



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 07:29 PM EST

PDB ID : 1RXS  
Title : E. coli uridine phosphorylase: 2'-deoxyuridine phosphate complex  
Authors : Caradoc-Davies, T.T.; Cutfield, S.M.; Lamont, I.L.; Cutfield, J.F.  
Deposited on : 2003-12-18  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

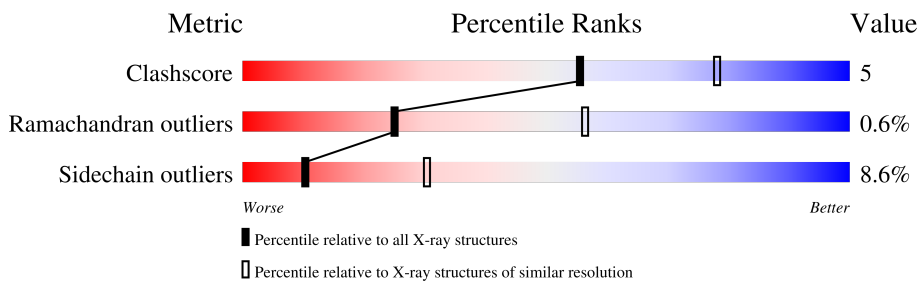
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)














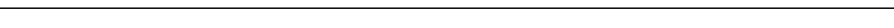








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	253	
1	B	253	
1	C	253	
1	D	253	
1	E	253	
1	F	253	
1	G	253	
1	H	253	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	253	 81% 13% . .
1	J	253	 81% 13% . .
1	K	253	 82% 13% . .
1	L	253	 77% 19% . .
1	M	253	 81% 11% . .
1	N	253	 81% 15% . .
1	O	253	 81% 14% . .
1	P	253	 80% 13% . .
1	Q	253	 81% 14% . .
1	R	253	 80% 16% . .
1	a	253	 87% 8% .
1	b	253	 86% 9% .
1	c	253	 86% 9% .
1	d	253	 89% 9% .
1	e	253	 86% 9% .
1	h	253	 86% 9% .
1	i	253	 86% 11% .
1	j	253	 86% 9% .
1	k	253	 87% 9% .
1	l	253	 87% 9% .
1	m	253	 89% 9% .
1	o	253	 89% 10% .

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
4	PO4	P	3121	-	-	X	-
5	DUR	B	2012	X	-	-	-
5	DUR	C	2022	X	-	-	-
5	DUR	D	2032	X	-	-	-
5	DUR	E	2042	X	-	-	-
5	DUR	F	2052	X	-	-	-
5	DUR	G	3052	X	-	-	-
5	DUR	H	2062	X	-	-	-
5	DUR	I	3072	X	-	-	-
5	DUR	J	2082	X	-	-	-
5	DUR	K	2092	X	-	-	-
5	DUR	M	3112	X	-	-	-
5	DUR	N	2102	X	-	-	-
5	DUR	O	2112	X	-	-	-
5	DUR	P	3122	X	-	-	-
5	DUR	Q	2122	X	-	-	-
5	DUR	R	2132	X	-	-	-
5	DUR	a	3012	X	-	-	-
5	DUR	b	3022	X	-	-	-
5	DUR	c	3032	X	-	-	-
5	DUR	e	3042	X	-	-	-
5	DUR	h	3062	X	-	-	-
5	DUR	i	2072	X	-	-	-
5	DUR	j	3082	X	-	-	-
5	DUR	k	3092	X	-	-	-
5	DUR	l	3102	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 57608 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	Total 1880	C 1178	N 328	O 363	S 11	0	0	0
1	a	242	Total 1817	C 1141	N 318	O 348	S 10	0	0	0
1	B	246	Total 1851	C 1162	N 323	O 355	S 11	0	0	0
1	b	242	Total 1817	C 1141	N 318	O 348	S 10	0	0	0
1	C	246	Total 1851	C 1162	N 323	O 355	S 11	0	0	0
1	c	242	Total 1817	C 1141	N 318	O 348	S 10	0	0	0
1	D	246	Total 1851	C 1162	N 323	O 355	S 11	0	0	0
1	d	250	Total 1880	C 1178	N 328	O 363	S 11	0	0	0
1	E	246	Total 1851	C 1162	N 323	O 355	S 11	0	0	0
1	e	242	Total 1817	C 1141	N 318	O 348	S 10	0	0	0
1	F	246	Total 1851	C 1162	N 323	O 355	S 11	0	0	0
1	R	246	Total 1851	C 1162	N 323	O 355	S 11	0	0	0
1	G	242	Total 1817	C 1141	N 318	O 348	S 10	0	0	0
1	P	242	Total 1817	C 1141	N 318	O 348	S 10	0	0	0
1	H	246	Total 1851	C 1162	N 323	O 355	S 11	0	0	0
1	h	242	Total 1817	C 1141	N 318	O 348	S 10	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	i	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	J	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	j	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	K	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	k	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	L	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	l	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	M	242	Total	C	N	O	S	0	0	0
			1817	1141	318	348	10			
1	m	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	N	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	Q	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	O	246	Total	C	N	O	S	0	0	0
			1851	1162	323	355	11			
1	o	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

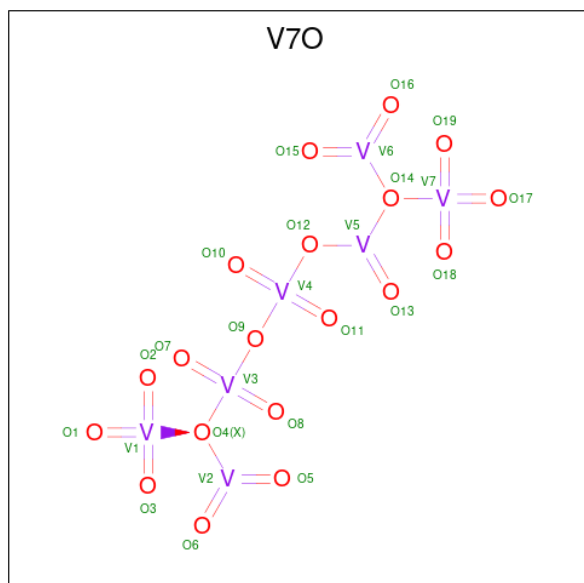
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	1	Total K 1 1	0	0
2	G	1	Total K 1 1	0	0
2	h	1	Total K 1 1	0	0
2	i	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	K	1	Total K 1 1	0	0
2	L	1	Total K 1 1	0	0
2	M	1	Total K 1 1	0	0
2	N	1	Total K 1 1	0	0
2	o	1	Total K 1 1	0	0

- Molecule 3 is META VANADATE (three-letter code: V7O) (formula:  $O_{19}V_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O V 11 8 3	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	V	0	0
			11	8	3		
3	b	1	Total	O	V	0	0
			11	8	3		
3	c	1	Total	O	V	0	0
			11	8	3		
3	D	1	Total	O	V	0	0
			11	8	3		
3	D	1	Total	O	V	0	0
			11	8	3		
3	e	1	Total	O	V	0	0
			11	8	3		
3	R	1	Total	O	V	0	0
			11	8	3		
3	H	1	Total	O	V	0	0
			11	8	3		
3	h	1	Total	O	V	0	0
			11	8	3		
3	I	1	Total	O	V	0	0
			11	8	3		
3	i	1	Total	O	V	0	0
			11	8	3		
3	J	1	Total	O	V	0	0
			11	8	3		
3	j	1	Total	O	V	0	0
			11	8	3		
3	k	1	Total	O	V	0	0
			11	8	3		
3	L	1	Total	O	V	0	0
			11	8	3		
3	M	1	Total	O	V	0	0
			11	8	3		
3	M	1	Total	O	V	0	0
			11	8	3		
3	Q	1	Total	O	V	0	0
			11	8	3		
3	o	1	Total	O	V	0	0
			11	8	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





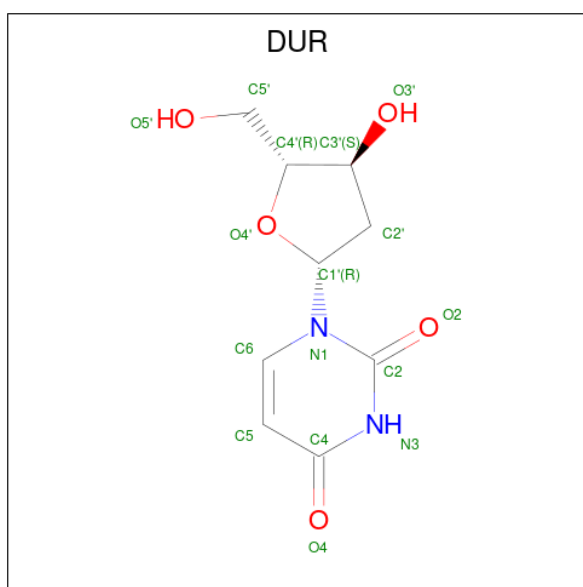
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	a	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	b	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	c	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	e	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	R	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	P	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0
4	h	1	Total O P 5 4 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	O	P	0	0
			5	4	1		
4	i	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	j	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		
4	k	1	Total	O	P	0	0
			5	4	1		
4	l	1	Total	O	P	0	0
			5	4	1		
4	M	1	Total	O	P	0	0
			5	4	1		
4	N	1	Total	O	P	0	0
			5	4	1		
4	Q	1	Total	O	P	0	0
			5	4	1		
4	O	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 2'-DEOXYURIDINE (three-letter code: DUR) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	a	1	Total 16	C 9	N 2	O 5	0	0
5	B	1	Total 16	C 9	N 2	O 5	0	0
5	b	1	Total 16	C 9	N 2	O 5	0	0
5	C	1	Total 16	C 9	N 2	O 5	0	0
5	c	1	Total 16	C 9	N 2	O 5	0	0
5	D	1	Total 16	C 9	N 2	O 5	0	0
5	E	1	Total 16	C 9	N 2	O 5	0	0
5	e	1	Total 16	C 9	N 2	O 5	0	0
5	F	1	Total 16	C 9	N 2	O 5	0	0
5	R	1	Total 16	C 9	N 2	O 5	0	0
5	G	1	Total 16	C 9	N 2	O 5	0	0
5	P	1	Total 16	C 9	N 2	O 5	0	0
5	H	1	Total 16	C 9	N 2	O 5	0	0
5	h	1	Total 16	C 9	N 2	O 5	0	0
5	I	1	Total 16	C 9	N 2	O 5	0	0
5	i	1	Total 16	C 9	N 2	O 5	0	0
5	J	1	Total 16	C 9	N 2	O 5	0	0
5	j	1	Total 16	C 9	N 2	O 5	0	0
5	K	1	Total 16	C 9	N 2	O 5	0	0
5	k	1	Total 16	C 9	N 2	O 5	0	0
5	l	1	Total 16	C 9	N 2	O 5	0	0
5	M	1	Total 16	C 9	N 2	O 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	N	O	0	0
			16	9	2	5		
5	Q	1	Total	C	N	O	0	0
			16	9	2	5		
5	O	1	Total	C	N	O	0	0
			16	9	2	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	a	52	Total	O	0	0
			52	52		
6	B	55	Total	O	0	0
			55	55		
6	b	48	Total	O	0	0
			48	48		
6	C	52	Total	O	0	0
			52	52		
6	c	54	Total	O	0	0
			54	54		
6	D	52	Total	O	0	0
			52	52		
6	d	56	Total	O	0	0
			56	56		
6	E	51	Total	O	0	0
			51	51		
6	e	49	Total	O	0	0
			49	49		
6	F	59	Total	O	0	0
			59	59		
6	R	52	Total	O	0	0
			52	52		
6	G	46	Total	O	0	0
			46	46		
6	P	51	Total	O	0	0
			51	51		
6	H	51	Total	O	0	0
			51	51		
6	h	55	Total	O	0	0
			55	55		

*Continued on next page...*

*Continued from previous page...*


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	51	Total O 51 51	0	0
6	i	56	Total O 56 56	0	0
6	J	52	Total O 52 52	0	0
6	j	51	Total O 51 51	0	0
6	K	50	Total O 50 50	0	0
6	k	53	Total O 53 53	0	0
6	L	58	Total O 58 58	0	0
6	l	51	Total O 51 51	0	0
6	M	48	Total O 48 48	0	0
6	m	53	Total O 53 53	0	0
6	N	58	Total O 58 58	0	0
6	Q	50	Total O 50 50	0	0
6	O	56	Total O 56 56	0	0
6	o	57	Total O 57 57	0	0

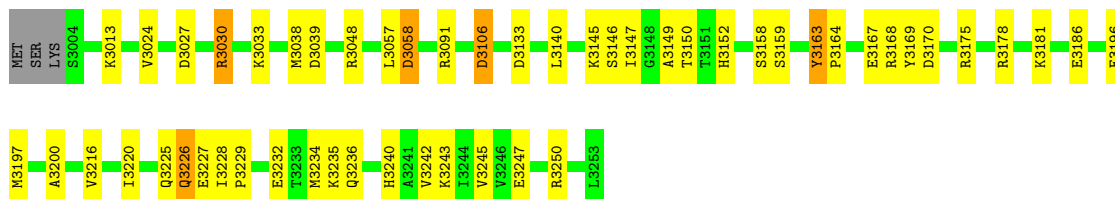
### 3 Residue-property plots [i](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


Note EDS failed to run properly.

- Molecule 1: Uridine phosphorylase

Chain A:  78% 19% ..




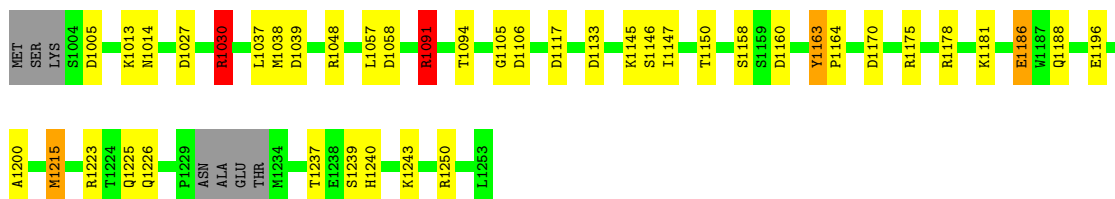
- Molecule 1: Uridine phosphorylase

Chain a:  87% 8% .




- Molecule 1: Uridine phosphorylase

Chain B:  81% 15% ..



- Molecule 1: Uridine phosphorylase

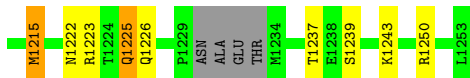
Chain b:  86% 9% .





- Molecule 1: Uridine phosphorylase

Chain C: 80% 15% ..



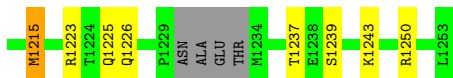
- Molecule 1: Uridine phosphorylase

Chain c: 86% 9% .



- Molecule 1: Uridine phosphorylase

Chain D: 81% 14% ..



- Molecule 1: Uridine phosphorylase

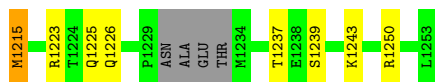
Chain d: 89% 9% .



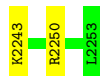
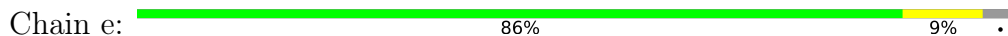
- Molecule 1: Uridine phosphorylase

Chain E: 81% 14% ..

