



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:48 PM UTC

PDB ID : 1RXS / pdb_00001rxs
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

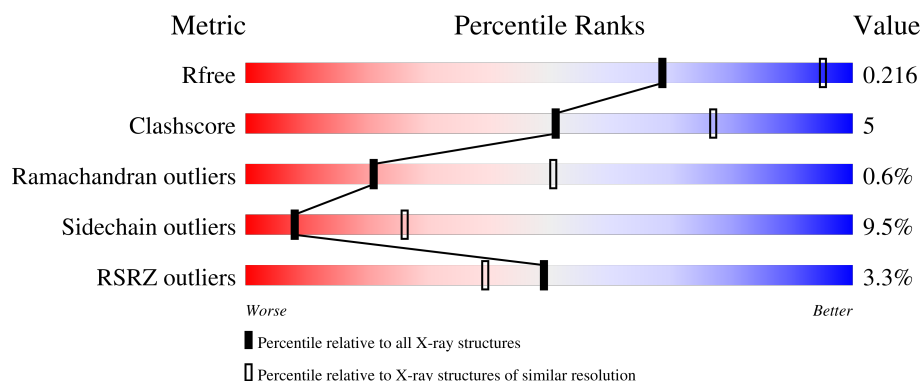
1 Overall quality at a glance

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.



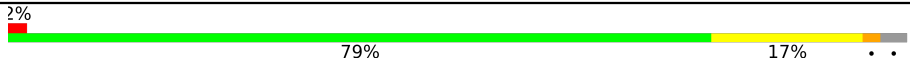
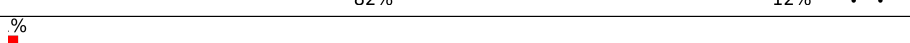
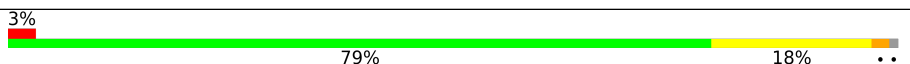
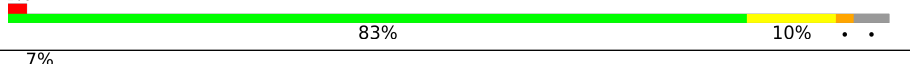
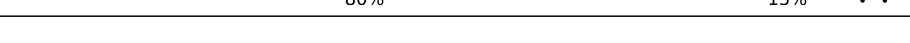
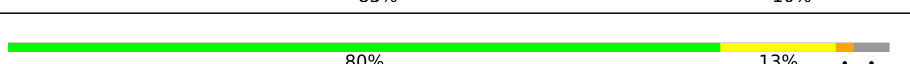
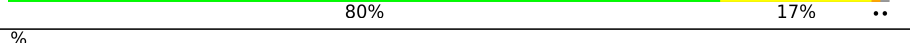
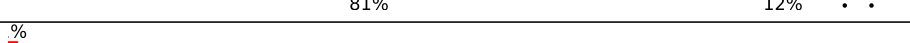
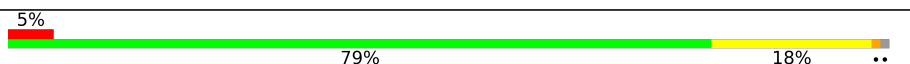
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	80% 16% ..
1	B	253	82% 12% ..
1	C	253	4% 79% 16% ..
1	D	253	4% 80% 15% ..
1	E	253	82% 14% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	253	
1	G	253	
1	H	253	
1	I	253	
1	J	253	
1	K	253	
1	L	253	
1	M	253	
1	N	253	
1	O	253	
1	P	253	
1	Q	253	
1	R	253	
1	a	253	
1	b	253	
1	c	253	
1	d	253	
1	e	253	
1	h	253	
1	i	253	
1	j	253	
1	k	253	
1	l	253	
1	m	253	
1	o	253	

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 (CCD ID: K) (formula: K).

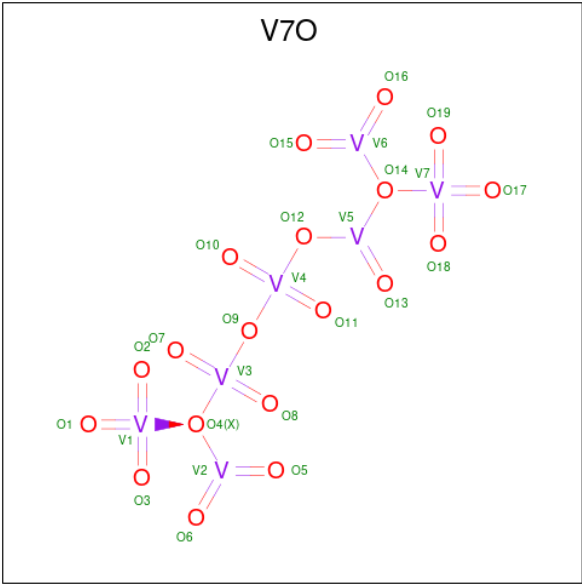
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is META VANADATE (CCD ID: V7O) (formula: O₁₉V₇).



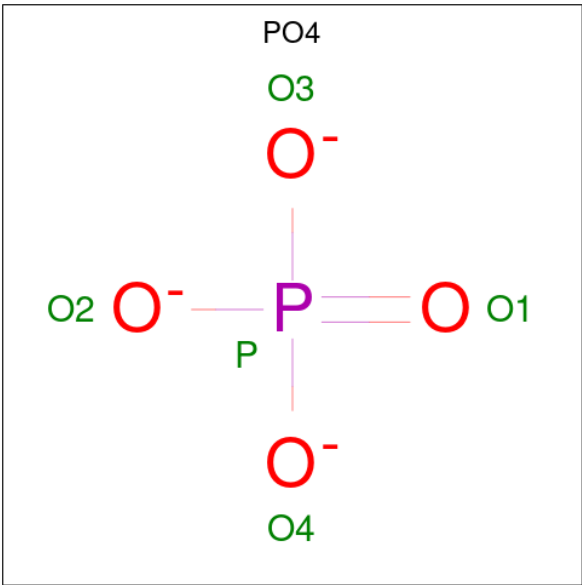
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			11	8	3		

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 (CCD ID: PO4) (formula: O₄P).



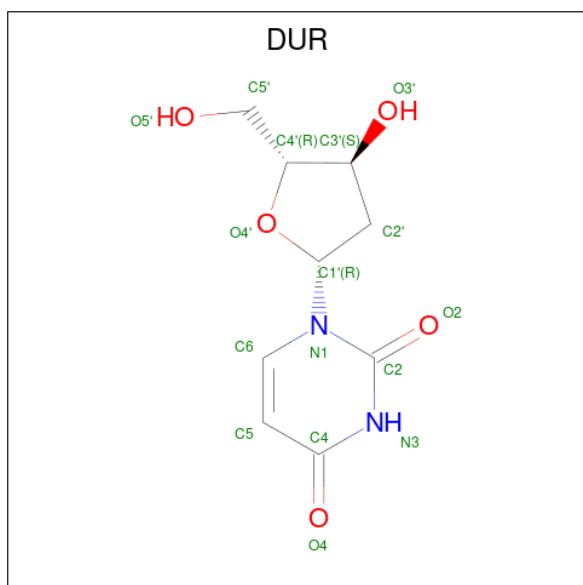
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	b	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	c	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	e	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	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 (CCD ID: DUR) (formula: $C_9H_{12}N_2O_5$).



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

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...

