wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2024 – 09:35 AM EDT

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)

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

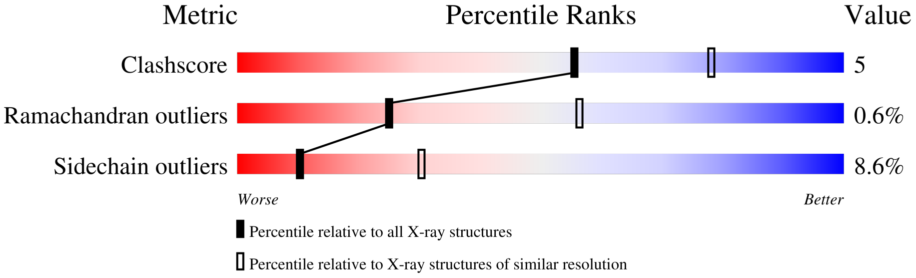
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 >=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 <=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	

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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	1880	1178	328	363	11	0	0	0
1	a	242	1817	1141	318	348	10	0	0	0
1	B	246	1851	1162	323	355	11	0	0	0
1	b	242	1817	1141	318	348	10	0	0	0
1	C	246	1851	1162	323	355	11	0	0	0
1	c	242	1817	1141	318	348	10	0	0	0
1	D	246	1851	1162	323	355	11	0	0	0
1	d	250	1880	1178	328	363	11	0	0	0
1	E	246	1851	1162	323	355	11	0	0	0
1	e	242	1817	1141	318	348	10	0	0	0
1	F	246	1851	1162	323	355	11	0	0	0
1	R	246	1851	1162	323	355	11	0	0	0
1	G	242	1817	1141	318	348	10	0	0	0
1	P	242	1817	1141	318	348	10	0	0	0
1	H	246	1851	1162	323	355	11	0	0	0
1	h	242	1817	1141	318	348	10	0	0	0

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

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

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

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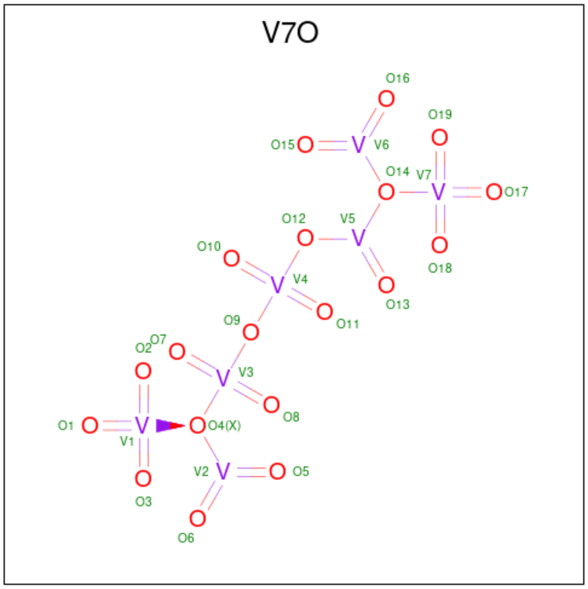
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	1	Total K 1 1	0	0
2	G	1	Total K 1 1	0	0
2	h	1	Total K 1 1	0	0
2	i	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	K	1	Total K 1 1	0	0
2	L	1	Total K 1 1	0	0
2	M	1	Total K 1 1	0	0
2	N	1	Total K 1 1	0	0
2	o	1	Total K 1 1	0	0

- 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

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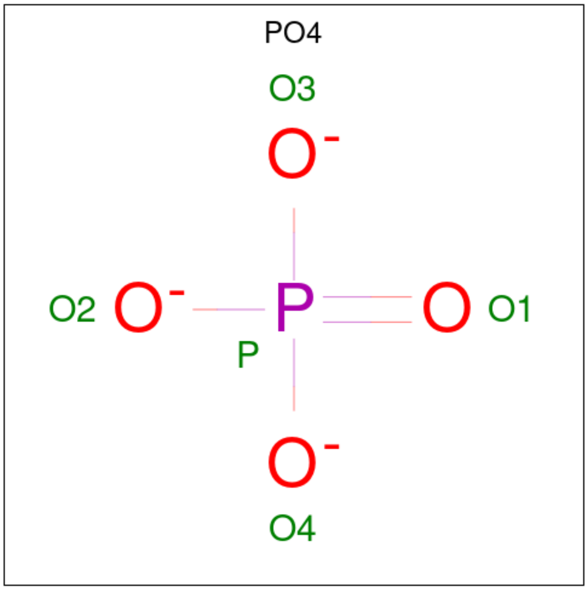
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O V 11 8 3	0	0
3	b	1	Total O V 11 8 3	0	0
3	c	1	Total O V 11 8 3	0	0
3	D	1	Total O V 11 8 3	0	0
3	D	1	Total O V 11 8 3	0	0
3	e	1	Total O V 11 8 3	0	0
3	R	1	Total O V 11 8 3	0	0
3	H	1	Total O V 11 8 3	0	0
3	h	1	Total O V 11 8 3	0	0
3	I	1	Total O V 11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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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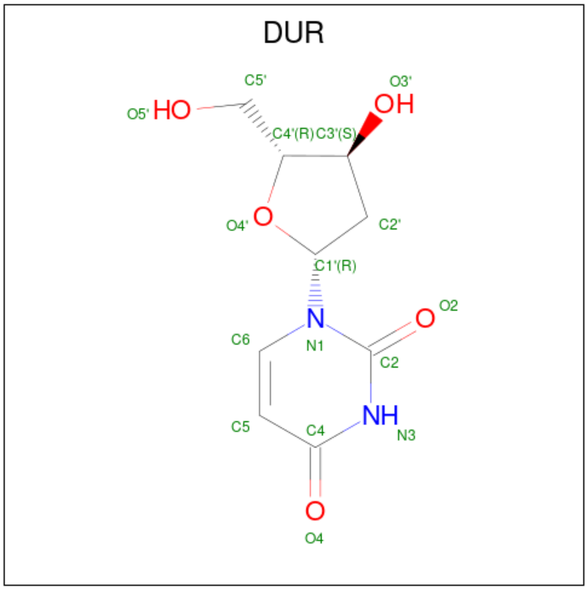
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total O P 5 4 1	0	0
4	i	1	Total O P 5 4 1	0	0
4	J	1	Total O P 5 4 1	0	0
4	j	1	Total O P 5 4 1	0	0
4	K	1	Total O P 5 4 1	0	0
4	k	1	Total O P 5 4 1	0	0
4	l	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	N	1	Total O P 5 4 1	0	0
4	Q	1	Total O P 5 4 1	0	0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

