2.36	0.60
1:I:270:HIS:CD2	1:I:283:LYS:HE2	2.37	0.60
1:M:270:HIS:CD2	1:M:283:LYS:HE2	2.36	0.60
1:A:58:ILE:HD12	1:A:175:LEU:HD21	1.83	0.60
1:E:37:VAL:O	1:E:37:VAL:HG12	2.02	0.60
1:M:118:TYR:CD1	1:M:119:PRO:HA	2.36	0.60
1:I:238:ASP:OD1	1:I:239:ALA:N	2.35	0.59
1:E:115:SER:HB2	10:E:567:HOH:O	2.02	0.59
3:G:688:G:HO5'	3:G:688:G:H8	1.48	0.59
1:M:415:ARG:HG2	1:M:415:ARG:HH11	1.65	0.59
1:I:277:ASN:ND2	1:I:278:LYS:HG2	2.18	0.59
1:M:334:TYR:CG	1:M:335:PRO:HD2	2.37	0.59
1:A:375:LYS:HD2	3:C:700:G:H5''	1.84	0.59
1:M:446:ASP:C	1:M:447:LEU:HD23	2.23	0.59
1:M:6:MET:HG2	1:M:280:TYR:HB3	1.84	0.59
1:M:166:THR:HG22	1:M:170:GLN:NE2	2.18	0.59
1:A:368:TRP:HB3	8:A:6030:IPA:H2	1.84	0.59
1:I:65:ASN:O	1:I:242:SER:HB3	2.02	0.59
1:M:341:SER:HA	1:M:363:PHE:CD2	2.38	0.59
1:I:166:THR:HG22	1:I:170:GLN:NE2	2.17	0.59
1:I:355:THR:HB	1:I:356:PRO:CD	2.32	0.59
1:M:455:ARG:HD3	1:M:455:ARG:O	2.03	0.59
1:E:177:GLU:O	1:E:289:GLY:HA3	2.03	0.59
1:I:341:SER:HA	1:I:363:PHE:CD2	2.38	0.59
1:A:95:MET:O	1:A:189:MET:HG2	2.03	0.58
1:M:235:THR:CG2	1:M:353:THR:HB	2.33	0.58
1:I:426:GLU:N	1:I:450:TYR:CE1	2.71	0.58
1:M:65:ASN:O	1:M:66:LYS:HB2	2.02	0.58
1:M:269:ASN:O	1:M:283:LYS:HA	2.04	0.58
1:M:398:HIS:O	1:M:402:ARG:HG3	2.03	0.58
1:I:6:MET:HG2	1:I:280:TYR:HB3	1.84	0.58
1:A:37:VAL:HG12	1:A:37:VAL:O	2.03	0.58
1:I:446:ASP:C	1:I:447:LEU:HD23	2.24	0.58
1:I:235:THR:CG2	1:I:353:THR:HB	2.34	0.58
1:M:355:THR:HB	1:M:356:PRO:CD	2.34	0.58
1:A:306:ARG:HG2	1:A:318:LEU:HD13	1.85	0.58
1:M:313:TYR:CD2	8:M:6019:IPA:H11	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TYR:CD1	1:A:328:ASP:HB2	2.38	0.58
1:I:8:PRO:HB2	1:I:11:GLU:HB2	1.85	0.58
1:I:234:TYR:CD1	1:I:328:ASP:HB2	2.39	0.58
1:A:397:ILE:HD13	1:A:421:ALA:HB2	1.85	0.57
1:I:232:PHE:HA	1:I:357:ALA:HB2	1.86	0.57
1:I:398:HIS:O	1:I:402:ARG:HG3	2.04	0.57
2:J:605:U:H2'	2:J:606:C:C6	2.38	0.57
1:A:289:GLY:HA2	2:B:600:G:N3	2.19	0.57
1:E:213:ASP:HB3	8:E:6014:IPA:H12	1.86	0.57
1:I:269:ASN:O	1:I:283:LYS:HA	2.04	0.57
1:A:177:GLU:O	1:A:289:GLY:HA3	2.04	0.57
1:I:342:LEU:O	1:I:345:GLN:HB3	2.05	0.57
1:E:425:GLY:HA2	10:E:505:HOH:O	2.03	0.57
2:N:605:U:H2'	2:N:606:C:C6	2.39	0.57
1:E:58:ILE:HD12	1:E:175:LEU:HD21	1.86	0.57
1:E:82:ALA:O	1:E:86:MET:HG2	2.04	0.57
1:I:439:VAL:HG23	1:I:442:GLY:H	1.70	0.57
1:M:11:GLU:O	1:M:12:VAL:HG23	2.05	0.57
1:I:11:GLU:O	1:I:12:VAL:HG23	2.04	0.57
1:M:439:VAL:HG23	1:M:442:GLY:H	1.68	0.57
1:A:82:ALA:O	1:A:86:MET:HG2	2.05	0.57
1:I:133:LYS:HD3	10:I:512:HOH:O	2.04	0.56
1:E:2:GLU:HG3	1:E:64:GLY:HA2	1.87	0.56
1:M:426:GLU:N	1:M:450:TYR:CE1	2.74	0.56
1:A:2:GLU:HG3	1:A:64:GLY:HA2	1.87	0.56
1:A:270:HIS:CD2	1:A:283:LYS:HE2	2.40	0.56
1:E:375:LYS:HD2	3:G:700:G:H5''	1.87	0.56
1:M:49:ARG:HH21	1:M:168:VAL:CG1	2.16	0.56
1:A:419:LEU:HD11	2:B:606:C:H4'	1.87	0.56
1:M:8:PRO:HB2	1:M:11:GLU:HB2	1.86	0.56
1:M:289:GLY:HA2	2:N:600:G:N3	2.20	0.56
1:M:65:ASN:O	1:M:242:SER:HB3	2.05	0.56
1:M:342:LEU:O	1:M:345:GLN:HB3	2.06	0.56
1:E:419:LEU:HD11	2:F:606:C:H4'	1.87	0.56
1:I:270:HIS:CE1	1:I:272:HIS:HE1	2.24	0.56
1:M:356:PRO:HG2	1:M:361:ALA:N	2.21	0.56
1:A:260:ASP:OD1	1:A:260:ASP:N	2.34	0.56
1:E:260:ASP:N	1:E:260:ASP:OD1	2.36	0.56
1:A:52:THR:CG2	1:A:53:ASP:N	2.69	0.55
1:E:397:ILE:HD13	1:E:421:ALA:HB2	1.88	0.55
1:I:426:GLU:HA	1:I:450:TYR:CD1	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:HD3	1:A:12:VAL:CG2	2.37	0.55
1:E:270:HIS:CD2	1:E:283:LYS:HE2	2.41	0.55
1:I:356:PRO:HG2	1:I:361:ALA:N	2.21	0.55
3:K:688:G:HO5'	3:K:688:G:H8	1.54	0.55
1:A:112:LEU:HD21	1:A:131:LEU:HB2	1.88	0.55
1:I:455:ARG:HD2	1:I:455:ARG:O	2.05	0.55
1:M:232:PHE:HB3	1:M:355:THR:O	2.07	0.55
1:A:451:SER:O	1:A:455:ARG:HD2	2.07	0.55
1:M:49:ARG:HE	1:M:168:VAL:CG1	2.19	0.55
1:I:397:ILE:HD11	1:I:420:LEU:HB3	1.88	0.54
1:A:120:TYR:CE1	1:A:144:LEU:HD13	2.42	0.54
1:I:49:ARG:HH21	1:I:168:VAL:CG1	2.19	0.54
1:I:120:TYR:HB3	1:I:125:LYS:HB3	1.89	0.54
1:E:218:TRP:CD1	1:E:390:PRO:HA	2.43	0.54
1:E:428:GLU:HB2	10:E:579:HOH:O	2.08	0.54