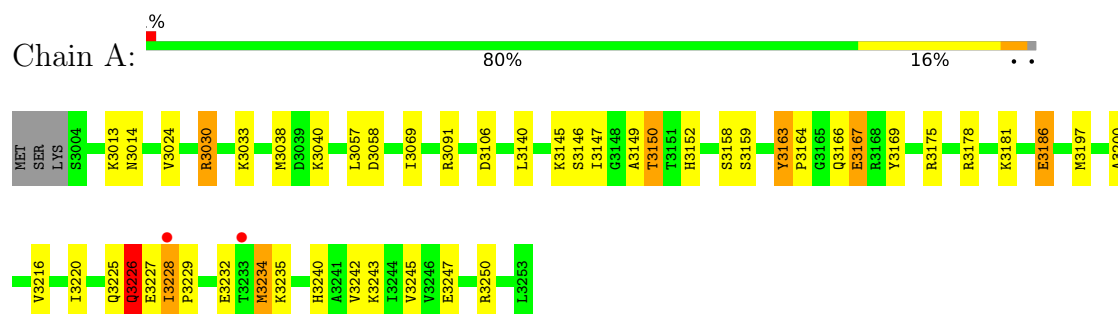
Continued from previous page...

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

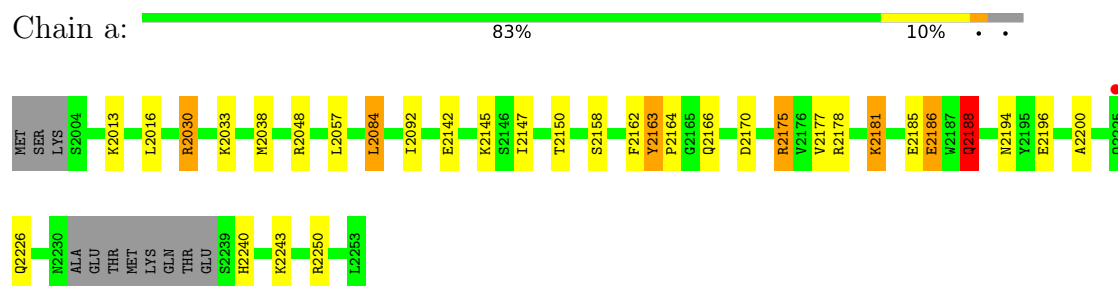
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

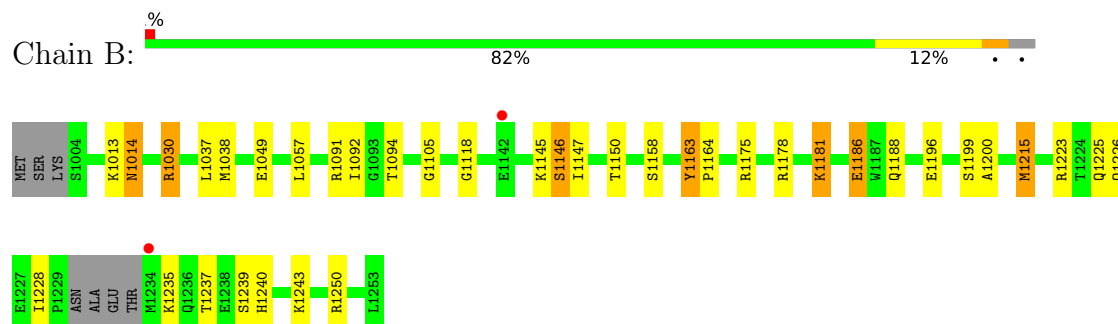
• Molecule 1: Uridine phosphorylase



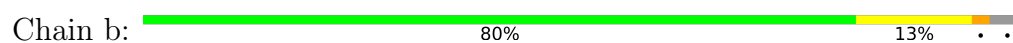
• Molecule 1: Uridine phosphorylase

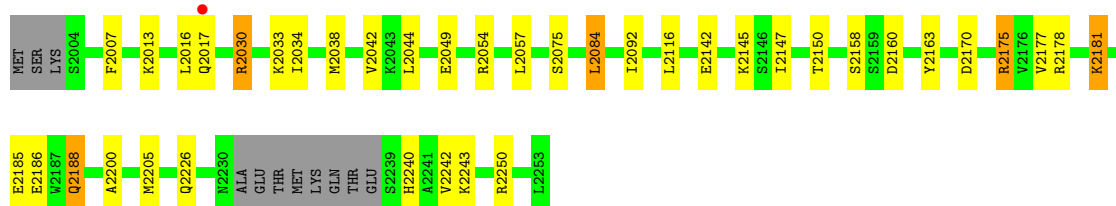


• Molecule 1: Uridine phosphorylase

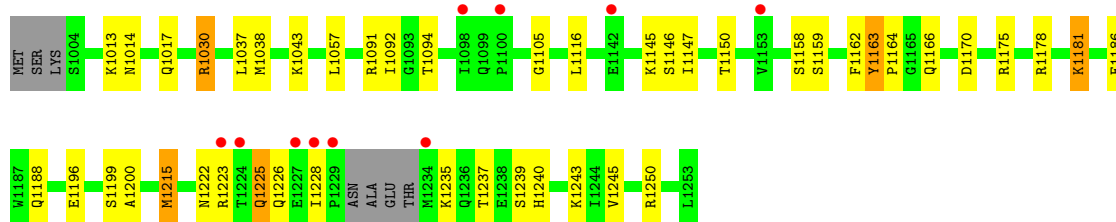
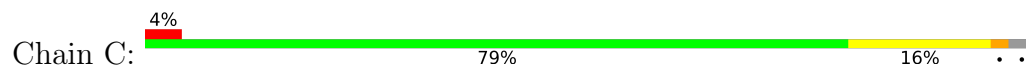


• Molecule 1: Uridine phosphorylase

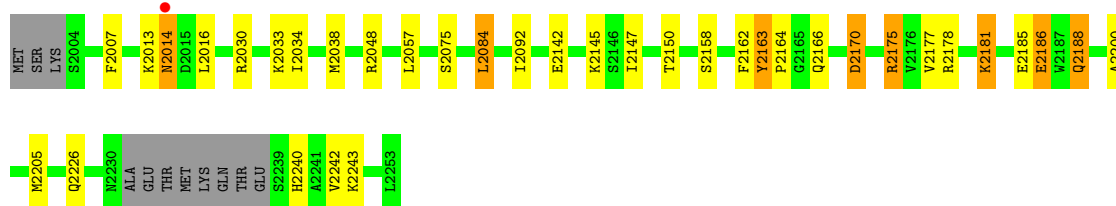
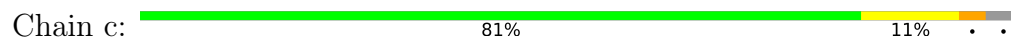




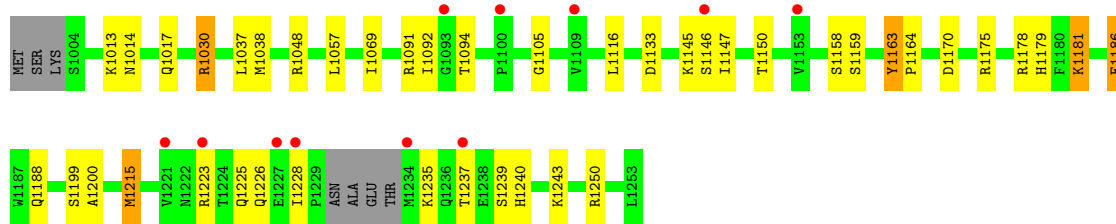
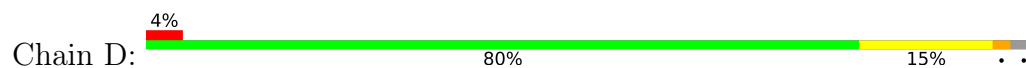
• Molecule 1: Uridine phosphorylase



