



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2025 – 02:33 PM JST

PDB ID : 8YQ0  
Title : Crystal structure of human phosphoribosyl pyrophosphate synthetase 1(PRPS1) chimera swapped with three residues from PRPS2  
Authors : Zhang, L.; Zhang, L.  
Deposited on : 2024-03-18  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

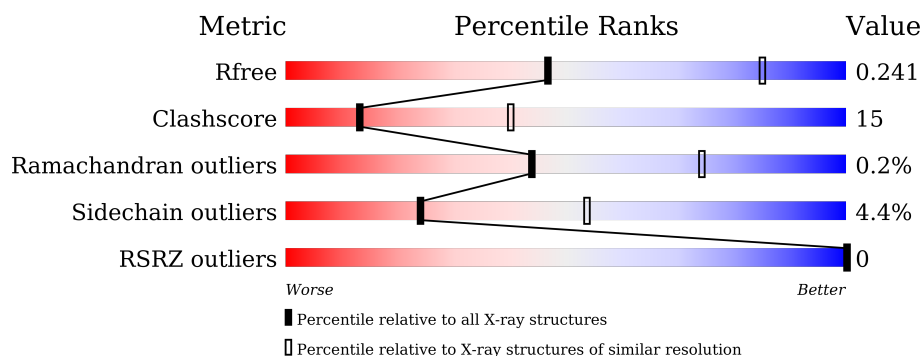
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.











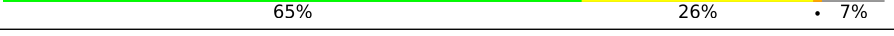

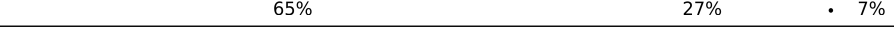

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	321	<div> <div>71%</div> <div>23%</div> <div>..</div> </div>
1	B	321	<div> <div>68%</div> <div>25%</div> <div>...</div> </div>
1	C	321	<div> <div>65%</div> <div>28%</div> <div>..</div> </div>
1	D	321	<div> <div>71%</div> <div>23%</div> <div>..</div> </div>
1	E	321	<div> <div>65%</div> <div>27%</div> <div>..</div> </div>
1	F	321	<div> <div>71%</div> <div>23%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	321	 62%30%•••
1	H	321	 69%22%•6%
1	I	321	 73%22%••
1	J	321	 73%19%•7%
1	K	321	 72%23%••
1	L	321	 62%30%•7%
1	M	321	 68%23%•7%
1	N	321	 66%29%••
1	O	321	 65%26%•7%
1	P	321	 75%20%••
1	Q	321	 65%27%•7%
1	R	321	 68%28%••

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 42231 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 Ribose-phosphate pyrophosphokinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2382	1496	418	451	17			
1	B	312	Total	C	N	O	S	0	0	0
			2382	1496	418	451	17			
1	C	309	Total	C	N	O	S	0	0	0
			2354	1479	412	446	17			
1	D	310	Total	C	N	O	S	0	0	0
			2362	1485	413	447	17			
1	E	312	Total	C	N	O	S	0	0	0
			2379	1494	418	450	17			
1	F	312	Total	C	N	O	S	0	0	0
			2382	1496	418	451	17			
1	G	311	Total	C	N	O	S	0	0	0
			2373	1491	417	448	17			
1	H	301	Total	C	N	O	S	0	0	0
			2291	1434	405	435	17			
1	I	313	Total	C	N	O	S	0	0	0
			2390	1500	419	454	17			
1	J	300	Total	C	N	O	S	0	1	0
			2295	1437	407	434	17			
1	K	311	Total	C	N	O	S	0	0	0
			2368	1488	414	449	17			
1	L	298	Total	C	N	O	S	0	0	0
			2267	1421	399	430	17			
1	M	298	Total	C	N	O	S	0	0	0
			2267	1421	399	430	17			
1	N	310	Total	C	N	O	S	0	0	0
			2362	1485	413	447	17			
1	O	298	Total	C	N	O	S	0	0	0
			2272	1424	402	429	17			
1	P	313	Total	C	N	O	S	0	0	0
			2390	1500	419	454	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	300	Total	C	N	O	S	0	0	0
			2285	1431	404	433	17			
1	R	313	Total	C	N	O	S	0	0	0
			2388	1499	419	453	17			

There are 72 discrepancies between the modelled and reference sequences:

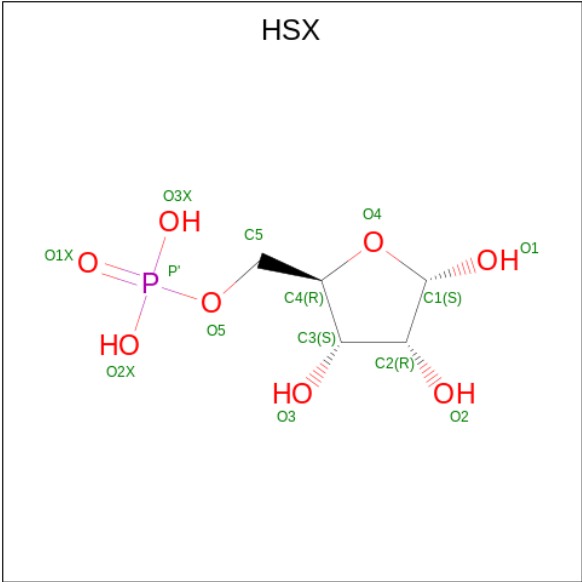
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P60891
A	103	VAL	-	insertion	UNP P60891
A	104	GLY	-	insertion	UNP P60891
A	105	GLU	-	insertion	UNP P60891
B	1	SER	-	expression tag	UNP P60891
B	103	VAL	-	insertion	UNP P60891
B	104	GLY	-	insertion	UNP P60891
B	105	GLU	-	insertion	UNP P60891
C	1	SER	-	expression tag	UNP P60891
C	103	VAL	-	insertion	UNP P60891
C	104	GLY	-	insertion	UNP P60891
C	105	GLU	-	insertion	UNP P60891
D	1	SER	-	expression tag	UNP P60891
D	103	VAL	-	insertion	UNP P60891
D	104	GLY	-	insertion	UNP P60891
D	105	GLU	-	insertion	UNP P60891
E	1	SER	-	expression tag	UNP P60891
E	103	VAL	-	insertion	UNP P60891
E	104	GLY	-	insertion	UNP P60891
E	105	GLU	-	insertion	UNP P60891
F	1	SER	-	expression tag	UNP P60891
F	103	VAL	-	insertion	UNP P60891
F	104	GLY	-	insertion	UNP P60891
F	105	GLU	-	insertion	UNP P60891
G	1	SER	-	expression tag	UNP P60891
G	103	VAL	-	insertion	UNP P60891
G	104	GLY	-	insertion	UNP P60891
G	105	GLU	-	insertion	UNP P60891
H	1	SER	-	expression tag	UNP P60891
H	103	VAL	-	insertion	UNP P60891
H	104	GLY	-	insertion	UNP P60891
H	105	GLU	-	insertion	UNP P60891
I	1	SER	-	expression tag	UNP P60891
I	103	VAL	-	insertion	UNP P60891

