



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:20 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

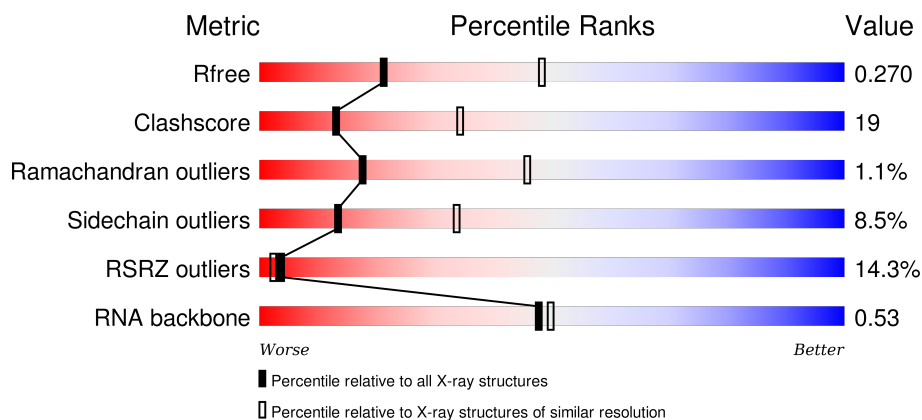
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.






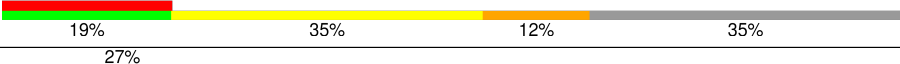
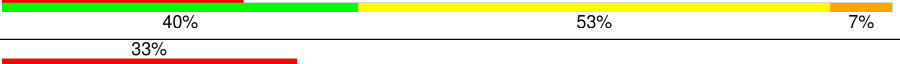


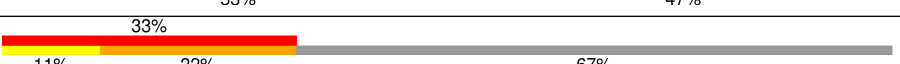
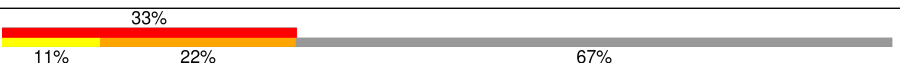



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)
RNA backbone	2183	1006 (3.14-2.38)

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

Mol	Chain	Length	Quality of chain
1	A	471	<div> <div>11%</div> <div>64%</div> <div>29%</div> <div>5%</div> </div>
1	E	471	<div> <div>10%</div> <div>64%</div> <div>30%</div> <div>5%</div> </div>
1	I	471	<div> <div>13%</div> <div>60%</div> <div>34%</div> <div>• •</div> </div>
1	M	471	<div> <div>15%</div> <div>58%</div> <div>35%</div> <div>• •</div> </div>

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
7	POP	A	5004	-	-	-	X
7	POP	G	5003	-	-	-	X
7	POP	I	5002	-	-	-	X
8	IPA	A	6009	-	-	-	X
8	IPA	A	6011	-	-	X	-
8	IPA	A	6028	-	-	-	X
8	IPA	A	6030	-	-	-	X
8	IPA	E	6014	-	-	X	X
8	IPA	E	6029	-	-	-	X
8	IPA	M	6019	-	-	X	-
9	GOL	J	8005	-	-	-	X
9	GOL	N	8010	-	-	-	X

2 Entry composition

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
1	A	461	Total	C	N	O	S	0	0	0
			3697	2370	610	695	22			
1	E	461	Total	C	N	O	S	0	0	0
			3697	2370	610	695	22			
1	I	461	Total	C	N	O	S	0	0	0
			3697	2370	610	695	22			
1	M	461	Total	C	N	O	S	0	0	0
			3697	2370	610	695	22			

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*GP*UP*CP*CP*GP*GP*AP*AP*A)-3').

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

- 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	I	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		
5	M	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		

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

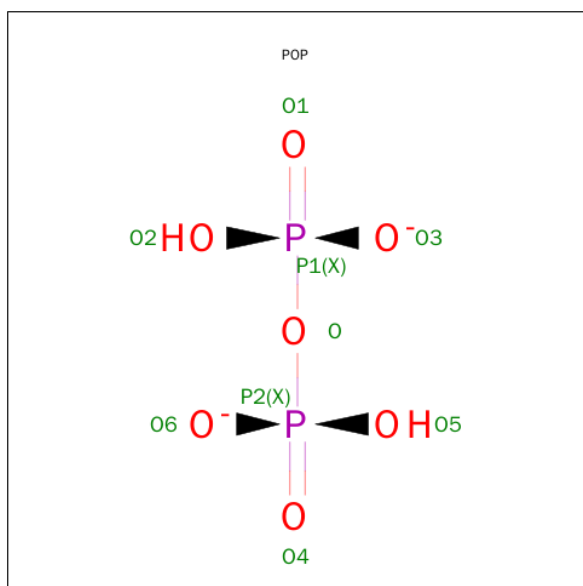
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total	Mn	0	0
			2	2		
6	A	2	Total	Mn	0	0
			2	2		
6	M	2	Total	Mn	0	0
			2	2		

Continued on next page...

Continued from previous page...

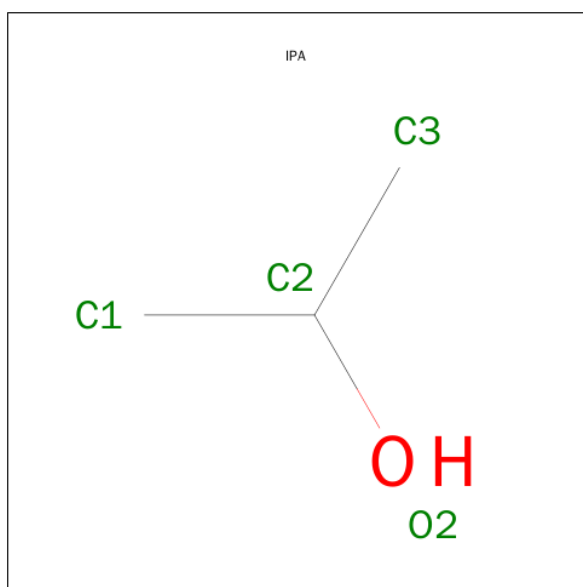
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	2	Total	Mn	0	0
			2	2		

- 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	0	0
			4	3	1		
8	A	1	Total	C	O	0	0
			4	3	1		
8	A	1	Total	C	O	0	0
			4	3	1		
8	A	1	Total	C	O	0	0
			4	3	1		
8	E	1	Total	C	O	0	0
			4	3	1		
8	E	1	Total	C	O	0	0
			4	3	1		
8	M	1	Total	C	O	0	0
			4	3	1		
8	M	1	Total	C	O	0	0
			4	3	1		

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



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

- Molecule 10 is water.

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

Continued on next page...

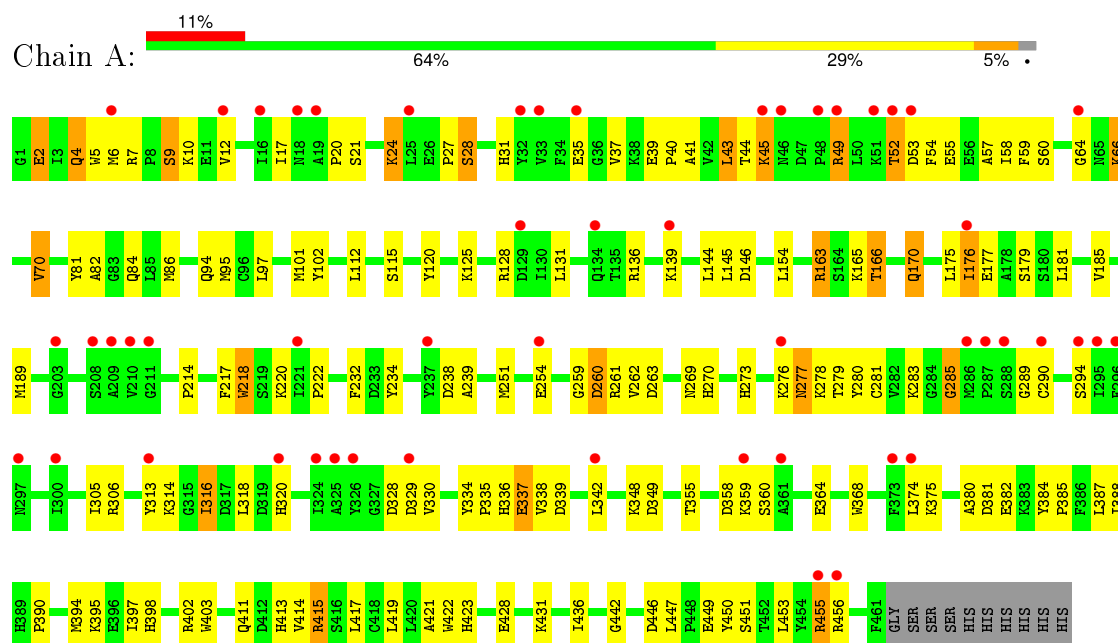
Continued from previous page...