1:I:232:PHE:HB3	1:I:355:THR:O	2.08	0.54
1:M:426:GLU:HA	1:M:450:TYR:CD1	2.43	0.54
1:M:12:VAL:O	1:M:12:VAL:CG1	2.55	0.54
1:E:23:THR:HG22	10:E:547:HOH:O	2.08	0.54
2:F:605:U:H2'	2:F:606:C:C6	2.43	0.54
1:E:112:LEU:HD21	1:E:131:LEU:HB2	1.89	0.53
1:M:120:TYR:HB3	1:M:125:LYS:HB3	1.89	0.53
1:M:133:LYS:HD3	10:M:511:HOH:O	2.08	0.53
1:A:66:LYS:HG2	1:A:349:ASP:O	2.08	0.53
1:I:118:TYR:O	1:I:180:SER:HB2	2.08	0.53
1:E:451:SER:O	1:E:455:ARG:HD2	2.09	0.53
2:J:598:A:H1'	4:L:805:G:N2	2.24	0.53
2:B:602:C:H2'	2:B:603:U:H6	1.73	0.53
2:B:605:U:H2'	2:B:606:C:C6	2.43	0.53
1:I:289:GLY:HA2	2:J:600:G:N3	2.23	0.53
1:M:232:PHE:HA	1:M:357:ALA:HB2	1.89	0.53
3:O:688:G:H8	3:O:688:G:HO5'	1.56	0.53
1:I:232:PHE:CE1	1:I:354:MET:CE	2.92	0.53
1:E:95:MET:O	1:E:189:MET:HG2	2.08	0.53
1:I:65:ASN:O	1:I:66:LYS:HB2	2.07	0.53
1:I:374:LEU:O	1:I:375:LYS:HB2	2.08	0.53
1:M:84:GLN:OE1	1:M:306:ARG:NH2	2.41	0.53
1:E:52:THR:CG2	1:E:53:ASP:N	2.72	0.53
1:M:270:HIS:CE1	1:M:272:HIS:HE1	2.27	0.53
1:I:230:PHE:O	1:I:231:ALA:HB2	2.08	0.53
1:I:270:HIS:CE1	1:I:272:HIS:CE1	2.96	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:381:ASP:HB3	1:M:384:TYR:O	2.08	0.53
1:I:84:GLN:OE1	1:I:306:ARG:NH2	2.42	0.53
7:I:5002:POP:O4	7:I:5002:POP:O1	2.25	0.53
1:M:232:PHE:CE1	1:M:354:MET:CE	2.92	0.52
1:E:238:ASP:OD1	1:E:239:ALA:N	2.42	0.52
1:M:277:ASN:HD22	1:M:278:LYS:HG2	1.74	0.52
1:M:234:TYR:HD1	1:M:328:ASP:HB2	1.74	0.52
1:I:277:ASN:HD22	1:I:278:LYS:N	2.08	0.52
1:I:436:ILE:O	1:I:442:GLY:HA3	2.10	0.52
1:E:37:VAL:O	1:E:37:VAL:CG1	2.57	0.52
1:I:381:ASP:HB3	1:I:384:TYR:O	2.11	0.51
1:I:320:HIS:HB2	1:I:334:TYR:CE1	2.46	0.51
1:M:230:PHE:O	1:M:231:ALA:HB2	2.10	0.51
1:M:277:ASN:HD22	1:M:278:LYS:N	2.08	0.51
2:B:597:C:O2	2:B:597:C:H2'	2.09	0.51
1:E:176:ILE:HG13	2:F:600:G:C8	2.45	0.51
1:E:414:VAL:CG1	1:E:436:ILE:HD13	2.40	0.51
1:I:449:GLU:HB2	10:I:513:HOH:O	2.11	0.51
1:A:238:ASP:OD1	1:A:239:ALA:N	2.43	0.51
2:F:597:C:H2'	2:F:597:C:O2	2.09	0.51
1:I:177:GLU:O	1:I:289:GLY:HA3	2.10	0.51
1:M:177:GLU:O	1:M:289:GLY:HA3	2.11	0.51
1:E:66:LYS:HG2	1:E:349:ASP:O	2.11	0.51
1:M:320:HIS:HB2	1:M:334:TYR:CE1	2.46	0.51
1:I:334:TYR:CD1	1:I:335:PRO:HD2	2.46	0.51
1:M:85:LEU:HA	1:M:88:LEU:HD12	1.93	0.51
1:A:374:LEU:N	10:A:540:HOH:O	2.44	0.50
1:A:37:VAL:O	1:A:37:VAL:CG1	2.60	0.50
1:E:24:LYS:HE3	10:E:524:HOH:O	2.12	0.50
1:I:251:MET:O	1:I:255:LYS:HG3	2.10	0.50
1:M:334:TYR:CD2	1:M:335:PRO:HD2	2.46	0.50
1:M:270:HIS:CE1	1:M:272:HIS:CE1	2.99	0.50
1:M:358:ASP:O	1:M:359:LYS:HB2	2.11	0.50
1:E:120:TYR:CE1	1:E:144:LEU:HD13	2.46	0.50
1:I:234:TYR:HD1	1:I:328:ASP:HB2	1.77	0.50
1:I:334:TYR:CD2	1:I:335:PRO:HD2	2.47	0.50
1:M:336:HIS:CB	8:M:6019:IPA:H31	2.40	0.50
1:E:39:GLU:OE2	1:E:165:LYS:HG3	2.11	0.50
1:I:334:TYR:CG	1:I:335:PRO:CD	2.94	0.50
1:M:238:ASP:HB2	1:M:286:MET:HB3	1.94	0.50
1:A:70:VAL:HG21	1:A:251:MET:HE3	1.91	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG11	1:A:251:MET:CE	2.42	0.50
1:E:236:GLY:HA2	7:G:5003:POP:O6	2.12	0.50
2:N:612:G:H5''	2:N:613:A:OP1	2.12	0.50
1:A:313:TYR:CD1	8:A:6011:IPA:H32	2.47	0.50
1:A:316:ILE:HD12	8:A:6011:IPA:H33	1.93	0.50
1:E:414:VAL:HG11	1:E:436:ILE:HD13	1.93	0.50
1:M:374:LEU:O	1:M:375:LYS:HB2	2.11	0.50
1:I:421:ALA:O	1:I:424:ASN:HB2	2.12	0.49
2:N:609:C:C4	2:N:610:C:H5	2.30	0.49
1:A:40:PRO:HD3	1:A:403:TRP:CH2	2.47	0.49
1:I:79:ASP:OD1	1:I:255:LYS:HE2	2.12	0.49
1:M:218:TRP:CD1	1:M:390:PRO:HA	2.47	0.49
1:E:217:PHE:CD1	8:E:6014:IPA:H31	2.47	0.49
1:M:54:PHE:CE1	1:M:58:ILE:CG2	2.95	0.49
1:M:118:TYR:O	1:M:180:SER:HB2	2.12	0.49
1:M:312:THR:HG22	1:M:313:TYR:CD1	2.48	0.49
1:M:334:TYR:CG	1:M:335:PRO:CD	2.95	0.49
1:E:154:LEU:HD22	1:E:177:GLU:HB3	1.95	0.49
2:J:612:G:H5''	2:J:613:A:OP1	2.13	0.49
1:M:251:MET:O	1:M:255:LYS:HG3	2.11	0.49
1:M:336:HIS:CD2	8:M:6019:IPA:H31	2.48	0.49
1:M:397:ILE:HD11	1:M:420:LEU:HB3	1.94	0.49
1:A:176:ILE:HG13	2:B:600:G:C8	2.47	0.49
1:A:336:HIS:HB2	8:A:6011:IPA:C1	2.42	0.49
2:B:598:A:C1'	4:D:805:G:N2	2.73	0.49
