Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:06 PM GMT

PDB ID	:	1RXU
Title	:	E. coli uridine phosphorylase: thymidine phosphate complex
Authors	:	Caradoc-Davies, T.T.; Cutfield, S.M.; Lamont, I.L.; Cutfield, J.F.
Deposited on	:	2003-12-18
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

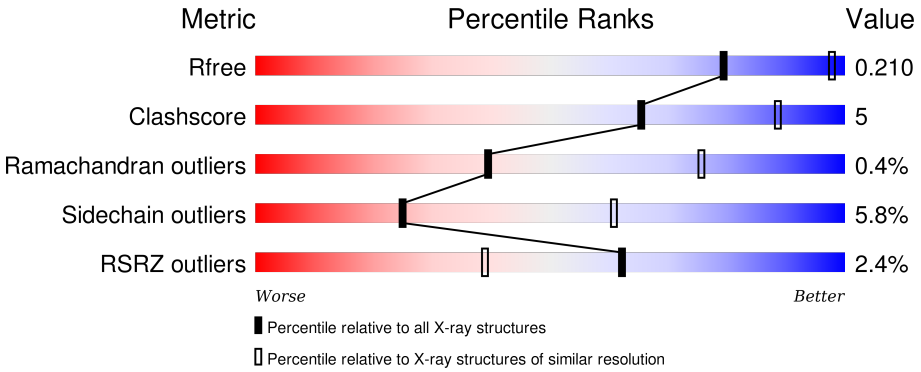
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	3% 80% 18%
1	B	253	2% 79% 19%
1	C	253	2% 78% 20%
1	D	253	3% 79% 19%
1	E	253	3% 80% 19%

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Mol	Chain	Length	Quality of chain
1	F	253	4% 79% 19%
1	G	253	3% 79% 19%
1	H	253	3% 78% 20%
1	I	253	2% 80% 18%
1	J	253	2% 81% 17%
1	K	253	2% 80% 19%
1	L	253	2% 78% 20%
1	M	253	3% 78% 20%
1	N	253	2% 78% 20%
1	O	253	3% 82% 16%
1	P	253	4% 82% 16%
1	Q	253	81% 17%
1	R	253	% 78% 21%

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
2	PO4	D	2041	-	-	X	-
2	PO4	E	2051	-	-	X	-
2	PO4	F	2061	-	-	X	-
2	PO4	H	2081	-	-	-	X
2	PO4	K	2111	-	-	X	-
2	PO4	O	2151	-	-	X	-
4	THM	A	2012	X	-	-	-
4	THM	B	2022	X	-	-	-
4	THM	C	2032	X	-	-	-
4	THM	D	2042	X	-	-	-
4	THM	E	2052	X	-	-	-
4	THM	F	2062	X	-	-	-
4	THM	G	2072	X	-	-	-
4	THM	H	2082	X	-	-	-
4	THM	I	2092	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	THM	J	2102	X	-	-	-
4	THM	K	2112	X	-	-	-
4	THM	L	2122	X	-	-	-
4	THM	M	2132	X	-	-	-
4	THM	N	2142	X	-	-	-
4	THM	O	2152	X	-	-	-
4	THM	P	2162	X	-	-	-
4	THM	Q	2172	X	-	-	-
4	THM	R	2182	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35307 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	B	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	C	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	D	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	E	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	F	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	G	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	H	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	I	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	J	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	K	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	L	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	M	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	N	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	O	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	P	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			

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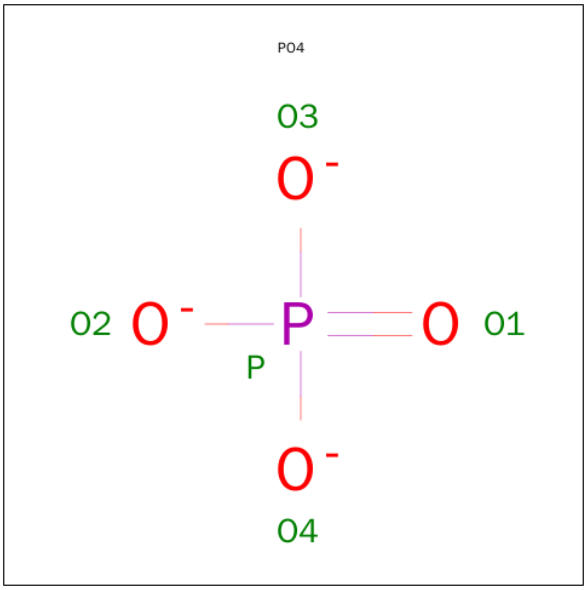
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			
1	R	250	Total	C	N	O	S	0	0	0
			1880	1178	328	363	11			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		

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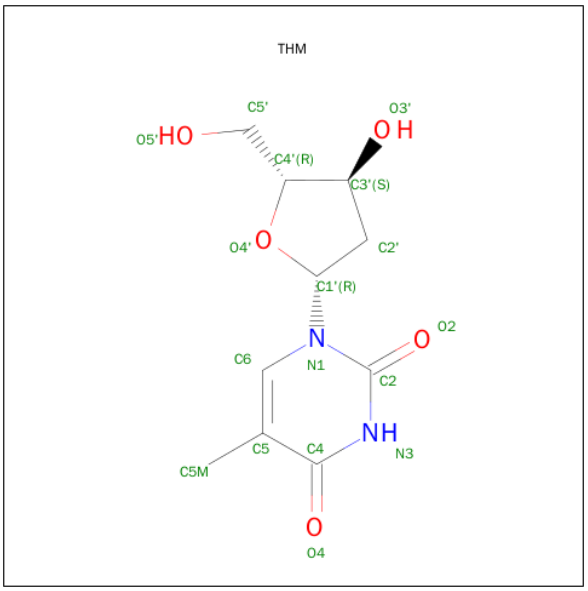
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0
2	M	1	Total O P 5 4 1	0	0
2	N	1	Total O P 5 4 1	0	0
2	O	1	Total O P 5 4 1	0	0
2	P	1	Total O P 5 4 1	0	0
2	Q	1	Total O P 5 4 1	0	0
2	R	1	Total O P 5 4 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total K 1 1	0	0
3	Q	1	Total K 1 1	0	0
3	K	1	Total K 1 1	0	0
3	I	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	A	1	Total K 1 1	0	0
3	O	1	Total K 1 1	0	0
3	F	1	Total K 1 1	0	0
3	M	1	Total K 1 1	0	0

- Molecule 4 is THYMIDINE (three-letter code: THM) (formula: $C_{10}H_{14}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	10	2	5		
4	B	1	Total	C	N	O	0	0
			17	10	2	5		
4	C	1	Total	C	N	O	0	0
			17	10	2	5		
4	D	1	Total	C	N	O	0	0
			17	10	2	5		
4	E	1	Total	C	N	O	0	0
			17	10	2	5		
4	F	1	Total	C	N	O	0	0
			17	10	2	5		
4	G	1	Total	C	N	O	0	0
			17	10	2	5		
4	H	1	Total	C	N	O	0	0
			17	10	2	5		
4	I	1	Total	C	N	O	0	0
			17	10	2	5		
4	J	1	Total	C	N	O	0	0
			17	10	2	5		
4	K	1	Total	C	N	O	0	0
			17	10	2	5		
4	L	1	Total	C	N	O	0	0
			17	10	2	5		
4	M	1	Total	C	N	O	0	0
			17	10	2	5		
4	N	1	Total	C	N	O	0	0
			17	10	2	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	1	Total C N O 17 10 2 5	0	0
4	P	1	Total C N O 17 10 2 5	0	0
4	Q	1	Total C N O 17 10 2 5	0	0
4	R	1	Total C N O 17 10 2 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	0	0
5	B	57	Total O 57 57	0	0
5	C	62	Total O 62 62	0	0
5	D	57	Total O 57 57	0	0
5	E	59	Total O 59 59	0	0
5	F	58	Total O 58 58	0	0
5	G	59	Total O 59 59	0	0
5	H	57	Total O 57 57	0	0
5	I	60	Total O 60 60	0	0
5	J	59	Total O 59 59	0	0
5	K	58	Total O 58 58	0	0
5	L	61	Total O 61 61	0	0
5	M	60	Total O 60 60	0	0
5	N	60	Total O 60 60	0	0
5	O	58	Total O 58 58	0	0