- Molecule 5 is 2'-DEOXYURIDINE (three-letter code: DUR) (formula: $C_9H_{12}N_2O_5$).



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

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

- Molecule 6 is water.

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

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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

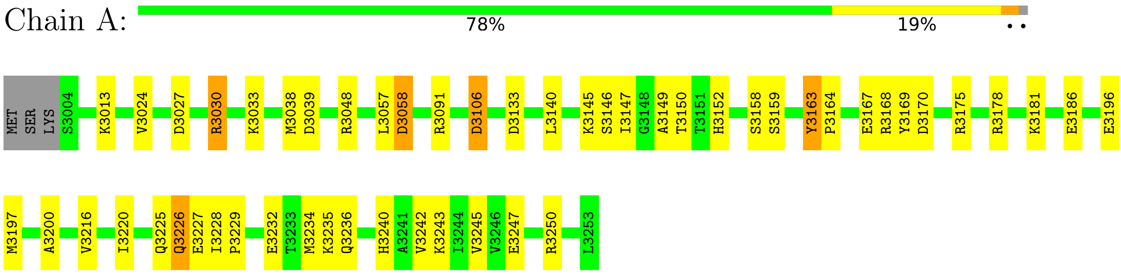
3 Residue-property plots ⓘ

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.

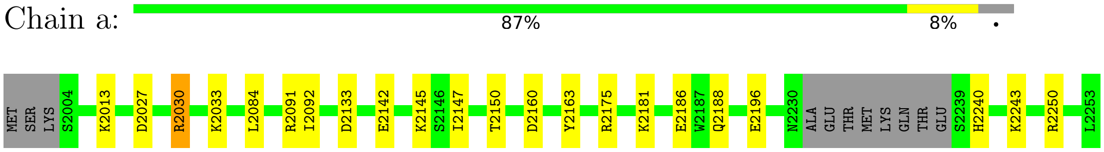
- Molecule 1: Uridine phosphorylase

Chain A:



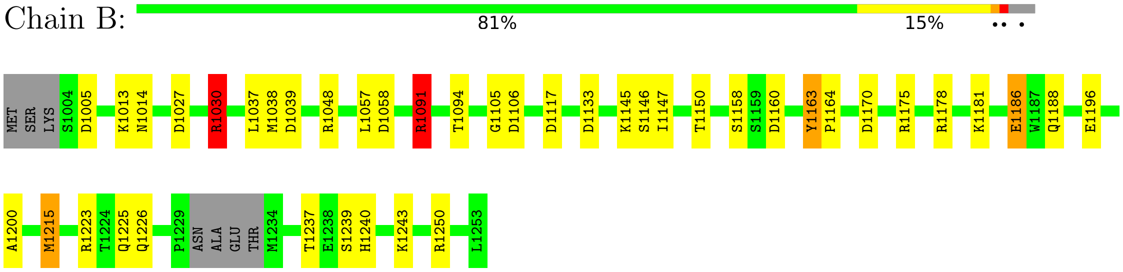
- Molecule 1: Uridine phosphorylase

Chain a:



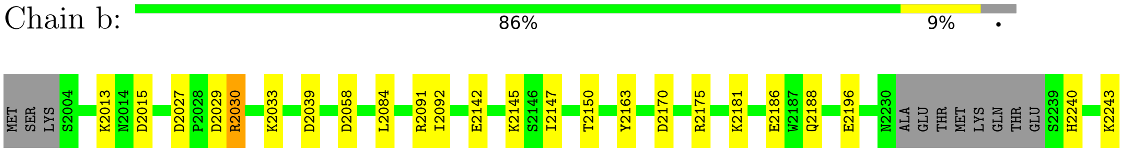
- Molecule 1: Uridine phosphorylase

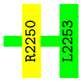
Chain B:



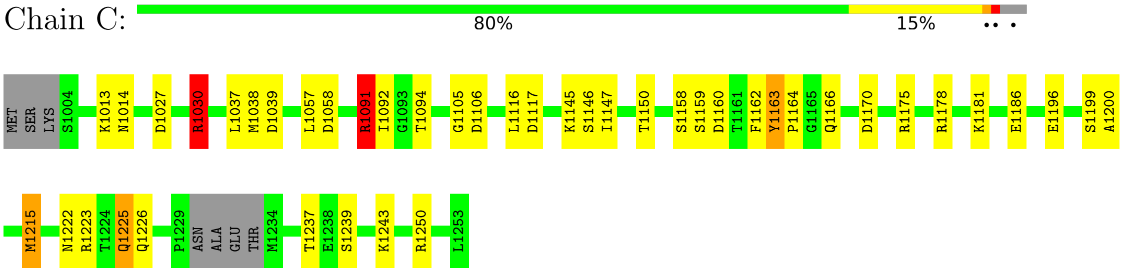
- Molecule 1: Uridine phosphorylase

Chain b:

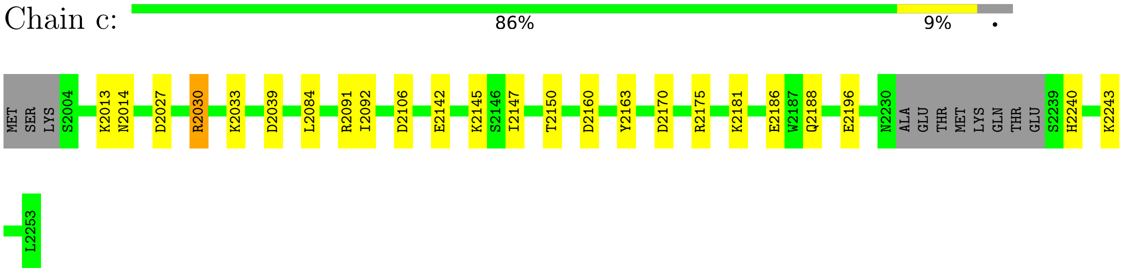




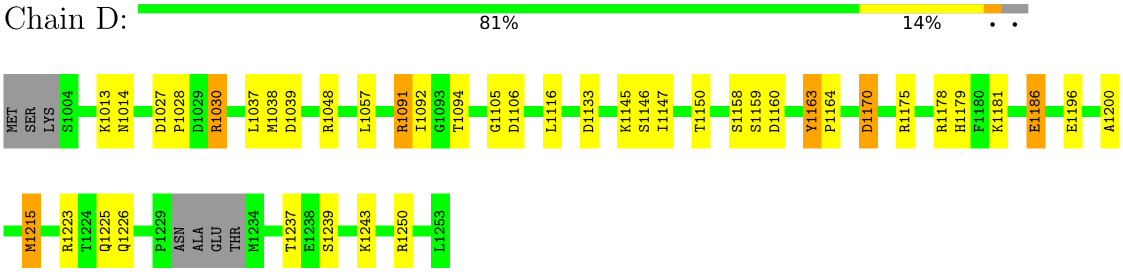
- Molecule 1: Uridine phosphorylase



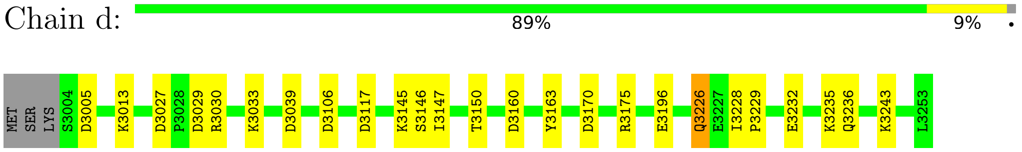
- Molecule 1: Uridine phosphorylase



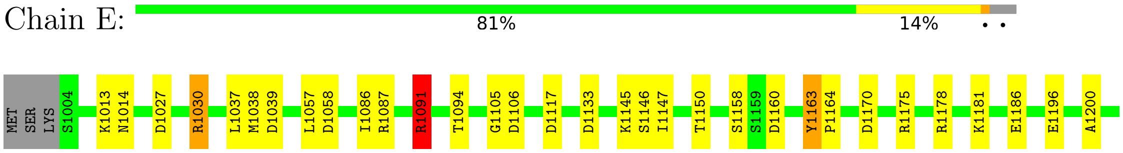
- Molecule 1: Uridine phosphorylase

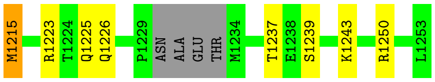


- Molecule 1: Uridine phosphorylase



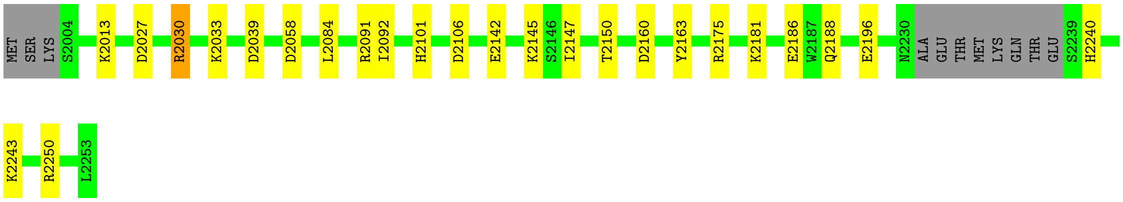
- Molecule 1: Uridine phosphorylase





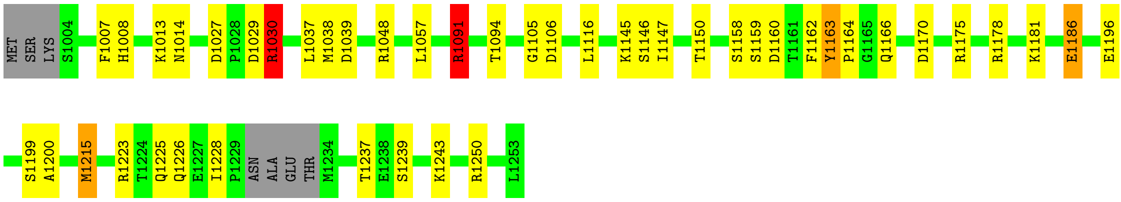
- Molecule 1: Uridine phosphorylase

Chain e:



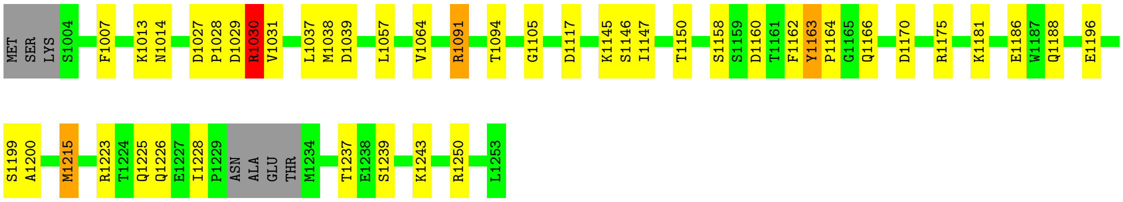
- Molecule 1: Uridine phosphorylase

Chain F:



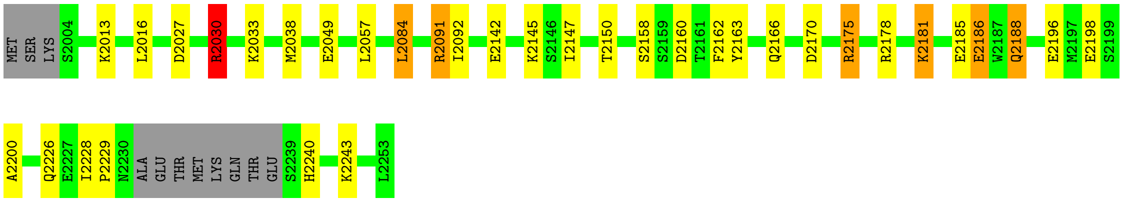
- Molecule 1: Uridine phosphorylase

Chain R:



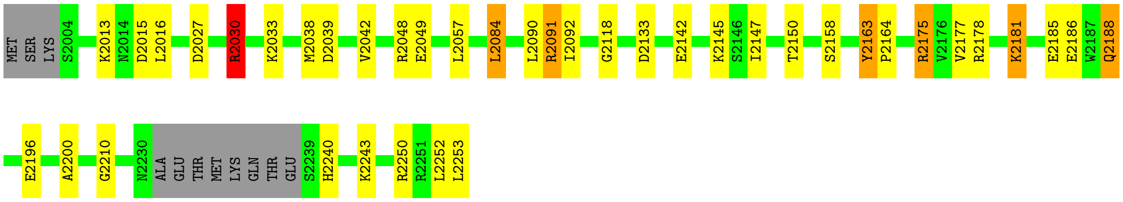
- Molecule 1: Uridine phosphorylase

Chain G:



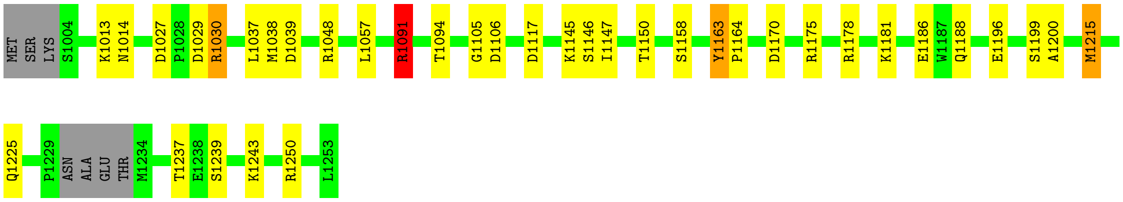
- Molecule 1: Uridine phosphorylase

Chain P:



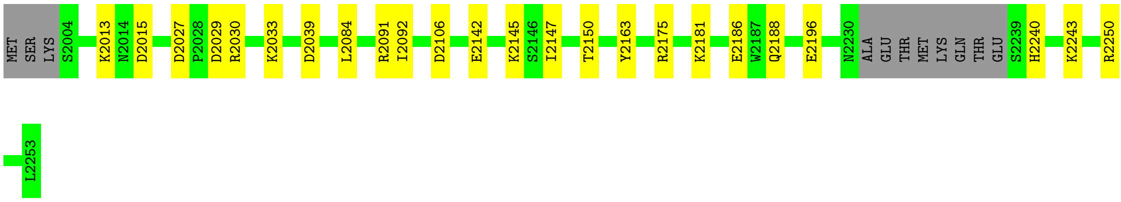
- Molecule 1: Uridine phosphorylase

Chain H:



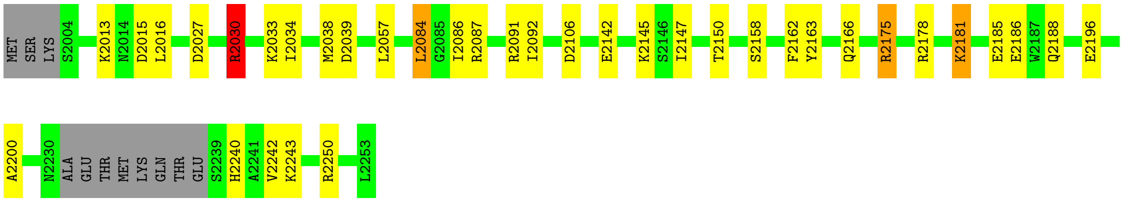
- Molecule 1: Uridine phosphorylase

Chain h:



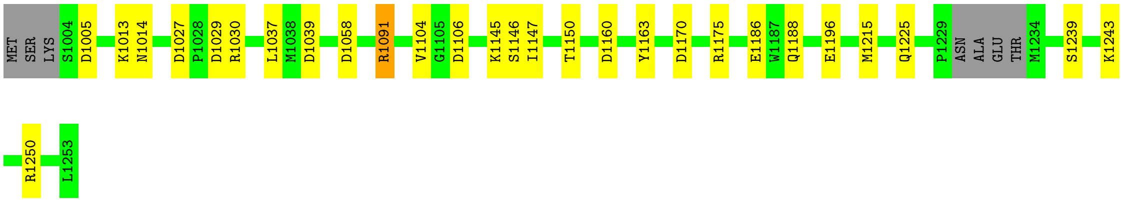
- Molecule 1: Uridine phosphorylase

Chain I:

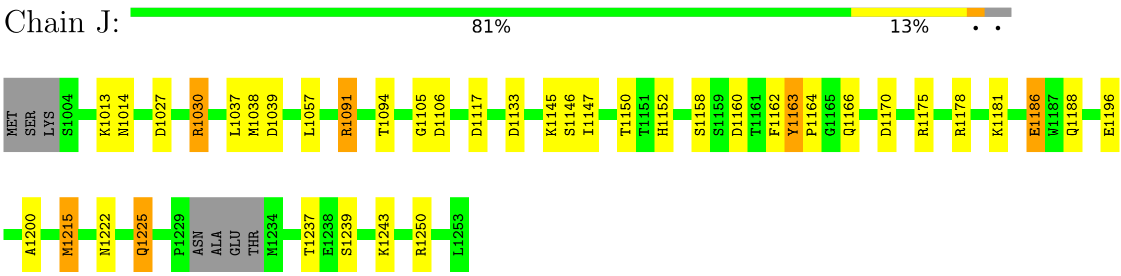


- Molecule 1: Uridine phosphorylase

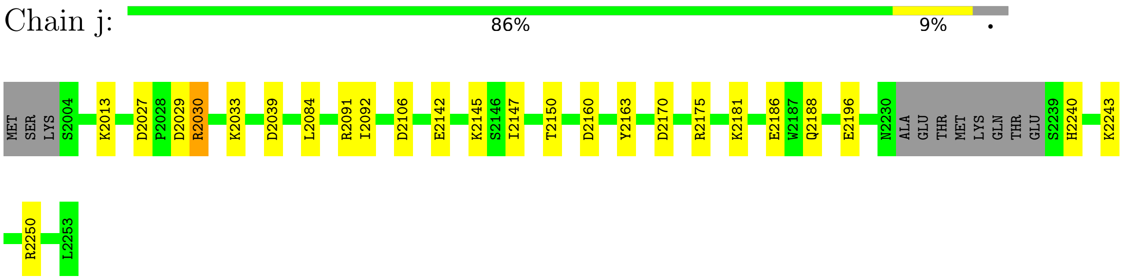
Chain i:



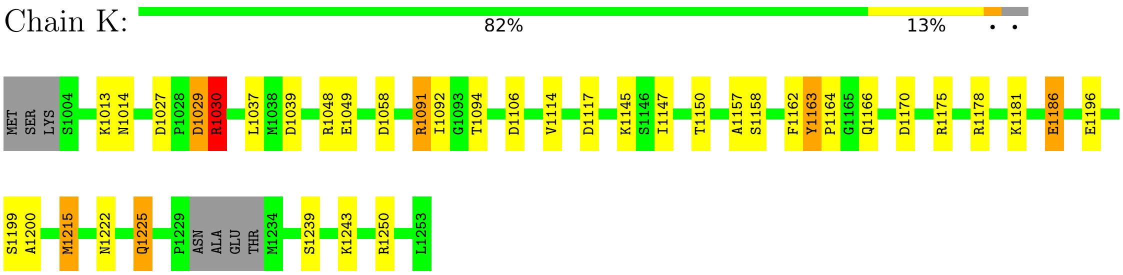
- Molecule 1: Uridine phosphorylase



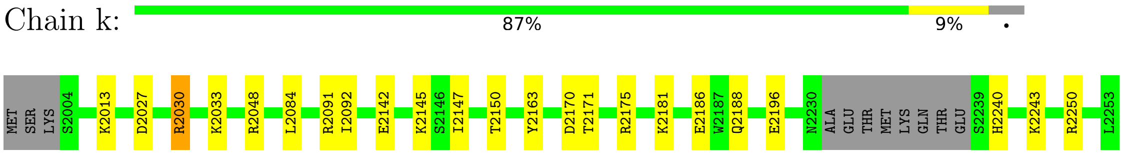
• Molecule 1: Uridine phosphorylase



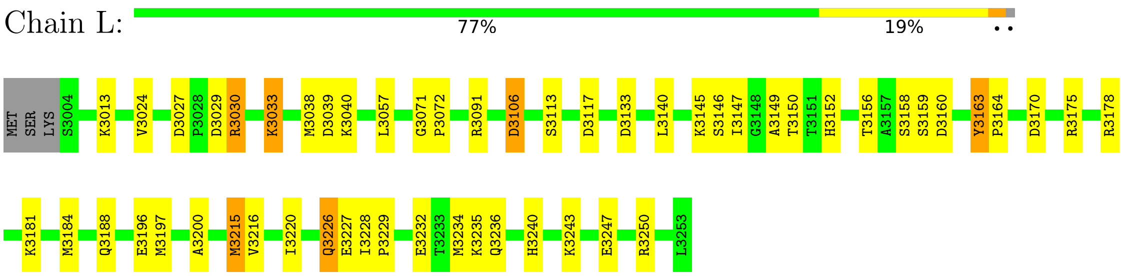
• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase

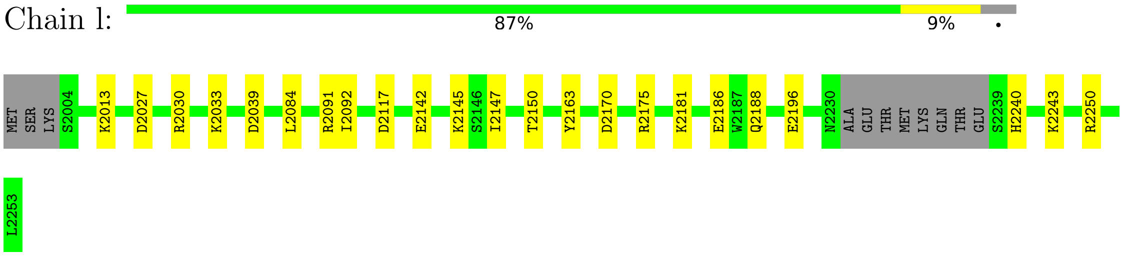


• Molecule 1: Uridine phosphorylase



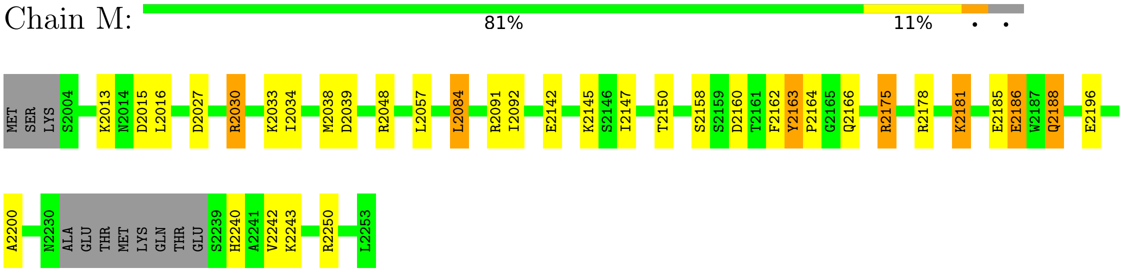
• Molecule 1: Uridine phosphorylase

Chain l:



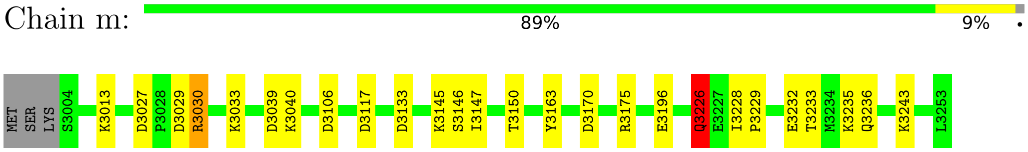
- Molecule 1: Uridine phosphorylase

Chain M:



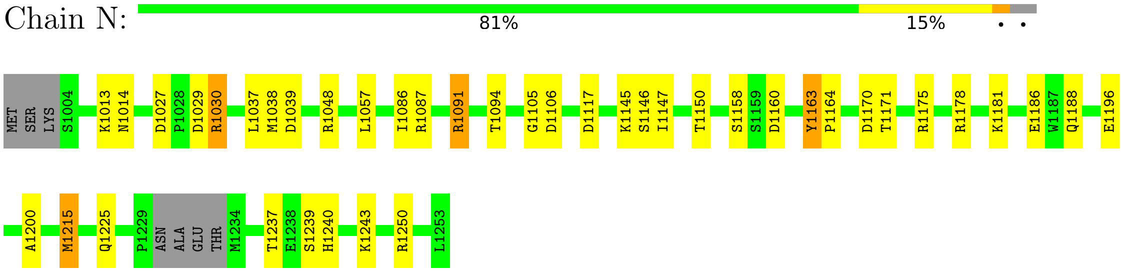
- Molecule 1: Uridine phosphorylase

Chain m:



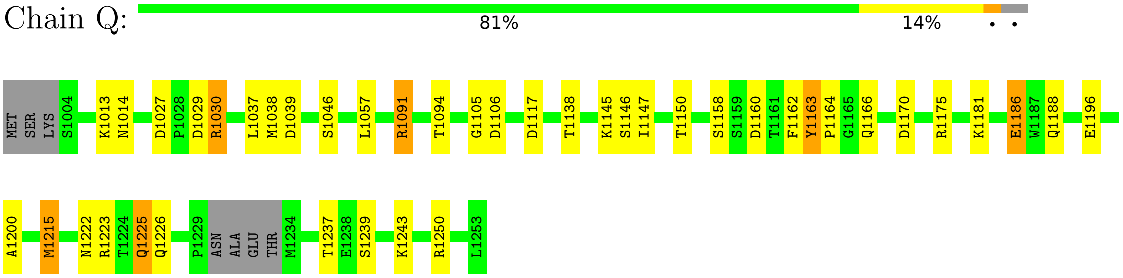
- Molecule 1: Uridine phosphorylase

Chain N:



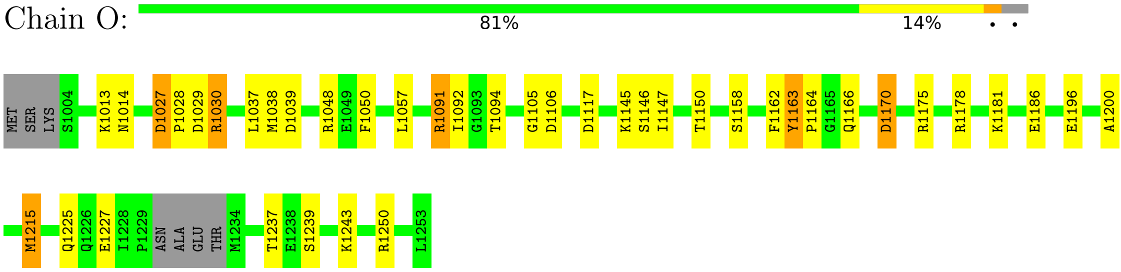
- Molecule 1: Uridine phosphorylase

Chain Q:



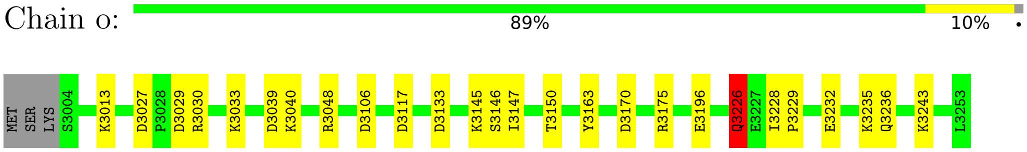
- Molecule 1: Uridine phosphorylase

Chain O:



- Molecule 1: Uridine phosphorylase

Chain o:



4 Data and refinement statistics ⓘ

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, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.99 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.218	Depositor
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.034	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
Total number of atoms	57608	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage'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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: DUR, K, PO4, V7O

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

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1851	0	1860	12	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	11	0	0	3	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	16	0	11	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	c	54	0	0	0	0
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.

The worst 5 of 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

The worst 5 of 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
1:e:2101:HIS:CE1	1:o:3226:GLN:CG[2_546]	1.93	0.27

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

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	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 508 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	2196	GLU
1	N	1091	ARG
1	i	1013	LYS
1	m	3243	LYS
1	Q	1239	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	3226	GLN

