



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 02:44 PM BST

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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) : 2.13

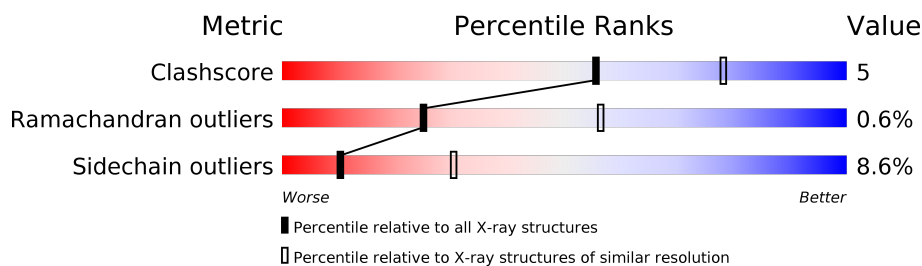
1 Overall quality at a glance

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	253	78% 19% ..
1	B	253	81% 15% ...
1	C	253	80% 15% ...
1	D	253	81% 14% ..
1	E	253	81% 14% ..
1	F	253	79% 16% ...
1	G	253	82% 11% ..
1	H	253	83% 13% ..

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

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

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).

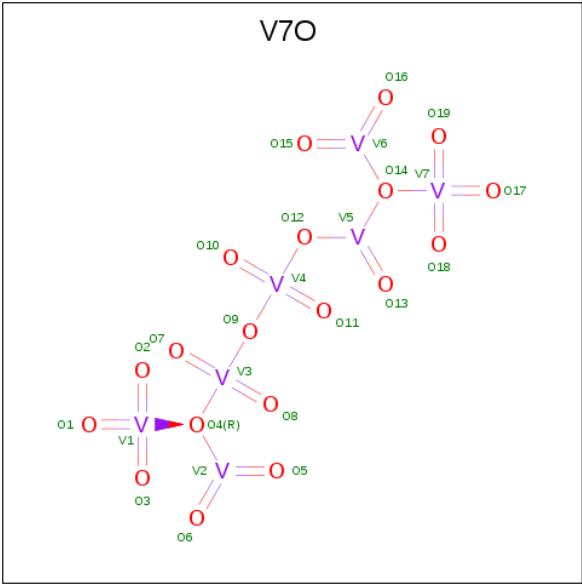
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	K	0	0
			1	1		
2	J	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	K	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	h	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	i	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		
2	N	1	Total	K	0	0
			1	1		
2	o	1	Total	K	0	0
			1	1		
2	R	1	Total	K	0	0
			1	1		
2	L	1	Total	K	0	0
			1	1		
2	M	1	Total	K	0	0
			1	1		

- Molecule 3 is META VANADATE (three-letter code: V7O) (formula: O₁₉V₇).



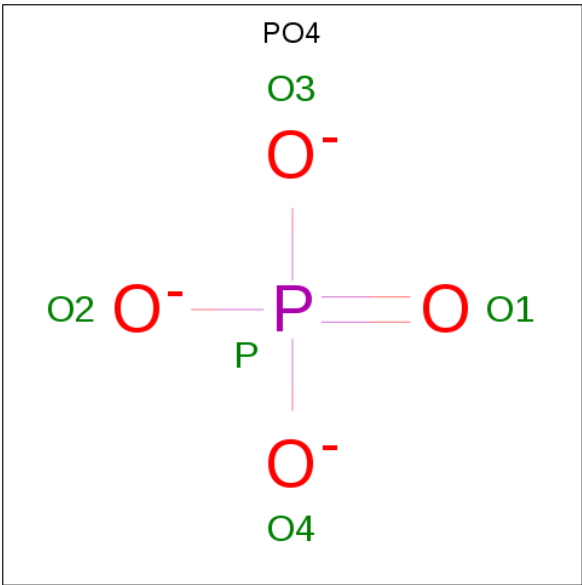
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			11	8	3		

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: O₄P).



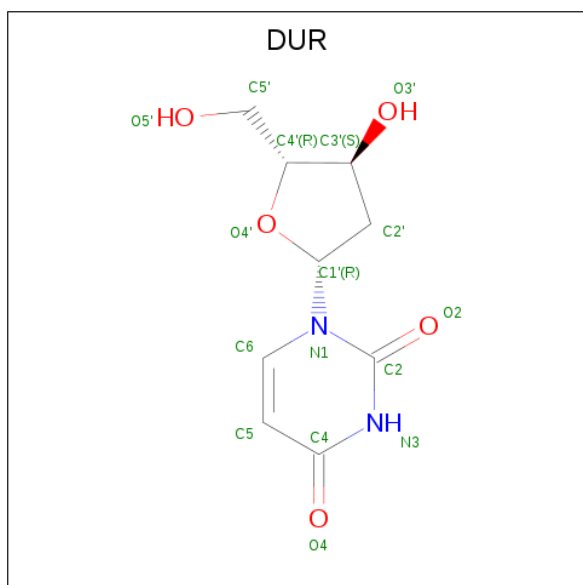
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	b	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	c	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	e	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total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

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: C₉H₁₂N₂O₅).