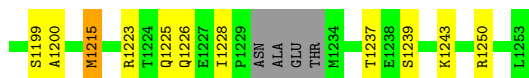
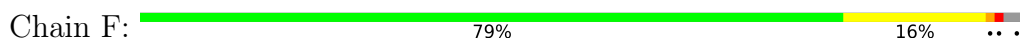




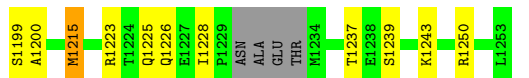
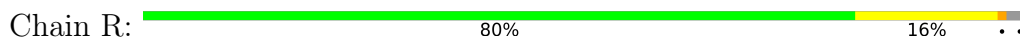
• Molecule 1: Uridine phosphorylase



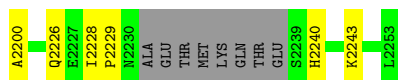
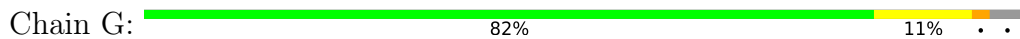
• Molecule 1: Uridine phosphorylase



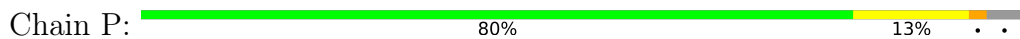
• Molecule 1: Uridine phosphorylase



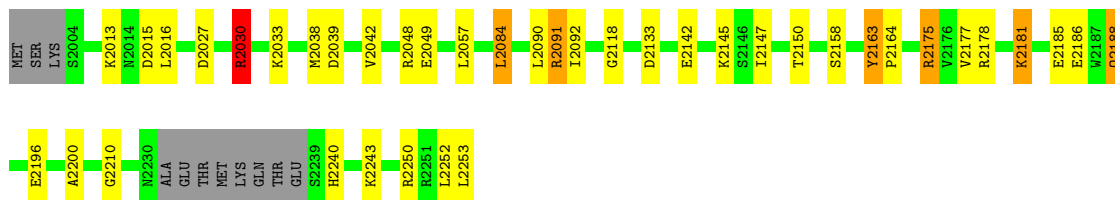
• Molecule 1: Uridine phosphorylase



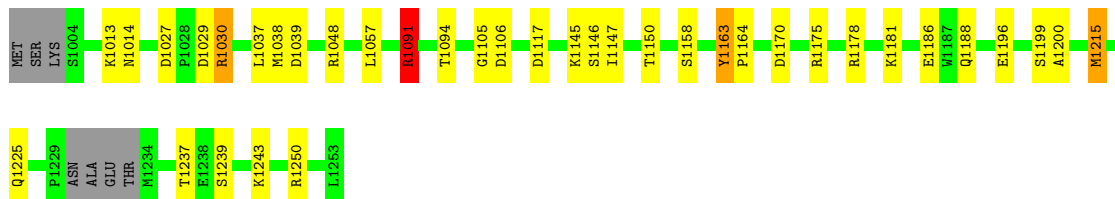
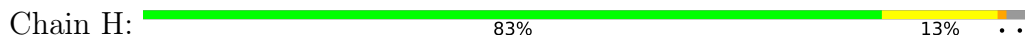
• Molecule 1: Uridine phosphorylase



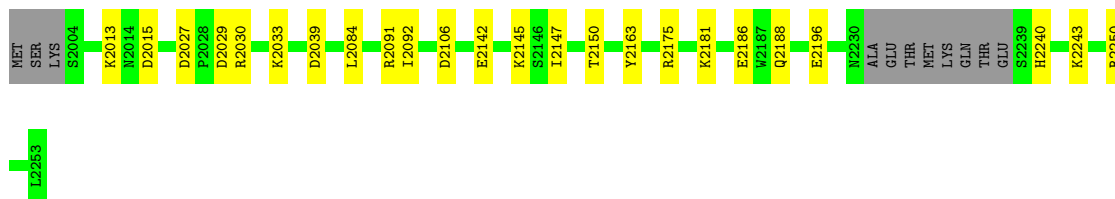




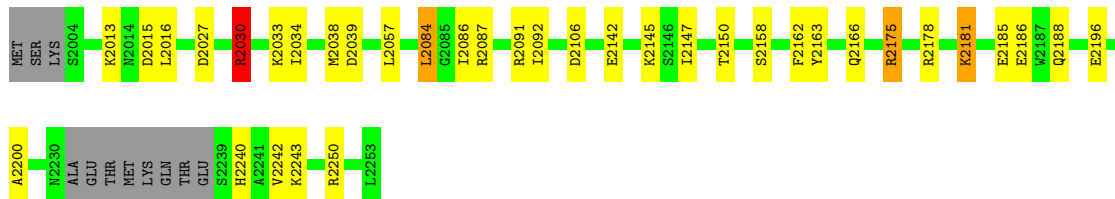
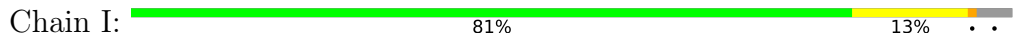
• Molecule 1: Uridine phosphorylase



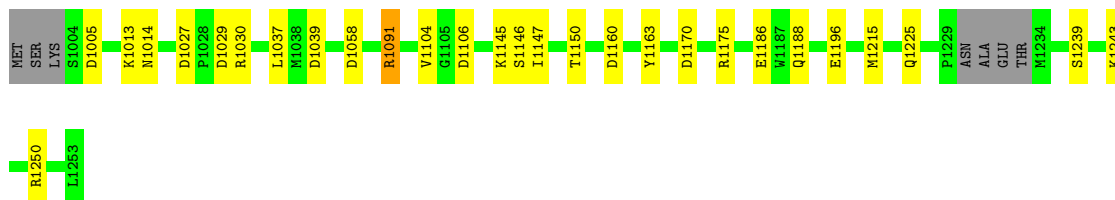
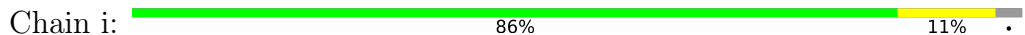
• Molecule 1: Uridine phosphorylase




• Molecule 1: Uridine phosphorylase

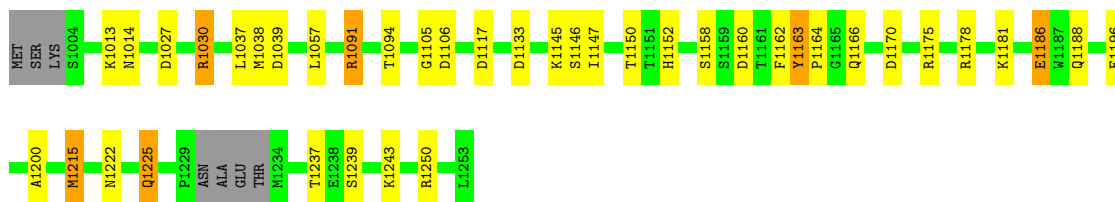


• Molecule 1: Uridine phosphorylase




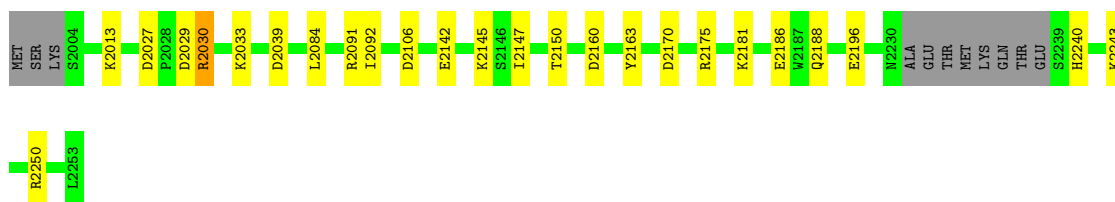
• Molecule 1: Uridine phosphorylase

Chain J:  81% 13% ..




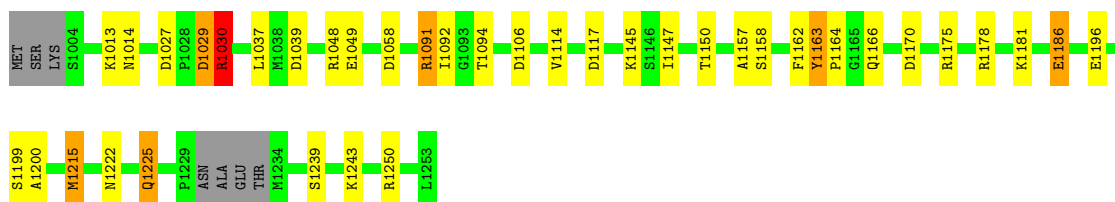
• Molecule 1: Uridine phosphorylase

Chain j:  86% 9% .




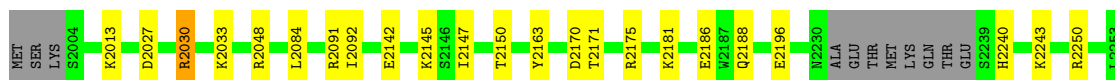
• Molecule 1: Uridine phosphorylase

Chain K:  82% 13% ..




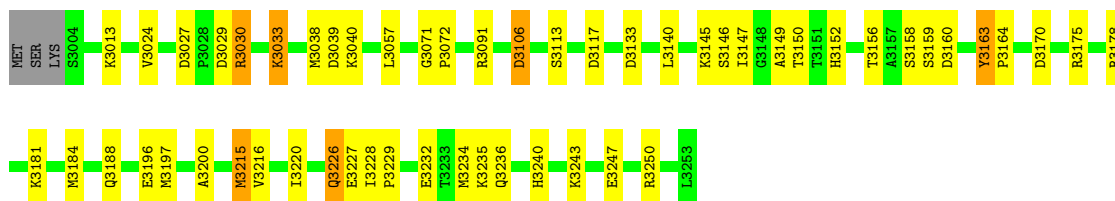
• Molecule 1: Uridine phosphorylase

Chain k:  87% 9% .




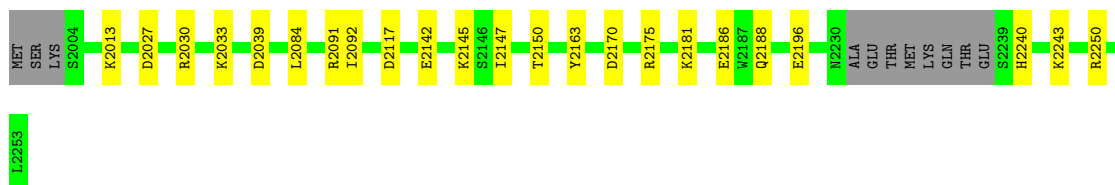
• Molecule 1: Uridine phosphorylase

Chain L:  77% 19% ..




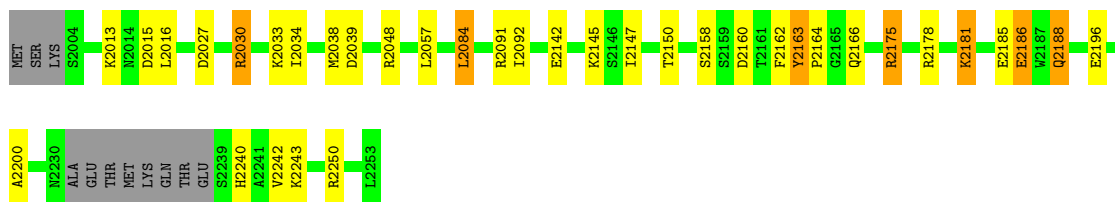
• Molecule 1: Uridine phosphorylase

Chain I:  87% 9%



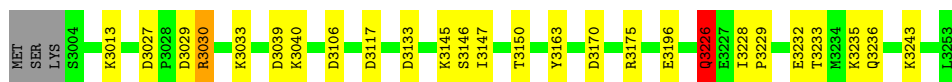
- Molecule 1: Uridine phosphorylase

Chain M:  81% 11%




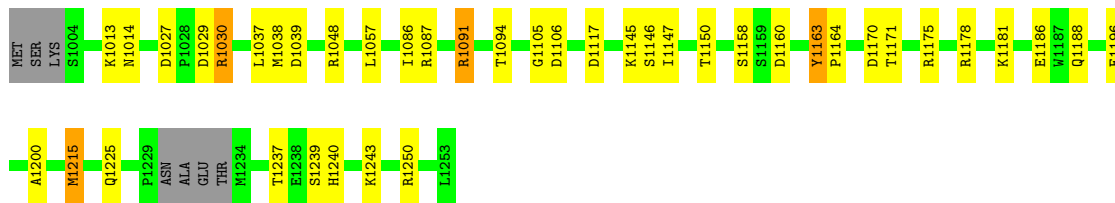
- Molecule 1: Uridine phosphorylase

Chain m:  89% 9%




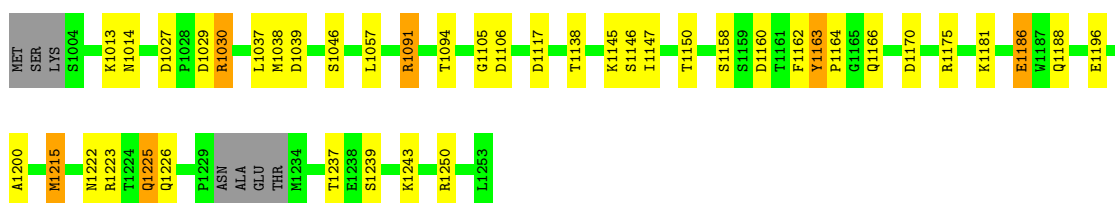
- Molecule 1: Uridine phosphorylase

Chain N:  81% 15%




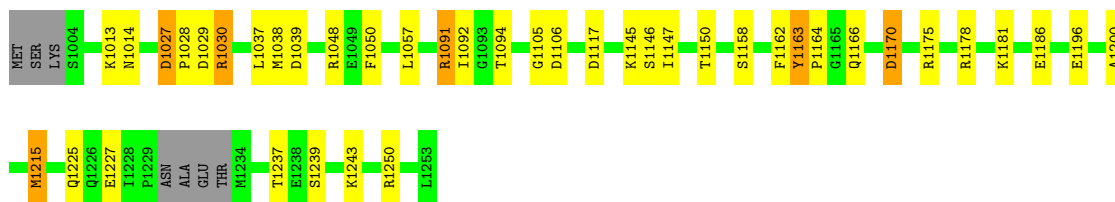
- Molecule 1: Uridine phosphorylase

Chain Q:  81% 14%




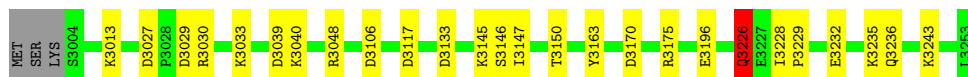
- Molecule 1: Uridine phosphorylase

Chain O:  81% 14% . .



• Molecule 1: Uridine phosphorylase

Chain o:  89% 10% .



## 4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.96Å 98.21Å 242.73Å 90.00° 109.09° 90.00°	Depositor
Resolution (Å)	26.75 – 2.80	Depositor
% Data completeness (in resolution range)	99.2 (26.75-2.80)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.80Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.176 , 0.218	Depositor
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtrriage
Anisotropy	0.034	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtrriage
Total number of atoms	57608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DUR, K, V7O, PO4

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	0.73	0/1912	0.87	8/2595 (0.3%)
1	B	0.68	0/1882	0.85	13/2552 (0.5%)
1	C	0.68	0/1882	0.81	8/2552 (0.3%)
1	D	0.59	0/1882	0.78	5/2552 (0.2%)
1	E	0.59	0/1882	0.80	9/2552 (0.4%)
1	F	0.66	0/1882	0.81	8/2552 (0.3%)
1	G	0.64	0/1848	0.86	4/2508 (0.2%)
1	H	0.64	0/1882	0.77	7/2552 (0.3%)
1	I	0.56	0/1848	0.81	6/2508 (0.2%)
1	J	0.59	0/1882	0.79	7/2552 (0.3%)
1	K	0.63	0/1882	0.78	8/2552 (0.3%)
1	L	0.61	1/1912 (0.1%)	0.81	8/2595 (0.3%)
1	M	0.54	0/1848	0.81	6/2508 (0.2%)
1	N	0.52	0/1882	0.76	8/2552 (0.3%)
1	O	0.55	0/1882	0.77	6/2552 (0.2%)
1	P	0.72	0/1848	0.87	8/2508 (0.3%)
1	Q	0.51	0/1882	0.77	7/2552 (0.3%)
1	R	0.65	0/1882	0.79	5/2552 (0.2%)
1	a	0.72	0/1848	0.89	5/2508 (0.2%)
1	b	0.70	0/1848	0.87	8/2508 (0.3%)
1	c	0.70	0/1848	0.85	7/2508 (0.3%)
1	d	0.61	0/1912	0.83	7/2595 (0.3%)
1	e	0.62	0/1848	0.84	7/2508 (0.3%)
1	h	0.55	0/1848	0.82	6/2508 (0.2%)
1	i	0.60	0/1882	0.81	9/2552 (0.4%)
1	j	0.69	0/1848	0.86	8/2508 (0.3%)
1	k	0.64	0/1848	0.84	5/2508 (0.2%)
1	l	0.55	0/1848	0.79	5/2508 (0.2%)
1	m	0.57	0/1912	0.80	8/2595 (0.3%)
1	o	0.56	0/1912	0.80	8/2595 (0.3%)
All	All	0.62	1/56202 (0.0%)	0.82	214/76247 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	3215	MET	CG-SD	-5.50	1.66	1.81