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Mol	Chain	Res	Type
1	m	3152	HIS
1	M	2230	ASN
1	m	3225	GLN
1	d	3225	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	j	3081	-	4,4,4	0.79	0	6,6,6	0.65	0
5	DUR	H	2062	-	17,17,17	1.76	3 (17%)	24,24,24	3.52	6 (25%)
3	V7O	M	5051	-	0,10,25	-	-	-		
5	DUR	c	3032	-	17,17,17	2.09	5 (29%)	24,24,24	4.39	11 (45%)
4	PO4	l	3101	-	4,4,4	0.84	0	6,6,6	0.51	0
5	DUR	C	2022	-	17,17,17	1.89	6 (35%)	24,24,24	4.19	10 (41%)
4	PO4	C	2021	-	4,4,4	0.83	0	6,6,6	0.51	0
4	PO4	K	2091	-	4,4,4	0.89	0	6,6,6	0.39	0
3	V7O	k	5043	-	0,10,25	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
3	V7O	Q	5053	-	0,10,25	-	-	-		
4	PO4	G	3051	-	4,4,4	0.86	0	6,6,6	0.62	0
3	V7O	R	5024	-	0,10,25	-	-	-		
4	PO4	e	3041	-	4,4,4	0.77	0	6,6,6	0.69	0
4	PO4	J	2081	-	4,4,4	0.82	0	6,6,6	0.45	0
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	-	-	-		
5	DUR	F	2052	-	17,17,17	1.87	6 (35%)	24,24,24	3.86	9 (37%)
4	PO4	a	3011	-	4,4,4	0.71	0	6,6,6	0.65	0
3	V7O	h	5033	-	0,10,25	-	-	-		
5	DUR	j	3082	-	17,17,17	1.87	3 (17%)	24,24,24	4.05	11 (45%)
5	DUR	Q	2122	-	17,17,17	1.75	4 (23%)	24,24,24	3.47	6 (25%)
4	PO4	b	3021	-	4,4,4	0.78	0	6,6,6	0.55	0
3	V7O	A	5011	-	0,10,25	-	-	-		
5	DUR	l	3102	-	17,17,17	1.74	3 (17%)	24,24,24	3.66	9 (37%)
3	V7O	D	5021	-	0,10,25	-	-	-		
3	V7O	e	5023	-	0,10,25	-	-	-		
5	DUR	O	2112	-	17,17,17	1.89	6 (35%)	24,24,24	3.48	6 (25%)
4	PO4	h	3061	-	4,4,4	0.86	0	6,6,6	0.49	0
5	DUR	M	3112	-	17,17,17	1.76	3 (17%)	24,24,24	3.81	7 (29%)
4	PO4	k	3091	-	4,4,4	0.80	0	6,6,6	0.80	0
3	V7O	o	5054	-	0,10,25	-	-	-		
3	V7O	c	5014	-	0,10,25	-	-	-		
4	PO4	B	2011	-	4,4,4	0.82	0	6,6,6	0.60	0
4	PO4	F	2051	-	4,4,4	0.84	0	6,6,6	0.35	0
3	V7O	M	5052	-	0,10,25	-	-	-		
5	DUR	b	3022	-	17,17,17	1.73	4 (23%)	24,24,24	3.94	9 (37%)
4	PO4	N	2101	-	4,4,4	0.88	0	6,6,6	0.53	0
5	DUR	D	2032	-	17,17,17	1.80	3 (17%)	24,24,24	3.76	8 (33%)
5	DUR	R	2132	-	17,17,17	1.91	4 (23%)	24,24,24	3.88	10 (41%)
5	DUR	P	3122	-	17,17,17	1.66	3 (17%)	24,24,24	4.00	11 (45%)
4	PO4	R	2131	-	4,4,4	0.90	0	6,6,6	0.36	0
5	DUR	k	3092	-	17,17,17	1.92	5 (29%)	24,24,24	3.79	7 (29%)
4	PO4	M	3111	-	4,4,4	0.81	0	6,6,6	0.79	0
5	DUR	E	2042	-	17,17,17	1.88	5 (29%)	24,24,24	3.79	8 (33%)
5	DUR	N	2102	-	17,17,17	1.75	4 (23%)	24,24,24	3.54	8 (33%)
5	DUR	i	2072	-	17,17,17	1.90	5 (29%)	24,24,24	3.69	8 (33%)
5	DUR	a	3012	-	17,17,17	1.98	4 (23%)	24,24,24	3.97	9 (37%)
3	V7O	L	5041	-	0,10,25	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	DUR	h	3062	-	17,17,17	1.94	6 (35%)	24,24,24	3.60	6 (25%)
4	PO4	D	2031	-	4,4,4	0.81	0	6,6,6	0.50	0
3	V7O	b	5013	-	0,10,25	-	-	-		
5	DUR	J	2082	-	17,17,17	2.05	4 (23%)	24,24,24	3.87	7 (29%)
5	DUR	B	2012	-	17,17,17	1.98	6 (35%)	24,24,24	3.84	8 (33%)
4	PO4	H	2061	-	4,4,4	0.83	0	6,6,6	0.53	0
5	DUR	e	3042	-	17,17,17	1.65	3 (17%)	24,24,24	3.74	7 (29%)
4	PO4	i	2071	-	4,4,4	0.82	0	6,6,6	0.48	0
4	PO4	O	2111	-	4,4,4	0.87	0	6,6,6	0.48	0
3	V7O	j	5044	-	0,10,25	-	-	-		
4	PO4	P	3121	-	4,4,4	0.85	0	6,6,6	0.52	0
3	V7O	B	5012	-	0,10,25	-	-	-		
5	DUR	I	3072	-	17,17,17	1.85	4 (23%)	24,24,24	3.75	7 (29%)
3	V7O	D	5022	-	0,10,25	-	-	-		
4	PO4	E	2041	-	4,4,4	0.77	0	6,6,6	0.63	0
4	PO4	Q	2121	-	4,4,4	0.94	0	6,6,6	0.54	0
3	V7O	H	5031	-	0,10,25	-	-	-		
4	PO4	I	3071	-	4,4,4	0.74	0	6,6,6	0.71	0
5	DUR	G	3052	-	17,17,17	1.72	3 (17%)	24,24,24	3.70	9 (37%)
4	PO4	c	3031	-	4,4,4	0.94	0	6,6,6	0.93	1 (16%)
3	V7O	I	5032	-	0,10,25	-	-	-		
3	V7O	i	5034	-	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	H	2062	-	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	C	2022	-	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	F	2052	-	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	j	3082	-	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	O	2112	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	D	2032	-	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	k	3092	-	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	N	2102	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	i	2072	-	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	h	3062	-	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	B	2012	-	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	I	3072	-	1/1/3/3	4/6/18/18	0/2/2/2
5	DUR	G	3052	-	1/1/3/3	4/6/18/18	0/2/2/2

The worst 5 of 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

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	a	3012	DUR	C1'

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Mol	Chain	Res	Type	Atom
5	B	2012	DUR	C1’
5	b	3022	DUR	C1’
5	C	2022	DUR	C1’
5	c	3032	DUR	C1’

5 of 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’

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
5	C	2022	DUR	1	0
4	C	2021	PO4	1	0
4	G	3051	PO4	1	0
3	J	5042	V7O	5	0
3	A	5011	V7O	1	0
3	D	5021	V7O	2	0
3	M	5052	V7O	4	0
5	P	3122	DUR	1	0
3	L	5041	V7O	1	0
4	O	2111	PO4	1	0
4	P	3121	PO4	2	0
3	B	5012	V7O	1	0
3	D	5022	V7O	3	0
3	H	5031	V7O	2	0
5	G	3052	DUR	1	0
3	I	5032	V7O	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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