1:I:277:ASN:HD22	1:I:278:LYS:HG2	1.77	0.49
2:F:602:C:H2'	2:F:603:U:H6	1.73	0.49
1:M:334:TYR:CD1	1:M:335:PRO:HD2	2.48	0.49
1:E:7:ARG:HD3	1:E:12:VAL:CG2	2.43	0.49
1:I:238:ASP:HB2	1:I:286:MET:HB3	1.95	0.49
2:B:604:C:H2'	2:B:605:U:C6	2.48	0.48
3:K:690:C:H2'	3:K:691:C:O4'	2.13	0.48
2:N:608:U:H2'	2:N:609:C:O4'	2.12	0.48
1:A:81:TYR:O	1:A:84:GLN:HB2	2.13	0.48
1:E:339:ASP:HB3	1:E:342:LEU:HD12	1.95	0.48
2:B:613:A:O5'	3:G:688:G:C5'	2.53	0.48
1:I:358:ASP:O	1:I:359:LYS:HB2	2.13	0.48
1:A:154:LEU:HD22	1:A:177:GLU:HB3	1.94	0.48
1:A:384:TYR:CE2	8:A:6028:IPA:H2	2.48	0.48
1:I:53:ASP:HB3	1:I:56:GLU:HB3	1.95	0.48
2:J:609:C:C4	2:J:610:C:H5	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:97:LEU:O	1:M:101:MET:HG3	2.13	0.48
1:E:216:LEU:HB2	8:E:6014:IPA:H13	1.94	0.48
1:M:225:MET:HE2	1:M:225:MET:HA	1.95	0.48
1:E:28:SER:HB2	1:E:402:ARG:C	2.33	0.48
1:I:9:SER:HA	1:I:279:THR:OG1	2.13	0.48
1:I:54:PHE:CE1	1:I:58:ILE:CG2	2.97	0.48
1:I:128:ARG:HG3	10:I:527:HOH:O	2.14	0.48
1:M:237:TYR:CG	1:M:328:ASP:HB3	2.48	0.48
1:A:146:ASP:HA	10:A:534:HOH:O	2.12	0.48
1:A:358:ASP:OD1	1:A:360:SER:HB3	2.13	0.48
1:I:49:ARG:HE	1:I:168:VAL:CG1	2.21	0.48
1:M:218:TRP:O	1:M:222:PRO:HD3	2.14	0.48
1:I:12:VAL:O	1:I:12:VAL:CG1	2.58	0.48
1:I:97:LEU:O	1:I:101:MET:HG3	2.12	0.48
1:A:232:PHE:HA	1:A:355:THR:O	2.14	0.48
1:I:237:TYR:CG	1:I:328:ASP:HB3	2.49	0.48
1:I:339:ASP:CG	1:I:341:SER:HG	2.17	0.48
1:M:411:GLN:HB3	10:M:496:HOH:O	2.14	0.48
1:I:40:PRO:HD3	1:I:403:TRP:CH2	2.49	0.47
1:I:312:THR:HG22	1:I:313:TYR:CD1	2.49	0.47
2:J:608:U:H2'	2:J:609:C:O4'	2.14	0.47
1:A:45:LYS:H	1:A:45:LYS:HG3	1.39	0.47
1:A:154:LEU:O	1:A:273:HIS:HA	2.14	0.47
1:A:166:THR:O	1:A:170:GLN:HB2	2.13	0.47
1:E:166:THR:O	1:E:170:GLN:HB2	2.15	0.47
2:F:604:C:H2'	2:F:605:U:C6	2.49	0.47
1:I:85:LEU:HA	1:I:88:LEU:HD12	1.95	0.47
1:M:11:GLU:O	1:M:12:VAL:CG2	2.62	0.47
3:O:690:C:H2'	3:O:691:C:O4'	2.14	0.47
1:A:5:TRP:O	1:A:280:TYR:HA	2.14	0.47
1:A:339:ASP:HB3	1:A:342:LEU:HD12	1.95	0.47
1:M:70:VAL:HG21	1:M:251:MET:SD	2.53	0.47
1:M:108:GLU:O	1:M:188:ARG:NH2	2.39	0.47
1:A:39:GLU:OE2	1:A:165:LYS:HG3	2.13	0.47
3:C:690:C:H5''	3:C:690:C:H6	1.80	0.47
1:E:45:LYS:H	1:E:45:LYS:HG3	1.39	0.47
1:I:97:LEU:HD23	1:I:138:THR:HB	1.95	0.47
1:A:387:LEU:HD11	8:A:6028:IPA:H33	1.96	0.47
1:A:398:HIS:O	1:A:402:ARG:HG3	2.14	0.47
4:H:805:G:H2'	4:H:806:G:O5'	2.15	0.47
1:M:436:ILE:O	1:M:442:GLY:HA3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:LEU:O	1:E:273:HIS:HA	2.13	0.47
1:M:226:GLU:HG2	1:M:322:LYS:HG3	1.95	0.47
3:C:700:G:H3'	10:C:165:HOH:O	2.14	0.47
1:E:422:TRP:CD1	1:E:453:LEU:HD13	2.50	0.47
3:G:690:C:H5''	3:G:690:C:H6	1.79	0.47
1:I:54:PHE:O	1:I:57:ALA:N	2.45	0.47
1:A:270:HIS:NE2	1:A:283:LYS:HE2	2.29	0.47
1:A:414:VAL:CG1	1:A:436:ILE:HD13	2.45	0.47
3:G:688:G:H8	3:G:688:G:O5'	1.98	0.47
1:E:70:VAL:HG11	1:E:251:MET:CE	2.45	0.47
1:I:11:GLU:O	1:I:12:VAL:CG2	2.62	0.47
1:M:53:ASP:HB3	1:M:56:GLU:HB3	1.97	0.47
1:A:411:GLN:HE22	1:A:446:ASP:N	2.12	0.47
1:E:81:TYR:O	1:E:84:GLN:HB2	2.14	0.47
1:E:277:ASN:ND2	1:E:278:LYS:HG3	2.30	0.47
1:E:5:TRP:O	1:E:280:TYR:HA	2.15	0.46
1:E:225:MET:HA	1:E:225:MET:HE2	1.97	0.46
1:E:270:HIS:NE2	1:E:283:LYS:HE2	2.30	0.46
1:I:142:GLN:OE1	1:I:142:GLN:HA	2.15	0.46
1:M:40:PRO:HD3	1:M:403:TRP:CH2	2.51	0.46
3:G:692:G:O2'	3:G:693:G:H5'	2.16	0.46
4:H:806:G:O2'	4:H:807:A:H5'	2.15	0.46
1:I:65:ASN:HB3	1:I:243:PRO:HD2	1.97	0.46
1:I:218:TRP:O	1:I:222:PRO:HD3	2.15	0.46
1:A:54:PHE:O	1:A:57:ALA:N	2.45	0.46
1:M:421:ALA:O	1:M:424:ASN:HB2	2.15	0.46
1:M:9:SER:HA	1:M:279:THR:OG1	2.15	0.46
1:M:253:LEU:CD1	1:M:265:ILE:CD1	2.85	0.46
1:M:339:ASP:OD2	1:M:342:LEU:HG	2.15	0.46
4:D:805:G:H2'	4:D:806:G:O5'	2.15	0.46
1:I:226:GLU:HG2	1:I:322:LYS:HG3	1.97	0.46
1:I:432:PHE:CZ	1:I:436:ILE:HD11	2.50	0.46
4:H:806:G:C2'	4:H:807:A:H5'	2.46	0.46
1:I:102:TYR:CE1	1:I:136:ARG:HA	2.51	0.46
1:M:54:PHE:CE1	1:M:58:ILE:HG21	2.51	0.46
1:E:232:PHE:HA	1:E:355:THR:O	2.16	0.46
1:I:108:GLU:O	1:I:188:ARG:NH2	2.38	0.46