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

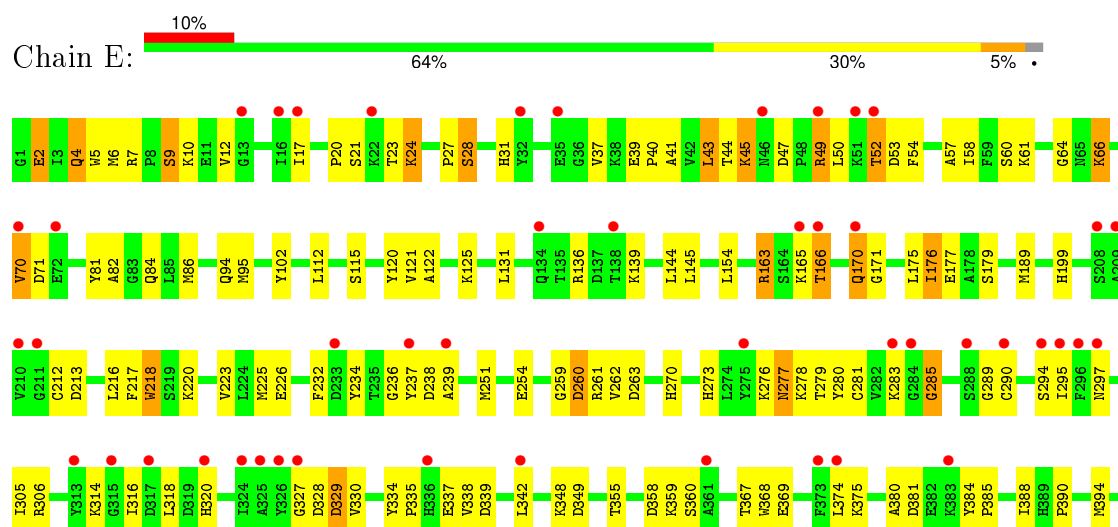
3 Residue-property plots [i](#)

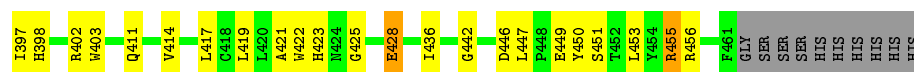
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Polymerase

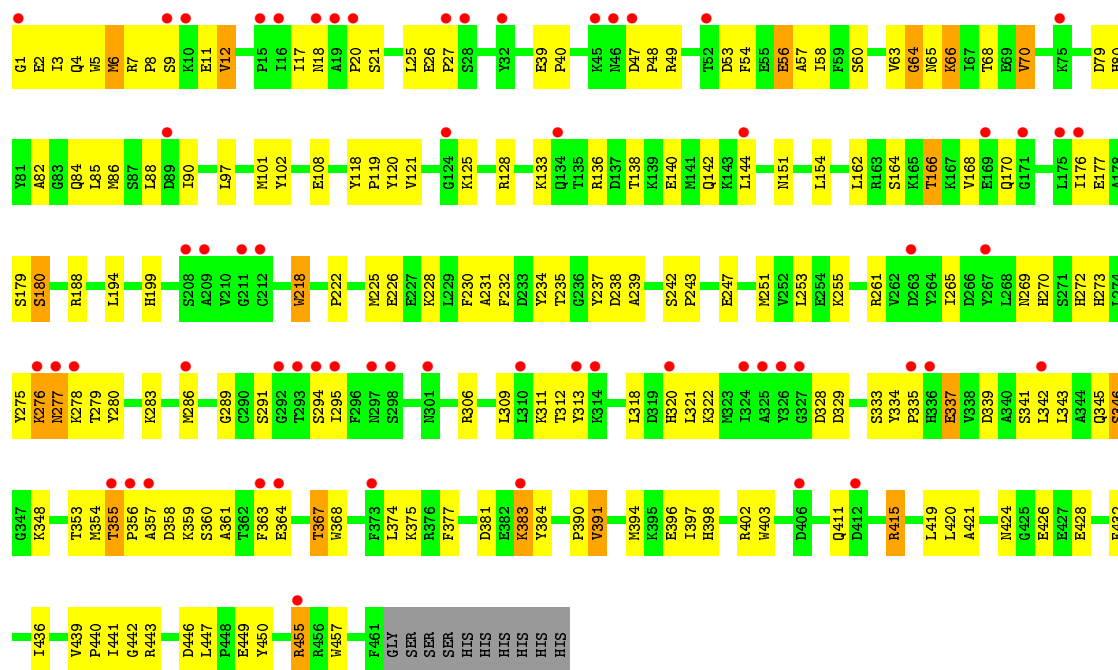


• Molecule 1: Polymerase

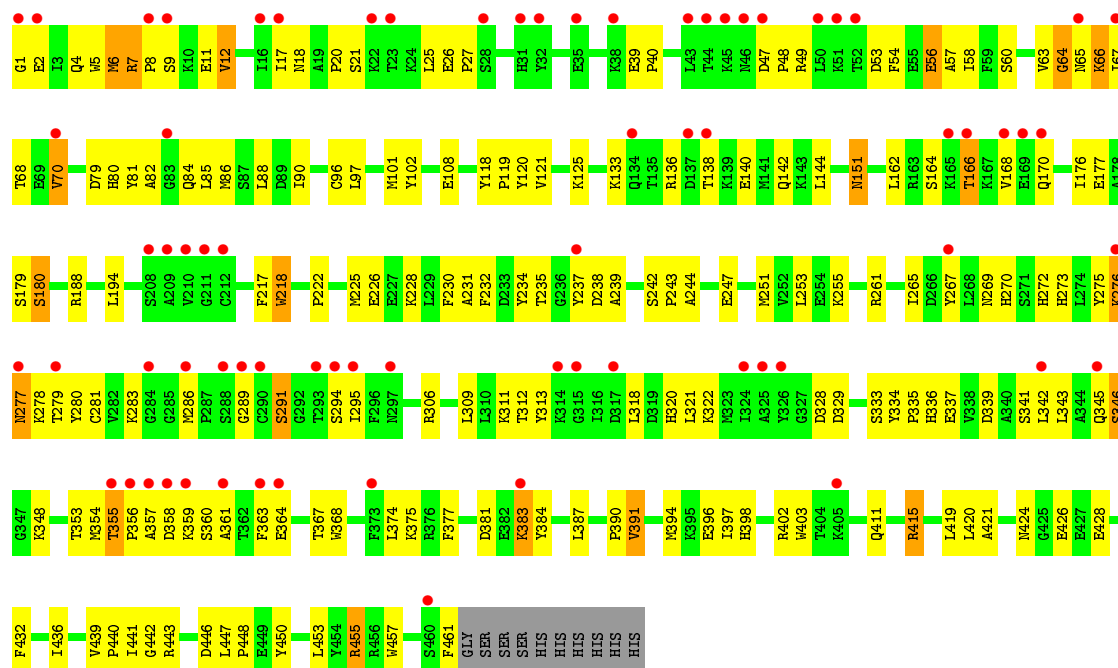




• Molecule 1: Polymerase

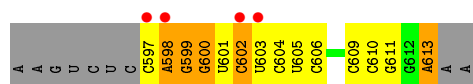


• Molecule 1: Polymerase



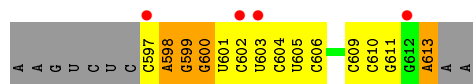
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain B: 