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	2027	ASP	CB-CG-OD2	11.16	128.35	118.30
1	b	2027	ASP	CB-CG-OD2	11.06	128.25	118.30
1	a	2027	ASP	CB-CG-OD2	10.15	127.44	118.30
1	l	2027	ASP	CB-CG-OD2	9.58	126.92	118.30
1	c	2027	ASP	CB-CG-OD2	9.57	126.92	118.30
1	I	2027	ASP	CB-CG-OD2	9.17	126.55	118.30
1	h	2027	ASP	CB-CG-OD2	9.00	126.40	118.30
1	b	2091	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	G	2027	ASP	CB-CG-OD2	8.78	126.20	118.30
1	k	2027	ASP	CB-CG-OD2	8.68	126.11	118.30
1	M	2027	ASP	CB-CG-OD2	8.62	126.06	118.30
1	a	2091	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	P	2027	ASP	CB-CG-OD2	8.32	125.79	118.30
1	h	2091	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	i	1027	ASP	CB-CG-OD2	8.11	125.60	118.30
1	D	1027	ASP	CB-CG-OD2	8.08	125.58	118.30
1	B	1117	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	3106	ASP	CB-CG-OD2	7.99	125.49	118.30
1	P	2091	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	j	2027	ASP	CB-CG-OD2	7.77	125.30	118.30
1	d	3039	ASP	CB-CG-OD2	7.74	125.27	118.30
1	J	1027	ASP	CB-CG-OD2	7.66	125.20	118.30
1	d	3160	ASP	CB-CG-OD2	7.34	124.91	118.30
1	R	1027	ASP	CB-CG-OD2	7.30	124.87	118.30
1	E	1170	ASP	CB-CG-OD2	7.27	124.84	118.30
1	Q	1027	ASP	CB-CG-OD2	7.23	124.81	118.30
1	J	1160	ASP	CB-CG-OD2	7.15	124.74	118.30
1	F	1039	ASP	CB-CG-OD2	7.15	124.73	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1027	ASP	CB-CG-OD2	7.12	124.71	118.30
1	E	1091	ARG	NE-CZ-NH1	-7.05	116.78	120.30
1	j	2039	ASP	CB-CG-OD2	7.00	124.60	118.30
1	Q	1117	ASP	CB-CG-OD2	6.99	124.59	118.30
1	k	2091	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	G	2091	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	C	1030	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	j	2091	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	K	1170	ASP	CB-CG-OD2	6.86	124.47	118.30
1	N	1027	ASP	CB-CG-OD2	6.81	124.43	118.30
1	B	1160	ASP	CB-CG-OD2	6.78	124.41	118.30
1	i	1170	ASP	CB-CG-OD2	6.77	124.39	118.30
1	B	1005	ASP	CB-CG-OD2	6.74	124.37	118.30
1	N	1170	ASP	CB-CG-OD2	6.73	124.36	118.30
1	e	2091	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	1170	ASP	CB-CG-OD2	6.67	124.30	118.30
1	C	1039	ASP	CB-CG-OD2	6.64	124.28	118.30
1	i	1091	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	C	1091	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	P	2030	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	3058	ASP	CB-CG-OD2	6.59	124.24	118.30
1	a	2030	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	O	1027	ASP	CB-CG-OD2	6.57	124.22	118.30
1	I	2091	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	i	1160	ASP	CB-CG-OD2	6.55	124.20	118.30
1	L	3039	ASP	CB-CG-OD2	6.54	124.19	118.30
1	d	3027	ASP	CB-CG-OD2	6.52	124.17	118.30
1	m	3039	ASP	CB-CG-OD2	6.52	124.17	118.30
1	E	1027	ASP	CB-CG-OD2	6.52	124.17	118.30
1	H	1039	ASP	CB-CG-OD2	6.49	124.14	118.30
1	F	1027	ASP	CB-CG-OD2	6.48	124.13	118.30
1	C	1106	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	3133	ASP	CB-CG-OD2	6.40	124.06	118.30
1	N	1106	ASP	CB-CG-OD2	6.39	124.05	118.30
1	L	3133	ASP	CB-CG-OD2	6.38	124.05	118.30
1	c	2030	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	R	1117	ASP	CB-CG-OD2	6.36	124.02	118.30
1	F	1029	ASP	CB-CG-OD2	6.33	123.99	118.30
1	G	2030	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	H	1029	ASP	CB-CG-OD2	6.30	123.97	118.30
1	i	1106	ASP	CB-CG-OD2	6.29	123.96	118.30
1	L	3106	ASP	CB-CG-OD2	6.27	123.95	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	3106	ASP	CB-CG-OD2	6.25	123.93	118.30
1	Q	1160	ASP	CB-CG-OD2	6.25	123.93	118.30
1	F	1106	ASP	CB-CG-OD2	6.23	123.91	118.30
1	o	3133	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	1030	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	o	3027	ASP	CB-CG-OD2	6.21	123.89	118.30
1	F	1160	ASP	CB-CG-OD2	6.20	123.88	118.30
1	Q	1170	ASP	CB-CG-OD2	6.19	123.87	118.30
1	J	1170	ASP	CB-CG-OD2	6.19	123.87	118.30
1	m	3117	ASP	CB-CG-OD2	6.18	123.86	118.30
1	H	1170	ASP	CB-CG-OD2	6.17	123.86	118.30
1	a	2133	ASP	CB-CG-OD2	6.17	123.85	118.30
1	P	2039	ASP	CB-CG-OD2	6.16	123.84	118.30
1	o	3106	ASP	CB-CG-OD2	6.16	123.84	118.30
1	J	1039	ASP	CB-CG-OD2	6.15	123.84	118.30
1	B	1091	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	H	1117	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	3039	ASP	CB-CG-OD2	6.13	123.81	118.30
1	m	3106	ASP	CB-CG-OD2	6.12	123.80	118.30
1	m	3027	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	1027	ASP	CB-CG-OD2	6.10	123.79	118.30
1	o	3039	ASP	CB-CG-OD2	6.10	123.79	118.30
1	H	1091	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	E	1117	ASP	CB-CG-OD2	6.09	123.78	118.30
1	b	2170	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	1048	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	P	2048	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	H	1027	ASP	CB-CG-OD2	6.05	123.75	118.30
1	O	1170	ASP	CB-CG-OD2	6.04	123.74	118.30
1	b	2029	ASP	CB-CG-OD2	6.02	123.72	118.30
1	j	2030	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	R	1160	ASP	CB-CG-OD2	6.01	123.71	118.30
1	l	2117	ASP	CB-CG-OD2	5.99	123.69	118.30
1	F	1030	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	P	2015	ASP	CB-CG-OD2	5.99	123.69	118.30
1	M	2160	ASP	CB-CG-OD2	5.98	123.68	118.30
1	l	2091	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	c	2091	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	b	2039	ASP	CB-CG-OD2	5.97	123.67	118.30
1	J	1117	ASP	CB-CG-OD2	5.96	123.66	118.30
1	I	2015	ASP	CB-CG-OD2	5.95	123.66	118.30
1	P	2048	ARG	NE-CZ-NH1	5.94	123.27	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	2170	ASP	CB-CG-OD2	5.92	123.63	118.30
1	Q	1106	ASP	CB-CG-OD2	5.91	123.62	118.30
1	m	3030	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	D	1039	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	1117	ASP	CB-CG-OD2	5.85	123.57	118.30
1	j	2106	ASP	CB-CG-OD2	5.84	123.56	118.30
1	o	3029	ASP	CB-CG-OD2	5.84	123.55	118.30
1	o	3170	ASP	CB-CG-OD2	5.83	123.55	118.30
1	M	2030	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	R	1029	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	1048	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	1133	ASP	CB-CG-OD2	5.80	123.52	118.30
1	O	1117	ASP	CB-CG-OD2	5.80	123.52	118.30
1	K	1027	ASP	CB-CG-OD2	5.76	123.49	118.30
1	j	2029	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	3027	ASP	CB-CG-OD2	5.76	123.48	118.30
1	m	3029	ASP	CB-CG-OD2	5.74	123.47	118.30
1	j	2160	ASP	CB-CG-OD2	5.73	123.46	118.30
1	O	1106	ASP	CB-CG-OD2	5.73	123.45	118.30
1	M	2091	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	k	2030	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	l	2039	ASP	CB-CG-OD2	5.70	123.43	118.30
1	i	1039	ASP	CB-CG-OD2	5.69	123.42	118.30
1	E	1160	ASP	CB-CG-OD2	5.69	123.42	118.30
1	O	1039	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	3170	ASP	CB-CG-OD2	5.67	123.40	118.30
1	b	2015	ASP	CB-CG-OD2	5.66	123.39	118.30
1	F	1091	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	B	1106	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	3048	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	l	2170	ASP	CB-CG-OD2	5.59	123.33	118.30
1	N	1039	ASP	CB-CG-OD2	5.58	123.33	118.30
1	N	1160	ASP	CB-CG-OD2	5.57	123.31	118.30
1	e	2058	ASP	CB-CG-OD2	5.56	123.31	118.30
1	h	2039	ASP	CB-CG-OD2	5.56	123.31	118.30
1	d	3029	ASP	CB-CG-OD2	5.55	123.29	118.30
1	h	2015	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	1058	ASP	CB-CG-OD2	5.54	123.29	118.30
1	h	2029	ASP	CB-CG-OD2	5.53	123.28	118.30
1	k	2048	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	a	2160	ASP	CB-CG-OD2	5.52	123.26	118.30
1	E	1058	ASP	CB-CG-OD2	5.50	123.25	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	1029	ASP	CB-CG-OD2	5.50	123.25	118.30
1	e	2106	ASP	CB-CG-OD2	5.50	123.25	118.30
1	o	3117	ASP	CB-CG-OD2	5.46	123.21	118.30
1	N	1048	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	K	1106	ASP	CB-CG-OD2	5.45	123.21	118.30
1	N	1117	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	1058	ASP	CB-CG-OD2	5.44	123.20	118.30
1	O	1029	ASP	CB-CG-OD2	5.44	123.19	118.30
1	m	3170	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	1160	ASP	CB-CG-OD2	5.43	123.19	118.30
1	M	2015	ASP	CB-CG-OD2	5.42	123.18	118.30
1	h	2106	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	1106	ASP	CB-CG-OD2	5.40	123.16	118.30
1	e	2039	ASP	CB-CG-OD2	5.38	123.14	118.30
1	b	2030	ARG	NE-CZ-NH2	5.37	122.99	120.30
1	i	1058	ASP	CB-CG-OD2	5.37	123.13	118.30
1	m	3030	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	e	2030	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	K	1029	ASP	CB-CG-OD2	5.35	123.11	118.30
1	E	1106	ASP	CB-CG-OD2	5.34	123.11	118.30
1	c	2160	ASP	CB-CG-OD2	5.33	123.10	118.30
1	c	2039	ASP	CB-CG-OD2	5.33	123.09	118.30
1	E	1039	ASP	CB-CG-OD2	5.33	123.09	118.30
1	M	2039	ASP	CB-CG-OD2	5.32	123.09	118.30
1	I	2039	ASP	CB-CG-OD2	5.31	123.08	118.30
1	J	1106	ASP	CB-CG-OD2	5.31	123.08	118.30
1	K	1039	ASP	CB-CG-OD2	5.30	123.07	118.30
1	K	1058	ASP	CB-CG-OD2	5.29	123.06	118.30
1	d	3117	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	1170	ASP	CB-CG-OD2	5.28	123.06	118.30
1	i	1029	ASP	CB-CG-OD2	5.28	123.05	118.30
1	L	3170	ASP	CB-CG-OD2	5.28	123.05	118.30
1	c	2106	ASP	CB-CG-OD2	5.28	123.05	118.30
1	k	2170	ASP	CB-CG-OD2	5.28	123.05	118.30
1	N	1029	ASP	CB-CG-OD2	5.27	123.05	118.30
1	L	3160	ASP	CB-CG-OD2	5.26	123.03	118.30
1	i	1005	ASP	CB-CG-OD2	5.24	123.01	118.30
1	H	1106	ASP	CB-CG-OD2	5.22	123.00	118.30
1	j	2170	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	1039	ASP	CB-CG-OD2	5.20	122.98	118.30
1	L	3029	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	1133	ASP	CB-CG-OD2	5.17	122.95	118.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	2133	ASP	CB-CG-OD2	5.15	122.93	118.30
1	Q	1039	ASP	CB-CG-OD2	5.15	122.93	118.30
1	b	2058	ASP	CB-CG-OD2	5.14	122.93	118.30
1	e	2160	ASP	CB-CG-OD2	5.13	122.92	118.30
1	I	2030	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	K	1030	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	1170	ASP	CB-CG-OD2	5.09	122.88	118.30
1	J	1133	ASP	CB-CG-OD2	5.08	122.88	118.30
1	R	1030	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	L	3117	ASP	CB-CG-OD2	5.06	122.85	118.30
1	L	3027	ASP	CB-CG-OD2	5.06	122.85	118.30
1	d	3170	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	3168	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	o	3048	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	c	2170	ASP	CB-CG-OD2	5.03	122.83	118.30
1	K	1117	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	1160	ASP	CB-CG-OD2	5.02	122.82	118.30
1	I	2106	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	o	3226	GLN	Peptide

## 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	1880	0	1884	27	0
1	B	1851	0	1860	12	0
1	C	1851	0	1860	19	0
1	D	1851	0	1860	20	0
1	E	1851	0	1860	11	0
1	F	1851	0	1860	20	0
1	G	1817	0	1822	16	1
1	H	1851	0	1860	12	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1817	0	1823	14	0
1	J	1851	0	1859	16	0
1	K	1851	0	1859	18	0
1	L	1880	0	1884	28	0
1	M	1817	0	1822	14	0
1	N	1851	0	1860	14	0
1	O	1851	0	1860	21	0
1	P	1817	0	1822	16	1
1	Q	1851	0	1860	15	0
1	R	1851	0	1860	16	1
1	a	1817	0	1823	0	0
1	b	1817	0	1822	0	0
1	c	1817	0	1822	0	1
1	d	1880	0	1884	0	1
1	e	1817	0	1822	0	5
1	h	1817	0	1822	0	0
1	i	1851	0	1859	0	2
1	j	1817	0	1823	0	0
1	k	1817	0	1822	0	1
1	l	1817	0	1823	0	0
1	m	1880	0	1885	0	2
1	o	1880	0	1884	0	5
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	R	1	0	0	0	0
2	h	1	0	0	0	0
2	i	1	0	0	0	0
2	o	1	0	0	0	0
3	A	11	0	0	1	0
3	B	11	0	0	1	0
3	D	22	0	0	4	0
3	H	11	0	0	2	0
3	I	11	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	11	0	0	5	0
3	L	11	0	0	1	0
3	M	22	0	0	4	0
3	Q	11	0	0	0	0
3	R	11	0	0	0	0
3	b	11	0	0	0	0
3	c	11	0	0	0	0
3	e	11	0	0	0	0
3	h	11	0	0	0	0
3	i	11	0	0	0	0
3	j	11	0	0	0	0
3	k	11	0	0	0	0
3	o	11	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	1	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0
4	K	5	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	0	0
4	O	5	0	0	1	0
4	P	5	0	0	2	0
4	Q	5	0	0	0	0
4	R	5	0	0	0	0
4	a	5	0	0	0	0
4	b	5	0	0	0	0
4	c	5	0	0	0	0
4	e	5	0	0	0	0
4	h	5	0	0	0	0
4	i	5	0	0	0	0
4	j	5	0	0	0	0
4	k	5	0	0	0	0
4	l	5	0	0	0	0
5	B	16	0	11	0	0
5	C	16	0	11	1	0
5	D	16	0	11	0	0
5	E	16	0	11	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	16	0	11	0	0
5	G	16	0	11	1	0
5	H	16	0	11	0	0
5	I	16	0	11	0	0
5	J	16	0	11	0	0
5	K	16	0	11	0	0
5	M	16	0	11	0	0
5	N	16	0	11	0	0
5	O	16	0	11	0	0
5	P	16	0	11	1	0
5	Q	16	0	11	0	0
5	R	16	0	11	0	0
5	a	16	0	11	0	0
5	b	16	0	11	0	0
5	c	16	0	11	0	0
5	e	16	0	11	0	0
5	h	16	0	11	0	0
5	i	16	0	11	0	0
5	j	16	0	11	0	0
5	k	16	0	11	0	0
5	l	16	0	11	0	0
6	A	54	0	0	2	0
6	B	55	0	0	0	1
6	C	52	0	0	3	0
6	D	52	0	0	4	0
6	E	51	0	0	1	0
6	F	59	0	0	2	0
6	G	46	0	0	4	0
6	H	51	0	0	1	0
6	I	51	0	0	5	0
6	J	52	0	0	2	0
6	K	50	0	0	3	0
6	L	58	0	0	1	0
6	M	48	0	0	3	0
6	N	58	0	0	1	0
6	O	56	0	0	6	0
6	P	51	0	0	4	0
6	Q	50	0	0	5	0
6	R	52	0	0	2	0
6	a	52	0	0	0	0
6	b	48	0	0	0	0
6	c	54	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	d	56	0	0	0	0
6	e	49	0	0	0	0
6	h	55	0	0	0	0
6	i	56	0	0	0	0
6	j	51	0	0	0	0
6	k	53	0	0	0	0
6	l	51	0	0	0	0
6	m	53	0	0	0	0
6	o	57	0	0	0	0
All	All	57608	0	55741	301	11

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 5.