1:I:231:ALA:C	1:I:232:PHE:CD2	2.90	0.46
1:M:79:ASP:OD1	1:M:255:LYS:HE2	2.16	0.46
1:A:277:ASN:ND2	1:A:278:LYS:HG3	2.30	0.45
1:E:238:ASP:O	1:E:285:GLY:HA2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:SER:HB2	1:A:402:ARG:C	2.37	0.45
1:A:334:TYR:CG	1:A:335:PRO:HD2	2.51	0.45
1:I:70:VAL:HG21	1:I:251:MET:SD	2.56	0.45
1:M:25:LEU:HB2	1:M:40:PRO:HG3	1.98	0.45
1:A:338:VAL:HG23	1:A:339:ASP:N	2.31	0.45
1:I:27:PRO:HD3	1:I:403:TRP:CZ3	2.50	0.45
1:I:394:MET:SD	1:I:421:ALA:HB1	2.57	0.45
1:M:231:ALA:C	1:M:232:PHE:CD2	2.89	0.45
1:E:436:ILE:O	1:E:442:GLY:HA3	2.16	0.45
2:N:609:C:H2'	2:N:610:C:H5'	1.98	0.45
1:A:238:ASP:O	1:A:285:GLY:HA2	2.16	0.45
1:A:431:LYS:HB2	1:A:431:LYS:HE2	1.76	0.45
1:E:446:ASP:C	1:E:447:LEU:HD23	2.37	0.45
1:M:97:LEU:HD23	1:M:138:THR:HB	1.99	0.45
1:A:218:TRP:CD1	1:A:390:PRO:HA	2.51	0.45
4:D:806:G:C2'	4:D:807:A:H5'	2.47	0.45
1:E:17:ILE:O	1:E:276:LYS:HA	2.16	0.45
1:A:411:GLN:HE22	1:A:446:ASP:H	1.63	0.45
1:M:339:ASP:CG	1:M:341:SER:HG	2.19	0.45
1:A:102:TYR:CE1	1:A:136:ARG:HA	2.51	0.45
1:I:275:TYR:HD2	1:I:275:TYR:O	1.99	0.45
1:E:334:TYR:CG	1:E:335:PRO:HD2	2.52	0.45
1:M:151:ASN:ND2	1:M:267:TYR:CD2	2.79	0.45
1:A:52:THR:HG23	1:A:53:ASP:N	2.32	0.44
1:I:225:MET:HE2	1:I:225:MET:HA	1.99	0.44
1:E:54:PHE:O	1:E:57:ALA:N	2.46	0.44
1:E:329:ASP:OD2	3:G:701:A:H5''	2.18	0.44
1:I:277:ASN:HD22	1:I:277:ASN:C	2.21	0.44
2:J:602:C:H2'	2:J:603:U:C6	2.53	0.44
1:M:102:TYR:CE1	1:M:136:ARG:HA	2.52	0.44
1:M:339:ASP:OD2	1:M:341:SER:OG	2.35	0.44
1:E:40:PRO:HD3	1:E:403:TRP:CH2	2.52	0.44
1:I:218:TRP:CD1	1:I:390:PRO:HA	2.52	0.44
1:A:436:ILE:O	1:A:442:GLY:HA3	2.17	0.44
1:E:358:ASP:OD1	1:E:360:SER:HB3	2.18	0.44
1:E:398:HIS:O	1:E:402:ARG:HG3	2.17	0.44
2:F:598:A:C3'	2:F:599:G:H5'	2.44	0.44
2:F:600:G:C2'	2:F:601:U:H5'	2.48	0.44
1:M:375:LYS:HD3	1:M:396:GLU:OE1	2.18	0.44
1:A:181:LEU:O	1:A:185:VAL:HG23	2.18	0.44
1:M:277:ASN:HD22	1:M:277:ASN:C	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HB3	1:A:395:LYS:HE2	1.70	0.44
1:A:446:ASP:C	1:A:447:LEU:HD23	2.38	0.44
1:E:394:MET:SD	1:E:421:ALA:HB1	2.57	0.44
1:M:275:TYR:HD2	1:M:275:TYR:O	2.00	0.44
1:M:397:ILE:CD1	1:M:421:ALA:HB2	2.46	0.44
1:E:305:ILE:HD11	1:E:330:VAL:HG11	1.99	0.44
1:I:339:ASP:OD2	1:I:342:LEU:HG	2.18	0.44
1:M:8:PRO:HB2	1:M:11:GLU:CB	2.48	0.44
1:A:364:GLU:HG2	10:A:555:HOH:O	2.18	0.44
1:A:422:TRP:CD1	1:A:453:LEU:HD13	2.52	0.44
1:E:102:TYR:CE1	1:E:136:ARG:HA	2.53	0.44
1:I:440:PRO:HA	1:I:443:ARG:NH1	2.33	0.44
1:M:7:ARG:NH1	1:M:11:GLU:HG2	2.30	0.44
1:M:276:LYS:HB3	1:M:277:ASN:H	1.60	0.44
1:A:17:ILE:O	1:A:276:LYS:HA	2.17	0.44
3:C:692:G:O2'	3:C:693:G:H5'	2.17	0.44
1:I:339:ASP:OD2	1:I:341:SER:OG	2.35	0.44
3:G:688:G:H1'	10:G:281:HOH:O	2.18	0.43
1:I:8:PRO:HB2	1:I:11:GLU:CB	2.47	0.43
1:I:358:ASP:HB2	1:I:360:SER:OG	2.18	0.43
1:A:414:VAL:HG11	1:A:436:ILE:HD13	2.00	0.43
1:E:338:VAL:HG23	1:E:339:ASP:N	2.33	0.43
1:I:17:ILE:O	1:I:276:LYS:HA	2.18	0.43
1:I:355:THR:CB	1:I:356:PRO:CD	2.96	0.43
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.75	0.43
2:B:600:G:C2'	2:B:601:U:H5'	2.49	0.43
4:D:806:G:O2'	4:D:807:A:H5'	2.18	0.43
1:E:411:GLN:HE22	1:E:446:ASP:N	2.17	0.43
1:I:54:PHE:CE1	1:I:58:ILE:HG21	2.53	0.43
1:I:222:PRO:HA	1:I:368:TRP:CZ2	2.54	0.43
1:M:2:GLU:HB3	1:M:64:GLY:HA2	2.00	0.43
1:M:228:LYS:O	1:M:333:SER:HB2	2.19	0.43
2:F:609:C:C2'	2:F:610:C:H5'	2.49	0.43
1:I:80:HIS:CE1	1:I:318:LEU:CB	3.01	0.43
1:A:49:ARG:HE	1:A:49:ARG:HB2	1.63	0.43
1:A:397:ILE:HG23	1:A:417:LEU:HD13	1.99	0.43
1:I:2:GLU:HB3	1:I:64:GLY:HA2	2.00	0.43
2:J:612:G:C5'	2:J:613:A:OP1	2.67	0.43
1:M:320:HIS:HB3	1:M:335:PRO:CG	2.49	0.43
3:C:688:G:H8	3:C:688:G:O5'	1.98	0.43
3:G:690:C:H6	3:G:690:C:C5'	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:609:C:H2'	2:J:610:C:H5'	2.00	0.43
1:M:54:PHE:O	1:M:57:ALA:N	2.45	0.43
1:M:222:PRO:HA	1:M:368:TRP:CZ2	2.54	0.43
1:M:276:LYS:HE2	1:M:276:LYS:HB2	1.79	0.43
1:A:27:PRO:HB3	1:A:31:HIS:CE1	2.54	0.42
1:E:4:GLN:HG2	1:E:283:LYS:HE3	2.01	0.42