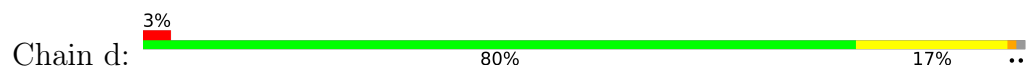
• Molecule 1: Uridine phosphorylase

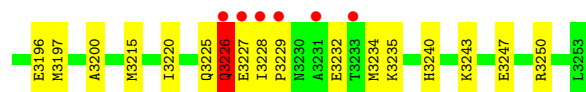


• Molecule 1: Uridine phosphorylase



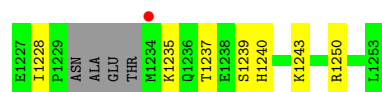
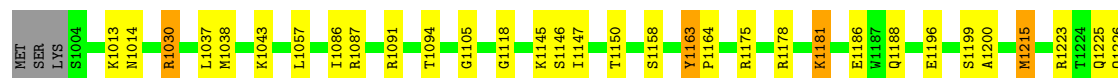
• Molecule 1: Uridine phosphorylase





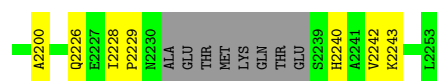
- Molecule 1: Uridine phosphorylase

Chain E: 82% 14% . .



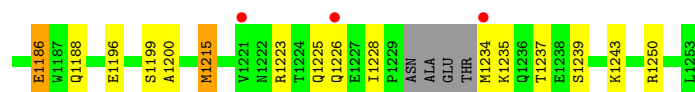
- Molecule 1: Uridine phosphorylase

Chain e: 81% 11% . .



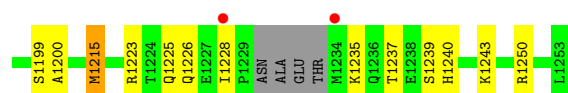
- Molecule 1: Uridine phosphorylase

Chain F: 79% 17% . .



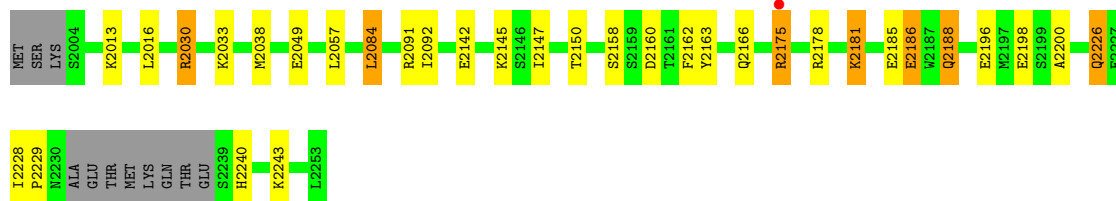
- Molecule 1: Uridine phosphorylase

Chain R: 80% 15% . .



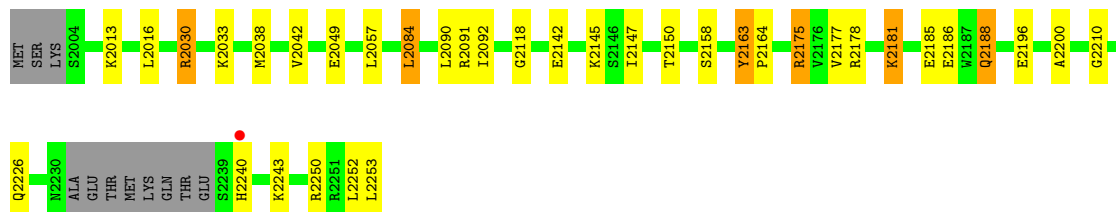
- Molecule 1: Uridine phosphorylase

Chain G:  83% 10% . .



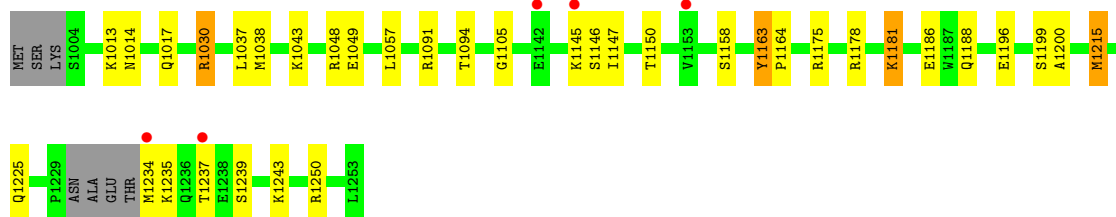
• Molecule 1: Uridine phosphorylase

Chain P:  81% 12% . .



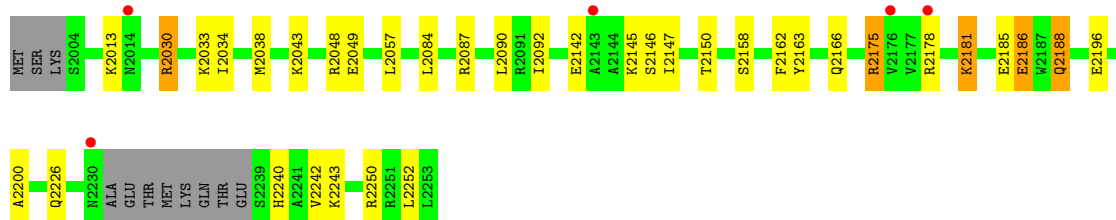
• Molecule 1: Uridine phosphorylase

Chain H:  83% 13% . .



• Molecule 1: Uridine phosphorylase

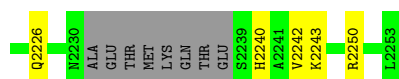
Chain h:  81% 12% . .



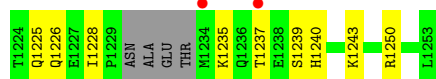
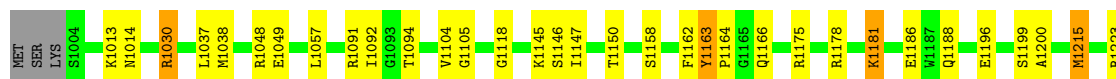
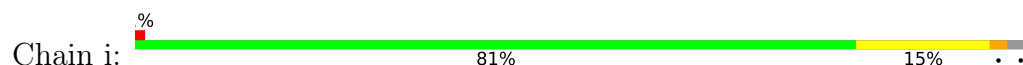
• Molecule 1: Uridine phosphorylase

Chain I:  82% 12% . .