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Chain	Residue	Modelled	Actual	Comment	Reference
I	104	GLY	-	insertion	UNP P60891
I	105	GLU	-	insertion	UNP P60891
J	1	SER	-	expression tag	UNP P60891
J	103	VAL	-	insertion	UNP P60891
J	104	GLY	-	insertion	UNP P60891
J	105	GLU	-	insertion	UNP P60891
K	1	SER	-	expression tag	UNP P60891
K	103	VAL	-	insertion	UNP P60891
K	104	GLY	-	insertion	UNP P60891
K	105	GLU	-	insertion	UNP P60891
L	1	SER	-	expression tag	UNP P60891
L	103	VAL	-	insertion	UNP P60891
L	104	GLY	-	insertion	UNP P60891
L	105	GLU	-	insertion	UNP P60891
M	1	SER	-	expression tag	UNP P60891
M	103	VAL	-	insertion	UNP P60891
M	104	GLY	-	insertion	UNP P60891
M	105	GLU	-	insertion	UNP P60891
N	1	SER	-	expression tag	UNP P60891
N	103	VAL	-	insertion	UNP P60891
N	104	GLY	-	insertion	UNP P60891
N	105	GLU	-	insertion	UNP P60891
O	1	SER	-	expression tag	UNP P60891
O	103	VAL	-	insertion	UNP P60891
O	104	GLY	-	insertion	UNP P60891
O	105	GLU	-	insertion	UNP P60891
P	1	SER	-	expression tag	UNP P60891
P	103	VAL	-	insertion	UNP P60891
P	104	GLY	-	insertion	UNP P60891
P	105	GLU	-	insertion	UNP P60891
Q	1	SER	-	expression tag	UNP P60891
Q	103	VAL	-	insertion	UNP P60891
Q	104	GLY	-	insertion	UNP P60891
Q	105	GLU	-	insertion	UNP P60891
R	1	SER	-	expression tag	UNP P60891
R	103	VAL	-	insertion	UNP P60891
R	104	GLY	-	insertion	UNP P60891
R	105	GLU	-	insertion	UNP P60891

- Molecule 2 is 5-O-phosphono-alpha-D-ribofuranose (three-letter code: HSX) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).

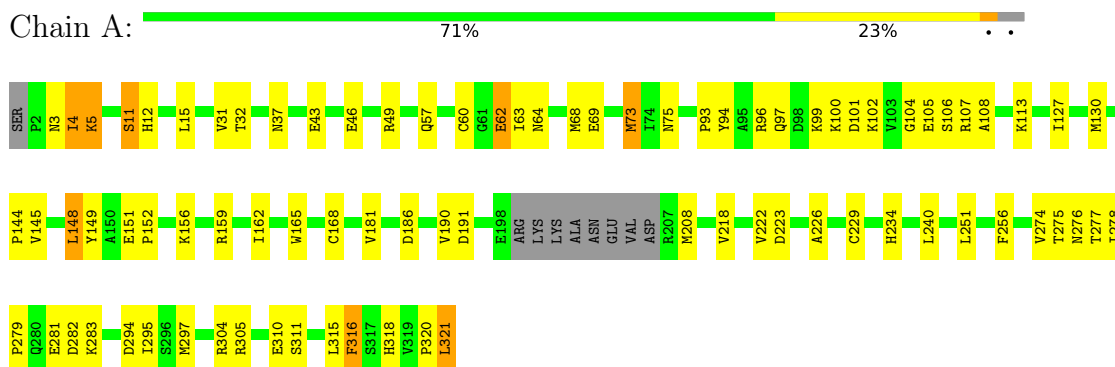


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			14	5	8	1		
2	F	1	Total	C	O	P	0	0
			14	5	8	1		
2	O	1	Total	C	O	P	0	0
			14	5	8	1		

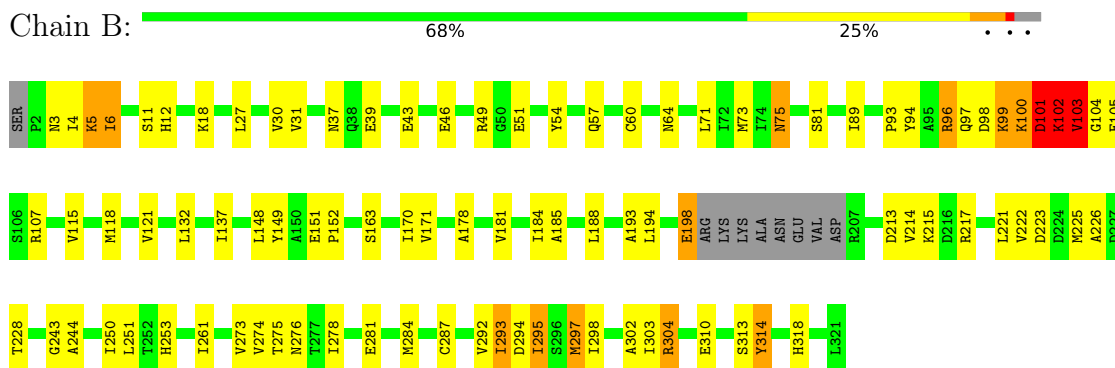
### 3 Residue-property plots [i](#)

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

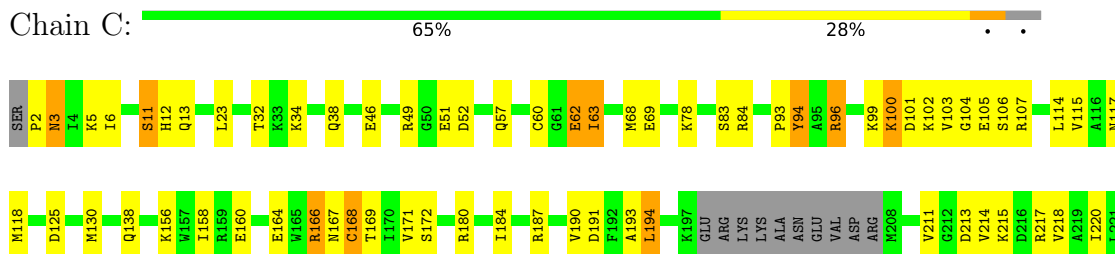
- Molecule 1: Ribose-phosphate pyrophosphokinase 1