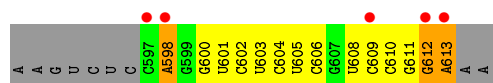
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain F: 




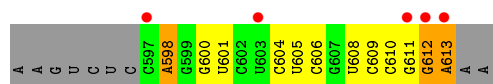
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain J: 



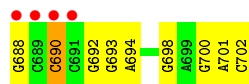
- Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP*CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain N: 



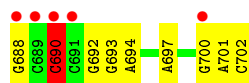
- Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*C)-3')

Chain C: 

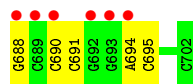
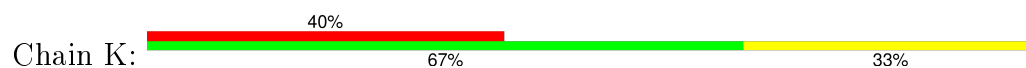


- Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*C)-3')

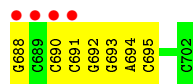
Chain G: 



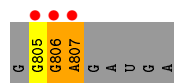
- Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*C)-3')



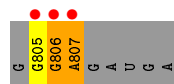
- Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*C)-3')



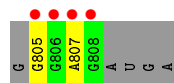
- Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



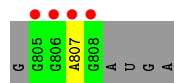
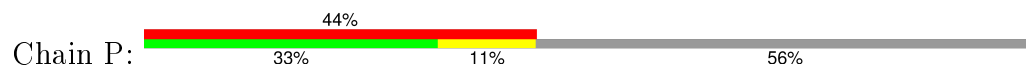
- Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')



- 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

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) 94.3 (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)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.224 , 0.277 0.212 , 0.270	Depositor DCC
R_{free} test set	3397 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.4	EDS
Estimated twinning fraction	0.398 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.63$, $\langle L^2 \rangle = 0.49$	Xtriage
Outliers	0 of 101191 reflections	Xtriage
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

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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 ⓘ