All (301) 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:G:2181:LYS:HD2	6:G:684:HOH:O	1.26	1.33
1:J:1178:ARG:HD3	3:J:5042:V7O:O15	1.29	1.26
3:H:5031:V7O:O17	3:I:5032:V7O:O13	1.67	1.11
1:L:3226:GLN:CG	1:L:3227:GLU:H	1.64	1.09
1:L:3226:GLN:HG2	1:L:3227:GLU:H	1.20	1.06
1:A:3226:GLN:CG	1:A:3227:GLU:H	1.67	1.04
1:A:3226:GLN:HG2	1:A:3227:GLU:H	1.23	1.04
3:J:5042:V7O:O18	1:L:3178:ARG:HD3	1.66	0.95
1:G:2175:ARG:NE	6:G:670:HOH:O	1.95	0.94
1:R:1181:LYS:HD2	6:R:631:HOH:O	1.69	0.92
3:D:5022:V7O:O18	1:F:1178:ARG:HD3	1.73	0.87
1:P:2181:LYS:HD2	6:P:735:HOH:O	1.74	0.87
1:J:1178:ARG:CD	3:J:5042:V7O:O15	2.21	0.85
1:L:3226:GLN:CG	1:L:3227:GLU:N	2.37	0.84
1:A:3226:GLN:CG	1:A:3227:GLU:N	2.38	0.83
1:A:3226:GLN:HG2	1:A:3227:GLU:N	1.98	0.78
1:L:3226:GLN:HG2	1:L:3227:GLU:N	1.97	0.77
1:D:1178:ARG:NH2	1:E:1181:LYS:O	2.16	0.76
1:I:2175:ARG:NE	6:I:876:HOH:O	2.18	0.76
1:K:1181:LYS:HD2	6:K:4154:HOH:O	1.86	0.76
1:I:2178:ARG:NH1	3:I:5032:V7O:O15	2.20	0.74
1:M:2178:ARG:NH2	1:N:1181:LYS:O	2.20	0.73
1:D:1048:ARG:NH1	6:D:330:HOH:O	2.15	0.73
1:K:1178:ARG:NH2	1:L:3181:LYS:O	2.23	0.70

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2178:ARG:NH2	1:H:1181:LYS:O	2.24	0.70
1:J:1178:ARG:NH2	1:K:1181:LYS:O	2.25	0.70
1:C:1181:LYS:HD2	6:C:261:HOH:O	1.90	0.69
1:L:3226:GLN:HG3	1:L:3227:GLU:H	1.58	0.68
1:L:3038:MET:HG2	1:L:3057:LEU:HD13	1.75	0.68
1:J:1181:LYS:O	1:L:3178:ARG:NH2	2.27	0.67
1:A:3226:GLN:HG3	1:A:3227:GLU:H	1.59	0.67
3:J:5042:V7O:O17	3:L:5041:V7O:O17	2.12	0.67
1:A:3178:ARG:NH2	1:B:1181:LYS:O	2.27	0.66
1:D:1178:ARG:HD3	3:D:5022:V7O:O15	1.97	0.65
1:D:1181:LYS:O	1:F:1178:ARG:NH2	2.28	0.65
1:Q:1158:SER:HB3	1:Q:1200:ALA:HB2	1.76	0.65
1:P:2158:SER:HB3	1:P:2200:ALA:HB2	1.79	0.65
1:F:1158:SER:HB3	1:F:1200:ALA:HB2	1.79	0.65
1:I:2038:MET:HG2	1:I:2057:LEU:HD13	1.78	0.65
1:G:2038:MET:HG2	1:G:2057:LEU:HD13	1.78	0.64
3:M:5052:V7O:O18	1:O:1178:ARG:HD3	1.97	0.64
1:B:1158:SER:HB3	1:B:1200:ALA:HB2	1.80	0.64
1:P:2038:MET:HG2	1:P:2057:LEU:HD13	1.79	0.64
1:K:1158:SER:HB3	1:K:1200:ALA:HB2	1.80	0.64
1:M:2048:ARG:NH1	6:M:1287:HOH:O	2.26	0.64
1:H:1048:ARG:HD2	6:H:773:HOH:O	1.98	0.63
1:P:2030:ARG:HD3	6:P:717:HOH:O	1.97	0.63
3:J:5042:V7O:O18	1:L:3178:ARG:CD	2.44	0.63
1:N:1178:ARG:NH2	1:O:1181:LYS:O	2.32	0.63
1:M:2181:LYS:HD2	6:M:1309:HOH:O	1.99	0.62
1:N:1181:LYS:HD2	6:N:1416:HOH:O	1.99	0.62
1:B:1178:ARG:NH2	1:C:1181:LYS:O	2.34	0.61
1:O:1170:ASP:HB3	6:O:1489:HOH:O	2.00	0.61
1:E:1158:SER:HB3	1:E:1200:ALA:HB2	1.83	0.60
1:A:3181:LYS:O	1:C:1178:ARG:NH2	2.35	0.60
1:G:2181:LYS:O	1:I:2178:ARG:NH2	2.35	0.60
1:I:2158:SER:HB3	1:I:2200:ALA:HB2	1.84	0.60
1:M:2181:LYS:O	1:O:1178:ARG:NH2	2.35	0.60
1:G:2186:GLU:HG3	6:I:877:HOH:O	2.02	0.60
1:Q:1046:SER:N	6:Q:1454:HOH:O	2.30	0.59
1:L:3163:TYR:HB2	1:L:3164:PRO:HD3	1.85	0.59
1:M:2186:GLU:HG3	6:O:1524:HOH:O	2.00	0.59
1:O:1158:SER:HB3	1:O:1200:ALA:HB2	1.82	0.59
1:C:1158:SER:HB3	1:C:1200:ALA:HB2	1.85	0.59
1:N:1158:SER:HB3	1:N:1200:ALA:HB2	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2158:SER:HB3	1:M:2200:ALA:HB2	1.85	0.59
1:J:1186:GLU:HG3	6:L:1207:HOH:O	2.03	0.58
3:D:5021:V7O:O16	3:D:5022:V7O:O13	2.22	0.58
1:O:1105:GLY:HA2	1:O:1237:THR:HG23	1.85	0.58
1:A:3158:SER:HB3	1:A:3200:ALA:HB2	1.85	0.58
1:A:3181:LYS:HE2	6:A:54:HOH:O	2.02	0.58
1:D:1158:SER:HB3	1:D:1200:ALA:HB2	1.86	0.58
1:F:1228:ILE:HD12	1:R:1007:PHE:HB2	1.86	0.58
1:H:1158:SER:HB3	1:H:1200:ALA:HB2	1.85	0.57
3:M:5051:V7O:O16	3:M:5052:V7O:O13	2.21	0.57
1:G:2158:SER:HB3	1:G:2200:ALA:HB2	1.88	0.55
6:A:55:HOH:O	1:B:1186:GLU:HG3	2.06	0.55
1:L:3247:GLU:O	1:L:3250:ARG:HB2	2.07	0.55
1:O:1227:GLU:OE2	6:O:1489:HOH:O	2.18	0.55
1:A:3058:ASP:OD2	1:A:3250:ARG:HD2	2.07	0.55
6:E:476:HOH:O	1:F:1186:GLU:HG3	2.07	0.55
1:J:1158:SER:HB3	1:J:1200:ALA:HB2	1.88	0.55
1:A:3220:ILE:HB	1:A:3234:MET:HG2	1.87	0.55
1:J:1105:GLY:HA2	1:J:1237:THR:HG23	1.88	0.55
1:E:1105:GLY:HA2	1:E:1237:THR:HG23	1.88	0.54
1:A:3186:GLU:HG3	6:C:263:HOH:O	2.07	0.54
1:D:1105:GLY:HA2	1:D:1237:THR:HG23	1.90	0.54
1:H:1038:MET:HG2	1:H:1057:LEU:HD13	1.89	0.54
1:O:1215:MET:HE3	6:O:1501:HOH:O	2.07	0.54
1:K:1030:ARG:HH21	1:K:1094:THR:HG23	1.73	0.53
3:M:5051:V7O:O17	3:M:5052:V7O:O13	2.26	0.53
1:O:1163:TYR:HB2	1:O:1164:PRO:CD	2.39	0.53
1:P:2210:GLY:N	6:P:708:HOH:O	2.41	0.53
1:R:1091:ARG:HG2	1:R:1215:MET:SD	2.48	0.53
1:R:1158:SER:HB3	1:R:1200:ALA:HB2	1.90	0.53
1:H:1178:ARG:NH2	1:I:2181:LYS:O	2.42	0.53
1:I:2185:GLU:HA	1:I:2188:GLN:HG3	1.91	0.53
1:A:3038:MET:HG2	1:A:3057:LEU:HD13	1.90	0.53
1:F:1105:GLY:HA2	1:F:1237:THR:HG23	1.91	0.53
1:Q:1091:ARG:HG2	1:Q:1215:MET:SD	2.49	0.53
1:F:1007:PHE:HB2	1:R:1228:ILE:HD12	1.91	0.53
1:M:2038:MET:HG2	1:M:2057:LEU:HD13	1.89	0.53
1:M:2175:ARG:NE	6:M:1295:HOH:O	2.40	0.53
1:Q:1186:GLU:HG3	6:Q:1580:HOH:O	2.09	0.53
3:A:5011:V7O:O16	3:B:5012:V7O:O13	2.27	0.53
1:O:1038:MET:HG2	1:O:1057:LEU:HD13	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:5084:HOH:O	1:K:1186:GLU:HG3	2.07	0.53
1:A:3140:LEU:HD22	1:A:3216:VAL:HB	1.91	0.52
1:K:1163:TYR:HB2	1:K:1164:PRO:CD	2.39	0.52
1:N:1030:ARG:HH21	1:N:1094:THR:HG23	1.75	0.52
1:L:3220:ILE:HB	1:L:3234:MET:HG2	1.90	0.52
1:N:1038:MET:HG2	1:N:1057:LEU:HD13	1.92	0.52
1:F:1030:ARG:HH21	1:F:1094:THR:HG23	1.76	0.52
1:O:1050:PHE:O	6:O:1510:HOH:O	2.18	0.52
1:N:1105:GLY:HA2	1:N:1237:THR:HG23	1.91	0.51
1:Q:1030:ARG:HH21	1:Q:1094:THR:HG23	1.75	0.51
1:C:1170:ASP:HB3	6:C:228:HOH:O	2.10	0.51
1:D:1170:ASP:HB3	6:D:332:HOH:O	2.10	0.51
1:I:2030:ARG:HD3	6:I:872:HOH:O	2.11	0.51
1:L:3149:ALA:HB2	1:L:3240:HIS:CE1	2.45	0.51
1:Q:1181:LYS:HD2	6:Q:1469:HOH:O	2.09	0.51
1:J:1030:ARG:HH21	1:J:1094:THR:HG23	1.76	0.51
1:R:1091:ARG:HB3	1:R:1215:MET:HG2	1.92	0.51
1:R:1030:ARG:HH21	1:R:1094:THR:HG23	1.75	0.51
4:P:3121:PO4:O4	5:P:3122:DUR:H2'2	2.11	0.51
1:B:1105:GLY:HA2	1:B:1237:THR:HG23	1.93	0.50
1:C:1163:TYR:HB2	1:C:1164:PRO:CD	2.41	0.50
1:M:2162:PHE:HA	1:M:2166:GLN:NE2	2.26	0.50
1:Q:1038:MET:HG2	1:Q:1057:LEU:HD13	1.94	0.50
1:P:2175:ARG:NE	6:P:721:HOH:O	2.32	0.50
1:L:3158:SER:HB3	1:L:3200:ALA:HB2	1.93	0.50
1:H:1030:ARG:HH21	1:H:1094:THR:HG23	1.76	0.50
1:G:2091:ARG:NH2	1:G:2198:GLU:OE1	2.44	0.50
1:O:1030:ARG:HH21	1:O:1094:THR:HG23	1.76	0.50
1:D:1186:GLU:HG3	6:F:580:HOH:O	2.11	0.49
1:J:1152:HIS:HA	6:J:5066:HOH:O	2.11	0.49
1:D:1163:TYR:HB2	1:D:1164:PRO:CD	2.41	0.49
1:P:2185:GLU:HA	1:P:2188:GLN:HG3	1.94	0.49
1:Q:1163:TYR:HB2	1:Q:1164:PRO:CD	2.43	0.49
1:C:1223:ARG:HA	1:C:1226:GLN:O	2.12	0.49
1:F:1038:MET:HG2	1:F:1057:LEU:HD13	1.93	0.49
1:L:3106:ASP:OD1	1:L:3152:HIS:HE1	1.96	0.49
1:R:1038:MET:HG2	1:R:1057:LEU:HD13	1.95	0.49
3:M:5051:V7O:O17	3:M:5052:V7O:O17	2.30	0.49
1:A:3106:ASP:OD1	1:A:3152:HIS:HE1	1.95	0.49
4:C:2021:PO4:O4	5:C:2022:DUR:H2'2	2.13	0.49
1:N:1163:TYR:HB2	1:N:1164:PRO:CD	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1163:TYR:HB2	1:B:1164:PRO:CD	2.43	0.48
1:N:1091:ARG:HG2	1:N:1215:MET:SD	2.52	0.48
1:A:3247:GLU:O	1:A:3250:ARG:HB2	2.13	0.48
1:L:3163:TYR:HB2	1:L:3164:PRO:CD	2.43	0.48
1:C:1091:ARG:HB3	1:C:1215:MET:HG2	1.96	0.48
1:E:1091:ARG:HG2	1:E:1215:MET:SD	2.54	0.48
1:I:2181:LYS:HD2	6:I:890:HOH:O	2.14	0.48
1:M:2185:GLU:HA	1:M:2188:GLN:HG3	1.94	0.48
1:Q:1138:THR:HG21	6:Q:1429:HOH:O	2.13	0.48
1:B:1030:ARG:HH21	1:B:1094:THR:HG23	1.78	0.47
1:K:1048:ARG:HD2	6:K:4142:HOH:O	2.15	0.47
1:C:1105:GLY:HA2	1:C:1237:THR:HG23	1.97	0.47
1:Q:1105:GLY:HA2	1:Q:1237:THR:HG23	1.97	0.47
1:I:2030:ARG:HB2	6:I:872:HOH:O	2.14	0.47
1:E:1178:ARG:NH2	1:F:1181:LYS:O	2.48	0.47
1:I:2162:PHE:HA	1:I:2166:GLN:NE2	2.30	0.47
1:J:1091:ARG:HB3	1:J:1215:MET:HG2	1.97	0.47
1:R:1162:PHE:HA	1:R:1166:GLN:NE2	2.30	0.46
1:G:2016:LEU:HD22	1:G:2084:LEU:HB3	1.96	0.46
4:G:3051:PO4:O4	5:G:3052:DUR:H2'2	2.15	0.46
1:A:3163:TYR:HB2	1:A:3164:PRO:CD	2.45	0.46
1:H:1163:TYR:HB2	1:H:1164:PRO:CD	2.45	0.46
1:K:1163:TYR:CB	1:K:1164:PRO:CD	2.93	0.46
1:E:1030:ARG:HH21	1:E:1094:THR:HG23	1.80	0.46
1:N:1163:TYR:HB2	1:N:1164:PRO:HD3	1.97	0.46
1:O:1163:TYR:CB	1:O:1164:PRO:CD	2.93	0.46
1:J:1162:PHE:HA	1:J:1166:GLN:NE2	2.31	0.46
1:C:1199:SER:HB3	1:C:1215:MET:CE	2.45	0.45
1:H:1091:ARG:HG2	1:H:1215:MET:SD	2.56	0.45
1:J:1038:MET:HG2	1:J:1057:LEU:HD13	1.98	0.45
1:C:1030:ARG:HH21	1:C:1094:THR:HG23	1.80	0.45
1:A:3226:GLN:HG3	1:A:3227:GLU:N	2.25	0.45
1:D:1030:ARG:HH21	1:D:1094:THR:HG23	1.81	0.45
1:J:1163:TYR:HB2	1:J:1164:PRO:CD	2.46	0.45
1:R:1223:ARG:HA	1:R:1226:GLN:O	2.16	0.45
1:Q:1091:ARG:HB3	1:Q:1215:MET:HG2	1.98	0.45
1:A:3167:GLU:HG2	1:A:3169:TYR:CE2	2.50	0.45
1:F:1163:TYR:HB2	1:F:1164:PRO:CD	2.46	0.45
1:P:2016:LEU:HD22	1:P:2084:LEU:HB3	1.97	0.45
1:I:2086:ILE:O	1:I:2087:ARG:NH1	2.49	0.45
1:C:1163:TYR:HB2	1:C:1164:PRO:HD3	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1038:MET:HG2	1:C:1057:LEU:HD13	1.98	0.45
1:F:1091:ARG:HB3	1:F:1215:MET:HG2	1.97	0.45
1:K:1029:ASP:OD2	6:K:4135:HOH:O	2.21	0.45
1:D:1038:MET:HG2	1:D:1057:LEU:HD13	2.00	0.44
1:A:3163:TYR:HB2	1:A:3164:PRO:HD3	1.99	0.44
1:B:1038:MET:HG2	1:B:1057:LEU:HD13	1.99	0.44
1:D:1091:ARG:HG2	1:D:1215:MET:SD	2.57	0.44
1:R:1170:ASP:HB3	6:R:598:HOH:O	2.17	0.44
1:E:1163:TYR:HB2	1:E:1164:PRO:CD	2.48	0.44
1:K:1222:ASN:HB3	1:K:1225:GLN:HE21	1.83	0.44
1:A:3242:VAL:O	1:A:3245:VAL:HG12	2.17	0.44
1:B:1091:ARG:HB3	1:B:1215:MET:HG2	2.00	0.44
1:C:1163:TYR:CB	1:C:1164:PRO:CD	2.96	0.44
1:D:1163:TYR:CB	1:D:1164:PRO:CD	2.96	0.44
1:R:1163:TYR:HB2	1:R:1164:PRO:CD	2.47	0.44
1:R:1199:SER:HB3	1:R:1215:MET:CE	2.47	0.44
1:K:1091:ARG:HG2	1:K:1215:MET:SD	2.58	0.44
1:L:3030:ARG:HE	1:L:3033:LYS:NZ	2.15	0.44
1:H:1105:GLY:HA2	1:H:1237:THR:HG23	2.00	0.44
1:A:3024:VAL:O	1:A:3091:ARG:HD2	2.17	0.44
1:B:1163:TYR:CB	1:B:1164:PRO:CD	2.95	0.44
1:L:3140:LEU:HD22	1:L:3216:VAL:HB	1.99	0.44
1:E:1223:ARG:HA	1:E:1226:GLN:O	2.17	0.43
1:P:2163:TYR:HB2	1:P:2164:PRO:CD	2.48	0.43
1:K:1048:ARG:HB3	1:K:1049:GLU:OE2	2.18	0.43
1:P:2253:LEU:HD23	1:P:2253:LEU:HA	1.84	0.43
1:J:1105:GLY:HA2	1:J:1237:THR:CG2	2.47	0.43
1:G:2049:GLU:HB3	1:P:2049:GLU:HB3	2.00	0.43
1:G:2030:ARG:HD3	6:G:666:HOH:O	2.18	0.43
1:L:3113:SER:HA	1:L:3156:THR:O	2.18	0.43
1:G:2228:ILE:HA	1:G:2229:PRO:HD3	1.93	0.43
1:O:1105:GLY:HA2	1:O:1237:THR:CG2	2.47	0.43
1:D:1181:LYS:HD2	6:D:365:HOH:O	2.18	0.43
1:O:1091:ARG:HG2	1:O:1215:MET:SD	2.58	0.43
1:A:3159:SER:O	1:A:3197:MET:HG2	2.18	0.43
1:F:1116:LEU:HB2	1:F:1159:SER:HA	2.01	0.43
1:A:3149:ALA:HB2	1:A:3240:HIS:CE1	2.54	0.43
1:N:1091:ARG:HB3	1:N:1215:MET:HG2	2.01	0.43
1:D:1091:ARG:HB3	1:D:1215:MET:HG2	2.01	0.42
1:I:2016:LEU:HD22	1:I:2084:LEU:HB3	2.00	0.42
1:M:2034:ILE:HG12	1:M:2242:VAL:HG13	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1031:VAL:HG13	1:R:1064:VAL:HG12	2.01	0.42
1:P:2163:TYR:CB	1:P:2164:PRO:CD	2.97	0.42
1:J:1091:ARG:HG2	1:J:1215:MET:SD	2.59	0.42
1:N:1163:TYR:CB	1:N:1164:PRO:CD	2.96	0.42
1:F:1223:ARG:HA	1:F:1226:GLN:O	2.19	0.42
1:C:1162:PHE:HA	1:C:1166:GLN:NE2	2.35	0.42
1:F:1163:TYR:CB	1:F:1164:PRO:CD	2.97	0.42
1:L:3091:ARG:HG2	1:L:3215:MET:SD	2.59	0.42
1:A:3225:GLN:HB3	1:A:3227:GLU:OE1	2.20	0.42
1:D:1091:ARG:HG3	1:D:1092:ILE:N	2.34	0.42
1:Q:1163:TYR:CB	1:Q:1164:PRO:CD	2.97	0.42
1:O:1027:ASP:HA	1:O:1028:PRO:HD2	1.94	0.42
1:A:3030:ARG:HB3	1:A:3030:ARG:CZ	2.49	0.42
1:E:1086:ILE:O	1:E:1087:ARG:NH2	2.52	0.42
1:L:3184:MET:O	1:L:3188:GLN:HG3	2.20	0.42
1:M:2016:LEU:HD22	1:M:2084:LEU:HB3	2.01	0.42
1:D:1116:LEU:HB2	1:D:1159:SER:HA	2.02	0.42
1:R:1105:GLY:HA2	1:R:1237:THR:HG23	2.02	0.42
1:K:1199:SER:HB3	1:K:1215:MET:CE	2.49	0.42
1:L:3149:ALA:HB2	1:L:3240:HIS:HE1	1.83	0.42
1:O:1163:TYR:HB2	1:O:1164:PRO:HD3	2.02	0.42
1:K:1114:VAL:HB	1:K:1157:ALA:HA	2.02	0.42
1:K:1199:SER:HB3	1:K:1215:MET:HE1	2.02	0.42
1:M:2163:TYR:HB2	1:M:2164:PRO:CD	2.50	0.42
1:O:1162:PHE:HA	1:O:1166:GLN:NE2	2.35	0.42
1:F:1048:ARG:NH1	6:F:543:HOH:O	2.46	0.42
1:P:2177:VAL:O	1:P:2178:ARG:C	2.58	0.42
1:L:3071:GLY:N	1:L:3072:PRO:CD	2.82	0.42
1:G:2185:GLU:HA	1:G:2188:GLN:HG3	2.01	0.41
1:H:1091:ARG:HB3	1:H:1215:MET:HG2	2.01	0.41
1:N:1086:ILE:O	1:N:1087:ARG:NH2	2.53	0.41
1:O:1091:ARG:HG3	1:O:1092:ILE:N	2.35	0.41
1:D:1133:ASP:OD2	6:D:359:HOH:O	2.22	0.41
1:H:1199:SER:HB3	1:H:1215:MET:CE	2.50	0.41
1:C:1116:LEU:HB2	1:C:1159:SER:HA	2.02	0.41
1:D:1179:HIS:ND1	3:D:5021:V7O:O12	2.38	0.41
1:P:2091:ARG:NH2	4:P:3121:PO4:O4	2.52	0.41
1:E:1105:GLY:HA2	1:E:1237:THR:CG2	2.50	0.41
1:Q:1162:PHE:HA	1:Q:1166:GLN:NE2	2.35	0.41
1:B:1223:ARG:HA	1:B:1226:GLN:O	2.21	0.41
1:F:1162:PHE:HA	1:F:1166:GLN:NE2	2.36	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2160:ASP:OD2	1:P:2118:GLY:HA3	2.21	0.41
1:L:3226:GLN:HG3	1:L:3227:GLU:N	2.25	0.41
1:O:1048:ARG:NH1	6:O:1487:HOH:O	2.42	0.41
1:E:1038:MET:HG2	1:E:1057:LEU:HD13	2.02	0.41
1:F:1091:ARG:HG2	1:F:1215:MET:SD	2.61	0.41
1:R:1163:TYR:HB2	1:R:1164:PRO:HD3	2.02	0.41
1:J:1222:ASN:HB3	1:J:1225:GLN:HE21	1.86	0.41
1:K:1091:ARG:HG3	1:K:1092:ILE:N	2.35	0.41
1:L:3024:VAL:O	1:L:3091:ARG:HD2	2.21	0.41
1:O:1091:ARG:NH1	4:O:2111:PO4:O4	2.54	0.41
1:A:3163:TYR:CB	1:A:3164:PRO:CD	2.99	0.41
1:F:1199:SER:HB3	1:F:1215:MET:CE	2.51	0.41
1:Q:1223:ARG:HA	1:Q:1226:GLN:O	2.21	0.41
1:C:1222:ASN:HB3	1:C:1225:GLN:HE21	1.86	0.40
1:L:3159:SER:O	1:L:3197:MET:HG2	2.21	0.40
1:F:1007:PHE:HD2	1:F:1008:HIS:CE1	2.39	0.40
1:G:2162:PHE:HA	1:G:2166:GLN:NE2	2.36	0.40
1:P:2090:LEU:HD11	1:P:2252:LEU:HD12	2.03	0.40
3:H:5031:V7O:O16	3:I:5032:V7O:O12	2.38	0.40
1:K:1162:PHE:HA	1:K:1166:GLN:NE2	2.36	0.40
1:G:2175:ARG:CD	6:G:670:HOH:O	2.61	0.40
1:I:2034:ILE:HG12	1:I:2242:VAL:HG13	2.04	0.40
1:C:1091:ARG:HG3	1:C:1092:ILE:N	2.35	0.40
1:C:1199:SER:HB3	1:C:1215:MET:HE1	2.04	0.40
1:D:1223:ARG:HA	1:D:1226:GLN:O	2.21	0.40
1:M:2163:TYR:CB	1:M:2164:PRO:CD	3.00	0.40
1:Q:1222:ASN:HB3	1:Q:1225:GLN:HE21	1.86	0.40
1:B:1091:ARG:HG2	1:B:1215:MET:SD	2.62	0.40
1:H:1163:TYR:HB2	1:H:1164:PRO:HD3	2.02	0.40
1:L:3163:TYR:CB	1:L:3164:PRO:CD	3.00	0.40
1:N:1171:THR:HB	6:Q:1374:HOH:O	2.20	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:1104:VAL:O	1:m:3226:GLN:NE2[2_546]	1.65	0.55
1:e:2101:HIS:CE1	1:o:3226:GLN:CD[2_546]	1.71	0.49
1:e:2101:HIS:NE2	1:o:3226:GLN:NE2[2_546]	1.79	0.41
1:d:3005:ASP:O	1:d:3226:GLN:OE1[2_656]	1.85	0.35