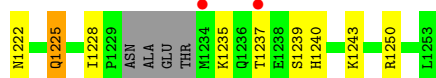
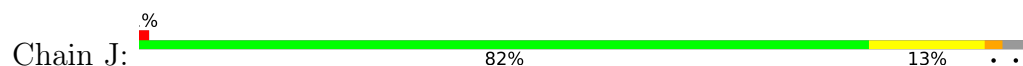




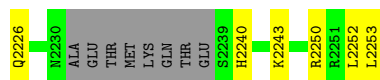
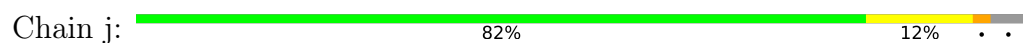
- Molecule 1: Uridine phosphorylase



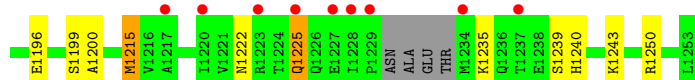
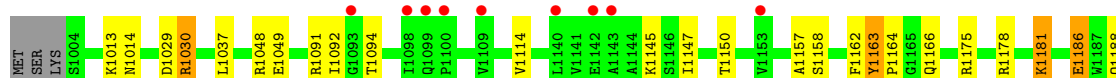
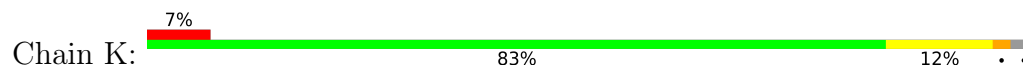
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

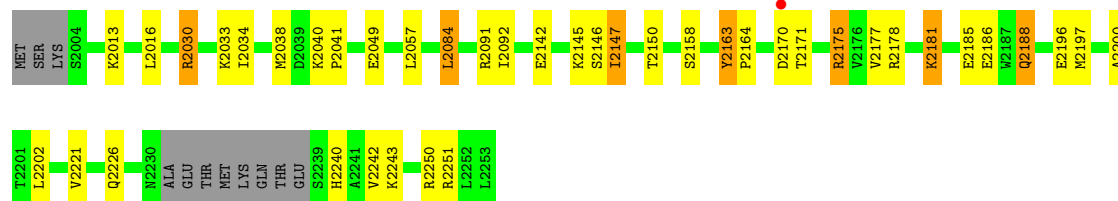


- Molecule 1: Uridine phosphorylase



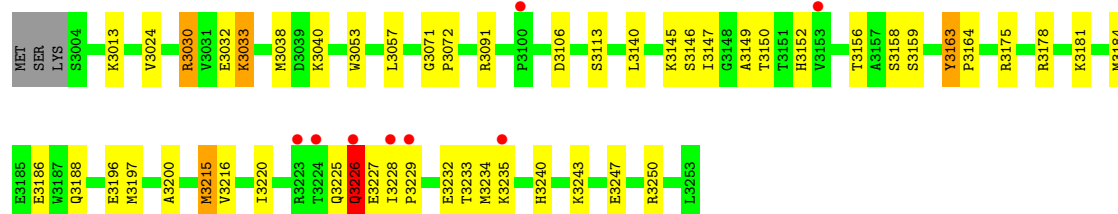
- Molecule 1: Uridine phosphorylase

Chain k:  79% 13% . .



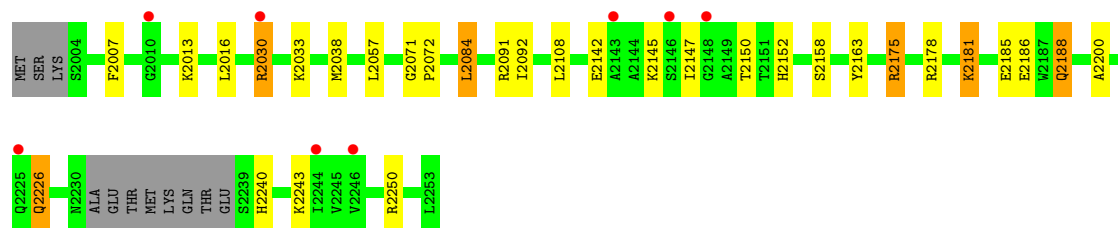
• Molecule 1: Uridine phosphorylase

Chain L:  79% 18% . .



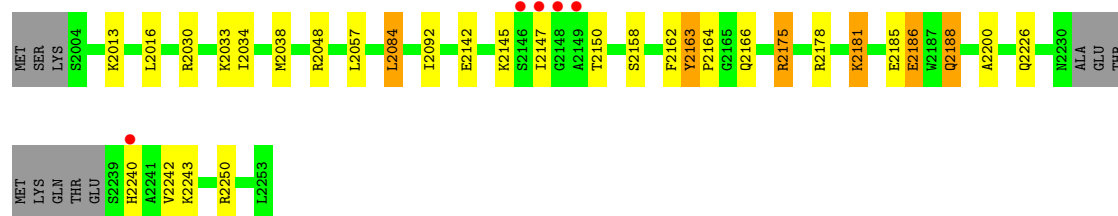
• Molecule 1: Uridine phosphorylase

Chain l:  83% 10% . .



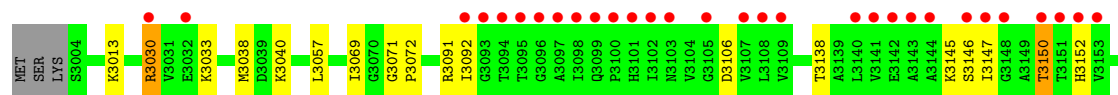
• Molecule 1: Uridine phosphorylase

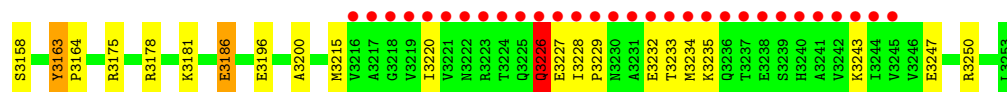
Chain M:  83% 10% . .



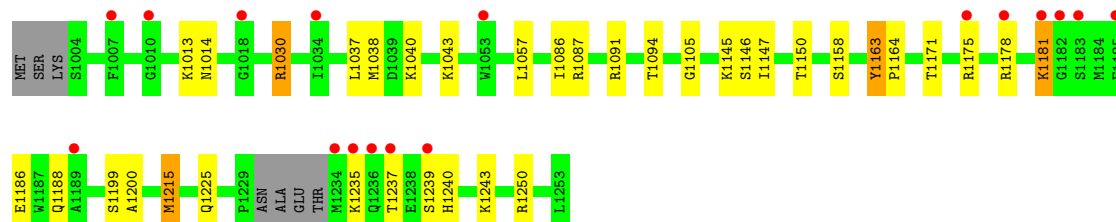
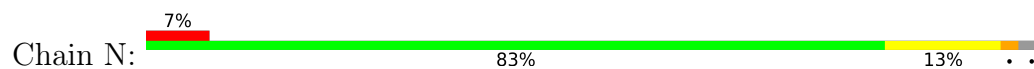
• Molecule 1: Uridine phosphorylase

Chain m:  83% 14% . .