- Molecule 1: Ribose-phosphate pyrophosphokinase 1



- Molecule 1: Ribose-phosphate pyrophosphokinase 1







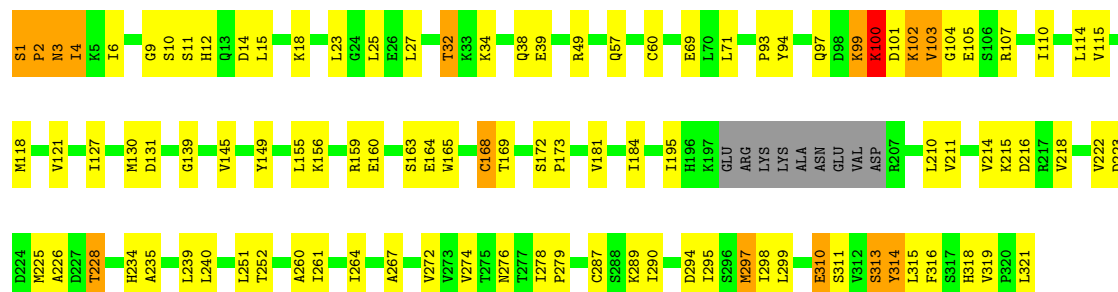
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain D: 71% 23% . .



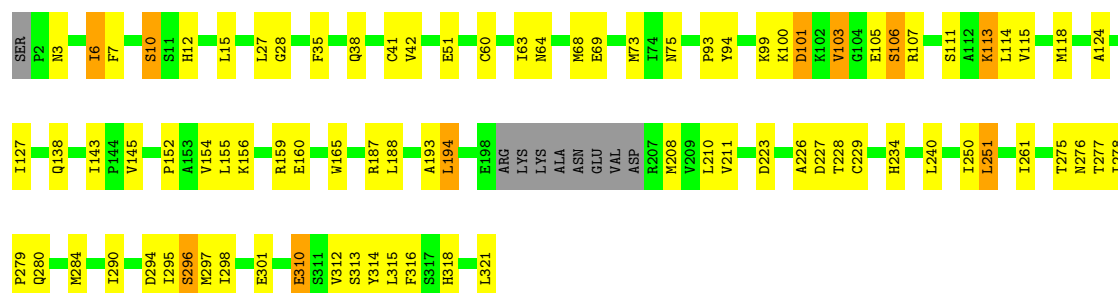
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain E: 65% 27% . .



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

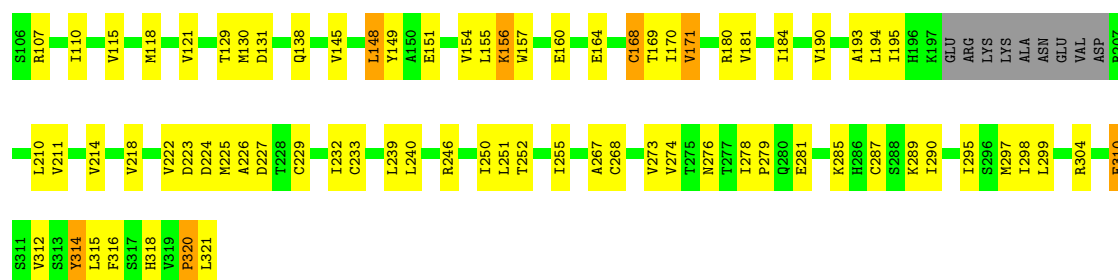
Chain F: 71% 23% . .



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

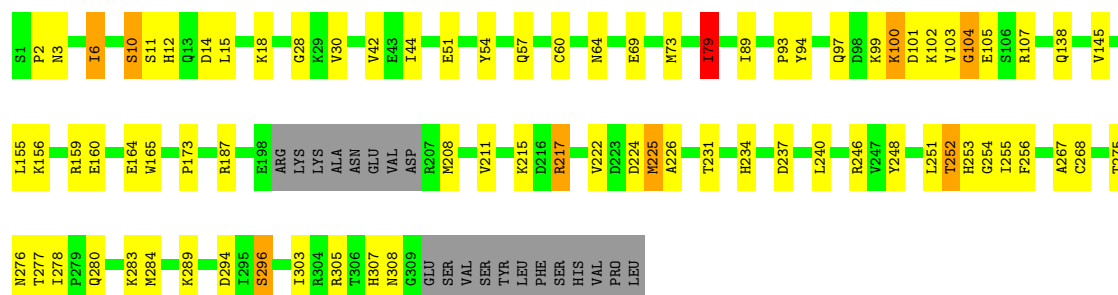
Chain G: 62% 30% . . .





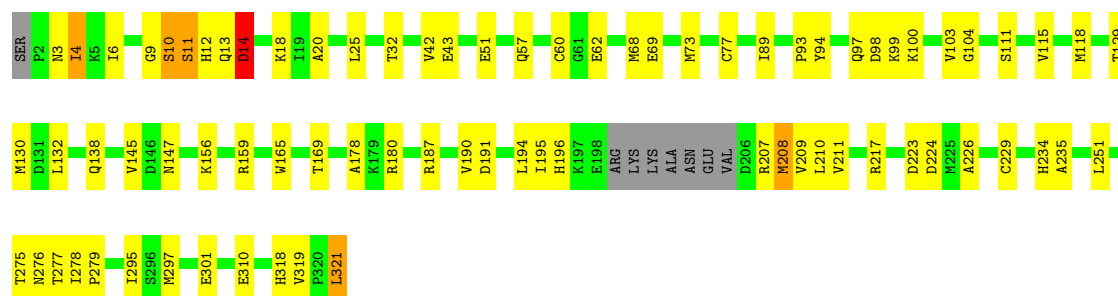
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain H: 69% 22% 6%



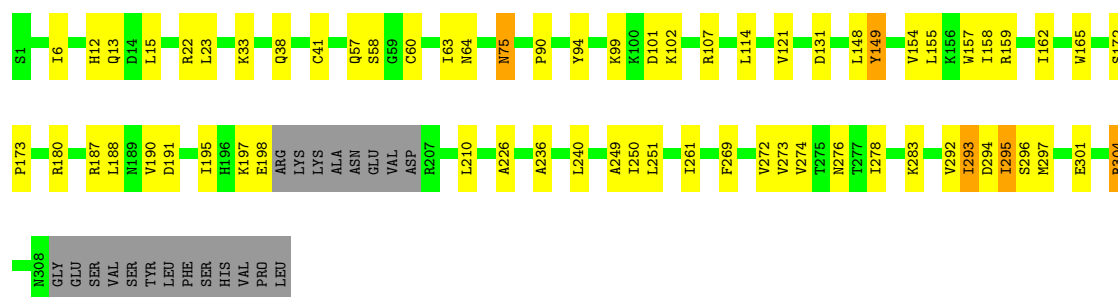
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain I: 73% 22% 2%