1:M:17:ILE:O	1:M:276:LYS:HA	2.19	0.42
1:E:43:LEU:HA	1:E:43:LEU:HD12	1.79	0.42
1:M:65:ASN:HB3	1:M:243:PRO:HD2	2.00	0.42
1:M:275:TYR:CE2	1:M:276:LYS:HE2	2.54	0.42
1:M:394:MET:SD	1:M:421:ALA:HB1	2.60	0.42
3:O:694:A:H2'	3:O:695:C:C6	2.54	0.42
3:O:694:A:H2'	3:O:695:C:H6	1.85	0.42
1:I:90:ILE:HD13	1:I:194:LEU:HD12	2.00	0.42
1:I:273:HIS:HB2	1:I:280:TYR:CZ	2.54	0.42
1:A:394:MET:SD	1:A:421:ALA:HB1	2.59	0.42
1:E:297:ASN:HB3	1:E:327:GLY:HA2	2.00	0.42
1:E:384:TYR:HA	1:E:385:PRO:HD3	1.83	0.42
1:M:7:ARG:O	1:M:7:ARG:HG3	2.19	0.42
1:M:142:GLN:OE1	1:M:142:GLN:HA	2.19	0.42
1:M:162:LEU:HD11	1:M:403:TRP:CD1	2.54	0.42
2:N:612:G:C5'	2:N:613:A:OP1	2.67	0.42
1:A:422:TRP:CZ2	1:A:423:HIS:CE1	3.07	0.42
1:E:179:SER:HB2	1:E:290:CYS:HA	2.00	0.42
1:E:422:TRP:CZ2	1:E:423:HIS:CE1	3.08	0.42
3:G:701:A:H2'	3:G:702:C:O4'	2.18	0.42
1:I:154:LEU:HD22	1:I:177:GLU:HB3	2.00	0.42
1:M:81:TYR:O	1:M:84:GLN:HB2	2.20	0.42
3:C:693:G:H2'	3:C:694:A:H8	1.85	0.42
3:C:701:A:H2'	3:C:702:C:O4'	2.19	0.42
1:E:120:TYR:HB3	1:E:125:LYS:HB3	2.01	0.42
1:E:306:ARG:CG	1:E:318:LEU:HD13	2.46	0.42
1:E:397:ILE:HG23	1:E:417:LEU:HD13	2.02	0.42
1:I:25:LEU:HB2	1:I:40:PRO:HG3	2.01	0.42
1:M:90:ILE:HD13	1:M:194:LEU:HD12	2.01	0.42
1:A:320:HIS:O	1:A:335:PRO:HD3	2.20	0.42
1:I:275:TYR:CE2	1:I:276:LYS:HE2	2.53	0.42
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.87	0.42
1:A:269:ASN:ND2	10:A:552:HOH:O	2.49	0.42
1:A:413:HIS:CD2	3:C:698:G:H4'	2.55	0.42
2:J:604:C:H2'	2:J:605:U:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:ARG:HD3	1:M:11:GLU:HG2	2.02	0.42
2:B:609:C:C2'	2:B:610:C:H5'	2.49	0.41
3:C:690:C:H6	3:C:690:C:C5'	2.32	0.41
1:E:388:ILE:HD12	8:E:6029:IPA:H13	2.03	0.41
1:I:320:HIS:HB3	1:I:335:PRO:CG	2.50	0.41
1:M:118:TYR:CG	1:M:119:PRO:HA	2.55	0.41
1:M:273:HIS:HB2	1:M:280:TYR:CZ	2.55	0.41
1:M:387:LEU:HD22	1:M:461:PHE:CZ	2.55	0.41
1:A:368:TRP:CB	8:A:6030:IPA:H2	2.49	0.41
1:A:449:GLU:O	1:A:450:TYR:C	2.57	0.41
1:I:397:ILE:CD1	1:I:421:ALA:HB2	2.46	0.41
1:A:35:GLU:O	1:A:402:ARG:HD2	2.20	0.41
2:B:605:U:H5	10:B:492:HOH:O	2.03	0.41
1:I:82:ALA:O	1:I:86:MET:HG2	2.20	0.41
1:M:232:PHE:CB	1:M:355:THR:O	2.69	0.41
1:M:237:TYR:O	1:M:238:ASP:C	2.59	0.41
1:M:383:LYS:HB3	1:M:384:TYR:CD1	2.56	0.41
1:A:4:GLN:HG2	1:A:283:LYS:HE3	2.02	0.41
1:M:27:PRO:HD3	1:M:403:TRP:CZ3	2.55	0.41
1:M:47:ASP:HA	1:M:48:PRO:HD3	1.89	0.41
1:M:140:GLU:O	1:M:140:GLU:HG3	2.18	0.41
1:M:318:LEU:HA	1:M:318:LEU:HD23	1.74	0.41
1:E:368:TRP:CB	8:E:6029:IPA:H2	2.34	0.41
1:M:355:THR:CB	1:M:356:PRO:CD	2.99	0.41
1:A:97:LEU:O	1:A:101:MET:HG3	2.21	0.41
1:A:218:TRP:O	1:A:222:PRO:HD3	2.21	0.41
3:G:693:G:H2'	3:G:694:A:H8	1.85	0.41
1:M:447:LEU:HD23	1:M:447:LEU:N	2.34	0.41
1:A:306:ARG:CG	1:A:318:LEU:HD13	2.51	0.41
1:A:384:TYR:HA	1:A:385:PRO:HD3	1.82	0.41
2:B:598:A:C3'	2:B:599:G:H5'	2.46	0.41
1:E:50:LEU:HD21	1:E:171:GLY:HA3	2.03	0.41
1:I:7:ARG:HD3	1:I:11:GLU:HG2	2.02	0.41
1:I:11:GLU:C	1:I:12:VAL:HG23	2.41	0.41
1:I:118:TYR:CG	1:I:119:PRO:HA	2.55	0.41
1:A:55:GLU:O	1:A:59:PHE:HD2	2.03	0.41
1:A:381:ASP:OD1	8:A:6027:IPA:H2	2.21	0.41
1:M:321:LEU:HD12	1:M:322:LYS:N	2.35	0.41
1:A:24:LYS:HB2	1:A:24:LYS:HE3	1.76	0.41
1:A:217:PHE:HD1	8:A:6009:IPA:H12	1.85	0.41
1:A:305:ILE:HD11	1:A:330:VAL:HG11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:PRO:HB3	1:E:31:HIS:CE1	2.55	0.41
1:E:52:THR:HG23	1:E:53:ASP:N	2.35	0.41
1:E:226:GLU:HG3	1:E:320:HIS:O	2.21	0.41
1:E:295:ILE:HG12	10:E:507:HOH:O	2.21	0.41
1:E:411:GLN:HE22	1:E:446:ASP:H	1.69	0.41
1:I:228:LYS:O	1:I:333:SER:HB2	2.21	0.41
1:I:275:TYR:O	1:I:275:TYR:CD2	2.74	0.41
2:J:604:C:H2'	2:J:605:U:C6	2.56	0.41
3:K:694:A:H2'	3:K:695:C:C6	2.56	0.41
1:M:82:ALA:O	1:M:86:MET:HG2	2.21	0.41
1:M:275:TYR:O	1:M:276:LYS:CB	2.69	0.41
2:N:604:C:H2'	2:N:605:U:C6	2.55	0.41
3:O:692:G:O2'	3:O:693:G:H5'	2.21	0.41
1:A:120:TYR:HB3	1:A:125:LYS:HB3	2.03	0.41
2:B:610:C:C2'	2:B:611:G:O5'	2.69	0.41
1:E:213:ASP:HB3	8:E:6014:IPA:C1	2.50	0.41
1:E:223:VAL:HG23	1:E:223:VAL:O	2.21	0.41