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
1:E:254:GLU:HG3	1:E:262:VAL:HG11	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: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:253:LEU:CD1	1:M:265:ILE:HD11	2.16	0.76
1:M:49:ARG:HE	1:M:168:VAL:HG11	1.50	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
2:J:600:G:O2'	2:J:601:U:H5'	1.89	0.72
1:I:49:ARG:HE	1:I:168:VAL:HG11	1.51	0.72
1:M:1:GLY:HA2	1:M:65:ASN:OD1	1.88	0.72
1:A:70:VAL:HG21	1:A:251:MET:CE	2.20	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:M:80:HIS:CE1	1:M:318:LEU:HB3	2.24	0.71
1:I:18:ASN:OD1	1:I:276:LYS:HG3	1.90	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:M:313:TYR:HD2	8:M:6019:IPA:H11	1.57	0.69
1:I:20:PRO:HG3	2:J:598:A:C4	2.27	0.69
1:M:7:ARG:HD2	1:M:12:VAL:CG2	2.22	0.69
1:M:217:PHE:HD1	8:M:6018:IPA:H32	1.56	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
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:E:37:VAL:HG13	1:E:165:LYS:HD2	1.76	0.68
1:A:337:GLU:HB2	10:A:571:HOH:O	1.93	0.68
1:I:415:ARG:HG2	1:I:415:ARG:HH11	1.58	0.68
3:C:694:A:N7	10:C:243:HOH:O	2.26	0.68
1:M:311:LYS:O	1:M:311:LYS:HG2	1.93	0.68
1:I:253:LEU:HD12	1:I:265:ILE:CD1	2.24	0.68
2:N:609:C:C4	2:N:610:C:C5	2.82	0.68
1:M:232:PHE:CE1	1:M:354:MET:HE2	2.29	0.68
1:A:381:ASP:HB3	1:A:384:TYR:O	1.94	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:I:311:LYS:O	1:I:311:LYS:HG2	1.95	0.66
1:E:270:HIS:CD2	1:E:283:LYS:HG2	2.27	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:M:20:PRO:HG3	2:N:598:A:C4	2.30	0.65
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: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:M:49:ARG:HH21	1:M:168:VAL:HG13	1.62	0.63
1:I:419:LEU:HD11	2:J:606:C:H4'	1.79	0.63
3:C:688:G:HO5'	3:C:688:G:H8	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:I:309:LEU:HD12	1:I:321:LEU:HD22	1.81	0.63
1:A:259:GLY:O	1:A:262:VAL:HG22	1.98	0.63
1:I:397:ILE:HD13	1:I:421:ALA:HB2	1.80	0.63
1:E:21:SER:HB2	1:E:44:THR:HG21	1.81	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:367:THR:HB	10:I:515:HOH:O	2.00	0.61
1:I:199:HIS:NE2	10:I:493:HOH:O	2.31	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:M:356:PRO:HG2	1:M:361:ALA:H	1.66	0.60
1:I:334:TYR:CG	1:I:335:PRO:HD2	2.35	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:E:37:VAL:O	1:E:37:VAL:HG12	2.02	0.60
1:A:58:ILE:HD12	1:A:175:LEU:HD21	1.83	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
3:G:688:G:H8	3:G:688:G:HO5'	1.48	0.59
1:E:115:SER:HB2	10:E:567:HOH:O	2.02	0.59
1:M:415:ARG:HG2	1:M:415:ARG:HH11	1.65	0.59
1:M:334:TYR:CG	1:M:335:PRO:HD2	2.37	0.59
1:I:277:ASN:ND2	1:I:278:LYS:HG2	2.18	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:I:65:ASN:O	1:I:242:SER:HB3	2.02	0.59
1:A:368:TRP:HB3	8:A:6030:IPA:H2	1.84	0.59
1:M:341:SER:HA	1:M:363:PHE:CD2	2.38	0.59
1:I:355:THR:HB	1:I:356:PRO:CD	2.32	0.59
1:I:166:THR:HG22	1:I:170:GLN:NE2	2.17	0.59
1:M:455:ARG:O	1:M:455:ARG:HD3	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:M:235:THR:CG2	1:M:353:THR:HB	2.33	0.58
1:A:95:MET:O	1:A:189:MET:HG2	2.03	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:I:426:GLU:N	1:I:450:TYR:CE1	2.71	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:M:313:TYR:CD2	8:M:6019:IPA:H11	2.38	0.58
1:A:306:ARG:HG2	1:A:318:LEU:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:PRO:HB2	1:I:11:GLU:HB2	1.85	0.58
1:A:234:TYR:CD1	1:A:328:ASP:HB2	2.38	0.58
1:I:234:TYR:CD1	1:I:328:ASP:HB2	2.39	0.58
1:I:232:PHE:HA	1:I:357:ALA:HB2	1.86	0.57
2:J:605:U:H2'	2:J:606:C:C6	2.38	0.57
1:I:398:HIS:O	1:I:402:ARG:HG3	2.04	0.57
1:A:397:ILE:HD13	1:A:421:ALA:HB2	1.85	0.57
1:E:213:ASP:HB3	8:E:6014:IPA:H12	1.86	0.57
1:A:289:GLY:HA2	2:B:600:G:N3	2.19	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
2:N:605:U:H2'	2:N:606:C:C6	2.39	0.57
1:E:425:GLY:HA2	10:E:505:HOH:O	2.03	0.57
1:M:11:GLU:O	1:M:12:VAL:HG23	2.05	0.57
1:I:439:VAL:HG23	1:I:442:GLY:H	1.70	0.57
1:E:82:ALA:O	1:E:86:MET:HG2	2.04	0.57
1:E:58:ILE:HD12	1:E:175:LEU:HD21	1.86	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:270:HIS:CD2	1:A:283:LYS:HE2	2.40	0.56
1:M:49:ARG:HH21	1:M:168:VAL:CG1	2.16	0.56
1:E:375:LYS:HD2	3:G:700:G:H5''	1.87	0.56
1:A:2:GLU:HG3	1:A:64:GLY:HA2	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:A:419:LEU:HD11	2:B:606:C:H4'	1.87	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: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:E:419:LEU:HD11	2:F:606:C:H4'	1.87	0.56
1:E:260:ASP:OD1	1:E:260:ASP:N	2.36	0.56
1:A:260:ASP:N	1:A:260:ASP:OD1	2.34	0.56
1:I:426:GLU:HA	1:I:450:TYR:CD1	2.42	0.55
1:E:397:ILE:HD13	1:E:421:ALA:HB2	1.88	0.55
1:A:52:THR:CG2	1:A:53:ASP:N	2.69	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:M:232:PHE:HB3	1:M:355:THR:O	2.07	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: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: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:A:120:TYR:CE1	1:A:144:LEU:HD13	2.42	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: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:E:112:LEU:HD21	1:E:131:LEU:HB2	1.89	0.53
1:I:118:TYR:O	1:I:180:SER:HB2	2.08	0.53
1:A:66:LYS:HG2	1:A:349:ASP:O	2.08	0.53
2:J:598:A:H1'	4:L:805:G:N2	2.24	0.53
1:E:451:SER:O	1:E:455:ARG:HD2	2.09	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
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
3:O:688:G:HO5'	3:O:688:G:H8	1.56	0.53
1:I:232:PHE:CE1	1:I:354:MET:CE	2.92	0.53
1:I:65:ASN:O	1:I:66:LYS:HB2	2.07	0.53
1:M:84:GLN:OE1	1:M:306:ARG:NH2	2.41	0.53
1:E:95:MET:O	1:E:189:MET:HG2	2.08	0.53
1:I:374:LEU:O	1:I:375:LYS:HB2	2.08	0.53
1:M:270:HIS:CE1	1:M:272:HIS:HE1	2.27	0.53
1:E:52:THR:CG2	1:E:53:ASP:N	2.72	0.53
1:I:270:HIS:CE1	1:I:272:HIS:CE1	2.96	0.53
1:I:230:PHE:O	1:I:231:ALA:HB2	2.08	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:M:277:ASN:HD22	1:M:278:LYS:HG2	1.74	0.52
1:E:238:ASP:OD1	1:E:239:ALA:N	2.42	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:277:ASN:HD22	1:M:278:LYS:N	2.08	0.51
1:M:230:PHE:O	1:M:231:ALA:HB2	2.10	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
2:B:597:C:O2	2:B:597:C:H2'	2.09	0.51
1:A:238:ASP:OD1	1:A:239:ALA:N	2.43	0.51
1:M:177:GLU:O	1:M:289:GLY:HA3	2.11	0.51
1:I:177:GLU:O	1:I:289:GLY:HA3	2.10	0.51
2:F:597:C:O2	2:F:597:C:H2'	2.09	0.51
1:M:320:HIS:HB2	1:M:334:TYR:CE1	2.46	0.51
1:E:66:LYS:HG2	1:E:349:ASP:O	2.11	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: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:A:37:VAL:CG1	1:A:37:VAL:O	2.60	0.50