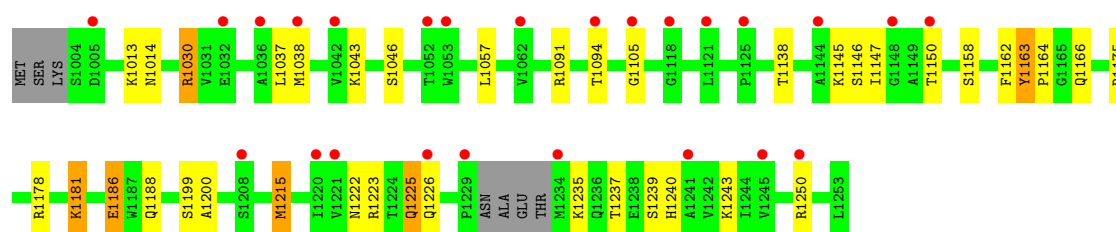
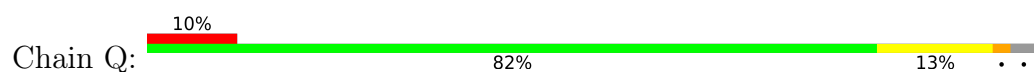




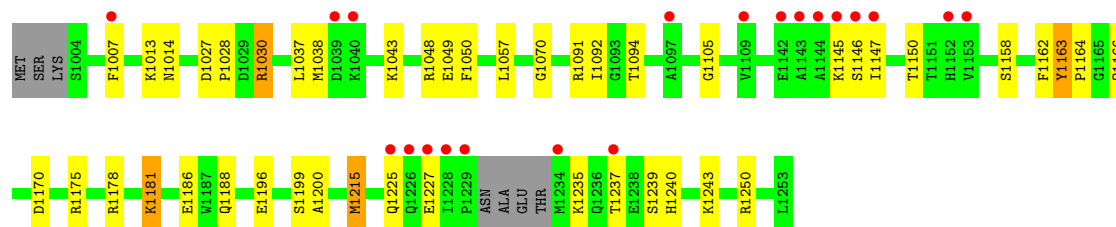
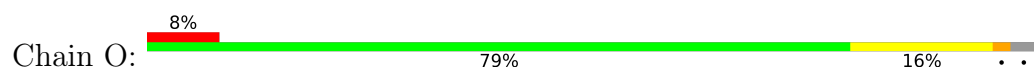
• Molecule 1: Uridine phosphorylase



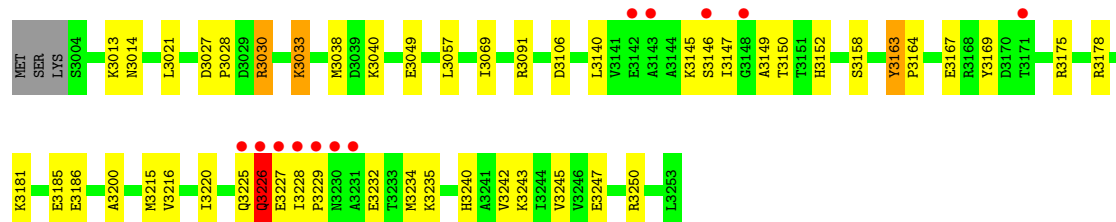
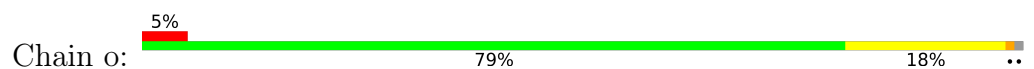
• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

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 26.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (26.75-2.80) 99.0 (26.75-2.80)	Depositor EDS
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 0.177 , 0.216	Depositor DCC
R_{free} test set	8725 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.9	EDS
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
F_o, F_c correlation	0.91	EDS
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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.92	3/1912 (0.2%)	1.04	2/2595 (0.1%)
1	B	0.84	0/1882	0.95	1/2552 (0.0%)
1	C	0.84	0/1882	0.94	0/2552
1	D	0.76	0/1882	0.92	0/2552
1	E	0.75	0/1882	0.93	0/2552
1	F	0.83	1/1882 (0.1%)	0.93	1/2552 (0.0%)
1	G	0.78	0/1848	1.00	0/2508
1	H	0.80	1/1882 (0.1%)	0.91	0/2552
1	I	0.71	0/1848	0.95	0/2508
1	J	0.72	0/1882	0.92	0/2552
1	K	0.76	0/1882	0.92	0/2552
1	L	0.76	1/1912 (0.1%)	0.97	0/2595
1	M	0.69	0/1848	0.96	0/2508
1	N	0.65	0/1882	0.91	0/2552
1	O	0.68	0/1882	0.91	1/2552 (0.0%)
1	P	0.88	0/1848	0.99	0/2508
1	Q	0.64	0/1882	0.88	0/2552
1	R	0.81	0/1882	0.94	0/2552
1	a	0.88	0/1848	1.03	3/2508 (0.1%)
1	b	0.86	0/1848	1.01	1/2508 (0.0%)
1	c	0.82	0/1848	1.00	2/2508 (0.1%)
1	d	0.79	1/1912 (0.1%)	0.97	0/2595
1	e	0.76	0/1848	0.96	0/2508
1	h	0.70	0/1848	0.96	0/2508
1	i	0.74	0/1882	0.94	0/2552
1	j	0.85	0/1848	1.00	1/2508 (0.0%)
1	k	0.81	1/1848 (0.1%)	0.98	1/2508 (0.0%)
1	l	0.67	0/1848	0.92	0/2508
1	m	0.72	1/1912 (0.1%)	0.93	0/2595
1	o	0.69	0/1912	0.95	0/2595
All	All	0.77	9/56202 (0.0%)	0.95	13/76247 (0.0%)

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3234	MET	SD-CE	6.53	1.95	1.79
1	H	1234	MET	SD-CE	5.86	1.94	1.79
1	A	3150	THR	CA-CB	5.82	1.61	1.53
1	L	3215	MET	CG-SD	-5.56	1.66	1.80
1	m	3150	THR	CA-CB	5.41	1.60	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	1070	GLY	N-CA-C	6.75	119.85	112.29
1	a	2194	ASN	N-CA-C	5.86	117.04	108.14
1	B	1014	ASN	N-CA-C	5.74	117.54	111.28
1	b	2170	ASP	CB-CA-C	-5.38	103.34	112.00
1	A	3167	GLU	N-CA-C	5.33	118.74	111.39

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	28	0
1	B	1851	0	1860	18	0
1	C	1851	0	1860	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1851	0	1860	25	0
1	E	1851	0	1860	14	0
1	F	1851	0	1860	29	0
1	G	1817	0	1822	16	1
1	H	1851	0	1860	14	0
1	I	1817	0	1823	17	0
1	J	1851	0	1859	20	0
1	K	1851	0	1859	19	0
1	L	1880	0	1884	30	0
1	M	1817	0	1822	15	0
1	N	1851	0	1860	27	0
1	O	1851	0	1860	25	0
1	P	1817	0	1822	18	1
1	Q	1851	0	1860	19	0
1	R	1851	0	1860	21	1
1	a	1817	0	1823	14	0
1	b	1817	0	1822	27	0
1	c	1817	0	1822	18	1
1	d	1880	0	1884	39	1
1	e	1817	0	1822	31	5
1	h	1817	0	1822	21	0
1	i	1851	0	1859	19	2
1	j	1817	0	1823	17	0
1	k	1817	0	1822	29	1
1	l	1817	0	1823	14	0
1	m	1880	0	1885	23	2
1	o	1880	0	1884	31	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1	0
3	R	11	0	0	2	0
3	b	11	0	0	2	0
3	c	11	0	0	2	0
3	e	11	0	0	2	0
3	h	11	0	0	3	0
3	i	11	0	0	2	0
3	j	11	0	0	0	0
3	k	11	0	0	0	0
3	o	11	0	0	1	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	1	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	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	l	5	0	0	1	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
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	3	0
6	K	50	0	0	3	0
6	L	58	0	0	2	0
6	M	48	0	0	3	0
6	N	58	0	0	1	0
6	O	56	0	0	5	0
6	P	51	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	50	0	0	6	0
6	R	52	0	0	3	0
6	a	52	0	0	4	0
6	b	48	0	0	4	0
6	c	54	0	0	5	0
6	d	56	0	0	4	0
6	e	49	0	0	5	0
6	h	55	0	0	7	0
6	i	56	0	0	3	0
6	j	51	0	0	3	0
6	k	53	0	0	6	0
6	l	51	0	0	3	0
6	m	53	0	0	2	0
6	o	57	0	0	3	0
All	All	57608	0	55741	586	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 586 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:b:2042:VAL:HG11	1:d:3250:ARG:NH2	1.18	1.50
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
1:m:3226:GLN:CG	1:m:3227:GLU:H	1.55	1.19
1:d:3226:GLN:CG	1:d:3227:GLU:H	1.57	1.18