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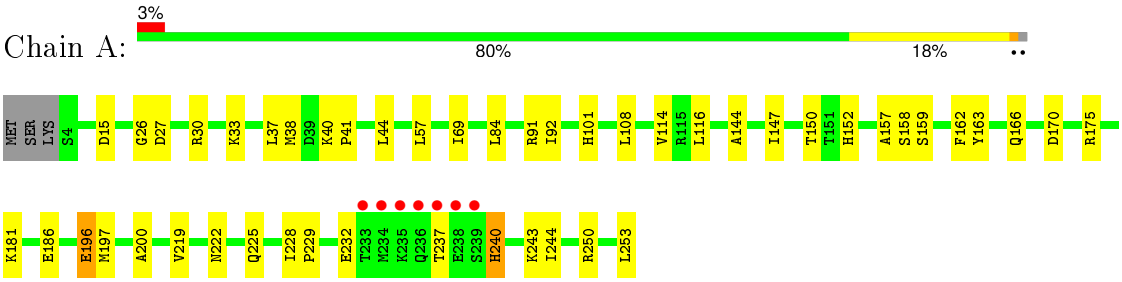
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	59	Total O 59 59	0	0
5	Q	61	Total O 61 61	0	0
5	R	58	Total O 58 58	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

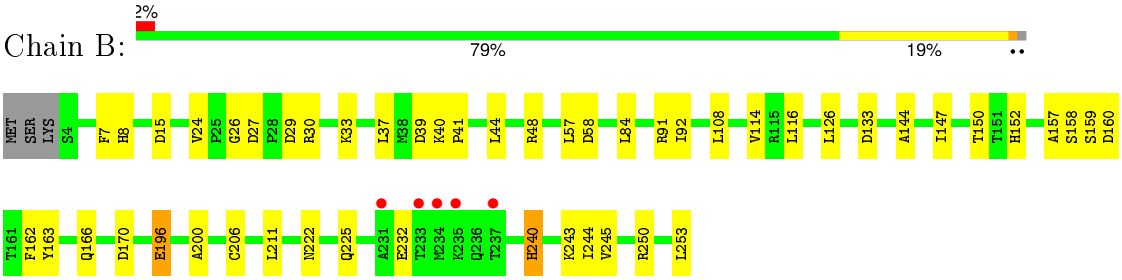
- Molecule 1: Uridine phosphorylase

Chain A:



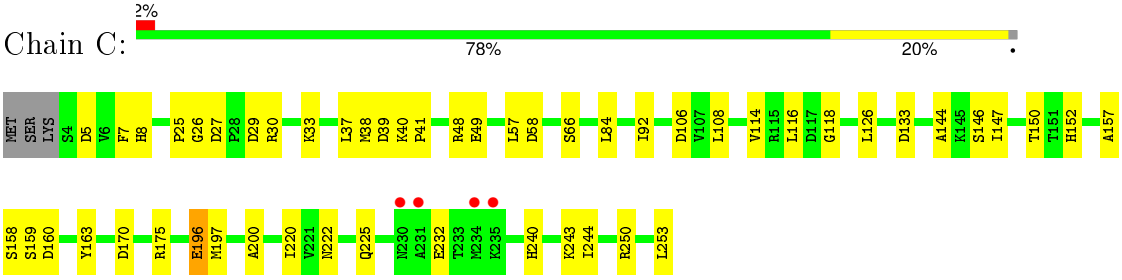
- Molecule 1: Uridine phosphorylase

Chain B:



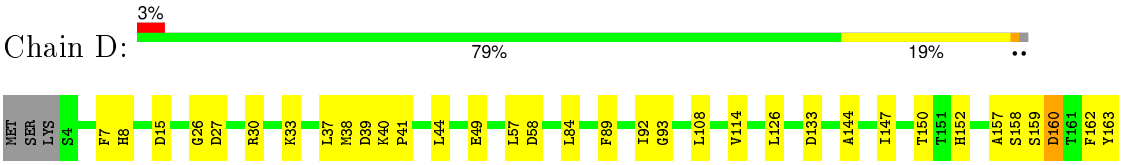
- Molecule 1: Uridine phosphorylase

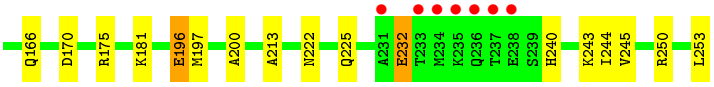
Chain C:



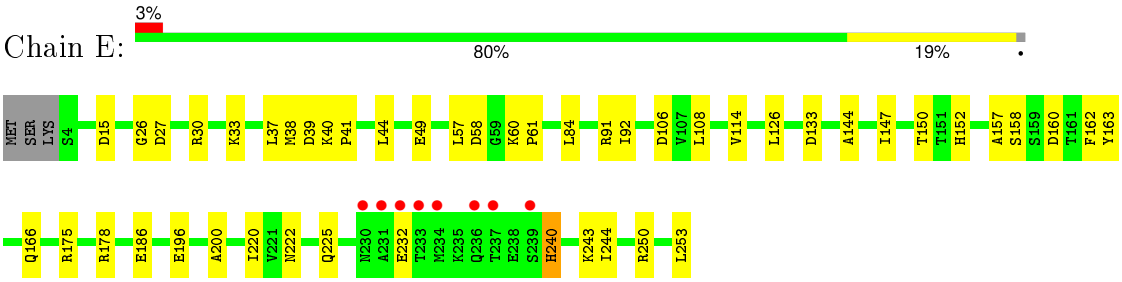
- Molecule 1: Uridine phosphorylase

Chain D:

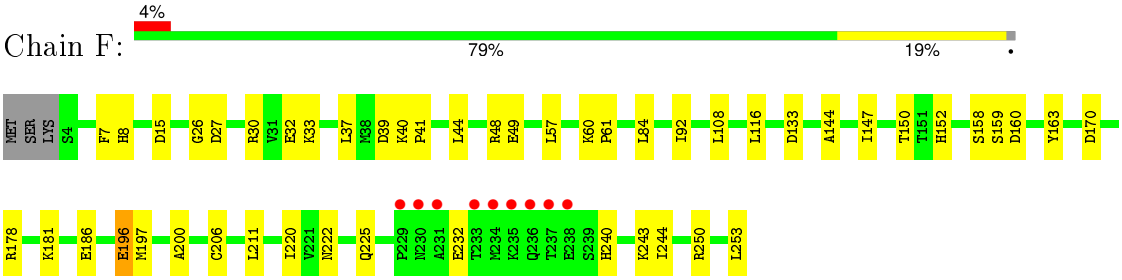




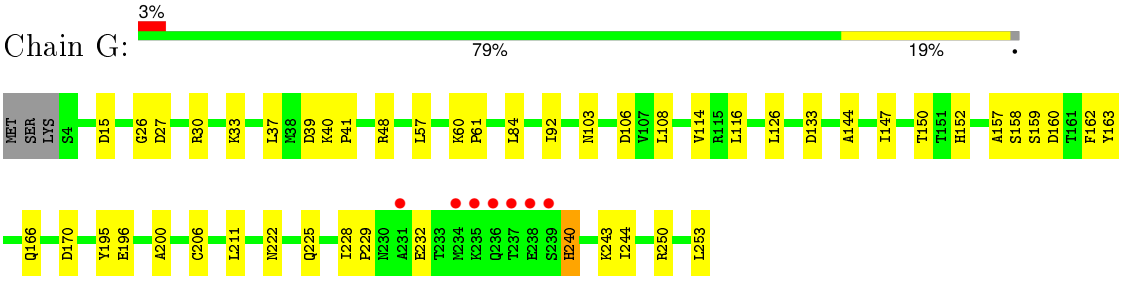
• Molecule 1: Uridine phosphorylase



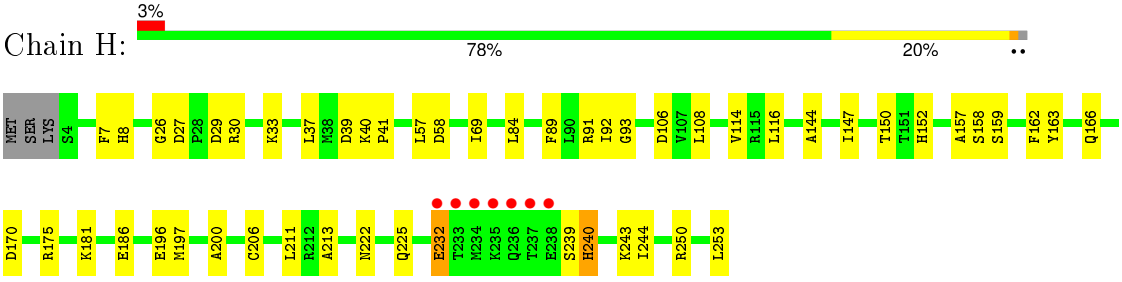
• Molecule 1: Uridine phosphorylase



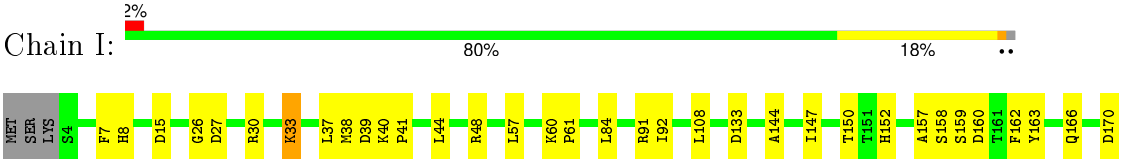
• Molecule 1: Uridine phosphorylase

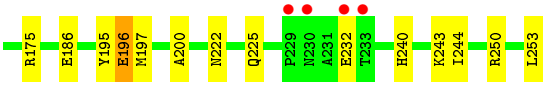


• Molecule 1: Uridine phosphorylase



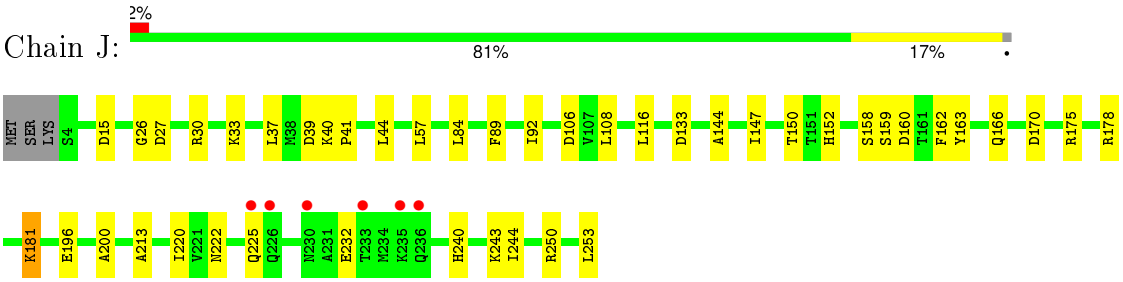
• Molecule 1: Uridine phosphorylase





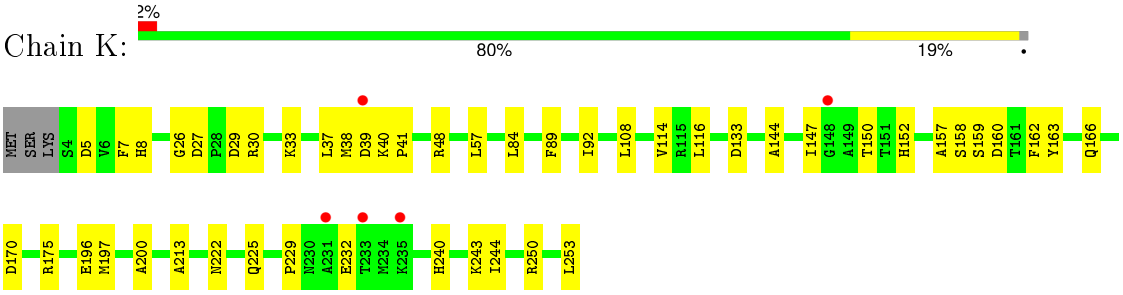
• Molecule 1: Uridine phosphorylase

Chain J:



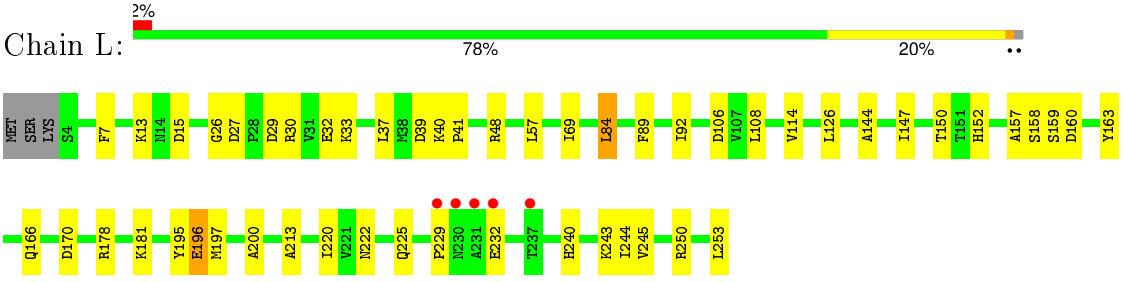
• Molecule 1: Uridine phosphorylase

Chain K:



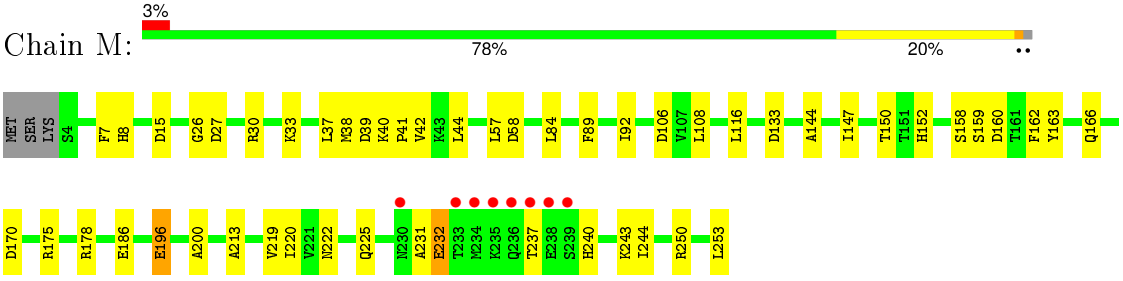
• Molecule 1: Uridine phosphorylase

Chain L:



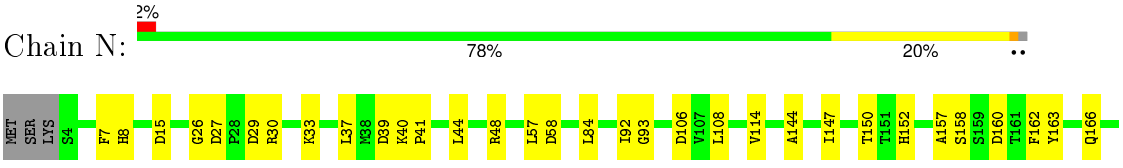
• Molecule 1: Uridine phosphorylase

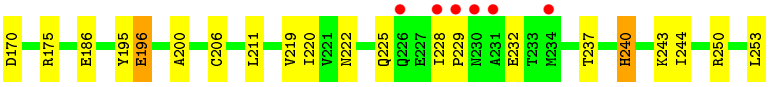
Chain M:



• Molecule 1: Uridine phosphorylase

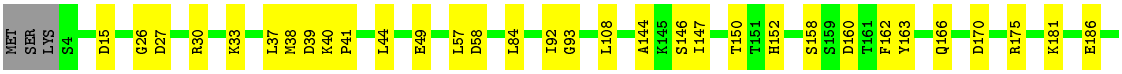
Chain N:

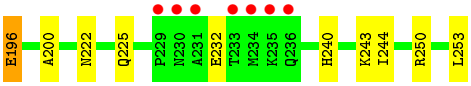




• Molecule 1: Uridine phosphorylase

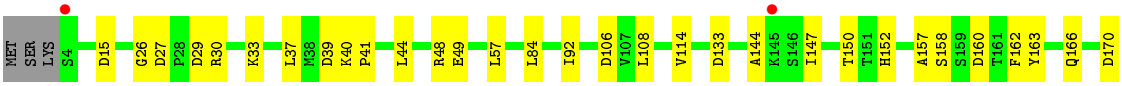
Chain O:

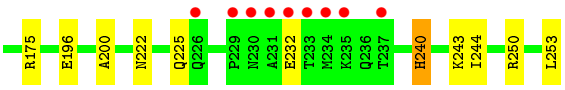




• Molecule 1: Uridine phosphorylase

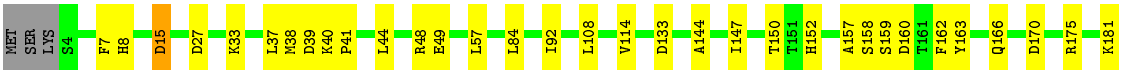
Chain P:

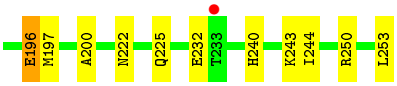




• Molecule 1: Uridine phosphorylase

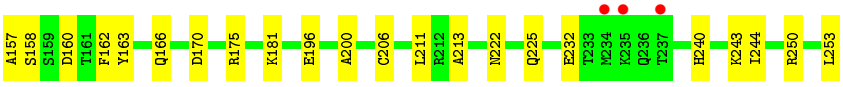
Chain Q:





• Molecule 1: Uridine phosphorylase

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	156.24Å 97.66Å 161.45Å 90.00° 118.23° 90.00°	Depositor
Resolution (Å)	25.00 – 3.10 24.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (25.00-3.10) 97.5 (24.92-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.212 , 0.229 0.193 , 0.210	Depositor DCC
R_{free} test set	3824 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.1	EDS
Estimated twinning fraction	0.001 for -h-l,k,h 0.001 for l,k,-h-l 0.021 for h,-k,-h-l 0.006 for -h-l,-k,l 0.006 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 76005 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	35307	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.81 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.4850e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

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	0.48	0/1912	0.74	3/2595 (0.1%)
1	B	0.51	0/1912	0.75	7/2595 (0.3%)
1	C	0.55	0/1912	0.77	8/2595 (0.3%)
1	D	0.49	0/1912	0.75	5/2595 (0.2%)
1	E	0.48	0/1912	0.74	6/2595 (0.2%)
1	F	0.45	0/1912	0.73	5/2595 (0.2%)
1	G	0.51	0/1912	0.75	7/2595 (0.3%)
1	H	0.51	0/1912	0.76	7/2595 (0.3%)
1	I	0.47	0/1912	0.74	6/2595 (0.2%)
1	J	0.48	0/1912	0.73	6/2595 (0.2%)
1	K	0.55	0/1912	0.75	6/2595 (0.2%)
1	L	0.56	0/1912	0.79	7/2595 (0.3%)
1	M	0.50	0/1912	0.75	6/2595 (0.2%)
1	N	0.49	0/1912	0.73	6/2595 (0.2%)
1	O	0.43	0/1912	0.72	4/2595 (0.2%)
1	P	0.42	0/1912	0.72	7/2595 (0.3%)
1	Q	0.47	0/1912	0.74	6/2595 (0.2%)
1	R	0.48	0/1912	0.76	8/2595 (0.3%)
All	All	0.49	0/34416	0.75	110/46710 (0.2%)

There are no bond length outliers.