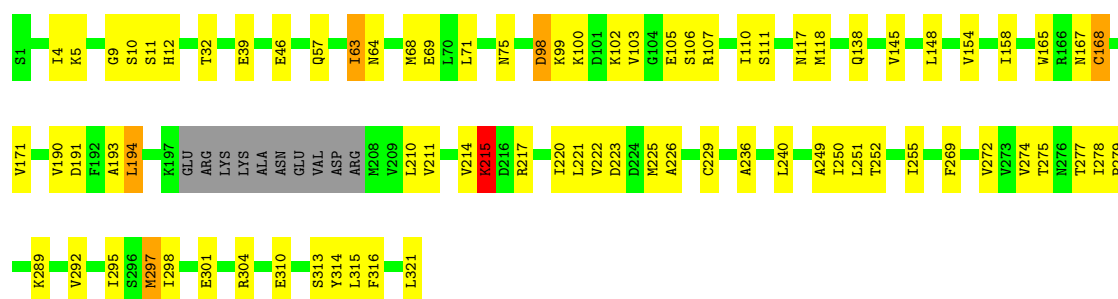
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain J: 73% 19% 7%



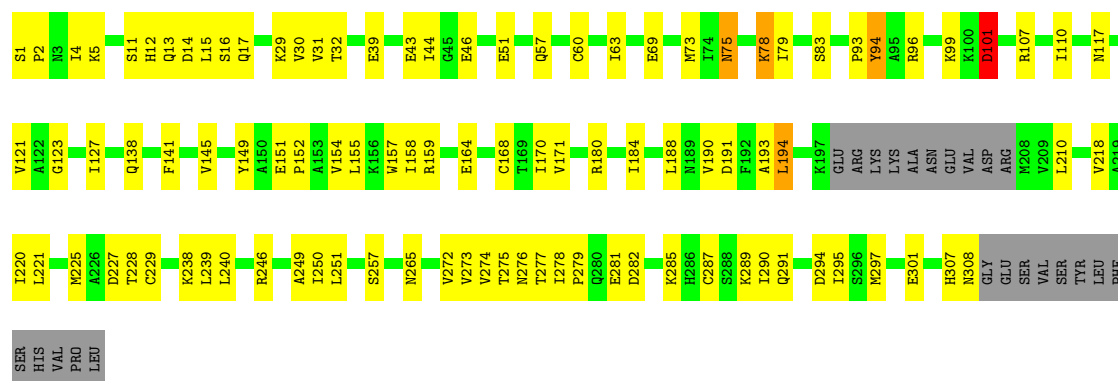
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain K:  72% 23% . .



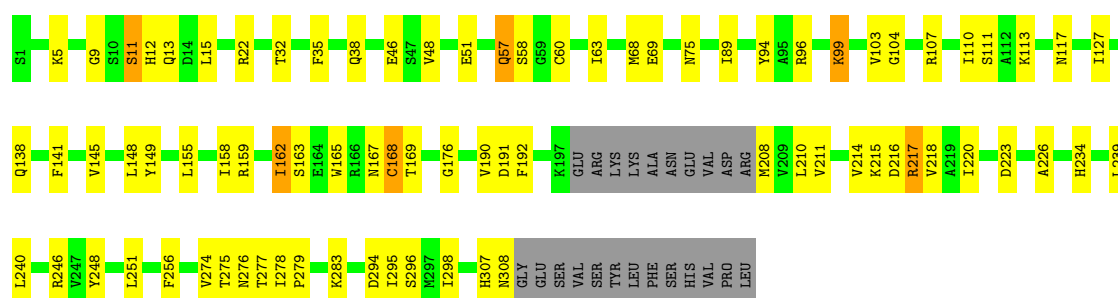
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain L:  62% 30% . 7%



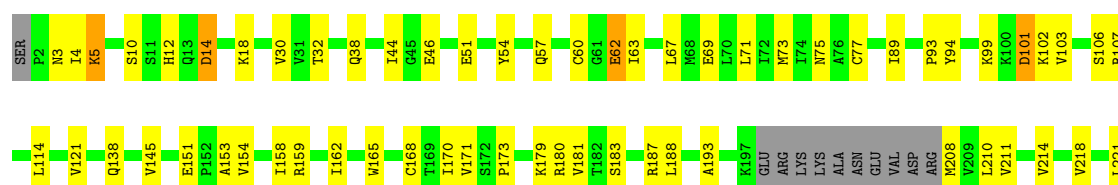
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain M:  68% 23% . 7%



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain N:  66% 29% . .





• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain O: 65% 26% 7%



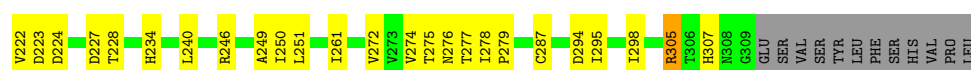
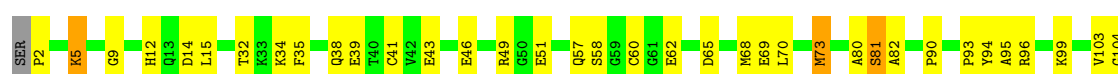
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain P: 75% 20% 5%



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

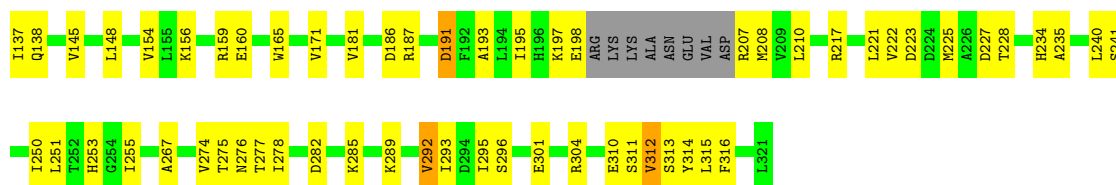
Chain Q: 65% 27% 7%



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain R: 68% 28% 4%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.08Å 108.08Å 659.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.10 50.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.01-3.10) 98.8 (50.01-3.10)	Depositor EDS
$R_{merge}$	0.54	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.196 , 0.250 0.198 , 0.241	Depositor DCC
$R_{free}$ test set	6691 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	42231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HSX