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...

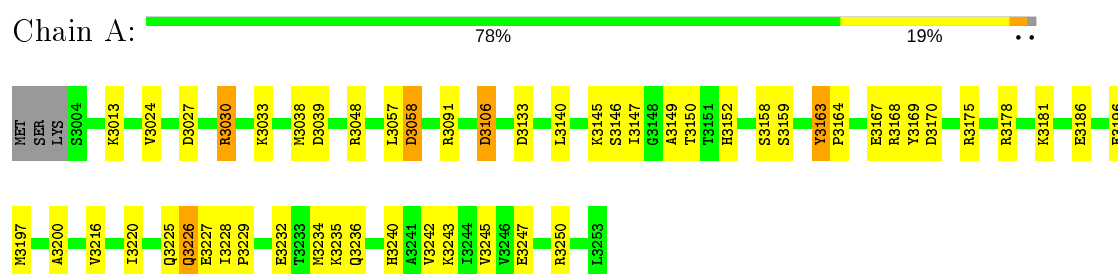
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	51	Total O 51 51	0	0
6	i	56	Total O 56 56	0	0
6	J	52	Total O 52 52	0	0
6	j	51	Total O 51 51	0	0
6	K	50	Total O 50 50	0	0
6	k	53	Total O 53 53	0	0
6	L	58	Total O 58 58	0	0
6	l	51	Total O 51 51	0	0
6	M	48	Total O 48 48	0	0
6	m	53	Total O 53 53	0	0
6	N	58	Total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

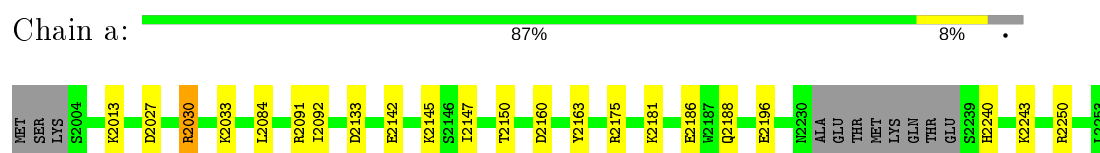
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

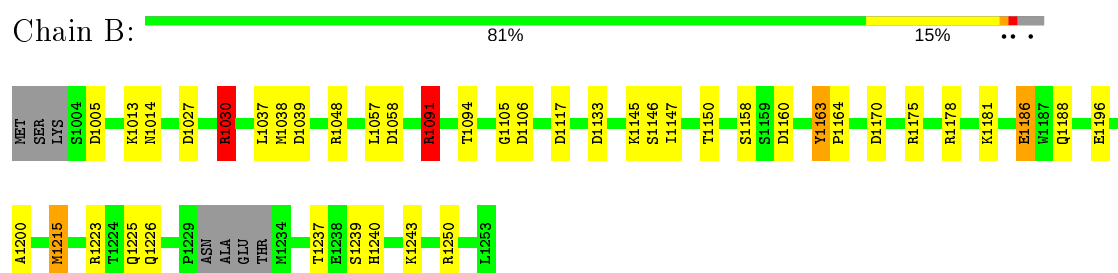
- Molecule 1: Uridine phosphorylase



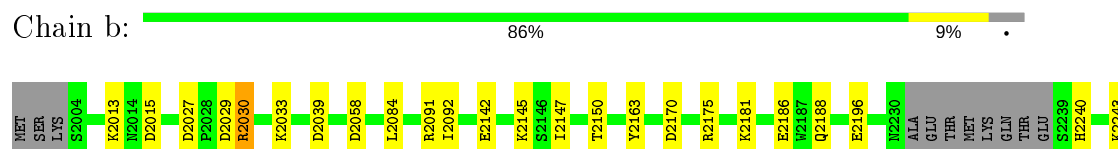
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