1:E:254:GLU:HG2	1:E:259:GLY:HA2	2.01	0.41
1:I:275:TYR:O	1:I:276:LYS:CB	2.69	0.41
1:M:432:PHE:CZ	1:M:436:ILE:HD11	2.55	0.41
2:N:604:C:H2'	2:N:605:U:O4'	2.21	0.41
2:F:598:A:H1'	4:H:805:G:C2	2.57	0.40
1:I:47:ASP:HA	1:I:48:PRO:HD3	1.87	0.40
1:I:270:HIS:NE2	1:I:283:LYS:HE2	2.36	0.40
1:M:226:GLU:HG3	1:M:320:HIS:O	2.20	0.40
1:A:95:MET:HE3	1:A:95:MET:HB2	1.94	0.40
1:A:179:SER:HB2	1:A:290:CYS:HA	2.02	0.40
1:A:254:GLU:HG2	1:A:259:GLY:HA2	2.02	0.40
1:A:382:GLU:HB2	8:A:6027:IPA:H33	2.03	0.40
1:E:212:CYS:HB2	8:E:6014:IPA:C3	2.51	0.40
1:E:237:TYR:CG	1:E:328:ASP:HB3	2.56	0.40
2:F:610:C:C2'	2:F:611:G:O5'	2.69	0.40
1:I:162:LEU:HD11	1:I:403:TRP:CD1	2.56	0.40
1:I:318:LEU:HD23	1:I:318:LEU:HA	1.75	0.40
1:M:11:GLU:C	1:M:12:VAL:HG23	2.42	0.40
1:M:448:PRO:HG2	1:M:453:LEU:HD21	2.02	0.40
1:A:20:PRO:HA	2:B:598:A:N1	2.36	0.40
1:E:334:TYR:CD2	1:E:335:PRO:HD2	2.55	0.40
1:I:375:LYS:HD3	1:I:396:GLU:OE1	2.21	0.40
1:M:67:ILE:HG23	1:M:244:ALA:HB3	2.04	0.40
1:A:58:ILE:HD11	1:A:59:PHE:CE2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PRO:O	1:A:390:PRO:HG3	2.22	0.40
1:E:61:LYS:HD2	1:E:239:ALA:CB	2.51	0.40
1:E:70:VAL:HG11	1:E:251:MET:HE3	2.03	0.40
1:E:121:VAL:CG1	1:E:122:ALA:N	2.85	0.40
1:E:367:THR:C	1:E:369:GLU:H	2.25	0.40
1:E:449:GLU:O	1:E:450:TYR:C	2.59	0.40
3:G:693:G:H2'	3:G:694:A:C8	2.57	0.40
1:M:270:HIS:NE2	1:M:283:LYS:HE2	2.36	0.40
1:E:145:LEU:HD23	1:E:145:LEU:HA	1.90	0.40
1:I:275:TYR:O	1:I:276:LYS:HB3	2.22	0.40
1:I:321:LEU:HD12	1:I:322:LYS:N	2.36	0.40
1:I:334:TYR:CD1	1:I:335:PRO:CD	3.05	0.40
1:I:337:GLU:OE2	1:I:337:GLU:C	2.60	0.40
1:I:355:THR:HB	1:I:356:PRO:HD3	2.03	0.40
1:I:383:LYS:HB3	1:I:384:TYR:CD1	2.57	0.40
1:I:411:GLN:HB3	10:I:546:HOH:O	2.22	0.40
1:M:334:TYR:CD1	1:M:335:PRO:CD	3.04	0.40
1:M:358:ASP:HB2	1:M:360:SER:OG	2.22	0.40
1:M:440:PRO:HA	1:M:443:ARG:NH1	2.36	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	
1	A	459/471 (98%)	434 (95%)	23 (5%)	2 (0%)	34	53
1	E	459/471 (98%)	432 (94%)	25 (5%)	2 (0%)	34	53
1	I	459/471 (98%)	406 (88%)	45 (10%)	8 (2%)	9	16
1	M	459/471 (98%)	407 (89%)	44 (10%)	8 (2%)	9	16
All	All	1836/1884 (98%)	1679 (91%)	137 (8%)	20 (1%)	14	25

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	GLY
1	E	285	GLY
1	I	12	VAL
1	I	64	GLY
1	I	70	VAL
1	I	164	SER
1	M	64	GLY
1	M	70	VAL
1	M	164	SER
1	I	66	LYS
1	M	12	VAL
1	M	66	LYS
1	I	276	LYS
1	I	355	THR
1	I	457	TRP
1	M	276	LYS
1	M	355	THR
1	M	457	TRP
1	E	70	VAL
1	A	70	VAL

5.3.2 Protein sidechains [i](#)

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	403/412 (98%)	368 (91%)	35 (9%)	10	18
1	E	403/412 (98%)	369 (92%)	34 (8%)	11	19
1	I	403/412 (98%)	369 (92%)	34 (8%)	11	19
1	M	403/412 (98%)	369 (92%)	34 (8%)	11	19
All	All	1612/1648 (98%)	1475 (92%)	137 (8%)	10	19

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	4	GLN
1	A	9	SER
1	A	10	LYS
1	A	24	LYS
1	A	28	SER
1	A	43	LEU
1	A	45	LYS
1	A	49	ARG
1	A	52	THR
1	A	66	LYS
1	A	94	GLN
1	A	139	LYS
1	A	163	ARG
1	A	166	THR
1	A	170	GLN
1	A	176	ILE
1	A	218	TRP
1	A	220	LYS
1	A	260	ASP
1	A	261	ARG
1	A	263	ASP
1	A	277	ASN
1	A	281	CYS
1	A	294	SER
1	A	314	LYS
1	A	316	ILE
1	A	329	ASP
1	A	337	GLU
1	A	348	LYS
1	A	359	LYS
1	A	415	ARG
1	A	428	GLU
1	A	455	ARG
1	A	456	ARG
1	E	2	GLU
1	E	4	GLN
1	E	9	SER
1	E	10	LYS
1	E	24	LYS
1	E	28	SER
1	E	43	LEU
1	E	45	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	49	ARG
1	E	52	THR
1	E	66	LYS
1	E	94	GLN
1	E	139	LYS
1	E	163	ARG
1	E	166	THR
1	E	170	GLN
1	E	176	ILE
1	E	218	TRP
1	E	220	LYS
1	E	260	ASP
1	E	261	ARG
1	E	263	ASP
1	E	277	ASN
1	E	281	CYS
1	E	294	SER
1	E	314	LYS
1	E	316	ILE
1	E	329	ASP
1	E	337	GLU
1	E	348	LYS
1	E	359	LYS
1	E	428	GLU
1	E	455	ARG
1	E	456	ARG
1	I	3	ILE
1	I	5	TRP
1	I	6	MET
1	I	21	SER
1	I	26	GLU
1	I	39	GLU
1	I	56	GLU
1	I	60	SER
1	I	63	VAL
1	I	68	THR
1	I	121	VAL
1	I	151	ASN
1	I	166	THR
1	I	176	ILE
1	I	179	SER
1	I	180	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	218	TRP
1	I	261	ARG
1	I	277	ASN