1:E:24:LYS:HE3	10:E:524:HOH:O	2.12	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:M:336:HIS:CB	8:M:6019:IPA:H31	2.40	0.50
1:I:334:TYR:CD2	1:I:335:PRO:HD2	2.47	0.50
1:I:234:TYR:HD1	1:I:328:ASP:HB2	1.77	0.50
1:E:39:GLU:OE2	1:E:165:LYS:HG3	2.11	0.50
1:M:238:ASP:HB2	1:M:286:MET:HB3	1.94	0.50
1:I:334:TYR:CG	1:I:335:PRO:CD	2.94	0.50
1:A:70:VAL:HG11	1:A:251:MET:CE	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG21	1:A:251:MET:HE3	1.91	0.50
2:N:612:G:H5''	2:N:613:A:OP1	2.12	0.50
1:E:236:GLY:HA2	7:G:5003:POP:O6	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
2:N:609:C:C4	2:N:610:C:H5	2.30	0.49
1:I:421:ALA:O	1:I:424:ASN:HB2	2.12	0.49
1:I:79:ASP:OD1	1:I:255:LYS:HE2	2.12	0.49
1:A:40:PRO:HD3	1:A:403:TRP:CH2	2.47	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:334:TYR:CG	1:M:335:PRO:CD	2.95	0.49
1:M:312:THR:HG22	1:M:313:TYR:CD1	2.48	0.49
1:M:118:TYR:O	1:M:180:SER:HB2	2.12	0.49
1:M:54:PHE:CE1	1:M:58:ILE:CG2	2.95	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: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:397:ILE:HD11	1:M:420:LEU:HB3	1.94	0.49
2:B:598:A:C1'	4:D:805:G:N2	2.73	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
1:I:277:ASN:HD22	1:I:278:LYS:HG2	1.77	0.49
1:M:334:TYR:CD1	1:M:335:PRO:HD2	2.48	0.49
2:F:602:C:H2'	2:F:603:U:H6	1.73	0.49
1:I:238:ASP:HB2	1:I:286:MET:HB3	1.95	0.49
1:E:7:ARG:HD3	1:E:12:VAL:CG2	2.43	0.49
2:N:608:U:H2'	2:N:609:C:O4'	2.12	0.48
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
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
2:J:609:C:C4	2:J:610:C:H5	2.31	0.48
1:M:97:LEU:O	1:M:101:MET:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:ASP:HB3	1:I:56:GLU:HB3	1.95	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:M:237:TYR:CG	1:M:328:ASP:HB3	2.48	0.48
1:I:54:PHE:CE1	1:I:58:ILE:CG2	2.97	0.48
1:I:9:SER:HA	1:I:279:THR:OG1	2.13	0.48
1:E:28:SER:HB2	1:E:402:ARG:C	2.33	0.48
1:I:128:ARG:HG3	10:I:527:HOH:O	2.14	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:A:358:ASP:OD1	1:A:360:SER:HB3	2.13	0.48
1:A:146:ASP:HA	10:A:534:HOH:O	2.12	0.48
1:I:12:VAL:CG1	1:I:12:VAL:O	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:339:ASP:CG	1:I:341:SER:HG	2.17	0.48
1:I:237:TYR:CG	1:I:328:ASP:HB3	2.49	0.48
1:M:411:GLN:HB3	10:M:496:HOH:O	2.14	0.48
2:J:608:U:H2'	2:J:609:C:O4'	2.14	0.47
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
1:M:11:GLU:O	1:M:12:VAL:CG2	2.62	0.47
1:A:154:LEU:O	1:A:273:HIS:HA	2.14	0.47
2:F:604:C:H2'	2:F:605:U:C6	2.49	0.47
3:O:690:C:H2'	3:O:691:C:O4'	2.14	0.47
1:A:166:THR:O	1:A:170:GLN:HB2	2.13	0.47
1:A:45:LYS:H	1:A:45:LYS:HG3	1.39	0.47
1:E:166:THR:O	1:E:170:GLN:HB2	2.15	0.47
1:I:85:LEU:HA	1:I:88:LEU:HD12	1.95	0.47
1:M:70:VAL:HG21	1:M:251:MET:SD	2.53	0.47
1:A:5:TRP:O	1:A:280:TYR:HA	2.14	0.47
1:M:108:GLU:O	1:M:188:ARG:NH2	2.39	0.47
1:A:339:ASP:HB3	1:A:342:LEU:HD12	1.95	0.47
1:A:39:GLU:OE2	1:A:165:LYS:HG3	2.13	0.47
1:I:97:LEU:HD23	1:I:138:THR:HB	1.95	0.47
1:E:45:LYS:HG3	1:E:45:LYS:H	1.39	0.47
3:C:690:C:H5''	3:C:690:C:H6	1.80	0.47
4:H:805:G:H2'	4:H:806:G:O5'	2.15	0.47
1:A:387:LEU:HD11	8:A:6028:IPA:H33	1.96	0.47
1:M:436:ILE:O	1:M:442:GLY:HA3	2.14	0.47
1:A:398:HIS:O	1:A:402:ARG:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:226:GLU:HG2	1:M:322:LYS:HG3	1.95	0.47
1:E:154:LEU:O	1:E:273:HIS:HA	2.13	0.47
3:C:700:G:H3'	10:C:165:HOH:O	2.14	0.47
1:I:54:PHE:O	1:I:57:ALA:N	2.45	0.47
3:G:690:C:H5''	3:G:690:C:H6	1.79	0.47
1:E:422:TRP:CD1	1:E:453:LEU:HD13	2.50	0.47
3:G:688:G:O5'	3:G:688:G:H8	1.98	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
1:I:11:GLU:O	1:I:12:VAL:CG2	2.62	0.47
1:E:70:VAL:HG11	1:E:251:MET:CE	2.45	0.47
1:M:53:ASP:HB3	1:M:56:GLU:HB3	1.97	0.47
1:E:277:ASN:ND2	1:E:278:LYS:HG3	2.30	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:5:TRP:O	1:E:280:TYR:HA	2.15	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:E:225:MET:HA	1:E:225:MET:HE2	1.97	0.46
1:M:40:PRO:HD3	1:M:403:TRP:CH2	2.51	0.46
1:I:65:ASN:HB3	1:I:243:PRO:HD2	1.97	0.46
4:H:806:G:O2'	4:H:807:A:H5'	2.15	0.46
1:I:218:TRP:O	1:I:222:PRO:HD3	2.15	0.46
3:G:692:G:O2'	3:G:693:G:H5'	2.16	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: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
1:M:9:SER:HA	1:M:279:THR:OG1	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:M:54:PHE:CE1	1:M:58:ILE:HG21	2.51	0.46
1:I:102:TYR:CE1	1:I:136:ARG:HA	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:M:79:ASP:OD1	1:M:255:LYS:HE2	2.16	0.46
1:I:231:ALA:C	1:I:232:PHE:CD2	2.90	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:I:70:VAL:HG21	1:I:251:MET:SD	2.56	0.45
1:A:28:SER:HB2	1:A:402:ARG:C	2.37	0.45
1:M:25:LEU:HB2	1:M:40:PRO:HG3	1.98	0.45
1:A:334:TYR:CG	1:A:335:PRO:HD2	2.51	0.45
1:I:394:MET:SD	1:I:421:ALA:HB1	2.57	0.45
1:I:27:PRO:HD3	1:I:403:TRP:CZ3	2.50	0.45
1:A:338:VAL:HG23	1:A:339:ASP:N	2.31	0.45
1:M:231:ALA:C	1:M:232:PHE:CD2	2.89	0.45
2:N:609:C:H2'	2:N:610:C:H5'	1.98	0.45
1:E:436:ILE:O	1:E:442:GLY:HA3	2.16	0.45
1:A:238:ASP:O	1:A:285:GLY:HA2	2.16	0.45
1:M:97:LEU:HD23	1:M:138:THR:HB	1.99	0.45
1:A:431:LYS:HE2	1:A:431:LYS:HB2	1.76	0.45
1:E:446:ASP:C	1:E:447:LEU:HD23	2.37	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:218:TRP:CD1	1:A:390:PRO:HA	2.51	0.45
1:M:339:ASP:CG	1:M:341:SER:HG	2.19	0.45
1:A:411:GLN:HE22	1:A:446:ASP:H	1.63	0.45
1:I:275:TYR:O	1:I:275:TYR:HD2	1.99	0.45
1:A:102:TYR:CE1	1:A:136:ARG:HA	2.51	0.45
1:M:151:ASN:ND2	1:M:267:TYR:CD2	2.79	0.45
1:E:334:TYR:CG	1:E:335:PRO:HD2	2.52	0.45
1:A:52:THR:HG23	1:A:53:ASP:N	2.32	0.44
1:I:225:MET:HA	1:I:225:MET:HE2	1.99	0.44
1:E:54:PHE:O	1:E:57:ALA:N	2.46	0.44
1:I:277:ASN:C	1:I:277:ASN:HD22	2.21	0.44
1:M:339:ASP:OD2	1:M:341:SER:OG	2.35	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:E:329:ASP:OD2	3:G:701:A:H5''	2.18	0.44
1:I:218:TRP:CD1	1:I:390:PRO:HA	2.52	0.44
1:E:40:PRO:HD3	1:E:403:TRP:CH2	2.52	0.44
2:F:600:G:C2'	2:F:601:U:H5'	2.48	0.44
2:F:598:A:C3'	2:F:599:G:H5'	2.44	0.44
1:M:375:LYS:HD3	1:M:396:GLU:OE1	2.18	0.44
1:E:398:HIS:O	1:E:402:ARG:HG3	2.17	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:M:277:ASN:HD22	1:M:277:ASN:C	2.21	0.44
1:A:181:LEU:O	1:A:185:VAL:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:394:MET:SD	1:E:421:ALA:HB1	2.57	0.44
1:A:446:ASP:C	1:A:447:LEU:HD23	2.38	0.44
1:A:395:LYS:HB3	1:A:395:LYS:HE2	1.70	0.44
1:M:8:PRO:HB2	1:M:11:GLU:CB	2.48	0.44
1:I:339:ASP:OD2	1:I:342:LEU:HG	2.18	0.44
1:E:305:ILE:HD11	1:E:330:VAL:HG11	1.99	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:E:102:TYR:CE1	1:E:136:ARG:HA	2.53	0.44
1:A:422:TRP:CD1	1:A:453:LEU:HD13	2.52	0.44