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	27	ASP	CB-CG-OD2	9.17	126.55	118.30
1	L	27	ASP	CB-CG-OD2	8.77	126.19	118.30
1	O	27	ASP	CB-CG-OD2	8.64	126.07	118.30
1	I	27	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	27	ASP	CB-CG-OD2	8.38	125.84	118.30
1	J	27	ASP	CB-CG-OD2	8.16	125.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	27	ASP	CB-CG-OD2	8.08	125.58	118.30
1	D	27	ASP	CB-CG-OD2	7.92	125.42	118.30
1	L	160	ASP	CB-CG-OD2	7.76	125.28	118.30
1	M	27	ASP	CB-CG-OD2	7.75	125.28	118.30
1	E	27	ASP	CB-CG-OD2	7.57	125.11	118.30
1	F	27	ASP	CB-CG-OD2	7.54	125.09	118.30
1	N	27	ASP	CB-CG-OD2	7.53	125.07	118.30
1	Q	27	ASP	CB-CG-OD2	7.39	124.95	118.30
1	G	27	ASP	CB-CG-OD2	7.20	124.78	118.30
1	R	133	ASP	CB-CG-OD2	7.08	124.67	118.30
1	D	170	ASP	CB-CG-OD2	6.87	124.48	118.30
1	K	27	ASP	CB-CG-OD2	6.74	124.36	118.30
1	M	133	ASP	CB-CG-OD2	6.72	124.35	118.30
1	C	27	ASP	CB-CG-OD2	6.71	124.34	118.30
1	G	160	ASP	CB-CG-OD2	6.71	124.34	118.30
1	F	160	ASP	CB-CG-OD2	6.71	124.34	118.30
1	H	27	ASP	CB-CG-OD2	6.69	124.32	118.30
1	H	91	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	D	160	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	133	ASP	CB-CG-OD2	6.59	124.23	118.30
1	E	133	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	27	ASP	CB-CG-OD2	6.49	124.14	118.30
1	P	170	ASP	CB-CG-OD2	6.35	124.01	118.30
1	H	39	ASP	CB-CG-OD2	6.32	123.98	118.30
1	I	160	ASP	CB-CG-OD2	6.31	123.98	118.30
1	C	160	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	29	ASP	CB-CG-OD2	6.27	123.94	118.30
1	J	133	ASP	CB-CG-OD2	6.26	123.94	118.30
1	I	170	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	160	ASP	CB-CG-OD2	6.22	123.89	118.30
1	C	133	ASP	CB-CG-OD2	6.19	123.87	118.30
1	L	170	ASP	CB-CG-OD2	6.12	123.81	118.30
1	M	39	ASP	CB-CG-OD2	6.12	123.80	118.30
1	F	133	ASP	CB-CG-OD2	6.09	123.78	118.30
1	N	160	ASP	CB-CG-OD2	6.08	123.78	118.30
1	K	170	ASP	CB-CG-OD2	6.08	123.77	118.30
1	G	170	ASP	CB-CG-OD2	6.02	123.72	118.30
1	Q	39	ASP	CB-CG-OD2	6.00	123.70	118.30
1	Q	170	ASP	CB-CG-OD2	6.00	123.70	118.30
1	I	133	ASP	CB-CG-OD2	5.98	123.68	118.30
1	G	133	ASP	CB-CG-OD2	5.96	123.66	118.30
1	P	106	ASP	CB-CG-OD2	5.93	123.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	160	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	170	ASP	CB-CG-OD2	5.92	123.63	118.30
1	M	170	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	39	ASP	CB-CG-OD2	5.92	123.62	118.30
1	J	170	ASP	CB-CG-OD2	5.92	123.62	118.30
1	N	106	ASP	CB-CG-OD2	5.91	123.61	118.30
1	J	39	ASP	CB-CG-OD2	5.90	123.61	118.30
1	E	39	ASP	CB-CG-OD2	5.88	123.59	118.30
1	F	170	ASP	CB-CG-OD2	5.88	123.59	118.30
1	N	170	ASP	CB-CG-OD2	5.85	123.57	118.30
1	P	133	ASP	CB-CG-OD2	5.82	123.54	118.30
1	Q	133	ASP	CB-CG-OD2	5.82	123.54	118.30
1	Q	160	ASP	CB-CG-OD2	5.78	123.50	118.30
1	K	133	ASP	CB-CG-OD2	5.75	123.47	118.30
1	M	160	ASP	CB-CG-OD2	5.75	123.47	118.30
1	G	106	ASP	CB-CG-OD2	5.74	123.46	118.30
1	Q	15	ASP	CB-CG-OD2	5.71	123.44	118.30
1	R	39	ASP	CB-CG-OD2	5.69	123.42	118.30
1	K	160	ASP	CB-CG-OD2	5.68	123.41	118.30
1	L	39	ASP	CB-CG-OD2	5.66	123.40	118.30
1	E	106	ASP	CB-CG-OD2	5.60	123.34	118.30
1	O	39	ASP	CB-CG-OD2	5.58	123.32	118.30
1	J	160	ASP	CB-CG-OD2	5.57	123.31	118.30
1	I	39	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	106	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	39	ASP	CB-CG-OD2	5.53	123.27	118.30
1	R	160	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	39	ASP	CB-CG-OD2	5.51	123.26	118.30
1	N	29	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	160	ASP	CB-CG-OD2	5.48	123.23	118.30
1	P	39	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	91	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	R	170	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	170	ASP	CB-CG-OD2	5.38	123.14	118.30
1	J	106	ASP	CB-CG-OD2	5.35	123.11	118.30
1	E	91	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	K	29	ASP	CB-CG-OD2	5.31	123.08	118.30
1	I	91	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	F	39	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	5	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	29	ASP	CB-CG-OD2	5.28	123.05	118.30
1	L	106	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	91	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	L	15	ASP	CB-CG-OD2	5.24	123.02	118.30
1	N	39	ASP	CB-CG-OD2	5.23	123.01	118.30
1	R	106	ASP	CB-CG-OD2	5.21	122.99	118.30
1	H	170	ASP	CB-CG-OD2	5.20	122.98	118.30
1	P	29	ASP	CB-CG-OD2	5.19	122.97	118.30
1	M	106	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	29	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	133	ASP	CB-CG-OD2	5.16	122.94	118.30
1	L	29	ASP	CB-CG-OD2	5.15	122.94	118.30
1	O	170	ASP	CB-CG-OD2	5.15	122.93	118.30
1	G	15	ASP	CB-CG-OD2	5.14	122.92	118.30
1	O	160	ASP	CB-CG-OD2	5.11	122.90	118.30
1	G	39	ASP	CB-CG-OD2	5.10	122.89	118.30
1	H	58	ASP	CB-CG-OD2	5.08	122.87	118.30
1	K	5	ASP	CB-CG-OD2	5.08	122.87	118.30
1	H	106	ASP	CB-CG-OD2	5.06	122.85	118.30
1	R	117	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	170	ASP	CB-CG-OD2	5.05	122.85	118.30
1	R	29	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1880	0	1884	22	2
1	B	1880	0	1884	21	0
1	C	1880	0	1884	22	1
1	D	1880	0	1884	23	1
1	E	1880	0	1884	19	0
1	F	1880	0	1884	28	0
1	G	1880	0	1884	20	1
1	H	1880	0	1884	19	9
1	I	1880	0	1884	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1880	0	1884	16	0
1	K	1880	0	1884	23	0
1	L	1880	0	1885	21	9
1	M	1880	0	1884	24	1
1	N	1880	0	1884	22	0
1	O	1880	0	1884	23	0
1	P	1880	0	1884	14	0
1	Q	1880	0	1884	17	0
1	R	1880	0	1884	19	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	3	0
2	E	5	0	0	2	0
2	F	5	0	0	2	0
2	G	5	0	0	1	0
2	H	5	0	0	1	0
2	I	5	0	0	0	0
2	J	5	0	0	1	0
2	K	5	0	0	3	0
2	L	5	0	0	0	0
2	M	5	0	0	1	0
2	N	5	0	0	1	0
2	O	5	0	0	3	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
4	A	17	0	13	0	0
4	B	17	0	13	0	0
4	C	17	0	13	2	0
4	D	17	0	13	0	0
4	E	17	0	13	1	0
4	F	17	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	17	0	13	0	0
4	H	17	0	13	0	0
4	I	17	0	13	0	0
4	J	17	0	13	1	0
4	K	17	0	13	0	0
4	L	17	0	13	1	0
4	M	17	0	13	1	0
4	N	17	0	13	1	0
4	O	17	0	13	1	0
4	P	17	0	13	0	0
4	Q	17	0	13	1	0
4	R	17	0	13	0	0
5	A	59	0	0	0	0
5	B	57	0	0	0	0
5	C	62	0	0	0	1
5	D	57	0	0	0	0
5	E	59	0	0	0	0
5	F	58	0	0	0	1
5	G	59	0	0	0	0
5	H	57	0	0	0	0
5	I	60	0	0	1	0
5	J	59	0	0	0	0
5	K	58	0	0	0	0
5	L	61	0	0	0	0
5	M	60	0	0	1	0
5	N	60	0	0	1	2
5	O	58	0	0	0	0
5	P	59	0	0	0	0
5	Q	61	0	0	0	0
5	R	58	0	0	1	0
All	All	35307	0	34147	342	14