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:2101:HIS:CE1	1:o:3226:GLN:CG[2_546]	1.93	0.27
1:c:2014:ASN:OD1	1:k:2171:THR:O[2_656]	1.96	0.24
1:i:1104:VAL:CB	1:m:3226:GLN:OE1[2_546]	1.99	0.21
1:G:2226:GLN:OE1	6:B:148:HOH:O[2_556]	2.06	0.14
1:e:2101:HIS:NE2	1:o:3226:GLN:CB[2_546]	2.09	0.11
1:e:2101:HIS:CE1	1:o:3226:GLN:NE2[2_546]	2.10	0.10
1:R:1039:ASP:OD2	1:P:2042:VAL:CG2[1_655]	2.11	0.09

## 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	248/253 (98%)	242 (98%)	3 (1%)	3 (1%)	13	39
1	B	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	34	66
1	C	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	34	66
1	D	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	34	66
1	E	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	34	66
1	F	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	34	66
1	G	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	34	66
1	H	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	34	66
1	I	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	34	66
1	J	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	34	66
1	K	242/253 (96%)	236 (98%)	5 (2%)	1 (0%)	34	66
1	L	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	13	39
1	M	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	34	66
1	N	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	34	66
1	O	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	34	66
1	P	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	34	66

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	34	66
1	R	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	34	66
1	a	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	34	66
1	b	238/253 (94%)	234 (98%)	3 (1%)	1 (0%)	34	66
1	c	238/253 (94%)	236 (99%)	1 (0%)	1 (0%)	34	66
1	d	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	13	39
1	e	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	34	66
1	h	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	34	66
1	i	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	34	66
1	j	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	34	66
1	k	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	34	66
1	l	238/253 (94%)	234 (98%)	3 (1%)	1 (0%)	34	66
1	m	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	13	39
1	o	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	13	39
All	All	7242/7590 (95%)	7100 (98%)	102 (1%)	40 (1%)	25	56

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3163	TYR
1	A	3229	PRO
1	b	2163	TYR
1	c	2163	TYR
1	d	3163	TYR
1	d	3229	PRO
1	e	2163	TYR
1	G	2163	TYR
1	P	2163	TYR
1	h	2163	TYR
1	i	1163	TYR
1	j	2163	TYR
1	K	1163	TYR
1	k	2163	TYR
1	L	3163	TYR
1	L	3229	PRO
1	M	2163	TYR
1	m	3229	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	o	3163	TYR
1	o	3229	PRO
1	A	3226	GLN
1	a	2163	TYR
1	B	1163	TYR
1	C	1163	TYR
1	D	1163	TYR
1	E	1163	TYR
1	F	1163	TYR
1	R	1163	TYR
1	I	2163	TYR
1	J	1163	TYR
1	L	3226	GLN
1	l	2163	TYR
1	m	3163	TYR
1	m	3226	GLN
1	N	1163	TYR
1	Q	1163	TYR
1	O	1163	TYR
1	o	3226	GLN
1	d	3226	GLN
1	H	1163	TYR

### 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	201/204 (98%)	187 (93%)	14 (7%)	15 40
1	B	198/204 (97%)	179 (90%)	19 (10%)	8 24
1	C	198/204 (97%)	181 (91%)	17 (9%)	10 30
1	D	198/204 (97%)	180 (91%)	18 (9%)	9 27
1	E	198/204 (97%)	181 (91%)	17 (9%)	10 30
1	F	198/204 (97%)	181 (91%)	17 (9%)	10 30
1	G	194/204 (95%)	178 (92%)	16 (8%)	11 33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	198/204 (97%)	180 (91%)	18 (9%)	9	27
1	I	194/204 (95%)	178 (92%)	16 (8%)	11	33
1	J	198/204 (97%)	180 (91%)	18 (9%)	9	27
1	K	198/204 (97%)	182 (92%)	16 (8%)	11	33
1	L	201/204 (98%)	186 (92%)	15 (8%)	13	37
1	M	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	N	198/204 (97%)	179 (90%)	19 (10%)	8	24
1	O	198/204 (97%)	181 (91%)	17 (9%)	10	30
1	P	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	Q	198/204 (97%)	180 (91%)	18 (9%)	9	27
1	R	198/204 (97%)	179 (90%)	19 (10%)	8	24
1	a	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	b	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	c	194/204 (95%)	178 (92%)	16 (8%)	11	33
1	d	201/204 (98%)	187 (93%)	14 (7%)	15	40
1	e	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	h	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	i	198/204 (97%)	180 (91%)	18 (9%)	9	27
1	j	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	k	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	l	194/204 (95%)	177 (91%)	17 (9%)	10	29
1	m	201/204 (98%)	183 (91%)	18 (9%)	9	28
1	o	201/204 (98%)	186 (92%)	15 (8%)	13	37
All	All	5907/6120 (96%)	5399 (91%)	508 (9%)	10	30