1:A:364:GLU:HG2	10:A:555:HOH:O	2.18	0.44
1:I:440:PRO:HA	1:I:443:ARG:NH1	2.33	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
1:A:17:ILE:O	1:A:276:LYS:HA	2.17	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:I:17:ILE:O	1:I:276:LYS:HA	2.18	0.43
1:E:338:VAL:HG23	1:E:339:ASP:N	2.33	0.43
1:A:414:VAL:HG11	1:A:436:ILE:HD13	2.00	0.43
1:I:355:THR:CB	1:I:356:PRO:CD	2.96	0.43
4:D:806:G:O2'	4:D:807:A:H5'	2.18	0.43
2:B:600:G:C2'	2:B:601:U:H5'	2.49	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:E:411:GLN:HE22	1:E:446:ASP:N	2.17	0.43
1:M:2:GLU:HB3	1:M:64:GLY:HA2	2.00	0.43
1:A:43:LEU:HA	1:A:43:LEU:HD12	1.75	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:M:320:HIS:HB3	1:M:335:PRO:CG	2.49	0.43
1:A:397:ILE:HG23	1:A:417:LEU:HD13	1.99	0.43
2:J:612:G:C5'	2:J:613:A:OP1	2.67	0.43
1:I:2:GLU:HB3	1:I:64:GLY:HA2	2.00	0.43
1:A:49:ARG:HE	1:A:49:ARG:HB2	1.63	0.43
3:C:688:G:O5'	3:C:688:G:H8	1.98	0.43
1:M:276:LYS:HE2	1:M:276:LYS:HB2	1.79	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:222:PRO:HA	1:M:368:TRP:CZ2	2.54	0.43
1:M:54:PHE:O	1:M:57:ALA:N	2.45	0.43
3:G:690:C:C5'	3:G:690:C:H6	2.31	0.43
1:E:4:GLN:HG2	1:E:283:LYS:HE3	2.01	0.42
1:A:27:PRO:HB3	1:A:31:HIS:CE1	2.54	0.42
1:M:17:ILE:O	1:M:276:LYS:HA	2.19	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:E:43:LEU:HA	1:E:43:LEU:HD12	1.79	0.42
1:I:273:HIS:HB2	1:I:280:TYR:CZ	2.54	0.42
1:I:90:ILE:HD13	1:I:194:LEU:HD12	2.00	0.42
1:M:7:ARG:HG3	1:M:7:ARG:O	2.19	0.42
1:E:384:TYR:HA	1:E:385:PRO:HD3	1.83	0.42
1:A:394:MET:SD	1:A:421:ALA:HB1	2.59	0.42
2:N:612:G:C5'	2:N:613:A:OP1	2.67	0.42
1:M:162:LEU:HD11	1:M:403:TRP:CD1	2.54	0.42
1:E:297:ASN:HB3	1:E:327:GLY:HA2	2.00	0.42
1:M:142:GLN:OE1	1:M:142:GLN:HA	2.19	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
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: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
3:C:693:G:H2'	3:C:694:A:H8	1.85	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:E:120:TYR:HB3	1:E:125:LYS:HB3	2.01	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
3:C:701:A:H2'	3:C:702:C:O4'	2.19	0.42
1:I:275:TYR:CE2	1:I:276:LYS:HE2	2.53	0.42
1:A:320:HIS:O	1:A:335:PRO:HD3	2.20	0.42
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.87	0.42
1:A:413:HIS:CD2	3:C:698:G:H4'	2.55	0.42
1:A:269:ASN:ND2	10:A:552:HOH:O	2.49	0.42
1:M:7:ARG:HD3	1:M:11:GLU:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:604:C:H2'	2:J:605:U:O4'	2.19	0.42
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
3:C:690:C:H6	3:C:690:C:C5'	2.32	0.41
2:B:609:C:C2'	2:B:610:C:H5'	2.49	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:I:397:ILE:CD1	1:I:421:ALA:HB2	2.46	0.41
1:A:449:GLU:O	1:A:450:TYR:C	2.57	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
2:B:605:U:H5	10:B:492:HOH:O	2.03	0.41
1:M:383:LYS:HB3	1:M:384:TYR:CD1	2.56	0.41
1:A:35:GLU:O	1:A:402:ARG:HD2	2.20	0.41
1:I:82:ALA:O	1:I:86:MET:HG2	2.20	0.41
1:A:4:GLN:HG2	1:A:283:LYS:HE3	2.02	0.41
1:M:318:LEU:HA	1:M:318:LEU:HD23	1.74	0.41
1:M:140:GLU:HG3	1:M:140:GLU:O	2.18	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: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:M:447:LEU:HD23	1:M:447:LEU:N	2.34	0.41
3:G:693:G:H2'	3:G:694:A:H8	1.85	0.41
1:A:218:TRP:O	1:A:222:PRO:HD3	2.21	0.41
1:A:97:LEU:O	1:A:101:MET:HG3	2.21	0.41
2:B:598:A:C3'	2:B:599:G:H5'	2.46	0.41
1:I:11:GLU:C	1:I:12:VAL:HG23	2.41	0.41
1:I:7:ARG:HD3	1:I:11:GLU:HG2	2.02	0.41
1:A:384:TYR:HA	1:A:385:PRO:HD3	1.82	0.41
1:I:118:TYR:CG	1:I:119:PRO:HA	2.55	0.41
1:A:306:ARG:CG	1:A:318:LEU:HD13	2.51	0.41
1:E:50:LEU:HD21	1:E:171:GLY:HA3	2.03	0.41
1:M:321:LEU:HD12	1:M:322:LYS:N	2.35	0.41
1:A:381:ASP:OD1	8:A:6027:IPA:H2	2.21	0.41
1:A:55:GLU:O	1:A:59:PHE:HD2	2.03	0.41
1:M:275:TYR:O	1:M:276:LYS:CB	2.69	0.41
1:E:27:PRO:HB3	1:E:31:HIS:CE1	2.55	0.41
1:I:275:TYR:CD2	1:I:275:TYR:O	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:604:C:H2'	2:N:605:U:C6	2.55	0.41
2:J:604:C:H2'	2:J:605:U:C6	2.56	0.41
1:E:52:THR:HG23	1:E:53:ASP:N	2.35	0.41
1:E:411:GLN:HE22	1:E:446:ASP:H	1.69	0.41
3:O:692:G:O2'	3:O:693:G:H5'	2.21	0.41
3:K:694:A:H2'	3:K:695:C:C6	2.56	0.41
1:A:305:ILE:HD11	1:A:330:VAL:HG11	2.03	0.41
1:M:82:ALA:O	1:M:86:MET:HG2	2.21	0.41
1:I:228:LYS:O	1:I:333:SER:HB2	2.21	0.41
1:E:295:ILE:HG12	10:E:507:HOH:O	2.21	0.41
1:E:226:GLU:HG3	1:E:320:HIS:O	2.21	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:E:213:ASP:HB3	8:E:6014:IPA:C1	2.50	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
2:N:604:C:H2'	2:N:605:U:O4'	2.21	0.41
1:M:432:PHE:CZ	1:M:436:ILE:HD11	2.55	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:223:VAL:HG23	1:E:223:VAL:O	2.21	0.41
1:M:226:GLU:HG3	1:M:320:HIS:O	2.20	0.40
1:I:270:HIS:NE2	1:I:283:LYS:HE2	2.36	0.40
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:E:212:CYS:HB2	8:E:6014:IPA:C3	2.51	0.40
1:M:11:GLU:C	1:M:12:VAL:HG23	2.42	0.40
1:A:254:GLU:HG2	1:A:259:GLY:HA2	2.02	0.40
1:I:318:LEU:HA	1:I:318:LEU:HD23	1.75	0.40
1:A:382:GLU:HB2	8:A:6027:IPA:H33	2.03	0.40
1:E:237:TYR:CG	1:E:328:ASP:HB3	2.56	0.40
1:A:95:MET:HE3	1:A:95:MET:HB2	1.94	0.40
1:I:162:LEU:HD11	1:I:403:TRP:CD1	2.56	0.40
2:F:610:C:C2'	2:F:611:G:O5'	2.69	0.40
1:M:448:PRO:HG2	1:M:453:LEU:HD21	2.02	0.40
1:A:179:SER:HB2	1:A:290:CYS:HA	2.02	0.40
1:A:20:PRO:HA	2:B:598:A:N1	2.36	0.40
1:I:375:LYS:HD3	1:I:396:GLU:OE1	2.21	0.40
1:E:334:TYR:CD2	1:E:335:PRO:HD2	2.55	0.40
1:M:67:ILE:HG23	1:M:244:ALA:HB3	2.04	0.40
1:M:270:HIS:NE2	1:M:283:LYS:HE2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:VAL:HG11	1:E:251:MET:HE3	2.03	0.40
1:A:58:ILE:HD11	1:A:59:PHE:CE2	2.57	0.40
1:E:61:LYS:HD2	1:E:239:ALA:CB	2.51	0.40
3:G:693:G:H2'	3:G:694:A:C8	2.57	0.40
1:A:214:PRO:O	1:A:390:PRO:HG3	2.22	0.40
1:E:121:VAL:CG1	1:E:122:ALA:N	2.85	0.40
1:E:449:GLU:O	1:E:450:TYR:C	2.59	0.40
1:E:367:THR:C	1:E:369:GLU:H	2.25	0.40
1:M:334:TYR:CD1	1:M:335:PRO:CD	3.04	0.40
1:I:321:LEU:HD12	1:I:322:LYS:N	2.36	0.40
1:I:275:TYR:O	1:I:276:LYS:HB3	2.22	0.40
1:I:355:THR:HB	1:I:356:PRO:HD3	2.03	0.40
1:I:334:TYR:CD1	1:I:335:PRO:CD	3.05	0.40
1:I:383:LYS:HB3	1:I:384:TYR:CD1	2.57	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
1:I:411:GLN:HB3	10:I:546:HOH:O	2.22	0.40
1:I:337:GLU:C	1:I:337:GLU:OE2	2.60	0.40
1:E:145:LEU:HD23	1:E:145:LEU:HA	1.90	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%)	39	72
1	E	459/471 (98%)	432 (94%)	25 (5%)	2 (0%)	39	72
1	I	459/471 (98%)	406 (88%)	45 (10%)	8 (2%)	11	32
1	M	459/471 (98%)	407 (89%)	44 (10%)	8 (2%)	11	32
All	All	1836/1884 (98%)	1679 (91%)	137 (8%)	20 (1%)	17	46