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (342) 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:K:39:ASP:OD2	1:M:42:VAL:CG1	1.76	1.34
1:F:32:GLU:OE2	1:O:146:SER:HA	1.25	1.33
1:F:32:GLU:OE2	1:O:146:SER:CA	1.78	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:GLU:OE2	1:O:146:SER:C	1.76	1.24
1:K:39:ASP:OD2	1:M:42:VAL:HG11	1.09	1.21
1:F:32:GLU:OE2	1:O:146:SER:O	1.80	1.00
1:F:32:GLU:CD	1:O:146:SER:O	2.03	0.96
1:G:30:ARG:NH2	2:G:2071:PO4:O2	2.09	0.86
1:H:93:GLY:HA2	2:H:2081:PO4:O2	1.79	0.82
1:K:39:ASP:OD2	1:M:42:VAL:HG13	1.79	0.82
1:F:32:GLU:OE1	1:O:146:SER:O	1.97	0.82
1:M:30:ARG:NH2	2:M:2131:PO4:O2	2.15	0.79
1:F:30:ARG:NH2	2:F:2061:PO4:O2	2.29	0.66
1:O:30:ARG:NH2	2:O:2151:PO4:O2	2.30	0.64
1:A:158:SER:HB3	1:A:200:ALA:HB2	1.80	0.63
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.81	0.63
1:C:48:ARG:NH2	2:D:2041:PO4:O3	2.25	0.63
1:H:158:SER:HB3	1:H:200:ALA:HB2	1.81	0.63
1:I:158:SER:HB3	1:I:200:ALA:HB2	1.81	0.62
1:R:158:SER:HB3	1:R:200:ALA:HB2	1.81	0.62
1:B:30:ARG:NH2	2:B:2021:PO4:O2	2.30	0.62
1:O:158:SER:HB3	1:O:200:ALA:HB2	1.82	0.61
1:D:30:ARG:NH2	2:D:2041:PO4:O2	2.33	0.61
1:C:30:ARG:NH2	2:C:2031:PO4:O2	2.34	0.61
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.83	0.61
1:L:158:SER:HB3	1:L:200:ALA:HB2	1.82	0.60
1:M:158:SER:HB3	1:M:200:ALA:HB2	1.83	0.60
1:J:158:SER:HB3	1:J:200:ALA:HB2	1.83	0.59
1:L:220:ILE:HD11	4:L:2122:THM:HM51	1.85	0.59
1:K:158:SER:HB3	1:K:200:ALA:HB2	1.84	0.59
1:N:158:SER:HB3	1:N:200:ALA:HB2	1.84	0.59
1:E:158:SER:HB3	1:E:200:ALA:HB2	1.86	0.58
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.85	0.58
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.86	0.57
1:Q:158:SER:HB3	1:Q:200:ALA:HB2	1.86	0.57
1:P:158:SER:HB3	1:P:200:ALA:HB2	1.85	0.57
1:G:158:SER:HB3	1:G:200:ALA:HB2	1.86	0.56
1:J:220:ILE:HD11	4:J:2102:THM:HM51	1.89	0.54
1:G:57:LEU:HB3	1:G:253:LEU:HD11	1.91	0.53
1:E:162:PHE:HA	1:E:166:GLN:NE2	2.24	0.53
1:K:48:ARG:HD3	1:L:69:ILE:HD11	1.91	0.52
1:E:57:LEU:HB3	1:E:253:LEU:HD11	1.92	0.52
1:O:222:ASN:HB3	1:O:225:GLN:HE21	1.74	0.52
1:B:162:PHE:HA	1:B:166:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:LEU:HB3	1:F:253:LEU:HD11	1.92	0.52
1:E:144:ALA:HA	1:E:244:ILE:HG12	1.92	0.52
2:E:2051:PO4:O3	1:F:48:ARG:NH2	2.40	0.52
1:B:57:LEU:HB3	1:B:253:LEU:HD11	1.92	0.51
1:L:57:LEU:HB3	1:L:253:LEU:HD11	1.92	0.51
1:R:7:PHE:HD1	1:R:8:HIS:CE1	2.27	0.51
1:A:57:LEU:HB3	1:A:253:LEU:HD11	1.91	0.51
1:L:222:ASN:HB3	1:L:225:GLN:HE21	1.76	0.51
1:E:49:GLU:HB3	1:F:49:GLU:HB3	1.91	0.51
1:E:222:ASN:HB3	1:E:225:GLN:HE21	1.76	0.51
1:H:57:LEU:HG	1:H:250:ARG:HG3	1.93	0.51
1:M:144:ALA:HA	1:M:244:ILE:HG12	1.92	0.51
1:K:7:PHE:CZ	1:L:229:PRO:HG2	2.45	0.51
1:Q:144:ALA:HA	1:Q:244:ILE:HG12	1.93	0.51
1:F:108:LEU:HD22	1:F:152:HIS:HB2	1.93	0.51
1:K:57:LEU:HB3	1:K:253:LEU:HD11	1.92	0.51
1:C:57:LEU:HB3	1:C:253:LEU:HD11	1.93	0.50
1:G:162:PHE:HA	1:G:166:GLN:NE2	2.26	0.50
1:C:222:ASN:HB3	1:C:225:GLN:HE21	1.76	0.50
1:I:162:PHE:HA	1:I:166:GLN:NE2	2.26	0.50
1:K:108:LEU:HD22	1:K:152:HIS:HB2	1.93	0.50
1:B:144:ALA:HA	1:B:244:ILE:HG12	1.93	0.50
1:H:26:GLY:H	1:H:30:ARG:NH2	2.09	0.50
1:R:57:LEU:HB3	1:R:253:LEU:HD11	1.93	0.50
1:J:144:ALA:HA	1:J:244:ILE:HG12	1.93	0.50
1:K:144:ALA:HA	1:K:244:ILE:HG12	1.94	0.50
1:E:40:LYS:N	1:E:41:PRO:HD3	2.27	0.50
1:C:38:MET:SD	1:C:57:LEU:HD13	2.51	0.49
1:N:144:ALA:HA	1:N:244:ILE:HG12	1.94	0.49
1:G:144:ALA:HA	1:G:244:ILE:HG12	1.93	0.49
1:J:30:ARG:NH2	2:J:2101:PO4:O2	2.43	0.49
1:A:40:LYS:N	1:A:41:PRO:HD3	2.28	0.49
1:K:38:MET:SD	1:K:57:LEU:HD13	2.53	0.49
1:I:57:LEU:HG	1:I:250:ARG:HG3	1.94	0.49
1:I:57:LEU:HB3	1:I:253:LEU:HD11	1.95	0.49
1:R:40:LYS:N	1:R:41:PRO:HD3	2.27	0.49
1:D:162:PHE:HA	1:D:166:GLN:NE2	2.28	0.49
1:M:108:LEU:HD22	1:M:152:HIS:HB2	1.95	0.49
1:E:57:LEU:HG	1:E:250:ARG:HG3	1.95	0.49
1:R:57:LEU:HG	1:R:250:ARG:HG3	1.95	0.49
1:O:144:ALA:HA	1:O:244:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:40:LYS:N	1:M:41:PRO:HD3	2.27	0.49
1:P:144:ALA:HA	1:P:244:ILE:HG12	1.94	0.49
1:C:108:LEU:HD22	1:C:152:HIS:HB2	1.93	0.49