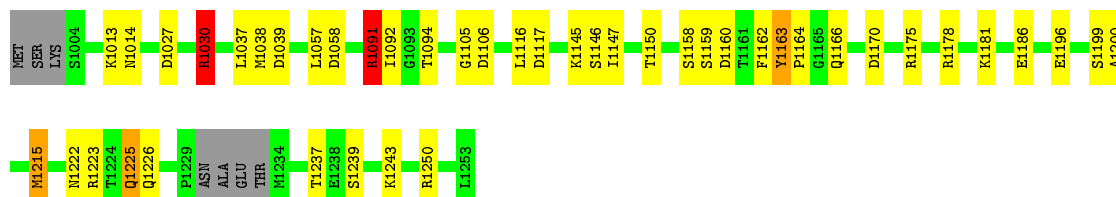
- Molecule 1: Uridine phosphorylase





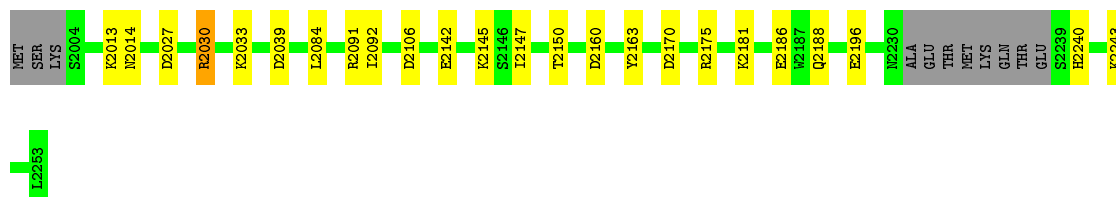
- Molecule 1: Uridine phosphorylase

Chain C: 80% 15% ..



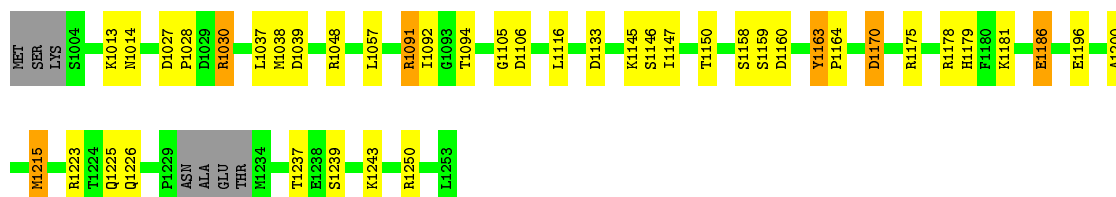
- Molecule 1: Uridine phosphorylase

Chain c: 86% 9% .



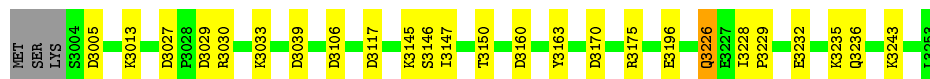
- Molecule 1: Uridine phosphorylase

Chain D: 81% 14% ..



- Molecule 1: Uridine phosphorylase

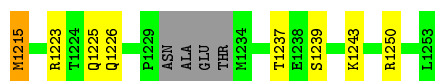
Chain d: 89% 9% .



- Molecule 1: Uridine phosphorylase

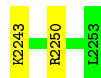
Chain E: 81% 14% ..





- Molecule 1: Uridine phosphorylase

Chain e: 86% 9% .



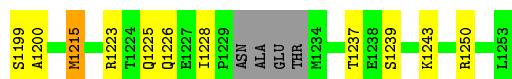
- Molecule 1: Uridine phosphorylase

Chain F: 79% 16% . . .



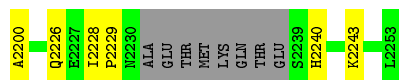
- Molecule 1: Uridine phosphorylase

Chain R: 80% 16% . . .



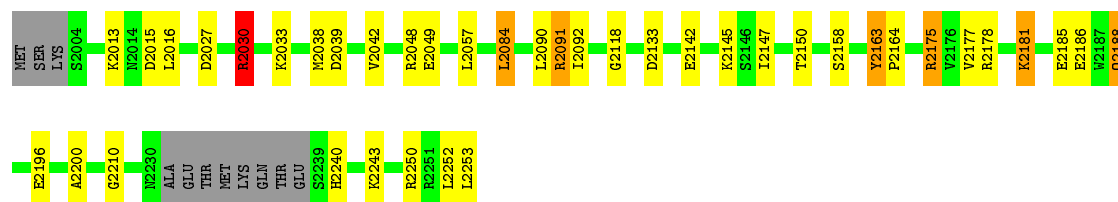
- Molecule 1: Uridine phosphorylase

Chain G: 82% 11% . . .



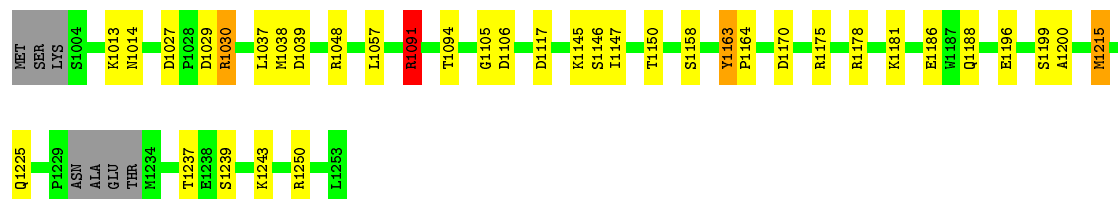
- Molecule 1: Uridine phosphorylase

Chain P: 80% 13% . . .