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%)	10	34
1	B	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	30	60
1	C	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	D	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	30	60
1	E	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	F	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	G	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60
1	H	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	30	60
1	I	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	30	60
1	J	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	K	242/253 (96%)	236 (98%)	5 (2%)	1 (0%)	30	60
1	L	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	10	34
1	M	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	30	60
1	N	242/253 (96%)	239 (99%)	2 (1%)	1 (0%)	30	60
1	O	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	30	60
1	P	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60
1	Q	242/253 (96%)	238 (98%)	3 (1%)	1 (0%)	30	60
1	R	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60
1	a	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60
1	b	238/253 (94%)	234 (98%)	3 (1%)	1 (0%)	30	60
1	c	238/253 (94%)	236 (99%)	1 (0%)	1 (0%)	30	60
1	d	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	10	34
1	e	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	60
1	h	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	30	60
1	i	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	30	60

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%)	30	60
1	k	238/253 (94%)	235 (99%)	2 (1%)	1 (0%)	30	60
1	l	238/253 (94%)	234 (98%)	3 (1%)	1 (0%)	30	60
1	m	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	10	34
1	o	248/253 (98%)	240 (97%)	5 (2%)	3 (1%)	10	34
All	All	7242/7590 (95%)	7100 (98%)	102 (1%)	40 (1%)	21	51

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%)	185 (92%)	16 (8%)	11	34
1	B	198/204 (97%)	177 (89%)	21 (11%)	6	22
1	C	198/204 (97%)	175 (88%)	23 (12%)	5	18
1	D	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	E	198/204 (97%)	177 (89%)	21 (11%)	6	22
1	F	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	G	194/204 (95%)	177 (91%)	17 (9%)	9	29
1	H	198/204 (97%)	177 (89%)	21 (11%)	6	22
1	I	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	J	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	K	198/204 (97%)	179 (90%)	19 (10%)	8	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	201/204 (98%)	183 (91%)	18 (9%)	9	28
1	M	194/204 (95%)	177 (91%)	17 (9%)	9	29
1	N	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	O	198/204 (97%)	177 (89%)	21 (11%)	6	22
1	P	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	Q	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	R	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	a	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	b	194/204 (95%)	177 (91%)	17 (9%)	9	29
1	c	194/204 (95%)	178 (92%)	16 (8%)	10	33
1	d	201/204 (98%)	184 (92%)	17 (8%)	10	31
1	e	194/204 (95%)	178 (92%)	16 (8%)	10	33
1	h	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	i	198/204 (97%)	178 (90%)	20 (10%)	7	23
1	j	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	k	194/204 (95%)	176 (91%)	18 (9%)	8	27
1	l	194/204 (95%)	177 (91%)	17 (9%)	9	29
1	m	201/204 (98%)	183 (91%)	18 (9%)	9	28
1	o	201/204 (98%)	185 (92%)	16 (8%)	11	34
All	All	5907/6120 (96%)	5348 (90%)	559 (10%)	8	26

5 of 559 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	2250	ARG
1	m	3226	GLN
1	M	2243	LYS
1	Q	1243	LYS
1	F	1175	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	3225	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	1103	ASN
1	L	3226	GLN
1	m	3225	GLN
1	Q	1103	ASN

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 oligosaccharides 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	l	3101	-	4,4,4	0.89	0	6,6,6	0.54	0
4	PO4	H	2061	-	4,4,4	0.87	0	6,6,6	0.56	0
4	PO4	j	3081	-	4,4,4	0.84	0	6,6,6	0.68	0
3	V7O	h	5033	-	0,10,25	-	-	-	-	-
4	PO4	D	2031	-	4,4,4	0.86	0	6,6,6	0.53	0
3	V7O	J	5042	-	0,10,25	-	-	-	-	-
4	PO4	B	2011	-	4,4,4	0.86	0	6,6,6	0.64	0
4	PO4	O	2111	-	4,4,4	0.92	0	6,6,6	0.50	0
5	DUR	b	3022	-	17,17,17	1.76	4 (23%)	24,24,24	3.78	9 (37%)
4	PO4	E	2041	-	4,4,4	0.82	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	K	2091	-	4,4,4	0.93	0	6,6,6	0.41	0
5	DUR	j	3082	-	17,17,17	1.89	3 (17%)	24,24,24	3.89	11 (45%)
5	DUR	F	2052	-	17,17,17	1.90	6 (35%)	24,24,24	3.66	9 (37%)
3	V7O	H	5031	-	0,10,25	-	-	-	-	-
5	DUR	l	3102	-	17,17,17	1.76	3 (17%)	24,24,24	3.50	9 (37%)
3	V7O	Q	5053	-	0,10,25	-	-	-	-	-
5	DUR	e	3042	-	17,17,17	1.67	3 (17%)	24,24,24	3.55	7 (29%)
4	PO4	b	3021	-	4,4,4	0.83	0	6,6,6	0.58	0
4	PO4	e	3041	-	4,4,4	0.81	0	6,6,6	0.73	0
4	PO4	P	3121	-	4,4,4	0.89	0	6,6,6	0.55	0
4	PO4	I	3071	-	4,4,4	0.78	0	6,6,6	0.75	0
4	PO4	c	3031	-	4,4,4	0.99	0	6,6,6	0.97	1 (16%)
4	PO4	G	3051	-	4,4,4	0.91	0	6,6,6	0.65	0
5	DUR	a	3012	-	17,17,17	2.01	5 (29%)	24,24,24	3.83	9 (37%)
5	DUR	G	3052	-	17,17,17	1.74	3 (17%)	24,24,24	3.54	9 (37%)
5	DUR	P	3122	-	17,17,17	1.69	3 (17%)	24,24,24	3.83	11 (45%)
5	DUR	M	3112	-	17,17,17	1.78	3 (17%)	24,24,24	3.64	7 (29%)
5	DUR	Q	2122	-	17,17,17	1.77	5 (29%)	24,24,24	3.27	6 (25%)
5	DUR	K	2092	-	17,17,17	1.88	5 (29%)	24,24,24	3.41	9 (37%)
3	V7O	k	5043	-	0,10,25	-	-	-	-	-
4	PO4	F	2051	-	4,4,4	0.89	0	6,6,6	0.37	0
3	V7O	A	5011	-	0,10,25	-	-	-	-	-
4	PO4	C	2021	-	4,4,4	0.87	0	6,6,6	0.54	0
3	V7O	L	5041	-	0,10,25	-	-	-	-	-
5	DUR	I	3072	-	17,17,17	1.88	4 (23%)	24,24,24	3.56	7 (29%)
4	PO4	h	3061	-	4,4,4	0.91	0	6,6,6	0.53	0
3	V7O	b	5013	-	0,10,25	-	-	-	-	-
3	V7O	M	5051	-	0,10,25	-	-	-	-	-
3	V7O	M	5052	-	0,10,25	-	-	-	-	-
5	DUR	B	2012	-	17,17,17	2.01	6 (35%)	24,24,24	3.66	8 (33%)
5	DUR	i	2072	-	17,17,17	1.92	6 (35%)	24,24,24	3.50	8 (33%)
4	PO4	M	3111	-	4,4,4	0.85	0	6,6,6	0.83	0
4	PO4	i	2071	-	4,4,4	0.87	0	6,6,6	0.51	0
5	DUR	h	3062	-	17,17,17	1.97	6 (35%)	24,24,24	3.39	6 (25%)
3	V7O	c	5014	-	0,10,25	-	-	-	-	-
4	PO4	a	3011	-	4,4,4	0.76	0	6,6,6	0.68	0
4	PO4	k	3091	-	4,4,4	0.84	0	6,6,6	0.84	0
5	DUR	k	3092	-	17,17,17	1.95	5 (29%)	24,24,24	3.62	7 (29%)
5	DUR	C	2022	-	17,17,17	1.92	7 (41%)	24,24,24	4.00	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	V7O	e	5023	-	0,10,25	-	-	-		
5	DUR	O	2112	-	17,17,17	1.92	6 (35%)	24,24,24	3.29	6 (25%)
4	PO4	N	2101	-	4,4,4	0.92	0	6,6,6	0.56	0
4	PO4	J	2081	-	4,4,4	0.87	0	6,6,6	0.48	0
3	V7O	D	5021	-	0,10,25	-	-	-		
3	V7O	o	5054	-	0,10,25	-	-	-		
5	DUR	c	3032	-	17,17,17	2.13	5 (29%)	24,24,24	4.23	11 (45%)
3	V7O	j	5044	-	0,10,25	-	-	-		
4	PO4	R	2131	-	4,4,4	0.95	0	6,6,6	0.38	0
3	V7O	D	5022	-	0,10,25	-	-	-		
3	V7O	B	5012	-	0,10,25	-	-	-		
3	V7O	R	5024	-	0,10,25	-	-	-		
5	DUR	R	2132	-	17,17,17	1.94	5 (29%)	24,24,24	3.71	10 (41%)
5	DUR	N	2102	-	17,17,17	1.77	4 (23%)	24,24,24	3.36	9 (37%)
5	DUR	H	2062	-	17,17,17	1.78	3 (17%)	24,24,24	3.35	6 (25%)
5	DUR	E	2042	-	17,17,17	1.91	5 (29%)	24,24,24	3.63	8 (33%)
4	PO4	Q	2121	-	4,4,4	0.99	0	6,6,6	0.57	0
5	DUR	D	2032	-	17,17,17	1.82	3 (17%)	24,24,24	3.59	8 (33%)
5	DUR	J	2082	-	17,17,17	2.07	5 (29%)	24,24,24	3.70	7 (29%)
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	M	3112	-	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	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	F	2052	-	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	Q	2122	-	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	G	3052	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DUR	K	2092	-	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	B	2012	-	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	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
5	DUR	C	2022	-	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	c	3032	-	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	H	2062	-	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	D	2032	-	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	N	2102	-	1/1/3/3	4/6/18/18	0/2/2/2