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 ⓘ

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%)	13	32
1	E	403/412 (98%)	369 (92%)	34 (8%)	14	34
1	I	403/412 (98%)	369 (92%)	34 (8%)	14	34
1	M	403/412 (98%)	369 (92%)	34 (8%)	14	34
All	All	1612/1648 (98%)	1475 (92%)	137 (8%)	13	34

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

Some 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 ⓘ

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
7	POP	A	5004	6	8,8,8	0.72	0	13,13,13	1.51	2 (15%)
8	IPA	A	6009	-	3,3,3	0.66	0	3,3,3	0.22	0
8	IPA	A	6011	-	3,3,3	0.54	0	3,3,3	0.37	0
8	IPA	A	6027	-	3,3,3	0.63	0	3,3,3	0.15	0
8	IPA	A	6028	-	3,3,3	0.66	0	3,3,3	0.26	0
8	IPA	A	6030	-	3,3,3	0.53	0	3,3,3	0.49	0
9	GOL	A	8012	-	5,5,5	0.35	0	5,5,5	0.39	0
8	IPA	E	6014	-	3,3,3	0.43	0	3,3,3	0.62	0
8	IPA	E	6029	-	3,3,3	0.56	0	3,3,3	0.23	0
9	GOL	E	8011	5	5,5,5	0.28	0	5,5,5	0.36	0
7	POP	G	5003	6	8,8,8	0.63	0	13,13,13	1.11	0
7	POP	I	5002	6	8,8,8	0.59	0	13,13,13	1.69	1 (7%)
9	GOL	J	8005	-	5,5,5	0.40	0	5,5,5	0.88	0
8	IPA	M	6018	-	3,3,3	0.63	0	3,3,3	0.25	0
8	IPA	M	6019	-	3,3,3	0.54	0	3,3,3	0.39	0
9	GOL	N	8010	-	5,5,5	0.36	0	5,5,5	0.88	0
7	POP	O	5001	6	8,8,8	0.56	0	13,13,13	0.95	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	A	5004	6	-	0/6/6/6	0/0/0/0
8	IPA	A	6009	-	-	0/0/0/0	0/0/0/0
8	IPA	A	6011	-	-	0/0/0/0	0/0/0/0
8	IPA	A	6027	-	-	0/0/0/0	0/0/0/0
8	IPA	A	6028	-	-	0/0/0/0	0/0/0/0
8	IPA	A	6030	-	-	0/0/0/0	0/0/0/0
9	GOL	A	8012	-	-	0/4/4/4	0/0/0/0
8	IPA	E	6014	-	-	0/0/0/0	0/0/0/0
8	IPA	E	6029	-	-	0/0/0/0	0/0/0/0
9	GOL	E	8011	5	-	0/4/4/4	0/0/0/0
7	POP	G	5003	6	-	0/6/6/6	0/0/0/0
7	POP	I	5002	6	-	0/6/6/6	0/0/0/0
9	GOL	J	8005	-	-	0/4/4/4	0/0/0/0
8	IPA	M	6018	-	-	0/0/0/0	0/0/0/0
8	IPA	M	6019	-	-	0/0/0/0	0/0/0/0
9	GOL	N	8010	-	-	0/4/4/4	0/0/0/0
7	POP	O	5001	6	-	0/6/6/6	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	5002	POP	P2-O-P1	-5.61	116.98	132.73
7	A	5004	POP	P2-O-P1	-3.30	123.46	132.73
7	A	5004	POP	O-P1-O1	2.45	115.33	107.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 34 short contacts:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	6018	IPA	1	0
8	M	6019	IPA	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.71	52 (11%) 7 4	37, 61, 92, 111	0
1	E	461/471 (97%)	0.67	47 (10%) 9 5	39, 60, 93, 110	0
1	I	461/471 (97%)	0.81	62 (13%) 4 3	40, 68, 115, 143	0
1	M	461/471 (97%)	0.84	72 (15%) 3 2	38, 68, 115, 143	0
2	B	17/26 (65%)	1.16	4 (23%) 1 1	47, 62, 135, 164	0
2	F	17/26 (65%)	1.46	4 (23%) 1 1	47, 62, 134, 164	0
2	J	17/26 (65%)	1.89	5 (29%) 1 0	53, 75, 166, 182	0
2	N	17/26 (65%)	1.68	5 (29%) 1 0	51, 76, 166, 182	0
3	C	15/15 (100%)	2.01	4 (26%) 1 0	49, 65, 124, 141	0
3	G	15/15 (100%)	2.23	5 (33%) 0 0	49, 65, 124, 141	0
3	K	15/15 (100%)	2.79	6 (40%) 0 0	52, 83, 145, 149	0
3	O	15/15 (100%)	2.55	4 (26%) 1 0	52, 84, 145, 149	0
4	D	3/9 (33%)	7.97	3 (100%) 0 0	168, 168, 172, 173	0
4	H	3/9 (33%)	9.56	3 (100%) 0 0	168, 168, 172, 173	0
4	L	4/9 (44%)	7.63	4 (100%) 0 0	146, 152, 157, 173	0
4	P	4/9 (44%)	8.67	4 (100%) 0 0	146, 152, 158, 173	0
All	All	1986/2084 (95%)	0.89	284 (14%) 4 2	37, 64, 114, 182	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	805	G	11.3
4	L	808	G	10.8
4	P	805	G	10.5
3	K	688	G	9.9
4	P	808	G	9.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	689	C	9.6
4	D	806	G	9.5
3	O	688	G	9.4
4	H	807	A	9.3
1	M	16	ILE	8.2
4	L	807	A	8.2
4	H	806	G	8.1
4	P	807	A	8.0
4	D	807	A	7.6
1	I	342	LEU	7.4
1	I	46	ASN	7.3
2	J	597	C	7.3
2	N	597	C	7.3
3	C	688	G	7.2
4	L	806	G	7.2
3	O	689	C	7.1
3	G	689	C	6.9
3	G	688	G	6.9
1	I	357	ALA	6.8
4	D	805	G	6.7
3	C	689	C	6.6
4	P	806	G	6.3
1	A	19	ALA	6.0
2	J	613	A	6.0
1	M	342	LEU	5.8
1	M	277	ASN	5.8
1	E	16	ILE	5.7
1	M	46	ASN	5.7
1	E	326	TYR	5.6
1	M	169	GLU	5.4
1	A	32	TYR	5.3
1	A	320	HIS	5.2
1	I	16	ILE	5.1
1	E	32	TYR	5.0
1	M	9	SER	5.0
1	I	363	PHE	5.0
1	A	326	TYR	5.0
1	M	134	GLN	4.9
1	M	356	PRO	4.9
1	E	49	ARG	4.8
1	M	32	TYR	4.7
1	M	166	THR	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	165	LYS	4.6
1	E	210	VAL	4.6
1	M	137	ASP	4.6
1	I	15	PRO	4.5
1	E	325	ALA	4.4
1	I	277	ASN	4.4
1	M	209	ALA	4.4
4	L	805	G	4.4
1	A	46	ASN	4.4
1	M	326	TYR	4.4
1	M	325	ALA	4.3
1	M	31	HIS	4.2
1	M	170	GLN	4.2
1	E	46	ASN	4.2
2	B	597	C	4.2
1	I	89	ASP	4.1
1	M	315	GLY	4.1
1	I	18	ASN	4.1
3	K	690	C	4.1
1	A	325	ALA	4.1
1	I	10	LYS	4.1
1	M	168	VAL	4.1
3	O	690	C	4.1
1	E	283	LYS	4.1
1	I	28	SER	4.0
1	A	210	VAL	4.0
1	E	295	ILE	4.0
1	M	52	THR	4.0
1	I	293	THR	4.0
1	M	212	CYS	4.0
1	E	17	ILE	4.0
1	A	52	THR	4.0
2	F	597	C	3.9
1	A	134	GLN	3.9
1	I	294	SER	3.9
1	A	295	ILE	3.9
1	M	17	ILE	3.9
1	M	211	GLY	3.9
1	I	47	ASP	3.8
1	M	357	ALA	3.8
1	E	211	GLY	3.8
3	G	690	C	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	32	TYR	3.8