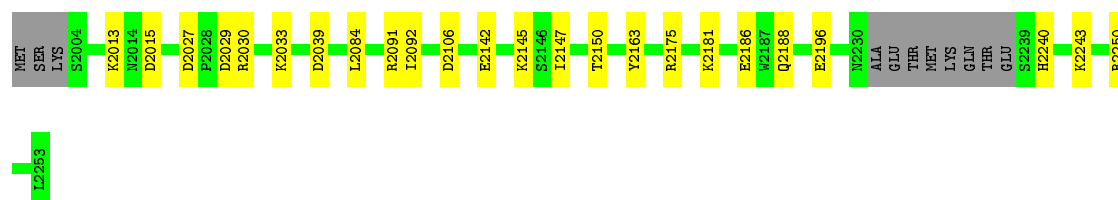
- Molecule 1: Uridine phosphorylase

Chain H: 83% 13% . .



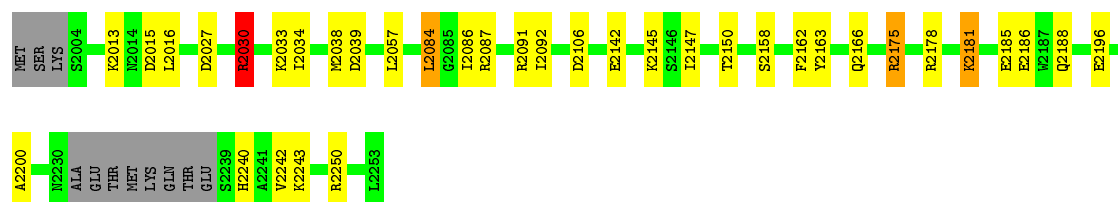
- Molecule 1: Uridine phosphorylase

Chain h: 86% 9% .



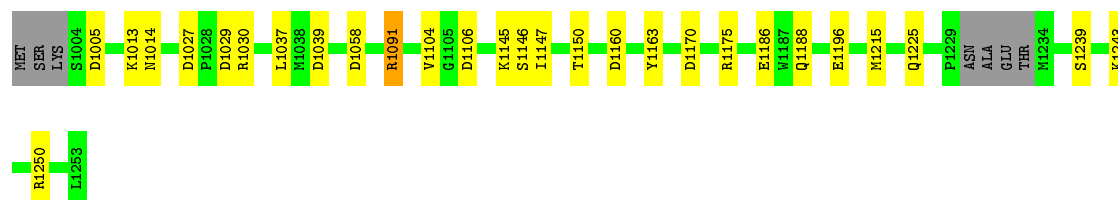
- Molecule 1: Uridine phosphorylase

Chain I: 81% 13% . .



- Molecule 1: Uridine phosphorylase

Chain i: 86% 11% .