The worst 5 of 113 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	5.17	1.47	1.35
5	i	2072	DUR	C6-C5	5.16	1.47	1.35
5	D	2032	DUR	C6-C5	5.09	1.46	1.35

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2022	DUR	C2'-C1'-N1	15.46	152.46	113.81
5	c	3032	DUR	C2'-C1'-N1	15.21	151.85	113.81
5	F	2052	DUR	C2'-C1'-N1	14.67	150.50	113.81
5	I	3072	DUR	C2'-C1'-N1	14.44	149.91	113.81
5	j	3082	DUR	C2'-C1'-N1	14.33	149.65	113.81

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	a	3012	DUR	C1'

Continued on next page...

Continued from previous page...

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.

28 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	l	3101	PO4	1	0
4	H	2061	PO4	1	0
3	h	5033	V7O	3	0
3	J	5042	V7O	5	0
4	O	2111	PO4	1	0
3	H	5031	V7O	2	0
3	Q	5053	V7O	1	0
4	P	3121	PO4	2	0
4	G	3051	PO4	1	0
5	G	3052	DUR	1	0
5	P	3122	DUR	1	0
3	A	5011	V7O	1	0
4	C	2021	PO4	1	0
3	L	5041	V7O	1	0
3	b	5013	V7O	2	0
3	M	5051	V7O	3	0
3	M	5052	V7O	4	0
3	c	5014	V7O	2	0
4	k	3091	PO4	1	0
5	C	2022	DUR	1	0
3	e	5023	V7O	2	0
3	D	5021	V7O	2	0
3	o	5054	V7O	1	0
3	D	5022	V7O	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5012	V7O	1	0
3	R	5024	V7O	2	0
3	I	5032	V7O	3	0
3	i	5034	V7O	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/253 (98%)	-0.35	2 (0%) 82 75	4, 15, 31, 46	0
1	B	246/253 (97%)	-0.42	2 (0%) 82 75	4, 14, 29, 63	0
1	C	246/253 (97%)	-0.05	10 (4%) 41 33	4, 14, 29, 63	0
1	D	246/253 (97%)	0.05	11 (4%) 38 30	4, 14, 29, 63	0
1	E	246/253 (97%)	-0.07	1 (0%) 88 84	4, 14, 29, 63	0
1	F	246/253 (97%)	-0.20	4 (1%) 70 61	4, 14, 29, 63	0
1	G	242/253 (95%)	-0.34	1 (0%) 88 84	6, 13, 25, 37	0
1	H	246/253 (97%)	-0.17	5 (2%) 65 56	4, 14, 29, 63	0
1	I	242/253 (95%)	-0.04	0 100 100	5, 13, 25, 37	0
1	J	246/253 (97%)	-0.16	2 (0%) 82 75	4, 14, 29, 63	0
1	K	246/253 (97%)	0.17	18 (7%) 21 15	4, 14, 29, 63	0
1	L	250/253 (98%)	0.19	8 (3%) 50 40	4, 15, 31, 46	0
1	M	242/253 (95%)	0.09	5 (2%) 63 54	5, 13, 25, 37	0
1	N	246/253 (97%)	0.60	17 (6%) 23 16	4, 14, 29, 63	0
1	O	246/253 (97%)	0.56	20 (8%) 18 13	4, 14, 29, 63	0
1	P	242/253 (95%)	-0.56	1 (0%) 88 84	6, 13, 25, 37	0
1	Q	246/253 (97%)	0.99	25 (10%) 12 9	4, 14, 29, 63	0
1	R	246/253 (97%)	-0.21	6 (2%) 59 49	4, 14, 29, 63	0
1	a	242/253 (95%)	-0.56	1 (0%) 88 84	6, 13, 25, 37	0
1	b	242/253 (95%)	-0.54	1 (0%) 88 84	5, 13, 25, 37	0
1	c	242/253 (95%)	-0.50	1 (0%) 88 84	5, 13, 25, 37	0
1	d	250/253 (98%)	-0.03	8 (3%) 50 40	4, 15, 31, 46	0
1	e	242/253 (95%)	-0.25	2 (0%) 82 75	6, 13, 25, 37	0
1	h	242/253 (95%)	0.32	5 (2%) 63 54	6, 13, 25, 37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	i	246/253 (97%)	-0.35	2 (0%) 82 75	4, 14, 29, 63	0
1	j	242/253 (95%)	-0.48	0 100 100	5, 13, 25, 37	0
1	k	242/253 (95%)	-0.38	1 (0%) 88 84	6, 13, 25, 37	0
1	l	242/253 (95%)	0.46	8 (3%) 49 39	5, 13, 25, 37	0
1	m	250/253 (98%)	0.82	60 (24%) 2 1	4, 15, 31, 46	0
1	o	250/253 (98%)	0.20	12 (4%) 35 28	4, 15, 31, 46	0
All	All	7352/7590 (96%)	-0.04	239 (3%) 49 39	4, 14, 28, 63	0