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	0.99	10/2417 (0.4%)	0.92	0/3269
1	B	0.97	8/2417 (0.3%)	0.90	0/3269
1	C	0.93	6/2389 (0.3%)	0.96	0/3232
1	D	0.81	2/2397 (0.1%)	0.88	0/3243
1	E	1.08	5/2414 (0.2%)	0.99	3/3266 (0.1%)
1	F	1.00	6/2417 (0.2%)	0.92	0/3269
1	G	1.00	9/2408 (0.4%)	0.98	4/3257 (0.1%)
1	H	1.03	9/2322 (0.4%)	0.93	1/3139 (0.0%)
1	I	0.83	2/2425 (0.1%)	0.90	0/3280
1	J	0.74	3/2329 (0.1%)	0.87	1/3148 (0.0%)
1	K	0.83	2/2403 (0.1%)	0.93	3/3252 (0.1%)
1	L	0.76	1/2298 (0.0%)	0.91	2/3108 (0.1%)
1	M	0.81	5/2298 (0.2%)	0.88	0/3108
1	N	0.82	3/2397 (0.1%)	0.91	0/3243
1	O	0.89	6/2303 (0.3%)	0.90	0/3113
1	P	0.72	2/2425 (0.1%)	0.91	1/3280 (0.0%)
1	Q	0.96	6/2316 (0.3%)	0.92	0/3130
1	R	0.84	0/2423	0.91	0/3278
All	All	0.90	85/42798 (0.2%)	0.92	15/57884 (0.0%)

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	168	CYS	CB-SG	-8.45	1.67	1.82
1	H	254	GLY	C-O	-8.27	1.10	1.23
1	N	77	CYS	CB-SG	-7.58	1.69	1.82
1	B	105	GLU	CD-OE2	-6.91	1.18	1.25
1	F	106	SER	CB-OG	-6.73	1.33	1.42

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3	ASN	CB-CA-C	9.05	128.51	110.40
1	G	100	LYS	N-CA-C	-7.23	91.49	111.00
1	L	101	ASP	C-N-CA	7.16	139.59	121.70
1	P	2	PRO	C-N-CA	6.42	137.75	121.70
1	G	99	LYS	CB-CA-C	-5.97	98.45	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2382	0	2421	70	0
1	B	2382	0	2421	96	0
1	C	2354	0	2388	95	0
1	D	2362	0	2402	72	0
1	E	2379	0	2419	97	0
1	F	2382	0	2421	76	0
1	G	2373	0	2415	105	0
1	H	2291	0	2334	62	0
1	I	2390	0	2425	63	0
1	J	2295	0	2345	49	0
1	K	2368	0	2409	77	0
1	L	2267	0	2313	90	0
1	M	2267	0	2313	76	0
1	N	2362	0	2402	67	0
1	O	2272	0	2319	73	0
1	P	2390	0	2425	62	0
1	Q	2285	0	2328	66	0
1	R	2388	0	2428	82	0
2	B	14	0	0	1	0
2	F	14	0	0	2	0
2	O	14	0	0	4	0
All	All	42231	0	42928	1243	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.



The worst 5 of 1243 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:H:225:MET:HE1	1:H:255:ILE:CD1	1.56	1.36
1:C:213:ASP:O	1:C:217:ARG:NH2	1.60	1.30
1:B:11:SER:HB2	1:B:57:GLN:OE1	1.36	1.25
1:I:11:SER:HB2	1:I:57:GLN:OE1	1.07	1.23
1:B:4:ILE:HG22	1:G:310:GLU:O	1.40	1.18

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/321 (96%)	296 (96%)	12 (4%)	0	100	100
1	B	308/321 (96%)	289 (94%)	15 (5%)	4 (1%)	10	36
1	C	305/321 (95%)	290 (95%)	15 (5%)	0	100	100
1	D	306/321 (95%)	289 (94%)	17 (6%)	0	100	100
1	E	308/321 (96%)	290 (94%)	16 (5%)	2 (1%)	22	53
1	F	308/321 (96%)	299 (97%)	8 (3%)	1 (0%)	37	68
1	G	307/321 (96%)	292 (95%)	14 (5%)	1 (0%)	37	68
1	H	297/321 (92%)	285 (96%)	12 (4%)	0	100	100
1	I	309/321 (96%)	297 (96%)	12 (4%)	0	100	100
1	J	297/321 (92%)	285 (96%)	12 (4%)	0	100	100
1	K	307/321 (96%)	292 (95%)	15 (5%)	0	100	100
1	L	294/321 (92%)	282 (96%)	12 (4%)	0	100	100
1	M	294/321 (92%)	278 (95%)	15 (5%)	1 (0%)	37	68
1	N	306/321 (95%)	291 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	294/321 (92%)	278 (95%)	16 (5%)	0	100	100
1	P	309/321 (96%)	298 (96%)	10 (3%)	1 (0%)	37	68
1	Q	296/321 (92%)	285 (96%)	11 (4%)	0	100	100
1	R	309/321 (96%)	300 (97%)	9 (3%)	0	100	100
All	All	5462/5778 (94%)	5216 (96%)	236 (4%)	10 (0%)	44	74

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	LYS
1	B	101	ASP
1	B	102	LYS
1	B	103	VAL
1	E	100	LYS

### 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	264/272 (97%)	253 (96%)	11 (4%)	25	56
1	B	264/272 (97%)	246 (93%)	18 (7%)	13	40
1	C	261/272 (96%)	244 (94%)	17 (6%)	14	41
1	D	262/272 (96%)	252 (96%)	10 (4%)	28	59
1	E	264/272 (97%)	249 (94%)	15 (6%)	17	46
1	F	264/272 (97%)	253 (96%)	11 (4%)	25	56
1	G	263/272 (97%)	248 (94%)	15 (6%)	17	46
1	H	253/272 (93%)	242 (96%)	11 (4%)	25	55
1	I	265/272 (97%)	248 (94%)	17 (6%)	14	42
1	J	254/272 (93%)	247 (97%)	7 (3%)	38	66
1	K	263/272 (97%)	253 (96%)	10 (4%)	28	59
1	L	251/272 (92%)	244 (97%)	7 (3%)	38	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	251/272 (92%)	241 (96%)	10 (4%)	27	58
1	N	262/272 (96%)	254 (97%)	8 (3%)	35	63
1	O	251/272 (92%)	244 (97%)	7 (3%)	38	66
1	P	265/272 (97%)	256 (97%)	9 (3%)	32	62
1	Q	252/272 (93%)	245 (97%)	7 (3%)	38	66
1	R	265/272 (97%)	248 (94%)	17 (6%)	14	42
All	All	4674/4896 (96%)	4467 (96%)	207 (4%)	24	54

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	99	LYS
1	L	78	LYS
1	R	217	ARG
1	I	207	ARG
1	J	304[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	12	HIS
1	N	12	HIS
1	Q	12	HIS
1	O	57	GLN
1	M	57	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

3 ligands are modelled in this entry.