- Molecule 1: Uridine phosphorylase


Al200	Al204	Al208	Al212	Al216	Al220	Al224	Al228	Al232	Al236	Al240	Al244	Al248	Al252	Al256	Al260	Al264	Al268	Al272	Al276	Al280	Al284	Al288	Al292	Al296	Al300	Al304	Al308	Al312	Al316	Al320	Al324	Al328	Al332	Al336	Al340	Al344	Al348	Al352	Al356	Al360	Al364	Al368	Al372	Al376	Al380	Al384	Al388	Al392	Al396	Al400	Al404	Al408	Al412	Al416	Al420	Al424	Al428	Al432	Al436	Al440	Al444	Al448	Al452	Al456	Al460	Al464	Al468	Al472	Al476	Al480	Al484	Al488	Al492	Al496	Al500	Al504	Al508	Al512	Al516	Al520	Al524	Al528	Al532	Al536	Al540	Al544	Al548	Al552	Al556	Al560	Al564	Al568	Al572	Al576	Al580	Al584	Al588	Al592	Al596	Al600	Al604	Al608	Al612	Al616	Al620	Al624	Al628	Al632	Al636	Al640	Al644	Al648	Al652	Al656	Al660	Al664	Al668	Al672	Al676	Al680	Al684	Al688	Al692	Al696	Al700	Al704	Al708	Al712	Al716	Al720	Al724	Al728	Al732	Al736	Al740	Al744	Al748	Al752	Al756	Al760	Al764	Al768	Al772	Al776	Al780	Al784	Al788	Al792	Al796	Al800	Al804	Al808	Al812	Al816	Al820	Al824	Al828	Al832	Al836	Al840	Al844	Al848	Al852	Al856	Al860	Al864	Al868	Al872	Al876	Al880	Al884	Al888	Al892	Al896	Al900	Al904	Al908	Al912	Al916	Al920	Al924	Al928	Al932	Al936	Al940	Al944	Al948	Al952	Al956	Al960	Al964	Al968	Al972	Al976	Al980	Al984	Al988	Al992	Al996	Al1000	Al1004	Al1008	Al1012	Al1016	Al1020	Al1024	Al1028	Al1032	Al1036	Al1040	Al1044	Al1048	Al1052	Al1056	Al1060	Al1064	Al1068	Al1072	Al1076	Al1080	Al1084	Al1088	Al1092	Al1096	Al1100	Al1104	Al1108	Al1112	Al1116	Al1120	Al1124	Al1128	Al1132	Al1136	Al1140	Al1144	Al1148	Al1152	Al1156	Al1160	Al1164	Al1168	Al1172	Al1176	Al1180	Al1184	Al1188	Al1192	Al1196	Al1200	Al1204	Al1208	Al1212	Al1216	Al1220	Al1224	Al1228	Al1232	Al1236	Al1240	Al1244	Al1248	Al1252	Al1256	Al1260	Al1264	Al1268	Al1272	Al1276	Al1280	Al1284	Al1288	Al1292	Al1296	Al1300	Al1304	Al1308	Al1312	Al1316	Al1320	Al1324	Al1328	Al1332	Al1336	Al1340	Al1344	Al1348	Al1352	Al1356	Al1360	Al1364	Al1368	Al1372	Al1376	Al1380	Al1384	Al1388	Al1392	Al1396	Al1400	Al1404	Al1408	Al1412	Al1416	Al1420	Al1424	Al1428	Al1432	Al1436	Al1440	Al1444	Al1448	Al1452	Al1456	Al1460	Al1464	Al1468	Al1472	Al1476	Al1480	Al1484	Al1488	Al1492	Al1496	Al1500	Al1504	Al1508	Al1512	Al1516	Al1520	Al1524	Al1528	Al1532	Al1536	Al1540	Al1544	Al1548	Al1552	Al1556	Al1560	Al1564	Al1568	Al1572	Al1576	Al1580	Al1584	Al1588	Al1592	Al1596	Al1600	Al1604	Al1608	Al1612	Al1616	Al1620	Al1624	Al1628	Al1632	Al1636	Al1640	Al1644	Al1648	Al1652	Al1656	Al1660	Al1664	Al1668	Al1672	Al1676	Al1680	Al1684	Al1688	Al1692	Al1696	Al1700	Al1704	Al1708	Al1712	Al1716	Al1720	Al1724	Al1728	Al1732	Al1736	Al1740	Al1744	Al1748	Al1752	Al1756</
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	----------

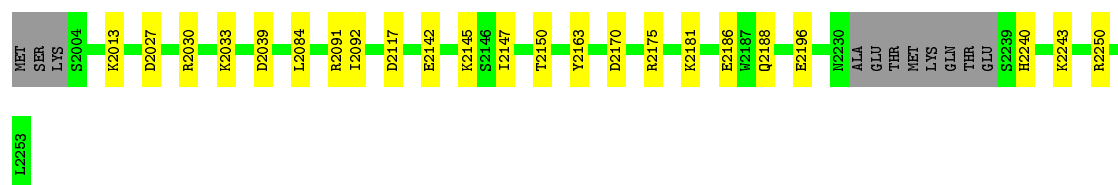
- | | |
|-------------------|-------------------|
| R2250 | L2253 |
| MET
SER
LYS | S2004 |
| K2013 | D2027 |
| P2028 | D2029 |
| R2030 | K2033 |
| D2039 | L2084 |
| R2091
I2092 | D2106 |
| E2142 | K2145 |
| S2146 | I2147 |
| T2150 | D2160 |
| V2163 | D2170 |
| R2175 | K2181 |
| E2186 | H2187 |
| Q2188 | E2196 |
| A2230 | ALA
GLU
THR |
| NET
LYS
GLN | NET
LYS
THR |
| S2239 | H2240 |
| V2243 | |

- | |
|-------|
| S1199 |
| A1200 |
| M1215 |
| M1222 |
| Q1225 |
| P1229 |
| ASN |
| ALA |
| GLU |
| THR |
| M1234 |
| S1239 |
| K1243 |
| R1250 |
| L1253 |
| MET |
| SER |
| LYS |
| S1004 |
| K1013 |
| M1014 |
| D1027 |
| P1028 |
| D1029 |
| R1030 |
| L1037 |
| M1038 |
| D1039 |
| R1048 |
| E1049 |
| D1058 |
| R1091 |
| I1092 |
| G1093 |
| T1094 |
| D1106 |
| V1114 |
| D1117 |
| K1145 |
| S1146 |
| I1147 |
| T1150 |
| A1157 |
| S1158 |
| F1162 |
| V1163 |
| P1164 |
| G1165 |
| Q1166 |
| D1170 |
| R1175 |
| R1178 |
| K1181 |
| E1186 |
| E1196 |


- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|
| MET | SER | LYS | S2004 | K2013 | D2027 | R2030 | K2033 | R2048 | L2084 | R2091 | L2092 | E2142 | K2145 | S2146 | L2147 | T2150 | Y2163 | D2170 | T2171 | R2175 | K2181 | E2186 | W2187 | Q2188 | E2196 | N2230 | ALA | GLU | THR | THR | MET | LYS | GLN | THR | GLU | S2239 | H2240 | K2243 | R2250 | L2252 |
|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|