1:K:7:PHE:HD1	1:K:8:HIS:CE1	2.31	0.49
1:I:158:SER:HA	1:I:196:GLU:O	2.13	0.49
1:H:159:SER:O	1:H:197:MET:HG2	2.13	0.49
1:J:222:ASN:HB3	1:J:225:GLN:HE21	1.75	0.49
1:O:57:LEU:HB3	1:O:253:LEU:HD11	1.95	0.49
1:A:144:ALA:HA	1:A:244:ILE:HG12	1.95	0.49
1:D:158:SER:HA	1:D:196:GLU:O	2.13	0.49
1:H:57:LEU:HB3	1:H:253:LEU:HD11	1.94	0.49
1:D:144:ALA:HA	1:D:244:ILE:HG12	1.95	0.49
1:F:144:ALA:HA	1:F:244:ILE:HG12	1.95	0.49
1:C:144:ALA:HA	1:C:244:ILE:HG12	1.95	0.48
1:N:57:LEU:HG	1:N:250:ARG:HG3	1.95	0.48
1:I:144:ALA:HA	1:I:244:ILE:HG12	1.95	0.48
1:J:40:LYS:N	1:J:41:PRO:HD3	2.28	0.48
1:Q:196:GLU:HA	4:Q:2172:THM:O2	2.14	0.48
1:D:40:LYS:N	1:D:41:PRO:HD3	2.28	0.48
1:J:108:LEU:HD22	1:J:152:HIS:HB2	1.95	0.48
1:G:57:LEU:HG	1:G:250:ARG:HG3	1.95	0.48
1:F:40:LYS:N	1:F:41:PRO:HD3	2.29	0.48
1:G:40:LYS:N	1:G:41:PRO:HD3	2.29	0.48
1:I:40:LYS:N	1:I:41:PRO:HD3	2.29	0.48
1:N:93:GLY:HA2	2:N:2141:PO4:O2	2.14	0.48
1:D:57:LEU:HG	1:D:250:ARG:HG3	1.95	0.48
1:F:222:ASN:HB3	1:F:225:GLN:HE21	1.79	0.48
1:Q:57:LEU:HB3	1:Q:253:LEU:HD11	1.95	0.48
1:L:40:LYS:N	1:L:41:PRO:HD3	2.29	0.48
1:J:57:LEU:HG	1:J:250:ARG:HG3	1.96	0.48
1:N:40:LYS:N	1:N:41:PRO:HD3	2.28	0.47
1:O:57:LEU:HG	1:O:250:ARG:HG3	1.96	0.47
1:H:144:ALA:HA	1:H:244:ILE:HG12	1.95	0.47
1:A:116:LEU:HB2	1:A:159:SER:HA	1.97	0.47
1:P:57:LEU:HG	1:P:250:ARG:HG3	1.96	0.47
1:P:57:LEU:HB3	1:P:253:LEU:HD11	1.96	0.47
1:O:108:LEU:HD22	1:O:152:HIS:HB2	1.96	0.47
1:K:30:ARG:NH2	2:K:2111:PO4:O2	2.47	0.47
1:D:38:MET:SD	1:D:57:LEU:HD13	2.54	0.47
1:Q:162:PHE:HA	1:Q:166:GLN:NE2	2.29	0.47
1:C:57:LEU:HG	1:C:250:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:57:LEU:HB3	1:N:253:LEU:HD11	1.95	0.47
1:L:57:LEU:HG	1:L:250:ARG:HG3	1.96	0.47
1:N:162:PHE:HA	1:N:166:GLN:NE2	2.30	0.47
1:M:38:MET:SD	1:M:57:LEU:HD13	2.54	0.47
1:K:114:VAL:HB	1:K:157:ALA:HA	1.96	0.47
1:A:219:VAL:O	1:A:237:THR:HG21	2.15	0.47
1:K:40:LYS:N	1:K:41:PRO:HD3	2.29	0.47
1:I:222:ASN:HB3	1:I:225:GLN:HE21	1.80	0.47
1:R:222:ASN:HB3	1:R:225:GLN:HE21	1.80	0.47
1:A:108:LEU:HD22	1:A:152:HIS:HB2	1.95	0.47
1:I:159:SER:O	1:I:197:MET:HG2	2.14	0.47
1:B:206:CYS:HB3	1:B:211:LEU:O	2.15	0.47
1:B:40:LYS:N	1:B:41:PRO:HD3	2.30	0.47
1:G:26:GLY:H	1:G:30:ARG:NH2	2.11	0.46
1:O:26:GLY:H	1:O:30:ARG:NH2	2.13	0.46
1:A:57:LEU:HG	1:A:250:ARG:HG3	1.96	0.46
1:J:57:LEU:HB3	1:J:253:LEU:HD11	1.97	0.46
1:M:57:LEU:HB3	1:M:253:LEU:HD11	1.96	0.46
1:A:26:GLY:H	1:A:30:ARG:NH2	2.13	0.46
1:I:108:LEU:HD22	1:I:152:HIS:HB2	1.97	0.46
1:H:40:LYS:N	1:H:41:PRO:HD3	2.29	0.46
1:E:15:ASP:HB3	1:E:44:LEU:HD13	1.97	0.46
1:N:26:GLY:H	1:N:30:ARG:NH2	2.12	0.46
1:Q:108:LEU:HD22	1:Q:152:HIS:HB2	1.97	0.46
1:F:57:LEU:HG	1:F:250:ARG:HG3	1.97	0.46
1:H:114:VAL:HB	1:H:157:ALA:HA	1.97	0.46
1:C:40:LYS:N	1:C:41:PRO:HD3	2.31	0.46
1:E:58:ASP:OD2	1:E:250:ARG:HG2	2.15	0.46
1:Q:38:MET:SD	1:Q:57:LEU:HD13	2.56	0.46
1:B:108:LEU:HD22	1:B:152:HIS:HB2	1.96	0.46
1:H:181:LYS:O	1:J:178:ARG:NH2	2.47	0.46
1:B:222:ASN:HB3	1:B:225:GLN:HE21	1.80	0.46
1:L:144:ALA:HA	1:L:244:ILE:HG12	1.96	0.46
1:R:144:ALA:HA	1:R:244:ILE:HG12	1.97	0.46
1:N:222:ASN:HB3	1:N:225:GLN:HE21	1.81	0.46
1:D:89:PHE:O	1:D:213:ALA:HA	2.16	0.46
1:L:159:SER:O	1:L:197:MET:HG2	2.15	0.46
1:D:26:GLY:H	1:D:30:ARG:NH2	2.13	0.46
1:B:58:ASP:OD2	1:B:250:ARG:HG2	2.16	0.46
1:P:162:PHE:HA	1:P:166:GLN:NE2	2.30	0.46
1:B:26:GLY:H	1:B:30:ARG:NH2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:GLY:H	1:E:30:ARG:NH2	2.14	0.46
1:D:57:LEU:HB3	1:D:253:LEU:HD11	1.97	0.45
2:K:2111:PO4:P	1:L:48:ARG:HH22	2.39	0.45
1:P:26:GLY:H	1:P:30:ARG:NH2	2.14	0.45
1:B:7:PHE:HD1	1:B:8:HIS:CE1	2.33	0.45
1:P:40:LYS:N	1:P:41:PRO:HD3	2.30	0.45
1:Q:49:GLU:HB3	1:R:49:GLU:HB3	1.97	0.45
1:P:108:LEU:HD22	1:P:152:HIS:HB2	1.98	0.45
1:J:15:ASP:HB3	1:J:44:LEU:HD13	1.99	0.45
1:A:30:ARG:NH2	2:A:2011:PO4:O2	2.47	0.45
1:F:206:CYS:HB3	1:F:211:LEU:O	2.16	0.45
1:G:108:LEU:HD22	1:G:152:HIS:HB2	1.98	0.45
1:M:222:ASN:HB3	1:M:225:GLN:HE21	1.79	0.45
1:A:222:ASN:HB3	1:A:225:GLN:HE21	1.81	0.45
1:L:158:SER:HA	1:L:196:GLU:O	2.16	0.45
1:O:38:MET:SD	1:O:57:LEU:HD13	2.57	0.45