1	I	276	LYS	3.8
1	I	356	PRO	3.8
2	F	603	U	3.7
1	I	325	ALA	3.7
1	I	1	GLY	3.7
1	E	294	SER	3.6
1	I	297	ASN	3.6
1	M	65	ASN	3.6
1	E	233	ASP	3.6
1	I	27	PRO	3.6
1	E	166	THR	3.6
1	M	8	PRO	3.6
1	M	293	THR	3.6
1	A	18	ASN	3.5
1	M	324	ILE	3.4
1	I	171	GLY	3.4
1	A	324	ILE	3.4
3	O	691	C	3.4
3	G	691	C	3.4
1	M	294	SER	3.4
1	E	361	ALA	3.4
1	M	22	LYS	3.4
1	A	33	VAL	3.4
1	M	295	ILE	3.3
1	I	278	LYS	3.3
1	M	44	THR	3.3
1	E	320	HIS	3.3
1	I	134	GLN	3.3
1	M	363	PHE	3.3
1	E	324	ILE	3.3
1	I	286	MET	3.3
1	A	139	LYS	3.3
1	E	170	GLN	3.3
1	A	211	GLY	3.2
1	I	324	ILE	3.2
1	A	64	GLY	3.2
1	A	209	ALA	3.2
1	M	38	LYS	3.2
2	N	612	G	3.2
1	I	295	ILE	3.1
1	A	208	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	134	GLN	3.1
1	A	342	LEU	3.1
1	I	212	CYS	3.1
1	I	52	THR	3.1
1	I	406	ASP	3.1
1	E	342	LEU	3.1
1	I	292	GLY	3.1
1	E	237	TYR	3.1
1	M	83	GLY	3.0
1	M	138	THR	3.0
1	E	288	SER	3.0
2	N	613	A	3.0
1	M	50	LEU	3.0
1	A	455	ARG	3.0
1	M	345	GLN	2.9
1	I	208	SER	2.9
2	B	598	A	2.9
2	F	612	G	2.9
1	E	22	LYS	2.9
1	E	52	THR	2.9
1	M	373	PHE	2.9
2	F	602	C	2.9
1	A	297	ASN	2.9
3	K	693	G	2.8
1	A	456	ARG	2.8
1	I	326	TYR	2.8
3	K	694	A	2.8
1	I	209	ALA	2.8
1	A	49	ARG	2.8
1	M	460	SER	2.8
1	I	211	GLY	2.8
1	A	51	LYS	2.8
1	M	297	ASN	2.8
1	M	51	LYS	2.8
2	J	609	C	2.8
1	A	203	GLY	2.8
3	K	692	G	2.8
1	I	9	SER	2.7
1	A	12	VAL	2.7
1	A	296	PHE	2.7
1	M	23	THR	2.7
1	M	208	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	209	ALA	2.7
1	E	296	PHE	2.7
1	A	35	GLU	2.7
1	I	124	GLY	2.7
2	J	612	G	2.7
1	A	176	ILE	2.7
1	M	267	TYR	2.7
1	I	335	PRO	2.6
1	I	144	LEU	2.6
1	A	294	SER	2.6
1	A	6	MET	2.6
1	I	169	GLU	2.6
1	A	286	MET	2.6
1	E	275	TYR	2.6
1	E	290	CYS	2.6
1	M	67	ILE	2.6
1	E	138	THR	2.5
1	E	327	GLY	2.5
2	J	598	A	2.5
1	I	355	THR	2.5
1	I	336	HIS	2.5
1	M	364	GLU	2.5
1	E	313	TYR	2.5
1	E	373	PHE	2.5
1	E	70	VAL	2.5
1	I	75	LYS	2.5
1	E	72	GLU	2.5
2	N	603	U	2.5
1	I	19	ALA	2.4
1	I	45	LYS	2.4
1	M	47	ASP	2.4
1	I	383	LYS	2.4
1	E	317	ASP	2.4
1	A	287	PRO	2.4
1	A	16	ILE	2.4
1	A	129	ASP	2.4
1	E	297	ASN	2.4
2	N	611	G	2.4
1	E	284	GLY	2.4
1	M	45	LYS	2.4
1	M	28	SER	2.4
1	A	25	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	176	ILE	2.4
1	M	290	CYS	2.4
1	E	383	LYS	2.4
1	I	314	LYS	2.4
1	I	364	GLU	2.4
1	A	359	LYS	2.4
1	M	355	THR	2.4
1	M	276	LYS	2.3
1	M	405	LYS	2.3
1	M	43	LEU	2.3
1	M	359	LYS	2.3
1	M	2	GLU	2.3
1	M	284	GLY	2.3
1	A	313	TYR	2.3
1	A	254	GLU	2.3
1	I	320	HIS	2.3
1	I	310	LEU	2.3
1	M	358	ASP	2.3
2	B	602	C	2.3
1	A	329	ASP	2.3
1	A	48	PRO	2.2
1	I	373	PHE	2.2
1	A	288	SER	2.2
1	E	51	LYS	2.2
1	A	45	LYS	2.2
1	E	13	GLY	2.2
1	I	175	LEU	2.2
1	A	221	ILE	2.2
3	G	700	G	2.2
3	C	690	C	2.2
2	B	603	U	2.2
1	A	276	LYS	2.2
3	C	691	C	2.2
1	E	165	LYS	2.2
1	E	336	HIS	2.2
1	M	288	SER	2.2
1	A	237	TYR	2.2
1	A	290	CYS	2.2
1	A	300	ILE	2.1
1	I	267	TYR	2.1
1	A	361	ALA	2.1
1	E	239	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	286	MET	2.1
1	E	208	SER	2.1
1	A	53	ASP	2.1
1	M	361	ALA	2.1
1	M	1	GLY	2.1
1	I	301	ASN	2.1
1	M	314	LYS	2.1
1	E	374	LEU	2.1
1	I	298	SER	2.1
1	I	327	GLY	2.1
1	E	315	GLY	2.1
1	M	383	LYS	2.1
1	E	35	GLU	2.0
1	M	279	THR	2.0
1	I	20	PRO	2.0
1	I	455	ARG	2.0
1	I	263	ASP	2.0
1	I	412	ASP	2.0
1	M	289	GLY	2.0
1	M	35	GLU	2.0
1	M	210	VAL	2.0
1	A	373	PHE	2.0
1	A	374	LEU	2.0
1	I	313	TYR	2.0
1	M	237	TYR	2.0
1	M	70	VAL	2.0
1	M	317	ASP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
8	IPA	A	6009	4/4	0.89	0.66	7.16	64,72,75,78	0
9	GOL	J	8005	6/6	0.91	0.56	5.92	47,55,64,73	0
8	IPA	A	6028	4/4	0.79	0.35	4.55	60,80,87,112	0
8	IPA	E	6029	4/4	0.79	0.45	3.95	67,75,80,84	0
7	POP	I	5002	9/9	0.77	0.45	3.84	97,119,129,136	9
8	IPA	A	6030	4/4	0.88	0.35	2.95	68,73,76,78	0
7	POP	G	5003	9/9	0.68	0.46	2.66	47,60,88,89	9
7	POP	A	5004	9/9	0.74	0.43	2.61	45,77,111,115	9
9	GOL	N	8010	6/6	0.92	0.54	2.50	55,71,72,86	0
8	IPA	E	6014	4/4	0.91	0.45	2.14	53,58,75,75	0
7	POP	O	5001	9/9	0.81	0.36	1.70	41,73,93,98	9
8	IPA	M	6018	4/4	0.91	0.38	0.97	47,52,58,72	0
8	IPA	M	6019	4/4	0.66	0.30	0.46	80,96,100,105	0
8	IPA	A	6027	4/4	0.76	0.21	-0.25	84,91,95,98	0
5	ZN	E	2003	1/1	0.97	0.14	-0.86	88,88,88,88	1
6	MN	A	3007	1/1	0.82	0.16	-1.37	91,91,91,91	0
6	MN	M	3002	1/1	0.98	0.12	-1.83	86,86,86,86	0
6	MN	E	3005	1/1	0.76	0.13	-2.13	87,87,87,87	0
6	MN	I	3003	1/1	0.94	0.17	-3.34	120,120,120,120	0
6	MN	M	3001	1/1	0.92	0.09	-4.53	127,127,127,127	0
9	GOL	A	8012	6/6	0.86	0.19	-	71,86,94,98	0
8	IPA	A	6011	4/4	0.74	0.58	-	65,88,92,106	0
6	MN	I	3004	1/1	0.96	0.22	-	90,90,90,90	0
5	ZN	M	2001	1/1	0.88	0.18	-	70,70,70,70	1
6	MN	A	3008	1/1	0.97	0.10	-	74,74,74,74	0
5	ZN	A	2004	1/1	0.96	0.10	-	81,81,81,81	1
9	GOL	E	8011	6/6	0.76	0.15	-	69,82,89,94	0
6	MN	E	3006	1/1	0.98	0.09	-	74,74,74,74	0
5	ZN	I	2002	1/1	0.92	0.16	-	70,70,70,70	1

6.5 Other polymers ⓘ

There are no such residues in this entry.