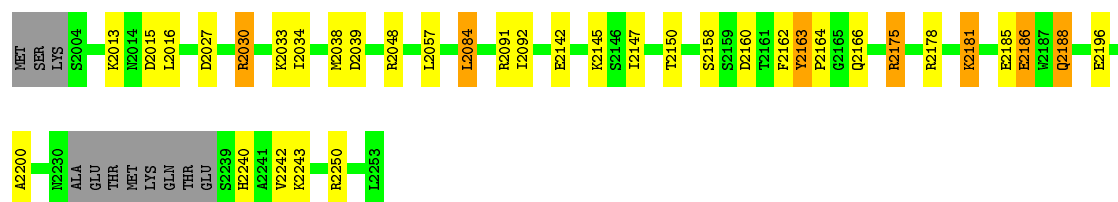
- | | | | |
|-------|-------|-------|-------|
| K3181 | K3188 | K3013 | MET |
| K3184 | K3196 | V3024 | SER |
| K3197 | K3197 | D3027 | LVS |
| A3200 | K3215 | P3028 | S3004 |
| B3216 | V3216 | D3029 | |
| I3220 | I3228 | R3030 | |
| Q3226 | P3229 | K3033 | |
| E3227 | E3232 | K3038 | |
| I3228 | M3234 | D3039 | |
| P3229 | K3235 | K3040 | |
| E3232 | Q3236 | L3057 | |
| M3234 | H3240 | G3071 | |
| K3235 | K3243 | P3072 | |
| Q3236 | E3247 | R3091 | |
| H3240 | R3250 | D3106 | |
| K3243 | L3253 | S3113 | |
| E3247 | | D3117 | |
| R3250 | | D3133 | |
| L3253 | | I3140 | |
| | | K3146 | |
| | | S3146 | |
| | | I3147 | |
| | | K3148 | |
| | | A3149 | |
| | | T3150 | |
| | | T3151 | |
| | | K3152 | |
| | | T3156 | |
| | | S3157 | |
| | | S3158 | |
| | | S3159 | |
| | | D3160 | |
| | | X3163 | |
| | | P3164 | |
| | | D3170 | |
| | | R3175 | |
| | | P3178 | |

Chain l:  87% 9%



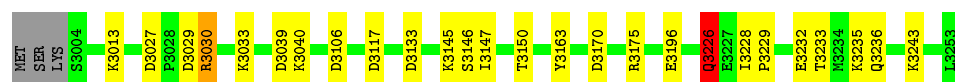
- Molecule 1: Uridine phosphorylase

Chain M:  81% 11%




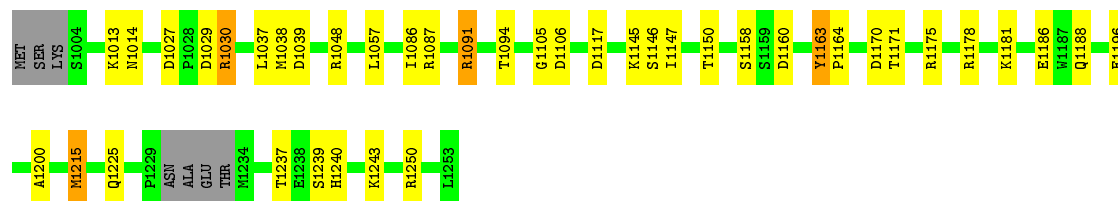
- Molecule 1: Uridine phosphorylase

Chain m:  89% 9%




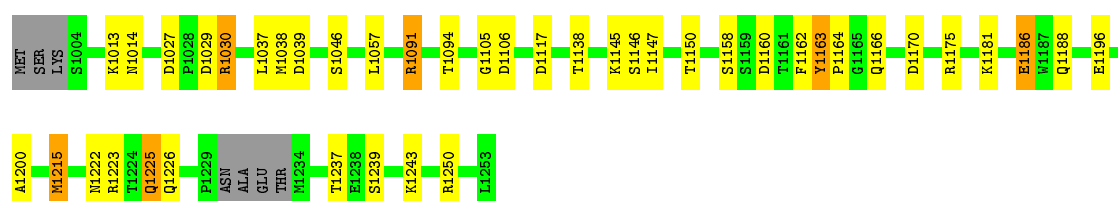
- Molecule 1: Uridine phosphorylase

Chain N:  81% 15%



- Molecule 1: Uridine phosphorylase

Chain Q:  81% 14%



- Molecule 1: Uridine phosphorylase

[illegible]