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	m	3153	VAL	6.7
1	Q	1229	PRO	6.1
1	m	3142	GLU	5.9
1	m	3093	GLY	5.8
1	m	3228	ILE	5.6

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	C	2021	5/5	0.40	0.28	147,148,148,148	0
4	PO4	Q	2121	5/5	0.51	0.21	131,131,132,132	0
4	PO4	R	2131	5/5	0.68	0.24	136,136,137,137	0
4	PO4	D	2031	5/5	0.69	0.25	135,135,135,136	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	E	2041	5/5	0.69	0.23	127,128,128,128	0
4	PO4	N	2101	5/5	0.71	0.21	126,126,126,127	0
4	PO4	I	3071	5/5	0.71	0.21	120,121,121,122	0
4	PO4	i	2071	5/5	0.73	0.24	127,128,128,128	0
4	PO4	O	2111	5/5	0.75	0.24	126,126,126,127	0
4	PO4	h	3061	5/5	0.76	0.18	124,125,125,125	0
5	DUR	N	2102	16/16	0.76	0.20	86,88,89,89	0
5	DUR	Q	2122	16/16	0.77	0.22	104,107,107,107	0
4	PO4	l	3101	5/5	0.78	0.17	107,107,108,108	0
4	PO4	H	2061	5/5	0.78	0.21	118,119,119,119	0
4	PO4	K	2091	5/5	0.78	0.20	114,114,115,115	0
4	PO4	J	2081	5/5	0.79	0.20	127,128,128,128	0
5	DUR	D	2032	16/16	0.79	0.15	68,72,73,74	0
5	DUR	I	3072	16/16	0.80	0.16	57,63,65,65	0
5	DUR	K	2092	16/16	0.80	0.19	77,81,83,83	0
5	DUR	C	2022	16/16	0.80	0.19	57,69,73,74	0
4	PO4	M	3111	5/5	0.80	0.22	106,106,107,108	0
3	V7O	o	5054	11/26	0.81	0.12	105,107,108,109	0
3	V7O	D	5021	11/26	0.81	0.13	91,94,95,96	0
5	DUR	O	2112	16/16	0.81	0.17	77,81,82,82	0
3	V7O	i	5034	11/26	0.82	0.12	86,88,90,91	0
4	PO4	G	3051	5/5	0.82	0.19	105,105,106,106	0
5	DUR	i	2072	16/16	0.82	0.16	72,75,77,77	0
5	DUR	J	2082	16/16	0.82	0.15	50,55,61,62	0
5	DUR	R	2132	16/16	0.83	0.16	63,67,70,71	0
5	DUR	l	3102	16/16	0.83	0.14	61,66,67,68	0
4	PO4	F	2051	5/5	0.83	0.21	108,109,109,110	0
5	DUR	E	2042	16/16	0.83	0.14	59,65,67,67	0
5	DUR	F	2052	16/16	0.83	0.16	57,62,66,67	0
5	DUR	h	3062	16/16	0.84	0.13	53,60,63,64	0
5	DUR	B	2012	16/16	0.84	0.16	44,51,55,55	0
3	V7O	R	5024	11/26	0.84	0.11	86,88,89,92	0
5	DUR	e	3042	16/16	0.85	0.15	55,62,66,67	0
5	DUR	k	3092	16/16	0.85	0.14	43,47,52,53	0
5	DUR	H	2062	16/16	0.85	0.14	57,60,61,62	0
3	V7O	H	5031	11/26	0.86	0.11	96,97,98,99	0
4	PO4	k	3091	5/5	0.86	0.20	106,106,107,107	0
3	V7O	c	5014	11/26	0.86	0.11	84,86,88,89	0
5	DUR	c	3032	16/16	0.86	0.13	38,43,49,50	0
3	V7O	j	5044	11/26	0.87	0.11	88,89,93,94	0
3	V7O	L	5041	11/26	0.87	0.12	91,94,95,95	0
5	DUR	G	3052	16/16	0.88	0.12	42,46,52,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	V7O	A	5011	11/26	0.88	0.11	78,83,84,88	0
5	DUR	a	3012	16/16	0.89	0.12	35,43,51,51	0
3	V7O	M	5051	11/26	0.89	0.10	87,89,90,90	0
4	PO4	B	2011	5/5	0.89	0.18	101,102,102,102	0
5	DUR	M	3112	16/16	0.90	0.11	55,58,61,61	0
4	PO4	a	3011	5/5	0.90	0.15	67,68,70,70	0
4	PO4	c	3031	5/5	0.91	0.15	74,74,75,75	0
4	PO4	j	3081	5/5	0.91	0.17	81,81,82,82	0
2	K	o	4151	1/1	0.91	0.09	66,66,66,66	0
3	V7O	Q	5053	11/26	0.91	0.10	88,91,94,95	0
5	DUR	j	3082	16/16	0.91	0.11	38,42,47,47	0
4	PO4	P	3121	5/5	0.91	0.17	94,94,95,95	0
5	DUR	b	3022	16/16	0.92	0.11	36,41,46,48	0
3	V7O	M	5052	11/26	0.92	0.12	74,76,78,78	0
2	K	N	4141	1/1	0.92	0.07	61,61,61,61	0
3	V7O	B	5012	11/26	0.92	0.11	73,76,78,78	0
5	DUR	P	3122	16/16	0.92	0.10	31,37,43,45	0
3	V7O	e	5023	11/26	0.92	0.10	70,73,74,74	0
3	V7O	h	5033	11/26	0.93	0.12	76,78,80,80	0
3	V7O	b	5013	11/26	0.93	0.10	63,66,68,69	0
4	PO4	e	3041	5/5	0.93	0.12	87,87,88,88	0
2	K	L	4121	1/1	0.94	0.08	58,58,58,58	0
2	K	R	4061	1/1	0.94	0.08	47,47,47,47	0
3	V7O	D	5022	11/26	0.94	0.09	74,77,78,79	0
2	K	h	4081	1/1	0.94	0.07	51,51,51,51	0
3	V7O	J	5042	11/26	0.94	0.10	69,73,74,77	0
4	PO4	b	3021	5/5	0.95	0.12	80,80,81,81	0
3	V7O	k	5043	11/26	0.95	0.09	64,67,69,70	0
3	V7O	I	5032	11/26	0.95	0.08	76,79,80,82	0
2	K	D	4041	1/1	0.96	0.06	64,64,64,64	0
2	K	K	4111	1/1	0.97	0.04	47,47,47,47	0
2	K	M	4131	1/1	0.97	0.06	55,55,55,55	0
2	K	A	4011	1/1	0.98	0.09	34,34,34,34	0
2	K	G	4071	1/1	0.98	0.03	40,40,40,40	0
2	K	E	4051	1/1	0.98	0.04	49,49,49,49	0
2	K	i	4091	1/1	0.98	0.06	45,45,45,45	0
2	K	J	4101	1/1	0.98	0.09	32,32,32,32	0
2	K	B	4021	1/1	0.99	0.04	36,36,36,36	0
2	K	C	4031	1/1	0.99	0.06	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.