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$
2	HSX	O	1001	-	14,14,14	0.77	0	20,21,21	0.94	0
2	HSX	F	1001	-	14,14,14	2.25	5 (35%)	20,21,21	1.79	7 (35%)
2	HSX	B	1001	-	14,14,14	1.03	0	20,21,21	1.49	2 (10%)

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
2	HSX	O	1001	-	-	6/6/22/22	0/1/1/1
2	HSX	F	1001	-	-	0/6/22/22	0/1/1/1
2	HSX	B	1001	-	-	3/6/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	HSX	O3-C3	4.23	1.52	1.43
2	F	1001	HSX	O4-C1	4.12	1.48	1.43
2	F	1001	HSX	O1-C1	2.58	1.47	1.39
2	F	1001	HSX	C3-C4	2.57	1.59	1.53
2	F	1001	HSX	C1-C2	2.12	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1001	HSX	O4-C1-C2	-3.98	99.57	104.46
2	B	1001	HSX	O5-P'-O1X	-3.69	96.13	106.47
2	F	1001	HSX	O1-C1-O4	3.16	115.18	111.13
2	F	1001	HSX	O3-C3-C4	2.62	118.62	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	HSX	P'-O5-C5	-2.54	111.30	118.30

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

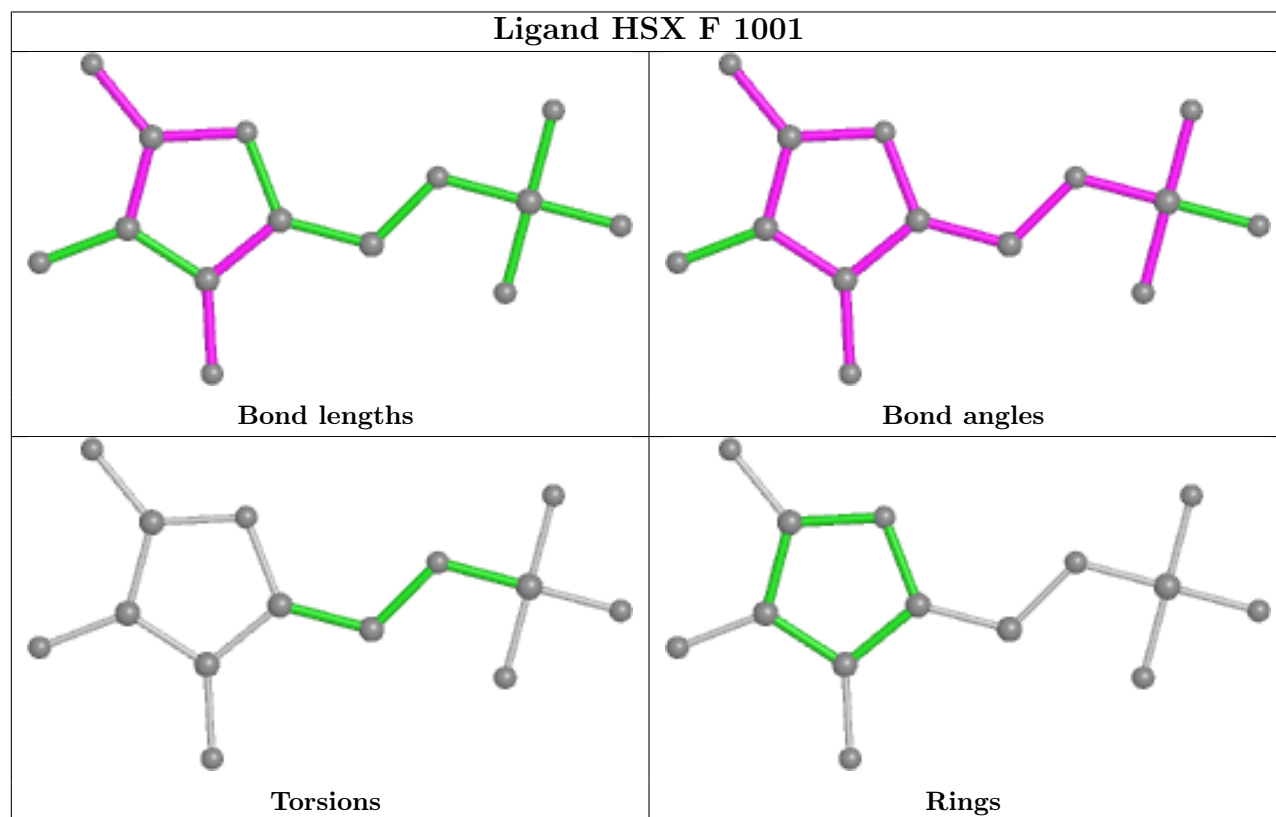
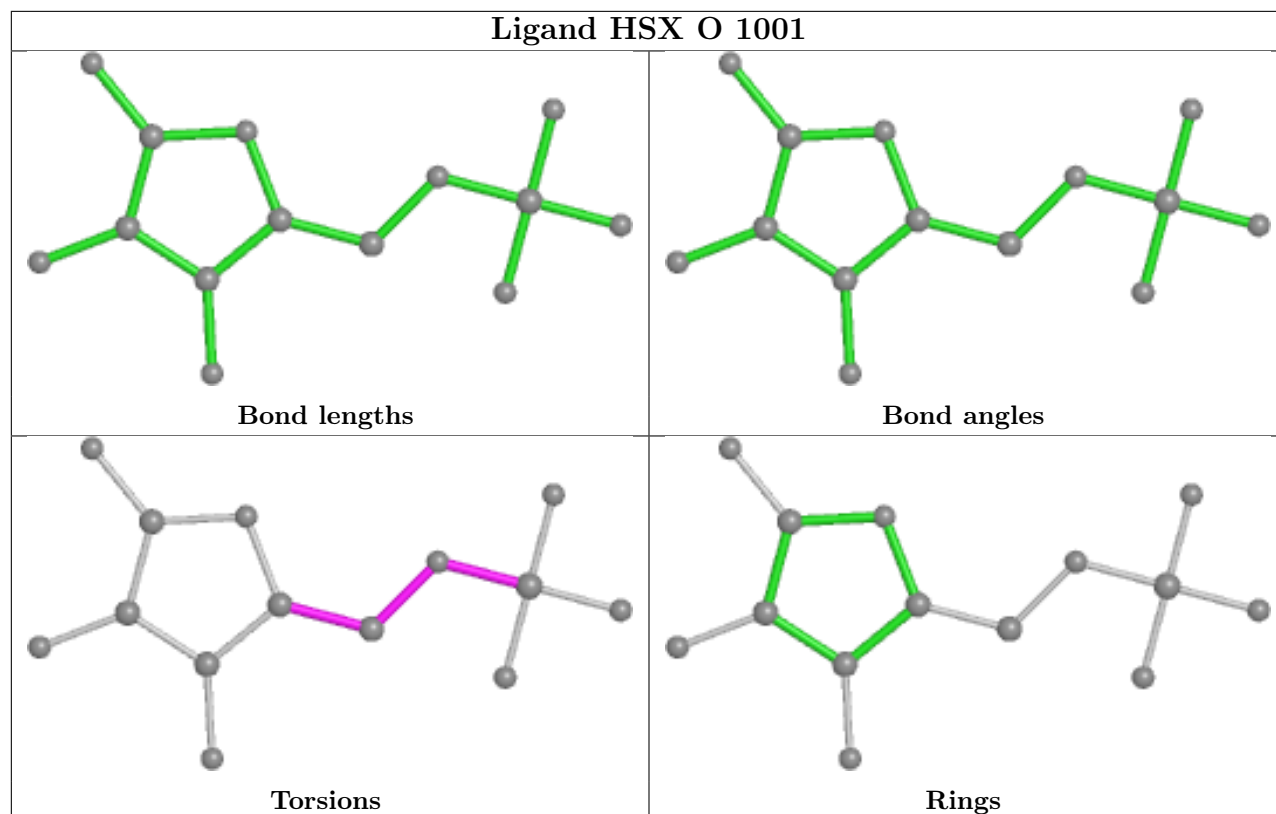
Mol	Chain	Res	Type	Atoms
2	B	1001	HSX	C3-C4-C5-O5
2	O	1001	HSX	C5-O5-P'-O3X
2	O	1001	HSX	C3-C4-C5-O5
2	B	1001	HSX	O4-C4-C5-O5
2	O	1001	HSX	O4-C4-C5-O5