1	I	291	SER
1	I	294	SER
1	I	295	ILE
1	I	329	ASP
1	I	337	GLU
1	I	346	SER
1	I	348	LYS
1	I	364	GLU
1	I	367	THR
1	I	383	LYS
1	I	391	VAL
1	I	415	ARG
1	I	428	GLU
1	I	441	ILE
1	I	455	ARG
1	M	5	TRP
1	M	6	MET
1	M	7	ARG
1	M	21	SER
1	M	26	GLU
1	M	39	GLU
1	M	56	GLU
1	M	60	SER
1	M	63	VAL
1	M	68	THR
1	M	121	VAL
1	M	151	ASN
1	M	166	THR
1	M	176	ILE
1	M	179	SER
1	M	180	SER
1	M	218	TRP
1	M	261	ARG
1	M	277	ASN
1	M	291	SER
1	M	294	SER
1	M	295	ILE
1	M	329	ASP
1	M	337	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	346	SER
1	M	348	LYS
1	M	364	GLU
1	M	367	THR
1	M	383	LYS
1	M	391	VAL
1	M	415	ARG
1	M	428	GLU
1	M	441	ILE
1	M	455	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	411	GLN
1	E	277	ASN
1	E	411	GLN
1	I	170	GLN
1	I	270	HIS
1	I	272	HIS
1	I	277	ASN
1	I	398	HIS
1	I	424	ASN
1	M	170	GLN
1	M	269	ASN
1	M	270	HIS
1	M	272	HIS
1	M	277	ASN
1	M	336	HIS
1	M	398	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	15/26 (57%)	2 (13%)	2 (13%)
2	F	15/26 (57%)	2 (13%)	2 (13%)
2	J	15/26 (57%)	2 (13%)	1 (6%)
2	N	15/26 (57%)	2 (13%)	1 (6%)
3	C	14/15 (93%)	1 (7%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	14/15 (93%)	1 (7%)	0
3	K	14/15 (93%)	0	0
3	O	14/15 (93%)	0	0
4	D	2/9 (22%)	2 (100%)	0
4	H	2/9 (22%)	2 (100%)	0
4	L	3/9 (33%)	1 (33%)	0
4	P	3/9 (33%)	1 (33%)	0
All	All	126/200 (63%)	16 (12%)	6 (4%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	599	G
2	B	600	G
3	C	690	C
4	D	806	G
4	D	807	A
2	F	599	G
2	F	600	G
3	G	690	C
4	H	806	G
4	H	807	A
2	J	611	G
2	J	612	G
4	L	807	A
2	N	611	G
2	N	612	G
4	P	807	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	598	A
2	B	599	G
2	F	598	A
2	F	599	G
2	J	598	A
2	N	598	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 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	$\# Z > 2$
8	IPA	A	6027	-	3,3,3	0.62	0	3,3,3	0.15	0
7	POP	G	5003	6	6,8,8	0.67	0	13,13,13	0.94	1 (7%)
8	IPA	A	6028	-	3,3,3	0.66	0	3,3,3	0.27	0
7	POP	I	5002	6	6,8,8	0.69	0	13,13,13	1.57	2 (15%)
7	POP	O	5001	6	6,8,8	0.61	0	13,13,13	1.08	1 (7%)
8	IPA	M	6018	-	3,3,3	0.63	0	3,3,3	0.26	0
8	IPA	E	6029	-	3,3,3	0.55	0	3,3,3	0.23	0
8	IPA	A	6009	-	3,3,3	0.66	0	3,3,3	0.22	0
8	IPA	A	6011	-	3,3,3	0.52	0	3,3,3	0.38	0
8	IPA	E	6014	-	3,3,3	0.41	0	3,3,3	0.66	0
8	IPA	M	6019	-	3,3,3	0.53	0	3,3,3	0.40	0
9	GOL	A	8012	-	5,5,5	0.38	0	5,5,5	0.46	0
8	IPA	A	6030	-	3,3,3	0.51	0	3,3,3	0.51	0
9	GOL	E	8011	5	5,5,5	0.32	0	5,5,5	0.41	0
9	GOL	J	8005	-	5,5,5	0.42	0	5,5,5	0.87	0
7	POP	A	5004	6	6,8,8	0.73	0	13,13,13	1.36	2 (15%)
9	GOL	N	8010	-	5,5,5	0.38	0	5,5,5	0.91	0

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	POP	G	5003	6	-	1/6/6/6	-
7	POP	I	5002	6	-	0/6/6/6	-
7	POP	O	5001	6	-	0/6/6/6	-
9	GOL	A	8012	-	-	0/4/4/4	-
9	GOL	J	8005	-	-	2/4/4/4	-
9	GOL	E	8011	5	-	2/4/4/4	-
7	POP	A	5004	6	-	3/6/6/6	-
9	GOL	N	8010	-	-	4/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	5002	POP	P2-O-P1	-4.62	116.98	132.83
7	O	5001	POP	O2-P1-O	2.73	113.79	104.64
7	A	5004	POP	P2-O-P1	-2.73	123.46	132.83
7	G	5003	POP	O6-P2-O	2.72	113.75	104.64
7	A	5004	POP	O5-P2-O	2.45	112.84	104.64
7	I	5002	POP	O3-P1-O	2.11	111.71	104.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5004	POP	P2-O-P1-O2
9	N	8010	GOL	O1-C1-C2-C3
9	E	8011	GOL	C1-C2-C3-O3
9	J	8005	GOL	O1-C1-C2-C3
9	N	8010	GOL	C1-C2-C3-O3
9	N	8010	GOL	O1-C1-C2-O2
7	A	5004	POP	P1-O-P2-O4
7	G	5003	POP	P2-O-P1-O2
9	E	8011	GOL	O2-C2-C3-O3
7	A	5004	POP	P2-O-P1-O1
9	J	8005	GOL	O1-C1-C2-O2
9	N	8010	GOL	O2-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	6027	IPA	2	0
7	G	5003	POP	1	0
8	A	6028	IPA	2	0
7	I	5002	POP	1	0
8	M	6018	IPA	1	0
8	E	6029	IPA	3	0
8	A	6009	IPA	1	0
8	A	6011	IPA	4	0
8	E	6014	IPA	11	0
8	M	6019	IPA	5	0
8	A	6030	IPA	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	461/471 (97%)	-0.06	14 (3%) 50 59	37, 61, 92, 111	0
1	E	461/471 (97%)	-0.05	15 (3%) 46 54	39, 60, 93, 110	0
1	I	461/471 (97%)	0.05	23 (4%) 28 35	40, 68, 115, 143	0