All (508) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3013	LYS
1	A	3030	ARG
1	A	3033	LYS
1	A	3145	LYS
1	A	3146	SER
1	A	3147	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	3150	THR
1	A	3175	ARG
1	A	3196	GLU
1	A	3228	ILE
1	A	3232	GLU
1	A	3235	LYS
1	A	3236	GLN
1	A	3243	LYS
1	a	2013	LYS
1	a	2030	ARG
1	a	2033	LYS
1	a	2084	LEU
1	a	2092	ILE
1	a	2142	GLU
1	a	2145	LYS
1	a	2147	ILE
1	a	2150	THR
1	a	2175	ARG
1	a	2181	LYS
1	a	2186	GLU
1	a	2188	GLN
1	a	2196	GLU
1	a	2240	HIS
1	a	2243	LYS
1	a	2250	ARG
1	B	1013	LYS
1	B	1014	ASN
1	B	1030	ARG
1	B	1037	LEU
1	B	1091	ARG
1	B	1145	LYS
1	B	1146	SER
1	B	1147	ILE
1	B	1150	THR
1	B	1175	ARG
1	B	1186	GLU
1	B	1188	GLN
1	B	1196	GLU
1	B	1215	MET
1	B	1225	GLN
1	B	1239	SER
1	B	1240	HIS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1243	LYS
1	B	1250	ARG
1	b	2013	LYS
1	b	2030	ARG
1	b	2033	LYS
1	b	2084	LEU
1	b	2092	ILE
1	b	2142	GLU
1	b	2145	LYS
1	b	2147	ILE
1	b	2150	THR
1	b	2175	ARG
1	b	2181	LYS
1	b	2186	GLU
1	b	2188	GLN
1	b	2196	GLU
1	b	2240	HIS
1	b	2243	LYS
1	b	2250	ARG
1	C	1013	LYS
1	C	1014	ASN
1	C	1030	ARG
1	C	1037	LEU
1	C	1091	ARG
1	C	1145	LYS
1	C	1146	SER
1	C	1147	ILE
1	C	1150	THR
1	C	1175	ARG
1	C	1186	GLU
1	C	1196	GLU
1	C	1215	MET
1	C	1225	GLN
1	C	1239	SER
1	C	1243	LYS
1	C	1250	ARG
1	c	2013	LYS
1	c	2030	ARG
1	c	2033	LYS
1	c	2084	LEU
1	c	2092	ILE
1	c	2142	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	c	2145	LYS
1	c	2147	ILE
1	c	2150	THR
1	c	2175	ARG
1	c	2181	LYS
1	c	2186	GLU
1	c	2188	GLN
1	c	2196	GLU
1	c	2240	HIS
1	c	2243	LYS
1	D	1013	LYS
1	D	1014	ASN
1	D	1028	PRO
1	D	1030	ARG
1	D	1037	LEU
1	D	1091	ARG
1	D	1145	LYS
1	D	1146	SER
1	D	1147	ILE
1	D	1150	THR
1	D	1175	ARG
1	D	1186	GLU
1	D	1196	GLU
1	D	1215	MET
1	D	1225	GLN
1	D	1239	SER
1	D	1243	LYS
1	D	1250	ARG
1	d	3013	LYS
1	d	3030	ARG
1	d	3033	LYS
1	d	3145	LYS
1	d	3146	SER
1	d	3147	ILE
1	d	3150	THR
1	d	3175	ARG
1	d	3196	GLU
1	d	3228	ILE
1	d	3232	GLU
1	d	3235	LYS
1	d	3236	GLN
1	d	3243	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	1013	LYS
1	E	1014	ASN
1	E	1030	ARG
1	E	1037	LEU
1	E	1091	ARG
1	E	1145	LYS
1	E	1146	SER
1	E	1147	ILE
1	E	1150	THR
1	E	1175	ARG
1	E	1186	GLU
1	E	1196	GLU
1	E	1215	MET
1	E	1225	GLN
1	E	1239	SER
1	E	1243	LYS
1	E	1250	ARG
1	e	2013	LYS
1	e	2030	ARG
1	e	2033	LYS
1	e	2084	LEU
1	e	2092	ILE
1	e	2142	GLU
1	e	2145	LYS
1	e	2147	ILE
1	e	2150	THR
1	e	2175	ARG
1	e	2181	LYS
1	e	2186	GLU
1	e	2188	GLN
1	e	2196	GLU
1	e	2240	HIS
1	e	2243	LYS
1	e	2250	ARG
1	F	1013	LYS
1	F	1014	ASN
1	F	1030	ARG
1	F	1037	LEU
1	F	1091	ARG
1	F	1145	LYS
1	F	1146	SER
1	F	1147	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	1150	THR
1	F	1175	ARG
1	F	1186	GLU
1	F	1196	GLU
1	F	1215	MET
1	F	1225	GLN
1	F	1239	SER
1	F	1243	LYS
1	F	1250	ARG
1	R	1013	LYS
1	R	1014	ASN
1	R	1028	PRO
1	R	1030	ARG
1	R	1037	LEU
1	R	1091	ARG
1	R	1145	LYS
1	R	1146	SER
1	R	1147	ILE
1	R	1150	THR
1	R	1175	ARG
1	R	1186	GLU
1	R	1188	GLN
1	R	1196	GLU
1	R	1215	MET
1	R	1225	GLN
1	R	1239	SER
1	R	1243	LYS
1	R	1250	ARG
1	G	2013	LYS
1	G	2030	ARG
1	G	2033	LYS
1	G	2084	LEU
1	G	2092	ILE
1	G	2142	GLU
1	G	2145	LYS
1	G	2147	ILE
1	G	2150	THR
1	G	2175	ARG
1	G	2181	LYS
1	G	2186	GLU
1	G	2188	GLN
1	G	2196	GLU

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	2240	HIS
1	G	2243	LYS
1	P	2013	LYS
1	P	2030	ARG
1	P	2033	LYS
1	P	2084	LEU
1	P	2092	ILE
1	P	2142	GLU
1	P	2145	LYS
1	P	2147	ILE
1	P	2150	THR
1	P	2175	ARG
1	P	2181	LYS
1	P	2186	GLU
1	P	2188	GLN
1	P	2196	GLU
1	P	2240	HIS
1	P	2243	LYS
1	P	2250	ARG
1	H	1013	LYS
1	H	1014	ASN
1	H	1030	ARG
1	H	1037	LEU
1	H	1091	ARG
1	H	1145	LYS
1	H	1146	SER
1	H	1147	ILE
1	H	1150	THR
1	H	1175	ARG
1	H	1186	GLU
1	H	1188	GLN
1	H	1196	GLU
1	H	1215	MET
1	H	1225	GLN
1	H	1239	SER
1	H	1243	LYS
1	H	1250	ARG
1	h	2013	LYS
1	h	2030	ARG
1	h	2033	LYS
1	h	2084	LEU
1	h	2092	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	h	2142	GLU
1	h	2145	LYS
1	h	2147	ILE
1	h	2150	THR
1	h	2175	ARG
1	h	2181	LYS
1	h	2186	GLU
1	h	2188	GLN
1	h	2196	GLU
1	h	2240	HIS
1	h	2243	LYS
1	h	2250	ARG
1	I	2013	LYS
1	I	2030	ARG
1	I	2033	LYS
1	I	2084	LEU
1	I	2092	ILE
1	I	2142	GLU
1	I	2145	LYS
1	I	2147	ILE
1	I	2150	THR
1	I	2175	ARG
1	I	2181	LYS
1	I	2186	GLU
1	I	2196	GLU
1	I	2240	HIS
1	I	2243	LYS
1	I	2250	ARG
1	i	1013	LYS
1	i	1014	ASN
1	i	1030	ARG
1	i	1037	LEU
1	i	1091	ARG
1	i	1145	LYS
1	i	1146	SER
1	i	1147	ILE
1	i	1150	THR
1	i	1175	ARG
1	i	1186	GLU
1	i	1188	GLN
1	i	1196	GLU
1	i	1215	MET

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	i	1225	GLN
1	i	1239	SER
1	i	1243	LYS
1	i	1250	ARG
1	J	1013	LYS
1	J	1014	ASN
1	J	1030	ARG
1	J	1037	LEU
1	J	1091	ARG
1	J	1145	LYS
1	J	1146	SER
1	J	1147	ILE
1	J	1150	THR
1	J	1175	ARG
1	J	1186	GLU
1	J	1188	GLN
1	J	1196	GLU
1	J	1215	MET
1	J	1225	GLN
1	J	1239	SER
1	J	1243	LYS
1	J	1250	ARG
1	j	2013	LYS
1	j	2030	ARG
1	j	2033	LYS
1	j	2084	LEU
1	j	2092	ILE
1	j	2142	GLU
1	j	2145	LYS
1	j	2147	ILE
1	j	2150	THR
1	j	2175	ARG
1	j	2181	LYS
1	j	2186	GLU
1	j	2188	GLN
1	j	2196	GLU
1	j	2240	HIS
1	j	2243	LYS
1	j	2250	ARG
1	K	1013	LYS
1	K	1014	ASN
1	K	1030	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	1037	LEU
1	K	1091	ARG
1	K	1145	LYS
1	K	1147	ILE
1	K	1150	THR
1	K	1175	ARG
1	K	1186	GLU
1	K	1196	GLU
1	K	1215	MET
1	K	1225	GLN
1	K	1239	SER
1	K	1243	LYS
1	K	1250	ARG
1	k	2013	LYS
1	k	2030	ARG
1	k	2033	LYS
1	k	2084	LEU
1	k	2092	ILE
1	k	2142	GLU
1	k	2145	LYS
1	k	2147	ILE
1	k	2150	THR
1	k	2175	ARG
1	k	2181	LYS
1	k	2186	GLU
1	k	2188	GLN
1	k	2196	GLU
1	k	2240	HIS
1	k	2243	LYS
1	k	2250	ARG
1	L	3013	LYS
1	L	3030	ARG
1	L	3033	LYS
1	L	3040	LYS
1	L	3145	LYS
1	L	3146	SER
1	L	3147	ILE
1	L	3150	THR
1	L	3175	ARG
1	L	3196	GLU
1	L	3228	ILE
1	L	3232	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	3235	LYS
1	L	3236	GLN
1	L	3243	LYS
1	l	2013	LYS
1	l	2030	ARG
1	l	2033	LYS
1	l	2084	LEU
1	l	2092	ILE
1	l	2142	GLU
1	l	2145	LYS
1	l	2147	ILE
1	l	2150	THR
1	l	2175	ARG
1	l	2181	LYS
1	l	2186	GLU
1	l	2188	GLN
1	l	2196	GLU
1	l	2240	HIS
1	l	2243	LYS
1	l	2250	ARG
1	M	2013	LYS
1	M	2030	ARG
1	M	2033	LYS
1	M	2084	LEU
1	M	2092	ILE
1	M	2142	GLU
1	M	2145	LYS
1	M	2147	ILE
1	M	2150	THR
1	M	2175	ARG
1	M	2181	LYS
1	M	2186	GLU
1	M	2188	GLN
1	M	2196	GLU
1	M	2240	HIS
1	M	2243	LYS
1	M	2250	ARG
1	m	3013	LYS
1	m	3030	ARG
1	m	3033	LYS
1	m	3040	LYS
1	m	3133	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	m	3145	LYS
1	m	3146	SER
1	m	3147	ILE
1	m	3150	THR
1	m	3175	ARG
1	m	3196	GLU
1	m	3226	GLN
1	m	3228	ILE
1	m	3232	GLU
1	m	3233	THR
1	m	3235	LYS
1	m	3236	GLN
1	m	3243	LYS
1	N	1013	LYS
1	N	1014	ASN
1	N	1030	ARG
1	N	1037	LEU
1	N	1091	ARG
1	N	1145	LYS
1	N	1146	SER
1	N	1147	ILE
1	N	1150	THR
1	N	1175	ARG
1	N	1186	GLU
1	N	1188	GLN
1	N	1196	GLU
1	N	1215	MET
1	N	1225	GLN
1	N	1239	SER
1	N	1240	HIS
1	N	1243	LYS
1	N	1250	ARG
1	Q	1013	LYS
1	Q	1014	ASN
1	Q	1030	ARG
1	Q	1037	LEU
1	Q	1091	ARG
1	Q	1145	LYS
1	Q	1146	SER
1	Q	1147	ILE
1	Q	1150	THR
1	Q	1175	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	1186	GLU
1	Q	1188	GLN
1	Q	1196	GLU
1	Q	1215	MET
1	Q	1225	GLN
1	Q	1239	SER
1	Q	1243	LYS
1	Q	1250	ARG
1	O	1013	LYS
1	O	1014	ASN
1	O	1030	ARG
1	O	1037	LEU
1	O	1091	ARG
1	O	1145	LYS
1	O	1146	SER
1	O	1147	ILE
1	O	1150	THR
1	O	1175	ARG
1	O	1186	GLU
1	O	1196	GLU
1	O	1215	MET
1	O	1225	GLN
1	O	1239	SER
1	O	1243	LYS
1	O	1250	ARG
1	o	3013	LYS
1	o	3030	ARG
1	o	3033	LYS
1	o	3040	LYS
1	o	3145	LYS
1	o	3146	SER
1	o	3147	ILE
1	o	3150	THR
1	o	3175	ARG
1	o	3196	GLU
1	o	3228	ILE
1	o	3232	GLU
1	o	3235	LYS
1	o	3236	GLN
1	o	3243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3152	HIS
1	A	3225	GLN
1	A	3226	GLN
1	A	3240	HIS
1	b	2017	GLN
1	d	3152	HIS
1	d	3225	GLN
1	d	3226	GLN
1	d	3240	HIS
1	e	2179	HIS
1	J	1225	GLN
1	K	1225	GLN
1	L	3152	HIS
1	L	3225	GLN
1	L	3226	GLN
1	L	3240	HIS
1	M	2230	ASN
1	m	3152	HIS
1	m	3225	GLN
1	m	3226	GLN
1	m	3240	HIS
1	o	3152	HIS
1	o	3225	GLN
1	o	3240	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 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 85 ligands modelled in this entry, 15 are monoatomic - leaving 70 for Mogul analysis.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	B	2011	-	4,4,4	0.82	0	6,6,6	0.60	0
3	V7O	M	5051	-	0,10,25	-	-	-	-	-
4	PO4	i	2071	-	4,4,4	0.82	0	6,6,6	0.48	0
3	V7O	D	5021	-	0,10,25	-	-	-	-	-
5	DUR	I	3072	-	17,17,17	1.85	4 (23%)	24,24,24	3.75	7 (29%)
5	DUR	a	3012	-	17,17,17	1.98	4 (23%)	24,24,24	3.97	9 (37%)
3	V7O	i	5034	-	0,10,25	-	-	-	-	-
5	DUR	G	3052	-	17,17,17	1.72	3 (17%)	24,24,24	3.70	9 (37%)
5	DUR	P	3122	-	17,17,17	1.66	3 (17%)	24,24,24	4.00	11 (45%)
5	DUR	i	2072	-	17,17,17	1.90	5 (29%)	24,24,24	3.69	8 (33%)
4	PO4	b	3021	-	4,4,4	0.78	0	6,6,6	0.55	0
5	DUR	l	3102	-	17,17,17	1.74	3 (17%)	24,24,24	3.66	9 (37%)
4	PO4	P	3121	-	4,4,4	0.85	0	6,6,6	0.52	0
4	PO4	M	3111	-	4,4,4	0.81	0	6,6,6	0.79	0
5	DUR	H	2062	-	17,17,17	1.76	3 (17%)	24,24,24	3.52	6 (25%)
5	DUR	e	3042	-	17,17,17	1.65	3 (17%)	24,24,24	3.74	7 (29%)
3	V7O	b	5013	-	0,10,25	-	-	-	-	-
4	PO4	G	3051	-	4,4,4	0.86	0	6,6,6	0.62	0
3	V7O	o	5054	-	0,10,25	-	-	-	-	-
3	V7O	M	5052	-	0,10,25	-	-	-	-	-
5	DUR	F	2052	-	17,17,17	1.87	6 (35%)	24,24,24	3.86	9 (37%)
3	V7O	R	5024	-	0,10,25	-	-	-	-	-
3	V7O	H	5031	-	0,10,25	-	-	-	-	-
5	DUR	B	2012	-	17,17,17	1.98	6 (35%)	24,24,24	3.84	8 (33%)
4	PO4	h	3061	-	4,4,4	0.86	0	6,6,6	0.49	0
4	PO4	O	2111	-	4,4,4	0.87	0	6,6,6	0.48	0
5	DUR	N	2102	-	17,17,17	1.75	4 (23%)	24,24,24	3.54	8 (33%)
3	V7O	j	5044	-	0,10,25	-	-	-	-	-
5	DUR	D	2032	-	17,17,17	1.80	3 (17%)	24,24,24	3.76	8 (33%)
4	PO4	J	2081	-	4,4,4	0.82	0	6,6,6	0.45	0
5	DUR	k	3092	-	17,17,17	1.92	5 (29%)	24,24,24	3.79	7 (29%)
4	PO4	Q	2121	-	4,4,4	0.94	0	6,6,6	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	H	2061	-	4,4,4	0.83	0	6,6,6	0.53	0
3	V7O	D	5022	-	0,10,25	-	-	-	-	-
5	DUR	C	2022	-	17,17,17	1.89	6 (35%)	24,24,24	4.19	10 (41%)
4	PO4	j	3081	-	4,4,4	0.79	0	6,6,6	0.65	0
4	PO4	e	3041	-	4,4,4	0.77	0	6,6,6	0.69	0
4	PO4	D	2031	-	4,4,4	0.81	0	6,6,6	0.50	0
3	V7O	A	5011	-	0,10,25	-	-	-	-	-
4	PO4	R	2131	-	4,4,4	0.90	0	6,6,6	0.36	0
5	DUR	b	3022	-	17,17,17	1.73	4 (23%)	24,24,24	3.94	9 (37%)
5	DUR	R	2132	-	17,17,17	1.91	4 (23%)	24,24,24	3.88	10 (41%)
5	DUR	M	3112	-	17,17,17	1.76	3 (17%)	24,24,24	3.81	7 (29%)
4	PO4	N	2101	-	4,4,4	0.88	0	6,6,6	0.53	0
3	V7O	h	5033	-	0,10,25	-	-	-	-	-
5	DUR	K	2092	-	17,17,17	1.85	5 (29%)	24,24,24	3.61	9 (37%)
3	V7O	J	5042	-	0,10,25	-	-	-	-	-
3	V7O	e	5023	-	0,10,25	-	-	-	-	-
4	PO4	F	2051	-	4,4,4	0.84	0	6,6,6	0.35	0
4	PO4	I	3071	-	4,4,4	0.74	0	6,6,6	0.71	0
3	V7O	Q	5053	-	0,10,25	-	-	-	-	-
5	DUR	j	3082	-	17,17,17	1.87	3 (17%)	24,24,24	4.05	11 (45%)
4	PO4	E	2041	-	4,4,4	0.77	0	6,6,6	0.63	0
3	V7O	k	5043	-	0,10,25	-	-	-	-	-
4	PO4	C	2021	-	4,4,4	0.83	0	6,6,6	0.51	0
4	PO4	k	3091	-	4,4,4	0.80	0	6,6,6	0.80	0
5	DUR	Q	2122	-	17,17,17	1.75	4 (23%)	24,24,24	3.47	6 (25%)
3	V7O	I	5032	-	0,10,25	-	-	-	-	-
5	DUR	E	2042	-	17,17,17	1.88	5 (29%)	24,24,24	3.79	8 (33%)
4	PO4	l	3101	-	4,4,4	0.84	0	6,6,6	0.51	0
5	DUR	c	3032	-	17,17,17	2.09	5 (29%)	24,24,24	4.39	11 (45%)
5	DUR	J	2082	-	17,17,17	2.05	4 (23%)	24,24,24	3.87	7 (29%)
4	PO4	a	3011	-	4,4,4	0.71	0	6,6,6	0.65	0
5	DUR	O	2112	-	17,17,17	1.89	6 (35%)	24,24,24	3.48	6 (25%)
5	DUR	h	3062	-	17,17,17	1.94	6 (35%)	24,24,24	3.60	6 (25%)
3	V7O	c	5014	-	0,10,25	-	-	-	-	-
3	V7O	L	5041	-	0,10,25	-	-	-	-	-
4	PO4	c	3031	-	4,4,4	0.94	0	6,6,6	0.93	1 (16%)
4	PO4	K	2091	-	4,4,4	0.89	0	6,6,6	0.39	0
3	V7O	B	5012	-	0,10,25	-	-	-	-	-