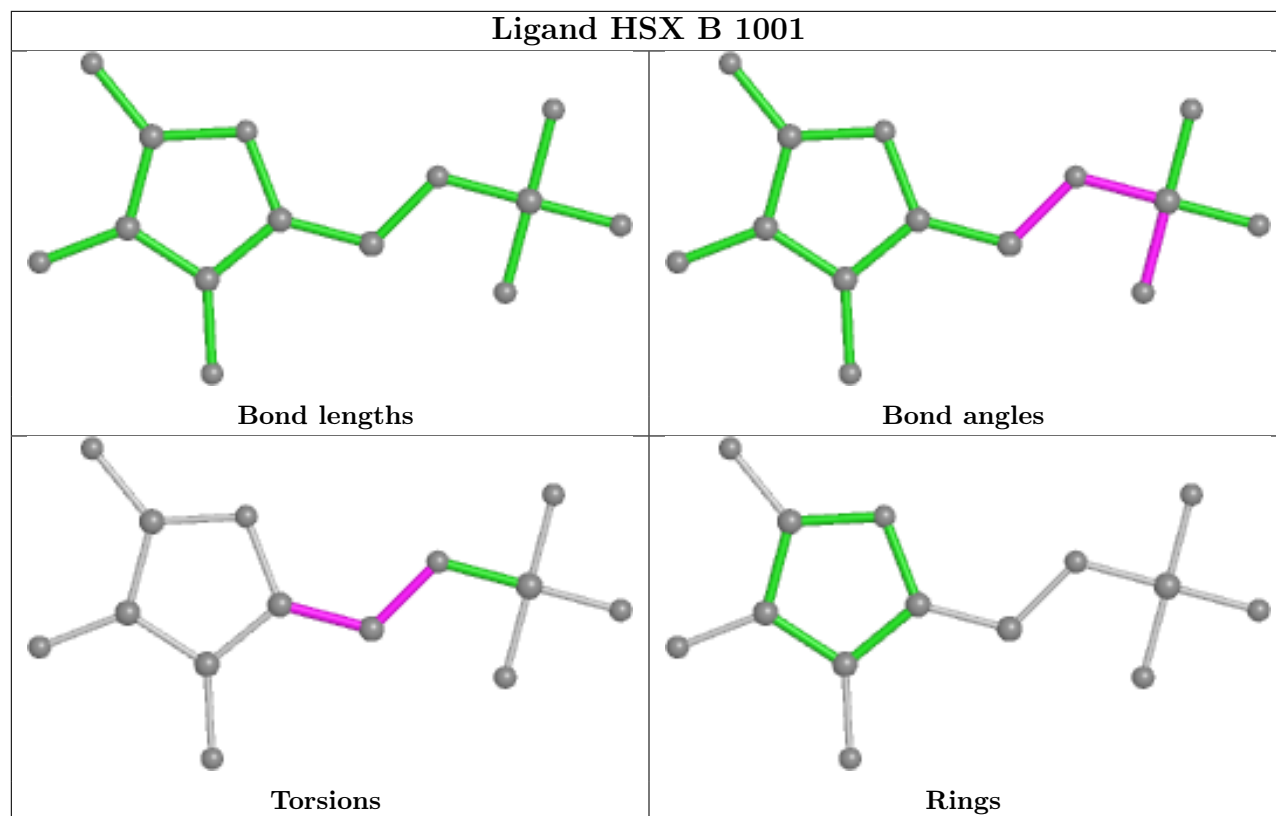
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1001	HSX	4	0
2	F	1001	HSX	2	0
2	B	1001	HSX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	312/321 (97%)	-1.65	0 100 100	30, 49, 75, 115	0
1	B	312/321 (97%)	-1.61	0 100 100	34, 54, 78, 111	0
1	C	309/321 (96%)	-1.64	0 100 100	33, 55, 78, 110	0
1	D	310/321 (96%)	-1.64	0 100 100	30, 56, 78, 113	0
1	E	312/321 (97%)	-1.61	0 100 100	35, 55, 81, 102	0
1	F	312/321 (97%)	-1.64	0 100 100	31, 49, 74, 113	0
1	G	311/321 (96%)	-1.63	0 100 100	30, 52, 75, 103	0
1	H	301/321 (93%)	-1.66	0 100 100	33, 50, 69, 111	0
1	I	313/321 (97%)	-1.57	0 100 100	30, 58, 88, 109	0
1	J	300/321 (93%)	-1.59	0 100 100	33, 56, 85, 110	1 (0%)
1	K	311/321 (96%)	-1.64	0 100 100	34, 52, 74, 107	0
1	L	298/321 (92%)	-1.59	0 100 100	30, 61, 84, 107	0
1	M	298/321 (92%)	-1.59	0 100 100	31, 55, 88, 108	0
1	N	310/321 (96%)	-1.59	0 100 100	30, 59, 85, 124	0
1	O	298/321 (92%)	-1.66	0 100 100	32, 51, 71, 100	0
1	P	313/321 (97%)	-1.60	0 100 100	34, 52, 76, 115	0
1	Q	300/321 (93%)	-1.56	0 100 100	38, 63, 86, 109	0
1	R	313/321 (97%)	-1.60	0 100 100	34, 52, 77, 116	0
All	All	5533/5778 (95%)	-1.61	0 100 100	30, 54, 81, 124	1 (0%)

There are no RSRZ outliers to report.