1	M	461/471 (97%)	0.13	34 (7%) 14 17	38, 68, 115, 143	0
2	B	17/26 (65%)	-0.65	0 100 100	47, 62, 135, 164	0
2	F	17/26 (65%)	-0.50	0 100 100	47, 62, 134, 164	0
2	J	17/26 (65%)	-0.22	0 100 100	53, 75, 166, 182	0
2	N	17/26 (65%)	-0.16	1 (5%) 22 27	51, 76, 166, 182	0
3	C	15/15 (100%)	-0.24	2 (13%) 3 4	49, 65, 124, 141	0
3	G	15/15 (100%)	-0.03	2 (13%) 3 4	49, 65, 124, 141	0
3	K	15/15 (100%)	0.03	2 (13%) 3 4	52, 83, 145, 149	0
3	O	15/15 (100%)	0.11	2 (13%) 3 4	52, 84, 145, 149	0
4	D	3/9 (33%)	1.79	2 (66%) 0 0	168, 168, 172, 173	0
4	H	3/9 (33%)	4.60	2 (66%) 0 0	168, 168, 172, 173	0
4	L	4/9 (44%)	1.67	1 (25%) 0 0	146, 152, 157, 173	0
4	P	4/9 (44%)	2.65	3 (75%) 0 0	146, 152, 158, 173	0
All	All	1986/2084 (95%)	0.02	103 (5%) 27 33	37, 64, 114, 182	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	805	G	7.0
1	E	284	GLY	6.8
1	I	357	ALA	5.6
1	I	342	LEU	5.2
4	H	806	G	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	285	GLY	4.9
1	M	134	GLN	4.8
4	P	805	G	4.7
1	M	285	GLY	4.6
1	M	284	GLY	4.1
1	A	19	ALA	4.0
1	M	32	TYR	3.9
3	G	689	C	3.8
1	I	134	GLN	3.8
1	E	283	LYS	3.7
1	M	65	ASN	3.6
1	A	67	ILE	3.6
1	M	38	LYS	3.6
1	E	134	GLN	3.5
3	C	688	G	3.5
1	E	49	ARG	3.5
3	K	689	C	3.4
3	K	688	G	3.3
1	M	363	PHE	3.3
1	A	64	GLY	3.3
1	A	32	TYR	3.3
1	M	342	LEU	3.3
3	O	689	C	3.2
1	I	46	ASN	3.2
3	O	688	G	3.2
4	L	808	G	3.2
1	M	396	GLU	3.1
1	I	32	TYR	3.1
1	M	165	LYS	3.0
1	M	17	ILE	3.0
1	E	16	ILE	2.9
1	M	204	VAL	2.9
1	M	345	GLN	2.9
4	P	806	G	2.9
1	A	134	GLN	2.8
3	C	689	C	2.8
1	M	22	LYS	2.8
1	A	139	LYS	2.8
1	I	406	ASP	2.7
1	A	357	ALA	2.7
1	I	363	PHE	2.7
1	A	320	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	89	ASP	2.7
1	E	138	THR	2.7
1	M	357	ALA	2.6
1	M	16	ILE	2.6
1	A	154	LEU	2.6
1	E	178	ALA	2.5
1	I	47	ASP	2.5
1	M	460	SER	2.5
1	M	46	ASN	2.4
1	I	15	PRO	2.4
1	I	356	PRO	2.4
1	E	233	ASP	2.4
1	M	29	ALA	2.4
4	D	806	G	2.4
1	I	396	GLU	2.4
1	A	256	ILE	2.4
3	G	688	G	2.4
1	A	396	GLU	2.4
1	M	343	LEU	2.3
2	N	597	C	2.3
1	I	67	ILE	2.3
1	I	345	GLN	2.3
1	E	361	ALA	2.3
1	I	276	LYS	2.3
1	M	2	GLU	2.3
1	I	1	GLY	2.3
1	I	75	LYS	2.3
1	I	154	LEU	2.3
1	M	31	HIS	2.2
1	M	43	LEU	2.2
1	M	286	MET	2.2
1	M	355	THR	2.2
1	M	441	ILE	2.2
1	M	71	ASP	2.2
1	I	314	LYS	2.2
1	A	359	LYS	2.2
1	E	13	GLY	2.2
1	I	10	LYS	2.2
1	I	285	GLY	2.2
4	D	805	G	2.2
4	P	808	G	2.2
1	M	315	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	49	ARG	2.2
1	M	9	SER	2.1
1	E	10	LYS	2.1
1	A	414	VAL	2.1
1	M	178	ALA	2.1
1	E	317	ASP	2.1
1	M	67	ILE	2.1
1	M	137	ASP	2.1
1	E	313	TYR	2.1
1	E	414	VAL	2.0
1	I	320	HIS	2.0
1	M	287	PRO	2.0
1	M	170	GLN	2.0
1	I	34	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
7	POP	I	5002	9/9	0.69	0.27	97,119,129,136	9
8	IPA	M	6019	4/4	0.73	0.41	80,96,100,105	0
8	IPA	A	6027	4/4	0.74	0.23	84,91,95,98	0
7	POP	A	5004	9/9	0.78	0.24	45,77,111,115	9
8	IPA	A	6011	4/4	0.78	0.77	65,88,92,106	0
7	POP	G	5003	9/9	0.79	0.19	47,60,88,89	9
7	POP	O	5001	9/9	0.80	0.24	41,73,93,98	9
9	GOL	A	8012	6/6	0.87	0.20	71,86,94,98	0
9	GOL	E	8011	6/6	0.88	0.16	69,82,89,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	GOL	N	8010	6/6	0.88	0.34	55,71,72,86	0
8	IPA	E	6029	4/4	0.90	0.57	67,75,80,84	0
8	IPA	E	6014	4/4	0.91	0.24	53,58,75,75	0
9	GOL	J	8005	6/6	0.91	0.21	47,55,64,73	0
8	IPA	A	6028	4/4	0.91	0.28	60,80,87,112	0
6	MN	A	3007	1/1	0.93	0.07	91,91,91,91	0
8	IPA	A	6009	4/4	0.93	0.13	64,72,75,78	0
6	MN	E	3005	1/1	0.94	0.05	87,87,87,87	0
6	MN	I	3003	1/1	0.94	0.05	120,120,120,120	0
6	MN	M	3001	1/1	0.94	0.06	127,127,127,127	0
5	ZN	M	2001	1/1	0.95	0.15	70,70,70,70	1
8	IPA	M	6018	4/4	0.96	0.17	47,52,58,72	0
8	IPA	A	6030	4/4	0.96	0.37	68,73,76,78	0
5	ZN	E	2003	1/1	0.97	0.17	88,88,88,88	1
6	MN	I	3004	1/1	0.98	0.09	90,90,90,90	0
5	ZN	A	2004	1/1	0.98	0.10	81,81,81,81	1
6	MN	M	3002	1/1	0.98	0.08	86,86,86,86	0
6	MN	E	3006	1/1	0.98	0.09	74,74,74,74	0
5	ZN	I	2002	1/1	0.98	0.14	70,70,70,70	1
6	MN	A	3008	1/1	0.99	0.08	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.