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
5	DUR	i	2072	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	I	3072	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	a	3012	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	P	3122	-	1/1/3/3	2/6/18/18	0/2/2/2
5	DUR	G	3052	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	l	3102	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	H	2062	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	e	3042	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	F	2052	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	B	2012	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	N	2102	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	D	2032	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	C	2022	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	R	2132	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	b	3022	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	M	3112	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	K	2092	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	j	3082	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	Q	2122	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	E	2042	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	c	3032	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	J	2082	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	O	2112	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	h	3062	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	k	3092	-	1/1/3/3	4/6/18/18	0/2/2/2

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	3012	DUR	C6-C5	5.38	1.47	1.35
5	J	2082	DUR	C6-C5	5.34	1.47	1.35
5	c	3032	DUR	C6-C5	5.16	1.47	1.35
5	i	2072	DUR	C6-C5	5.16	1.47	1.35
5	D	2032	DUR	C6-C5	5.08	1.46	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2042	DUR	C6-C5	5.07	1.46	1.35
5	O	2112	DUR	C6-C5	4.99	1.46	1.35
5	C	2022	DUR	C6-C5	4.99	1.46	1.35
5	R	2132	DUR	C6-C5	4.99	1.46	1.35
5	h	3062	DUR	C6-C5	4.95	1.46	1.35
5	I	3072	DUR	C6-C5	4.92	1.46	1.35
5	F	2052	DUR	C6-C5	4.86	1.46	1.35
5	Q	2122	DUR	C6-C5	4.84	1.46	1.35
5	j	3082	DUR	C6-C5	4.79	1.46	1.35
5	l	3102	DUR	C6-C5	4.76	1.46	1.35
5	M	3112	DUR	C6-C5	4.71	1.46	1.35
5	N	2102	DUR	C6-C5	4.71	1.46	1.35
5	B	2012	DUR	C6-C5	4.67	1.45	1.35
5	H	2062	DUR	C6-C5	4.66	1.45	1.35
5	K	2092	DUR	C6-C5	4.63	1.45	1.35
5	k	3092	DUR	C6-C5	4.63	1.45	1.35
5	b	3022	DUR	C6-C5	4.61	1.45	1.35
5	P	3122	DUR	C6-C5	4.60	1.45	1.35
5	e	3042	DUR	C6-C5	4.38	1.45	1.35
5	G	3052	DUR	C6-C5	4.27	1.45	1.35
5	c	3032	DUR	C2'-C1'	3.68	1.62	1.52
5	G	3052	DUR	C2'-C1'	3.55	1.62	1.52
5	a	3012	DUR	C2'-C1'	3.53	1.62	1.52
5	j	3082	DUR	C2'-C1'	3.48	1.62	1.52
5	P	3122	DUR	C2'-C1'	3.41	1.61	1.52
5	k	3092	DUR	C2'-C1'	3.37	1.61	1.52
5	J	2082	DUR	C2'-C1'	3.26	1.61	1.52
5	H	2062	DUR	C2'-C1'	3.23	1.61	1.52
5	J	2082	DUR	C2-N1	3.23	1.43	1.38
5	R	2132	DUR	C2'-C1'	3.13	1.61	1.52
5	b	3022	DUR	C2'-C1'	3.11	1.61	1.52
5	I	3072	DUR	C2'-C1'	3.09	1.61	1.52
5	i	2072	DUR	C2'-C1'	3.08	1.61	1.52
5	F	2052	DUR	C2'-C1'	3.05	1.60	1.52
5	B	2012	DUR	C2'-C1'	3.03	1.60	1.52
5	h	3062	DUR	C2-N3	3.01	1.43	1.38
5	e	3042	DUR	C2'-C1'	2.95	1.60	1.52
5	K	2092	DUR	C2'-C1'	2.91	1.60	1.52
5	l	3102	DUR	C2'-C1'	2.90	1.60	1.52
5	D	2032	DUR	C2'-C1'	2.89	1.60	1.52
5	h	3062	DUR	C2'-C1'	2.89	1.60	1.52
5	h	3062	DUR	C4-N3	2.88	1.43	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2012	DUR	C2-N1	2.79	1.42	1.38
5	M	3112	DUR	C2'-C1'	2.78	1.60	1.52
5	E	2042	DUR	C2'-C1'	2.78	1.60	1.52
5	N	2102	DUR	C2'-C1'	2.76	1.60	1.52
5	O	2112	DUR	C2'-C1'	2.75	1.60	1.52
5	K	2092	DUR	C2-N1	2.75	1.42	1.38
5	C	2022	DUR	C2'-C1'	2.72	1.60	1.52
5	B	2012	DUR	C4-N3	2.71	1.43	1.38
5	B	2012	DUR	C5-C4	2.70	1.49	1.43
5	R	2132	DUR	C2-N1	2.66	1.42	1.38
5	M	3112	DUR	C2-N1	2.63	1.42	1.38
5	E	2042	DUR	C2-N1	2.59	1.42	1.38
5	R	2132	DUR	C4-N3	2.57	1.43	1.38
5	c	3032	DUR	C2-N1	2.56	1.42	1.38
5	O	2112	DUR	C2-N3	2.52	1.42	1.38
5	Q	2122	DUR	C2'-C1'	2.52	1.59	1.52
5	C	2022	DUR	C2-N1	2.51	1.42	1.38
5	F	2052	DUR	C4-N3	2.51	1.43	1.38
5	k	3092	DUR	C4-N3	2.50	1.43	1.38
5	I	3072	DUR	C2-N3	2.47	1.42	1.38
5	a	3012	DUR	C2-N3	2.43	1.42	1.38
5	N	2102	DUR	C2-N1	2.42	1.42	1.38
5	O	2112	DUR	C4-N3	2.40	1.42	1.38
5	c	3032	DUR	C2-N3	2.40	1.42	1.38
5	C	2022	DUR	C2-N3	2.40	1.42	1.38
5	c	3032	DUR	C2'-C3'	2.39	1.59	1.52
5	C	2022	DUR	C5-C4	2.36	1.48	1.43
5	O	2112	DUR	C2-N1	2.34	1.42	1.38
5	h	3062	DUR	C5-C4	2.30	1.48	1.43
5	K	2092	DUR	C4-N3	2.28	1.42	1.38
5	P	3122	DUR	C2'-C3'	2.27	1.58	1.52
5	E	2042	DUR	C5-C4	2.27	1.48	1.43
5	E	2042	DUR	C2-N3	2.26	1.42	1.38
5	i	2072	DUR	C2-N3	2.25	1.42	1.38
5	k	3092	DUR	C2'-C3'	2.24	1.58	1.52
5	e	3042	DUR	C2-N1	2.24	1.42	1.38
5	b	3022	DUR	C4-N3	2.23	1.42	1.38
5	j	3082	DUR	C2'-C3'	2.23	1.58	1.52
5	k	3092	DUR	C5-C4	2.22	1.48	1.43
5	i	2072	DUR	C2-N1	2.21	1.42	1.38
5	J	2082	DUR	C5-C4	2.20	1.48	1.43
5	F	2052	DUR	C2-N3	2.18	1.41	1.38

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2012	DUR	C2'-C3'	2.18	1.58	1.52
5	F	2052	DUR	C2-N1	2.16	1.41	1.38
5	Q	2122	DUR	C4-N3	2.14	1.42	1.38
5	a	3012	DUR	C4-N3	2.13	1.42	1.38
5	D	2032	DUR	C2-N1	2.13	1.41	1.38
5	O	2112	DUR	C5-C4	2.09	1.48	1.43
5	F	2052	DUR	C5-C4	2.08	1.48	1.43
5	i	2072	DUR	C5-C4	2.08	1.48	1.43
5	Q	2122	DUR	C5-C4	2.08	1.48	1.43
5	C	2022	DUR	C2'-C3'	2.08	1.58	1.52
5	G	3052	DUR	C2-N1	2.06	1.41	1.38
5	I	3072	DUR	C4-N3	2.04	1.42	1.38
5	b	3022	DUR	C2'-C3'	2.04	1.58	1.52
5	N	2102	DUR	C4-N3	2.03	1.42	1.38
5	K	2092	DUR	C5-C4	2.03	1.48	1.43
5	l	3102	DUR	C2'-C3'	2.02	1.58	1.52
5	H	2062	DUR	C2-N1	2.01	1.41	1.38
5	h	3062	DUR	C2-N1	2.00	1.41	1.38

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2022	DUR	C2'-C1'-N1	16.80	152.46	113.77
5	c	3032	DUR	C2'-C1'-N1	16.53	151.85	113.77
5	F	2052	DUR	C2'-C1'-N1	15.95	150.50	113.77
5	I	3072	DUR	C2'-C1'-N1	15.69	149.91	113.77
5	j	3082	DUR	C2'-C1'-N1	15.58	149.65	113.77
5	h	3062	DUR	C2'-C1'-N1	15.54	149.56	113.77
5	P	3122	DUR	C2'-C1'-N1	15.46	149.37	113.77
5	B	2012	DUR	C2'-C1'-N1	15.40	149.24	113.77
5	b	3022	DUR	C2'-C1'-N1	15.35	149.12	113.77
5	J	2082	DUR	C2'-C1'-N1	15.32	149.05	113.77
5	i	2072	DUR	C2'-C1'-N1	15.32	149.05	113.77
5	K	2092	DUR	C2'-C1'-N1	15.31	149.02	113.77
5	e	3042	DUR	C2'-C1'-N1	15.29	148.99	113.77
5	M	3112	DUR	C2'-C1'-N1	15.29	148.98	113.77
5	R	2132	DUR	C2'-C1'-N1	15.22	148.82	113.77
5	k	3092	DUR	C2'-C1'-N1	15.13	148.60	113.77
5	D	2032	DUR	C2'-C1'-N1	15.08	148.51	113.77
5	a	3012	DUR	C2'-C1'-N1	14.92	148.14	113.77
5	Q	2122	DUR	C2'-C1'-N1	14.90	148.08	113.77
5	O	2112	DUR	C2'-C1'-N1	14.81	147.87	113.77