### 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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

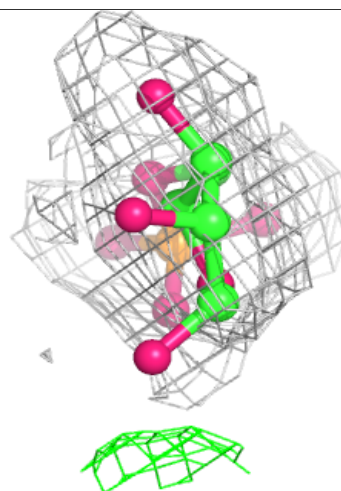
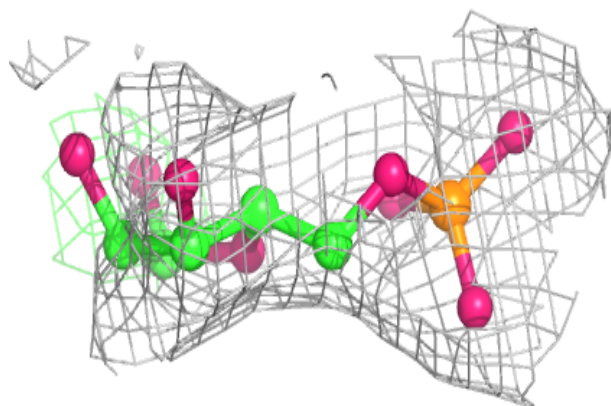
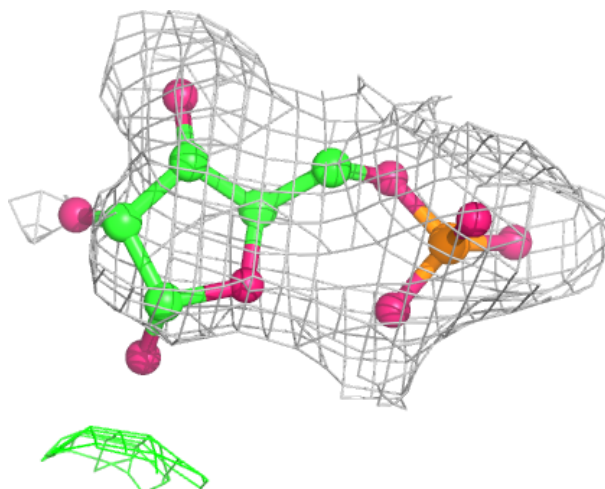
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HSX	B	1001	14/14	0.95	0.05	83,105,119,136	0
2	HSX	F	1001	14/14	0.98	0.05	76,93,120,129	0
2	HSX	O	1001	14/14	0.98	0.04	78,97,121,144	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

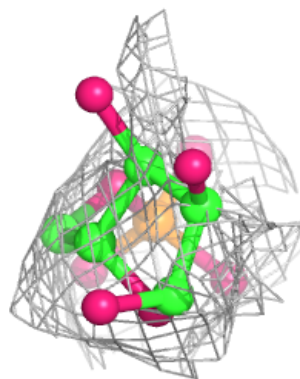
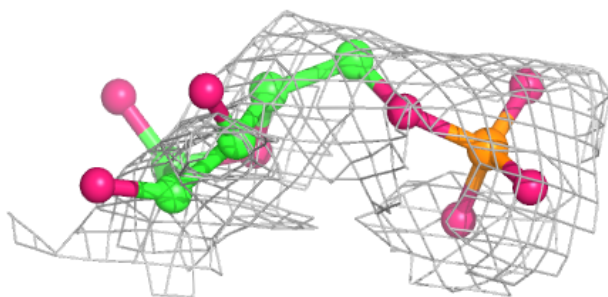
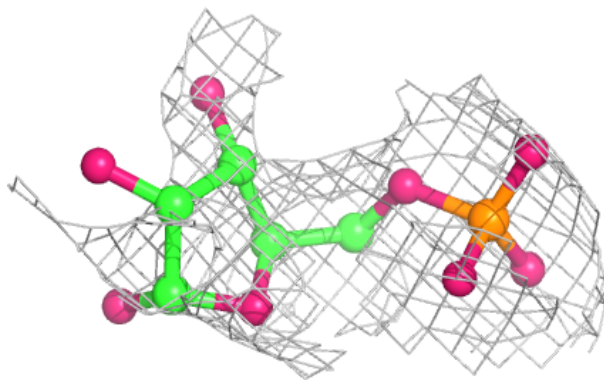
**Electron density around HSX B 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

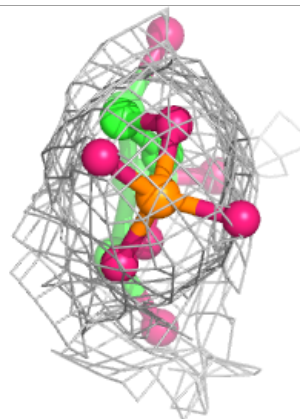
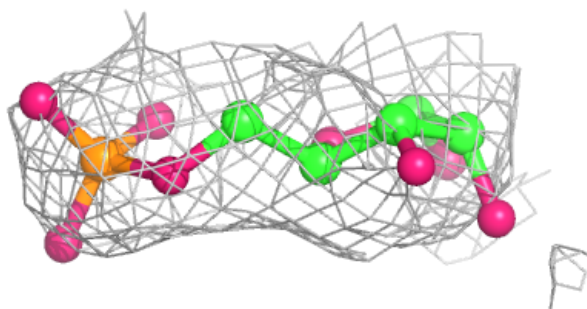
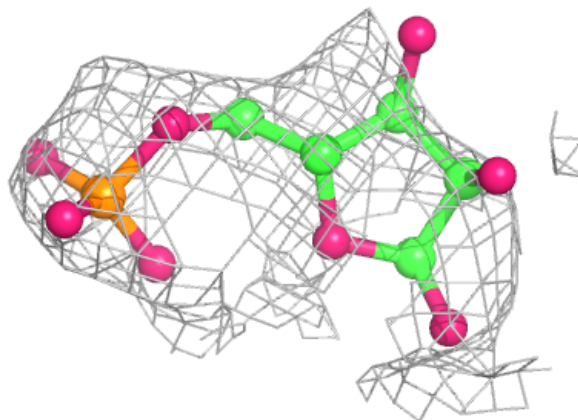


**Electron density around HSX F 1001:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HSX O 1001:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.