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| MET | SER | LYS | S3004 | K3013 | D8027 | P3028 | D8029 | R3030 | K3033 | D8039 | K3040 | R3048 | D8106 | D8117 | D8133 | K3145 | S3146 | I3147 | T3150 | Y3163 | D8170 | R3175 | E3196 | Q3226 | E3227 | T3228 | P3229 | E3232 | K3235 | Q3236 | K3243 | I3253 |
|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, V7O, DUR

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(°)	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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	2186	GLU
1	I	2243	LYS
1	Q	1188	GLN
1	H	1014	ASN
1	h	2092	ILE

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

Mol	Chain	Res	Type
1	J	1225	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	3225	GLN
1	o	3225	GLN
1	K	1225	GLN
1	L	3152	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	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
4	PO4	R	2131	-	4,4,4	0.90	0	6,6,6	0.36	0
4	PO4	h	3061	-	4,4,4	0.86	0	6,6,6	0.49	0
5	DUR	j	3082	-	14,17,17	2.04	4 (28%)	14,24,24	4.78	7 (50%)
4	PO4	P	3121	-	4,4,4	0.85	0	6,6,6	0.52	0
5	DUR	J	2082	-	14,17,17	2.27	4 (28%)	14,24,24	4.68	5 (35%)
4	PO4	K	2091	-	4,4,4	0.89	0	6,6,6	0.39	0
3	V7O	e	5023	-	0,10,25	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DUR	h	3062	-	14,17,17	2.35	5 (35%)	14,24,24	4.66	5 (35%)
5	DUR	K	2092	-	14,17,17	2.13	3 (21%)	14,24,24	4.51	6 (42%)
4	PO4	J	2081	-	4,4,4	0.82	0	6,6,6	0.45	0
5	DUR	c	3032	-	14,17,17	2.40	6 (42%)	14,24,24	5.28	8 (57%)
3	V7O	M	5052	-	0,10,25	0.00	-	-	-	-
5	DUR	C	2022	-	14,17,17	2.18	6 (42%)	14,24,24	5.22	8 (57%)
4	PO4	a	3011	-	4,4,4	0.71	0	6,6,6	0.65	0
3	V7O	H	5031	-	0,10,25	0.00	-	-	-	-
4	PO4	O	2111	-	4,4,4	0.87	0	6,6,6	0.48	0
3	V7O	M	5051	-	0,10,25	0.00	-	-	-	-
3	V7O	i	5034	-	0,10,25	0.00	-	-	-	-
3	V7O	L	5041	-	0,10,25	0.00	-	-	-	-
4	PO4	D	2031	-	4,4,4	0.81	0	6,6,6	0.50	0
5	DUR	N	2102	-	14,17,17	2.05	3 (21%)	14,24,24	4.36	5 (35%)
5	DUR	l	3102	-	14,17,17	1.96	4 (28%)	14,24,24	4.46	7 (50%)
4	PO4	l	3101	-	4,4,4	0.84	0	6,6,6	0.51	0
5	DUR	P	3122	-	14,17,17	1.98	4 (28%)	14,24,24	4.87	7 (50%)
5	DUR	D	2032	-	14,17,17	2.09	4 (28%)	14,24,24	4.61	6 (42%)
4	PO4	M	3111	-	4,4,4	0.81	0	6,6,6	0.79	0
5	DUR	F	2052	-	14,17,17	2.26	4 (28%)	14,24,24	4.83	6 (42%)
5	DUR	O	2112	-	14,17,17	2.25	5 (35%)	14,24,24	4.39	5 (35%)
4	PO4	i	2071	-	4,4,4	0.82	0	6,6,6	0.48	0
3	V7O	J	5042	-	0,10,25	0.00	-	-	-	-
4	PO4	B	2011	-	4,4,4	0.82	0	6,6,6	0.60	0
5	DUR	G	3052	-	14,17,17	2.01	3 (21%)	14,24,24	4.62	7 (50%)
5	DUR	M	3112	-	14,17,17	1.96	3 (21%)	14,24,24	4.69	5 (35%)
4	PO4	E	2041	-	4,4,4	0.77	0	6,6,6	0.63	0
3	V7O	D	5022	-	0,10,25	0.00	-	-	-	-
3	V7O	Q	5053	-	0,10,25	0.00	-	-	-	-
5	DUR	R	2132	-	14,17,17	2.27	4 (28%)	14,24,24	4.70	7 (50%)
3	V7O	B	5012	-	0,10,25	0.00	-	-	-	-
4	PO4	G	3051	-	4,4,4	0.86	0	6,6,6	0.62	0
3	V7O	D	5021	-	0,10,25	0.00	-	-	-	-
5	DUR	a	3012	-	14,17,17	2.31	4 (28%)	14,24,24	4.79	6 (42%)
5	DUR	I	3072	-	14,17,17	2.18	4 (28%)	14,24,24	4.70	6 (42%)
3	V7O	h	5033	-	0,10,25	0.00	-	-	-	-
5	DUR	b	3022	-	14,17,17	2.18	5 (35%)	14,24,24	4.87	6 (42%)
4	PO4	N	2101	-	4,4,4	0.88	0	6,6,6	0.53	0
3	V7O	j	5044	-	0,10,25	0.00	-	-	-	-