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2042	DUR	C2'-C1'-N1	14.79	147.84	113.77
5	G	3052	DUR	C2'-C1'-N1	14.74	147.72	113.77
5	l	3102	DUR	C2'-C1'-N1	14.61	147.43	113.77
5	N	2102	DUR	C2'-C1'-N1	14.58	147.34	113.77
5	H	2062	DUR	C2'-C1'-N1	14.40	146.92	113.77
5	c	3032	DUR	O4'-C1'-C2'	-6.93	93.16	106.25
5	C	2022	DUR	O4'-C1'-C2'	-6.52	93.94	106.25
5	j	3082	DUR	N3-C2-N1	6.36	123.33	114.89
5	P	3122	DUR	O4'-C1'-C2'	-6.00	94.91	106.25
5	b	3022	DUR	O4'-C1'-C2'	-6.00	94.92	106.25
5	a	3012	DUR	O4'-C1'-C2'	-5.94	95.03	106.25
5	M	3112	DUR	O4'-C1'-C2'	-5.76	95.37	106.25
5	E	2042	DUR	O4'-C1'-C2'	-5.75	95.39	106.25
5	c	3032	DUR	N3-C2-N1	5.70	122.46	114.89
5	B	2012	DUR	O4'-C1'-C2'	-5.66	95.55	106.25
5	c	3032	DUR	C6-N1-C2	-5.47	113.99	120.99
5	J	2082	DUR	O4'-C1'-C2'	-5.46	95.94	106.25
5	k	3092	DUR	N3-C2-N1	5.34	121.97	114.89
5	R	2132	DUR	O4'-C1'-C2'	-5.30	96.24	106.25
5	e	3042	DUR	O4'-C1'-C2'	-5.23	96.36	106.25
5	j	3082	DUR	O4'-C1'-C2'	-5.21	96.40	106.25
5	E	2042	DUR	N3-C2-N1	5.19	121.78	114.89
5	C	2022	DUR	N3-C2-N1	5.18	121.77	114.89
5	a	3012	DUR	C6-N1-C2	-5.16	114.39	120.99
5	a	3012	DUR	N3-C2-N1	5.11	121.67	114.89
5	k	3092	DUR	O4'-C1'-C2'	-5.06	96.69	106.25
5	l	3102	DUR	N3-C2-N1	5.02	121.56	114.89
5	M	3112	DUR	N3-C2-N1	4.97	121.48	114.89
5	P	3122	DUR	C6-N1-C2	-4.91	114.71	120.99
5	b	3022	DUR	C6-N1-C2	-4.89	114.73	120.99
5	D	2032	DUR	N3-C2-N1	4.85	121.33	114.89
5	i	2072	DUR	N3-C2-N1	4.84	121.31	114.89
5	P	3122	DUR	N3-C2-N1	4.83	121.30	114.89
5	a	3012	DUR	O4'-C1'-N1	4.81	116.47	107.86
5	B	2012	DUR	N3-C2-N1	4.77	121.23	114.89
5	G	3052	DUR	O4'-C1'-C2'	-4.75	97.27	106.25
5	D	2032	DUR	O4'-C1'-C2'	-4.75	97.27	106.25
5	J	2082	DUR	N3-C2-N1	4.72	121.16	114.89
5	F	2052	DUR	O4'-C1'-C2'	-4.70	97.37	106.25
5	I	3072	DUR	O4'-C1'-C2'	-4.66	97.44	106.25
5	F	2052	DUR	N3-C2-N1	4.55	120.92	114.89
5	i	2072	DUR	O4'-C1'-C2'	-4.52	97.72	106.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	3072	DUR	N3-C2-N1	4.49	120.86	114.89
5	Q	2122	DUR	N3-C2-N1	4.47	120.83	114.89
5	e	3042	DUR	N3-C2-N1	4.45	120.79	114.89
5	R	2132	DUR	N3-C2-N1	4.42	120.76	114.89
5	l	3102	DUR	O4'-C1'-C2'	-4.41	97.92	106.25
5	J	2082	DUR	C6-N1-C2	-4.39	115.38	120.99
5	E	2042	DUR	O4'-C1'-N1	4.38	115.69	107.86
5	H	2062	DUR	O4'-C1'-C2'	-4.32	98.09	106.25
5	j	3082	DUR	O2-C2-N3	-4.30	113.50	121.50
5	N	2102	DUR	N3-C2-N1	4.26	120.55	114.89
5	D	2032	DUR	C6-N1-C2	-4.26	115.55	120.99
5	R	2132	DUR	C6-N1-C2	-4.26	115.55	120.99
5	j	3082	DUR	C6-N1-C2	-4.24	115.57	120.99
5	H	2062	DUR	N3-C2-N1	4.21	120.48	114.89
5	J	2082	DUR	O2-C2-N3	-4.16	113.76	121.50
5	b	3022	DUR	O4'-C1'-N1	4.12	115.22	107.86
5	k	3092	DUR	C6-N1-C2	-4.10	115.74	120.99
5	C	2022	DUR	C5'-C4'-C3'	4.04	125.02	114.81
5	c	3032	DUR	O4'-C4'-C5'	-4.00	100.56	109.21
5	l	3102	DUR	C6-N1-C2	-3.99	115.89	120.99
5	O	2112	DUR	N3-C2-N1	3.98	120.17	114.89
5	O	2112	DUR	O4'-C1'-C2'	-3.97	98.76	106.25
5	R	2132	DUR	O4'-C1'-N1	3.96	114.95	107.86
5	G	3052	DUR	O4'-C4'-C5'	-3.93	100.72	109.21
5	E	2042	DUR	C6-N1-C2	-3.89	116.01	120.99
5	K	2092	DUR	N3-C2-N1	3.88	120.04	114.89
5	c	3032	DUR	O4'-C1'-N1	3.83	114.70	107.86
5	H	2062	DUR	O4'-C1'-N1	3.80	114.66	107.86
5	G	3052	DUR	O4'-C1'-N1	3.77	114.61	107.86
5	K	2092	DUR	O4'-C1'-C2'	-3.76	99.14	106.25
5	h	3062	DUR	O4'-C1'-C2'	-3.76	99.15	106.25
5	b	3022	DUR	N3-C2-N1	3.75	119.87	114.89
5	G	3052	DUR	C6-N1-C2	-3.72	116.23	120.99
5	G	3052	DUR	N3-C2-N1	3.70	119.81	114.89
5	F	2052	DUR	C6-N1-C2	-3.68	116.28	120.99
5	l	3102	DUR	O4'-C1'-N1	3.67	114.43	107.86
5	B	2012	DUR	O2-C2-N3	-3.62	114.77	121.50
5	i	2072	DUR	C6-N1-C2	-3.61	116.38	120.99
5	C	2022	DUR	C6-N1-C2	-3.60	116.39	120.99
5	M	3112	DUR	C6-N1-C2	-3.56	116.44	120.99
5	P	3122	DUR	O4'-C1'-N1	3.55	114.21	107.86
5	c	3032	DUR	O2-C2-N3	-3.53	114.93	121.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	2102	DUR	O4'-C1'-C2'	-3.51	99.61	106.25
5	N	2102	DUR	C6-N1-C2	-3.49	116.53	120.99
5	h	3062	DUR	C5'-C4'-C3'	3.47	123.57	114.81
5	j	3082	DUR	O4'-C4'-C5'	-3.45	101.76	109.21
5	I	3072	DUR	C6-N1-C2	-3.44	116.59	120.99
5	H	2062	DUR	C6-N1-C2	-3.37	116.68	120.99
5	M	3112	DUR	O2-C2-N3	-3.35	115.26	121.50
5	j	3082	DUR	O4'-C1'-N1	3.30	113.76	107.86
5	h	3062	DUR	N3-C2-N1	3.29	119.26	114.89
5	R	2132	DUR	O2-C2-N3	-3.28	115.40	121.50
5	D	2032	DUR	O4'-C1'-N1	3.27	113.71	107.86
5	e	3042	DUR	O2-C2-N3	-3.26	115.43	121.50
5	e	3042	DUR	O4'-C1'-N1	3.25	113.66	107.86
5	B	2012	DUR	O4'-C1'-N1	3.19	113.56	107.86
5	N	2102	DUR	O2-C2-N3	-3.18	115.59	121.50
5	P	3122	DUR	O2-C2-N3	-3.15	115.63	121.50
5	F	2052	DUR	C5'-C4'-C3'	3.14	122.75	114.81
5	k	3092	DUR	O4'-C1'-N1	3.13	113.46	107.86
5	b	3022	DUR	C5-C6-N1	3.12	127.04	121.81
5	k	3092	DUR	O3'-C3'-C2'	3.08	121.93	110.90
5	c	3032	DUR	C5'-C4'-C3'	3.07	122.58	114.81
5	Q	2122	DUR	O4'-C1'-C2'	-3.07	100.45	106.25
5	K	2092	DUR	O2-C2-N3	-3.07	115.79	121.50
5	h	3062	DUR	O4'-C4'-C5'	-3.06	102.59	109.21
5	l	3102	DUR	O2-C2-N3	-3.05	115.81	121.50
5	J	2082	DUR	O4'-C1'-N1	3.05	113.31	107.86
5	M	3112	DUR	O4'-C1'-N1	3.04	113.30	107.86
5	e	3042	DUR	C6-N1-C2	-3.03	117.11	120.99
5	I	3072	DUR	C5'-C4'-C3'	3.03	122.47	114.81
5	R	2132	DUR	C1'-N1-C2	3.01	123.58	117.64
5	B	2012	DUR	C5'-C4'-C3'	3.00	122.39	114.81
5	O	2112	DUR	O4'-C1'-N1	2.91	113.07	107.86
5	N	2102	DUR	O4'-C1'-N1	2.90	113.05	107.86
5	B	2012	DUR	C6-N1-C2	-2.89	117.29	120.99
5	D	2032	DUR	O2-C2-N3	-2.88	116.14	121.50
5	Q	2122	DUR	C6-N1-C2	-2.85	117.34	120.99
5	G	3052	DUR	C5'-C4'-C3'	2.84	121.99	114.81
5	F	2052	DUR	O4'-C4'-C5'	-2.84	103.08	109.21
5	O	2112	DUR	C6-N1-C2	-2.81	117.40	120.99
5	D	2032	DUR	C5'-C4'-C3'	2.80	121.89	114.81
5	E	2042	DUR	O2-C2-N3	-2.78	116.32	121.50
5	c	3032	DUR	C1'-N1-C2	2.77	123.10	117.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2062	DUR	O2-C2-N3	-2.77	116.34	121.50
5	k	3092	DUR	O2-C2-N3	-2.76	116.35	121.50
5	a	3012	DUR	C5-C4-N3	-2.72	110.78	114.84
5	e	3042	DUR	C5'-C4'-C3'	2.69	121.61	114.81
5	K	2092	DUR	C5'-C4'-C3'	2.67	121.55	114.81
5	i	2072	DUR	O2-C2-N3	-2.66	116.54	121.50
5	c	3032	DUR	C5-C6-N1	2.64	126.23	121.81
5	G	3052	DUR	O2-C2-N3	-2.61	116.64	121.50
5	C	2022	DUR	O2-C2-N3	-2.58	116.70	121.50
5	c	3032	DUR	O3'-C3'-C2'	2.56	120.05	110.90
5	F	2052	DUR	O2-C2-N3	-2.56	116.74	121.50
5	b	3022	DUR	O2-C2-N3	-2.53	116.79	121.50
5	P	3122	DUR	O3'-C3'-C2'	2.53	119.95	110.90
5	K	2092	DUR	O4'-C4'-C5'	-2.53	103.75	109.21
5	a	3012	DUR	O2-C2-N3	-2.52	116.80	121.50
5	R	2132	DUR	C5'-C4'-C3'	2.50	121.12	114.81
5	C	2022	DUR	O4'-C1'-N1	2.49	112.31	107.86
5	i	2072	DUR	O4'-C1'-N1	2.48	112.30	107.86
5	K	2092	DUR	C6-N1-C2	-2.47	117.83	120.99
5	l	3102	DUR	C5'-C4'-C3'	2.43	120.96	114.81
5	j	3082	DUR	O3'-C3'-C2'	2.43	119.59	110.90
5	E	2042	DUR	C5'-C4'-C3'	2.39	120.85	114.81
5	P	3122	DUR	O4-C4-C5	2.35	129.30	125.16
5	P	3122	DUR	C5-C6-N1	2.34	125.73	121.81
5	N	2102	DUR	C1'-N1-C2	2.34	122.25	117.64
5	I	3072	DUR	O4'-C4'-C5'	-2.33	104.18	109.21
5	B	2012	DUR	O4'-C4'-C5'	-2.32	104.20	109.21
5	P	3122	DUR	O4'-C4'-C5'	-2.31	104.21	109.21
5	j	3082	DUR	C5'-C4'-C3'	2.31	120.66	114.81
5	i	2072	DUR	O3'-C3'-C2'	2.31	119.15	110.90
5	F	2052	DUR	C1'-N1-C2	2.30	122.17	117.64
5	b	3022	DUR	O4'-C4'-C5'	-2.30	104.25	109.21
5	i	2072	DUR	C5'-C4'-C3'	2.30	120.61	114.81
5	E	2042	DUR	O4'-C4'-C5'	-2.28	104.29	109.21
5	I	3072	DUR	O4'-C1'-N1	2.28	111.93	107.86
5	K	2092	DUR	C1'-N1-C2	2.27	122.11	117.64
5	R	2132	DUR	O4'-C4'-C5'	-2.26	104.33	109.21
5	h	3062	DUR	C6-N1-C2	-2.25	118.12	120.99
5	j	3082	DUR	C1'-N1-C2	2.23	122.03	117.64
5	a	3012	DUR	C5-C6-N1	2.23	125.54	121.81
5	O	2112	DUR	C5'-C4'-C3'	2.22	120.43	114.81
5	R	2132	DUR	C5-C6-N1	2.22	125.52	121.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	2122	DUR	O3'-C3'-C2'	2.21	118.81	110.90
5	D	2032	DUR	O4'-C4'-C5'	-2.20	104.46	109.21
5	P	3122	DUR	C1'-N1-C6	2.20	125.88	121.55
5	Q	2122	DUR	O2-C2-N3	-2.18	117.43	121.50
5	F	2052	DUR	O4'-C1'-N1	2.16	111.73	107.86
5	C	2022	DUR	O4'-C4'-C5'	-2.14	104.58	109.21
5	a	3012	DUR	O3'-C3'-C2'	2.14	118.56	110.90
5	M	3112	DUR	O3'-C3'-C2'	2.13	118.53	110.90
5	G	3052	DUR	O3'-C3'-C2'	2.12	118.47	110.90
5	C	2022	DUR	O4'-C4'-C3'	-2.10	100.78	105.67
4	c	3031	PO4	O4-P-O2	2.06	114.57	107.97
5	N	2102	DUR	C5'-C4'-C3'	2.05	119.99	114.81
5	b	3022	DUR	C1'-N1-C2	2.05	121.67	117.64
5	J	2082	DUR	O3'-C3'-C4'	-2.04	102.29	110.10
5	l	3102	DUR	O4'-C4'-C5'	-2.04	104.80	109.21
5	j	3082	DUR	C4-N3-C2	-2.03	123.90	126.58
5	l	3102	DUR	O3'-C3'-C2'	2.02	118.11	110.90
5	K	2092	DUR	O4'-C1'-N1	2.00	111.44	107.86
5	C	2022	DUR	O3'-C3'-C4'	-2.00	102.45	110.10

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	a	3012	DUR	C1'
5	B	2012	DUR	C1'
5	b	3022	DUR	C1'
5	C	2022	DUR	C1'
5	c	3032	DUR	C1'
5	D	2032	DUR	C1'
5	E	2042	DUR	C1'
5	e	3042	DUR	C1'
5	F	2052	DUR	C1'
5	R	2132	DUR	C1'
5	G	3052	DUR	C1'
5	P	3122	DUR	C1'
5	H	2062	DUR	C1'
5	h	3062	DUR	C1'
5	I	3072	DUR	C1'
5	i	2072	DUR	C1'
5	J	2082	DUR	C1'
5	j	3082	DUR	C1'
5	K	2092	DUR	C1'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
5	k	3092	DUR	C1'
5	l	3102	DUR	C1'
5	M	3112	DUR	C1'
5	N	2102	DUR	C1'
5	Q	2122	DUR	C1'
5	O	2112	DUR	C1'

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	3112	DUR	C2'-C1'-N1-C2
5	k	3092	DUR	C3'-C4'-C5'-O5'
5	Q	2122	DUR	C3'-C4'-C5'-O5'
5	k	3092	DUR	O4'-C4'-C5'-O5'
5	Q	2122	DUR	O4'-C4'-C5'-O5'
5	F	2052	DUR	C3'-C4'-C5'-O5'
5	h	3062	DUR	C3'-C4'-C5'-O5'
5	I	3072	DUR	C3'-C4'-C5'-O5'
5	J	2082	DUR	C3'-C4'-C5'-O5'
5	K	2092	DUR	C3'-C4'-C5'-O5'
5	N	2102	DUR	C3'-C4'-C5'-O5'
5	O	2112	DUR	C3'-C4'-C5'-O5'
5	M	3112	DUR	C2'-C1'-N1-C6
5	b	3022	DUR	C2'-C1'-N1-C2
5	C	2022	DUR	C2'-C1'-N1-C2
5	c	3032	DUR	C2'-C1'-N1-C2
5	E	2042	DUR	C2'-C1'-N1-C2
5	e	3042	DUR	C2'-C1'-N1-C2
5	P	3122	DUR	C2'-C1'-N1-C2
5	I	3072	DUR	C2'-C1'-N1-C2
5	J	2082	DUR	C2'-C1'-N1-C2
5	k	3092	DUR	C2'-C1'-N1-C2
5	I	3072	DUR	O4'-C4'-C5'-O5'
5	i	2072	DUR	C3'-C4'-C5'-O5'
5	K	2092	DUR	O4'-C4'-C5'-O5'
5	F	2052	DUR	O4'-C4'-C5'-O5'
5	h	3062	DUR	O4'-C4'-C5'-O5'
5	i	2072	DUR	O4'-C4'-C5'-O5'
5	J	2082	DUR	O4'-C4'-C5'-O5'
5	N	2102	DUR	O4'-C4'-C5'-O5'
5	C	2022	DUR	C2'-C1'-N1-C6
5	E	2042	DUR	C2'-C1'-N1-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	e	3042	DUR	C2'-C1'-N1-C6
5	P	3122	DUR	C2'-C1'-N1-C6
5	J	2082	DUR	C2'-C1'-N1-C6
5	a	3012	DUR	C2'-C1'-N1-C2
5	B	2012	DUR	C2'-C1'-N1-C2
5	D	2032	DUR	C2'-C1'-N1-C2
5	F	2052	DUR	C2'-C1'-N1-C2
5	R	2132	DUR	C2'-C1'-N1-C2
5	H	2062	DUR	C2'-C1'-N1-C2
5	h	3062	DUR	C2'-C1'-N1-C2
5	i	2072	DUR	C2'-C1'-N1-C2
5	j	3082	DUR	C2'-C1'-N1-C2
5	O	2112	DUR	C2'-C1'-N1-C2
5	O	2112	DUR	O4'-C4'-C5'-O5'
5	l	3102	DUR	C3'-C4'-C5'-O5'
5	M	3112	DUR	C3'-C4'-C5'-O5'
5	e	3042	DUR	O4'-C4'-C5'-O5'
5	H	2062	DUR	O4'-C4'-C5'-O5'
5	l	3102	DUR	O4'-C4'-C5'-O5'
5	M	3112	DUR	O4'-C4'-C5'-O5'
5	a	3012	DUR	C3'-C4'-C5'-O5'
5	c	3032	DUR	C3'-C4'-C5'-O5'
5	e	3042	DUR	C3'-C4'-C5'-O5'
5	H	2062	DUR	C3'-C4'-C5'-O5'
5	j	3082	DUR	C3'-C4'-C5'-O5'
5	F	2052	DUR	C2'-C1'-N1-C6
5	G	3052	DUR	C2'-C1'-N1-C2
5	K	2092	DUR	C2'-C1'-N1-C2
5	a	3012	DUR	O4'-C4'-C5'-O5'
5	R	2132	DUR	C3'-C4'-C5'-O5'
5	B	2012	DUR	C2'-C1'-N1-C6
5	b	3022	DUR	C2'-C1'-N1-C6
5	c	3032	DUR	C2'-C1'-N1-C6
5	D	2032	DUR	C2'-C1'-N1-C6
5	H	2062	DUR	C2'-C1'-N1-C6
5	I	3072	DUR	C2'-C1'-N1-C6
5	i	2072	DUR	C2'-C1'-N1-C6
5	K	2092	DUR	C2'-C1'-N1-C6
5	k	3092	DUR	C2'-C1'-N1-C6
5	O	2112	DUR	C2'-C1'-N1-C6
5	l	3102	DUR	C2'-C1'-N1-C2
5	Q	2122	DUR	C2'-C1'-N1-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	j	3082	DUR	O4'-C4'-C5'-O5'
5	c	3032	DUR	O4'-C4'-C5'-O5'
5	R	2132	DUR	O4'-C4'-C5'-O5'
5	B	2012	DUR	C3'-C4'-C5'-O5'
5	a	3012	DUR	C2'-C1'-N1-C6
5	R	2132	DUR	C2'-C1'-N1-C6
5	G	3052	DUR	C2'-C1'-N1-C6
5	h	3062	DUR	C2'-C1'-N1-C6
5	j	3082	DUR	C2'-C1'-N1-C6
5	Q	2122	DUR	C2'-C1'-N1-C6
5	N	2102	DUR	C2'-C1'-N1-C2
5	E	2042	DUR	O4'-C4'-C5'-O5'
5	l	3102	DUR	C2'-C1'-N1-C6
5	E	2042	DUR	C3'-C4'-C5'-O5'
5	G	3052	DUR	C3'-C4'-C5'-O5'
5	G	3052	DUR	O4'-C4'-C5'-O5'
5	N	2102	DUR	C2'-C1'-N1-C6
5	D	2032	DUR	O4'-C4'-C5'-O5'
5	B	2012	DUR	O4'-C4'-C5'-O5'
5	C	2022	DUR	C3'-C4'-C5'-O5'
5	D	2032	DUR	C3'-C4'-C5'-O5'
5	C	2022	DUR	O4'-C4'-C5'-O5'
5	b	3022	DUR	C3'-C4'-C5'-O5'
5	b	3022	DUR	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	5051	V7O	3	0
3	D	5021	V7O	2	0
5	G	3052	DUR	1	0
5	P	3122	DUR	1	0
4	P	3121	PO4	2	0
4	G	3051	PO4	1	0
3	M	5052	V7O	4	0
3	H	5031	V7O	2	0
4	O	2111	PO4	1	0
3	D	5022	V7O	3	0
5	C	2022	DUR	1	0
3	A	5011	V7O	1	0
3	J	5042	V7O	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2021	PO4	1	0
3	I	5032	V7O	3	0
3	L	5041	V7O	1	0
3	B	5012	V7O	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.