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	B	2012	-	14,17,17	2.30	5 (35%)	14,24,24	4.73	6 (42%)
4	PO4	F	2051	-	4,4,4	0.84	0	6,6,6	0.35	0
5	DUR	Q	2122	-	14,17,17	2.09	3 (21%)	14,24,24	4.36	5 (35%)
5	DUR	E	2042	-	14,17,17	2.14	4 (28%)	14,24,24	4.59	6 (42%)
5	DUR	k	3092	-	14,17,17	2.27	4 (28%)	14,24,24	4.64	5 (35%)
3	V7O	o	5054	-	0,10,25	0.00	-	-	-	-
4	PO4	c	3031	-	4,4,4	0.94	0	6,6,6	0.93	1 (16%)
3	V7O	R	5024	-	0,10,25	0.00	-	-	-	-
4	PO4	Q	2121	-	4,4,4	0.94	0	6,6,6	0.54	0
5	DUR	H	2062	-	14,17,17	2.06	4 (28%)	14,24,24	4.31	4 (28%)
3	V7O	b	5013	-	0,10,25	0.00	-	-	-	-
3	V7O	A	5011	-	0,10,25	0.00	-	-	-	-
5	DUR	i	2072	-	14,17,17	2.17	3 (21%)	14,24,24	4.59	6 (42%)
4	PO4	e	3041	-	4,4,4	0.77	0	6,6,6	0.69	0
3	V7O	c	5014	-	0,10,25	0.00	-	-	-	-
4	PO4	H	2061	-	4,4,4	0.83	0	6,6,6	0.53	0
3	V7O	k	5043	-	0,10,25	0.00	-	-	-	-
4	PO4	I	3071	-	4,4,4	0.74	0	6,6,6	0.71	0
5	DUR	e	3042	-	14,17,17	1.84	3 (21%)	14,24,24	4.63	5 (35%)
3	V7O	I	5032	-	0,10,25	0.00	-	-	-	-
4	PO4	b	3021	-	4,4,4	0.78	0	6,6,6	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DUR	j	3082	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	Q	2122	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	J	2082	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	h	3062	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	K	2092	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	F	2052	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	C	2022	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	l	3102	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	N	2102	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	c	3032	-	1/1/3/3	2/3/18/18	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DUR	P	3122	-	1/1/3/3	0/3/18/18	0/2/2/2
5	DUR	D	2032	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	O	2112	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	G	3052	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	M	3112	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	a	3012	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	R	2132	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	E	2042	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	I	3072	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	b	3022	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	B	2012	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	k	3092	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	H	2062	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	i	2072	-	1/1/3/3	2/3/18/18	0/2/2/2
5	DUR	e	3042	-	1/1/3/3	2/3/18/18	0/2/2/2

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	h	3062	DUR	C4-N3	6.13	1.43	1.33
5	B	2012	DUR	C4-N3	5.96	1.43	1.33
5	R	2132	DUR	C4-N3	5.81	1.43	1.33
5	F	2052	DUR	C4-N3	5.75	1.43	1.33
5	k	3092	DUR	C4-N3	5.74	1.43	1.33

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2022	DUR	C2'-C1'-N1	16.56	152.46	114.27
5	c	3032	DUR	C2'-C1'-N1	16.29	151.85	114.27
5	F	2052	DUR	C2'-C1'-N1	15.71	150.50	114.27
5	I	3072	DUR	C2'-C1'-N1	15.45	149.91	114.27
5	j	3082	DUR	C2'-C1'-N1	15.34	149.65	114.27

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	3052	DUR	C1'
5	h	3062	DUR	C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
5	I	3072	DUR	C1'
5	c	3032	DUR	C1'
5	C	2022	DUR	C1'

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	2122	DUR	C3'-C4'-C5'-O5'
5	k	3092	DUR	C3'-C4'-C5'-O5'
5	Q	2122	DUR	O4'-C4'-C5'-O5'
5	k	3092	DUR	O4'-C4'-C5'-O5'
5	h	3062	DUR	C3'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2021	PO4	1	0
4	P	3121	PO4	2	0
3	M	5052	V7O	4	0
5	C	2022	DUR	1	0
3	H	5031	V7O	2	0
4	O	2111	PO4	1	0
3	M	5051	V7O	3	0
3	L	5041	V7O	1	0
5	P	3122	DUR	1	0
3	J	5042	V7O	5	0
5	G	3052	DUR	1	0
3	D	5022	V7O	3	0
3	B	5012	V7O	1	0
4	G	3051	PO4	1	0
3	D	5021	V7O	2	0
3	A	5011	V7O	1	0
3	I	5032	V7O	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.