1:J:116:LEU:HB2	1:J:159:SER:HA	1.98	0.45
1:M:116:LEU:HB2	1:M:159:SER:HA	1.98	0.45
2:O:2151:PO4:O3	1:P:48:ARG:NH2	2.48	0.45
1:D:108:LEU:HD22	1:D:152:HIS:HB2	1.97	0.45
1:K:222:ASN:HB3	1:K:225:GLN:HE21	1.82	0.45
1:R:30:ARG:HH22	2:R:2181:PO4:P	2.40	0.45
1:R:108:LEU:HD22	1:R:152:HIS:HB2	1.98	0.45
1:L:114:VAL:HB	1:L:157:ALA:HA	1.99	0.45
1:R:162:PHE:HA	1:R:166:GLN:NE2	2.31	0.45
1:B:240:HIS:O	1:B:244:ILE:HD12	2.16	0.45
1:M:57:LEU:HG	1:M:250:ARG:HG3	1.99	0.45
1:P:222:ASN:HB3	1:P:225:GLN:HE21	1.81	0.45
1:G:222:ASN:HB3	1:G:225:GLN:HE21	1.81	0.45
1:F:26:GLY:H	1:F:30:ARG:NH2	2.15	0.44
1:N:158:SER:HA	1:N:196:GLU:O	2.18	0.44
1:Q:48:ARG:HD3	1:R:69:ILE:HD11	1.99	0.44
1:A:162:PHE:HA	1:A:166:GLN:NE2	2.32	0.44
1:G:126:LEU:HB3	1:L:126:LEU:HD23	2.00	0.44
1:D:181:LYS:O	1:F:178:ARG:NH2	2.48	0.44
1:R:25:PRO:O	1:R:66:SER:HA	2.17	0.44
1:Q:40:LYS:N	1:Q:41:PRO:HD3	2.32	0.44
1:A:38:MET:SD	1:A:57:LEU:HD13	2.57	0.44
1:Q:57:LEU:HG	1:Q:250:ARG:HG3	1.98	0.44
1:N:166:GLN:HG2	1:N:195:TYR:CD1	2.53	0.44
1:E:220:ILE:HD11	4:E:2052:THM:HM51	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:178:ARG:NH2	1:O:181:LYS:O	2.46	0.44
1:E:108:LEU:HD22	1:E:152:HIS:HB2	1.98	0.44
1:K:57:LEU:HG	1:K:250:ARG:HG3	1.98	0.44
1:C:196:GLU:HA	4:C:2032:THM:O2	2.18	0.44
1:O:40:LYS:N	1:O:41:PRO:HD3	2.33	0.44
1:M:231:ALA:HB3	5:M:538:HOH:O	2.17	0.44
1:M:26:GLY:H	1:M:30:ARG:NH2	2.15	0.44
1:A:159:SER:O	1:A:197:MET:HG2	2.18	0.44
1:M:7:PHE:HD1	1:M:8:HIS:CE1	2.35	0.44
1:C:26:GLY:H	1:C:30:ARG:NH2	2.15	0.44
1:J:162:PHE:HA	1:J:166:GLN:NE2	2.32	0.44
1:L:26:GLY:H	1:L:30:ARG:NH2	2.16	0.44
1:G:126:LEU:HD23	1:L:126:LEU:HB3	2.00	0.44
1:H:162:PHE:HA	1:H:166:GLN:NE2	2.33	0.44
1:C:114:VAL:HB	1:C:157:ALA:HA	1.99	0.44
1:I:26:GLY:H	1:I:30:ARG:NH2	2.15	0.44
1:C:159:SER:O	1:C:197:MET:HG2	2.17	0.44
1:C:118:GLY:HA3	1:D:160:ASP:OD2	2.17	0.44
1:N:114:VAL:HB	1:N:157:ALA:HA	2.00	0.43
1:B:57:LEU:HG	1:B:250:ARG:HG3	1.99	0.43
1:D:58:ASP:OD2	1:D:250:ARG:HG2	2.18	0.43
1:K:89:PHE:O	1:K:213:ALA:HA	2.18	0.43
1:K:162:PHE:HA	1:K:166:GLN:NE2	2.33	0.43
1:P:240:HIS:O	1:P:244:ILE:HD12	2.18	0.43
1:N:58:ASP:OD2	1:N:250:ARG:HG2	2.18	0.43
1:N:108:LEU:HD22	1:N:152:HIS:HB2	1.99	0.43
1:Q:222:ASN:HB3	1:Q:225:GLN:HE21	1.84	0.43
1:O:196:GLU:HA	4:O:2152:THM:O2	2.18	0.43
1:M:162:PHE:HA	1:M:166:GLN:NE2	2.33	0.43
1:Q:158:SER:HA	1:Q:196:GLU:O	2.18	0.43
2:E:2051:PO4:P	1:F:48:ARG:HH22	2.41	0.43
1:I:38:MET:SD	1:I:57:LEU:HD13	2.59	0.43
1:Q:114:VAL:HB	1:Q:157:ALA:HA	2.00	0.43
1:L:108:LEU:HD22	1:L:152:HIS:HB2	2.00	0.43
1:G:48:ARG:HD3	1:H:69:ILE:HD11	2.00	0.43
1:B:126:LEU:HD23	1:C:126:LEU:HB3	1.99	0.43
1:D:126:LEU:HD23	1:E:126:LEU:HD23	2.00	0.43
1:I:7:PHE:HD1	1:I:8:HIS:CE1	2.37	0.43
1:G:240:HIS:O	1:G:244:ILE:HD12	2.18	0.43
1:N:48:ARG:NH1	5:N:1328:HOH:O	2.50	0.43
1:K:159:SER:O	1:K:197:MET:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:VAL:HB	1:E:157:ALA:HA	2.00	0.43
1:O:49:GLU:HB3	1:P:49:GLU:HB3	1.99	0.43
1:D:15:ASP:HB3	1:D:44:LEU:HD13	2.01	0.43
1:H:108:LEU:HD22	1:H:152:HIS:HB2	2.00	0.43
1:A:40:LYS:HE2	1:I:33:LYS:HE2	2.01	0.42
1:H:7:PHE:HD1	1:H:8:HIS:CE1	2.37	0.42
1:E:240:HIS:O	1:E:244:ILE:HD12	2.19	0.42
1:D:222:ASN:HB3	1:D:225:GLN:HE21	1.84	0.42
1:M:220:ILE:HD11	4:M:2132:THM:HM51	2.00	0.42
1:E:38:MET:SD	1:E:57:LEU:HD13	2.59	0.42
1:O:162:PHE:HA	1:O:166:GLN:NE2	2.34	0.42
1:A:69:ILE:HD11	1:B:48:ARG:HD3	2.01	0.42
1:H:89:PHE:O	1:H:213:ALA:HA	2.19	0.42
1:O:93:GLY:HA2	2:O:2151:PO4:O2	2.19	0.42
1:M:158:SER:HA	1:M:196:GLU:O	2.20	0.42
1:C:220:ILE:HD11	4:C:2032:THM:HM51	2.01	0.42
1:D:114:VAL:HB	1:D:157:ALA:HA	2.01	0.42
1:G:116:LEU:HB2	1:G:159:SER:HA	2.00	0.42
1:J:181:LYS:O	1:L:178:ARG:NH2	2.50	0.42
1:K:26:GLY:H	1:K:30:ARG:NH2	2.17	0.42
1:F:15:ASP:HB3	1:F:44:LEU:HD13	2.02	0.42
1:G:228:ILE:HA	1:G:229:PRO:HD3	1.96	0.42
1:H:206:CYS:HB3	1:H:211:LEU:O	2.20	0.42
1:C:49:GLU:HB3	1:D:49:GLU:HB3	2.02	0.42
1:Q:159:SER:O	1:Q:197:MET:HG2	2.19	0.42
1:B:158:SER:HA	1:B:196:GLU:O	2.20	0.42
1:F:116:LEU:HB2	1:F:159:SER:HA	2.02	0.42
1:R:129:PRO:O	1:R:131:VAL:HG12	2.20	0.42
1:D:93:GLY:HA2	2:D:2041:PO4:O2	2.19	0.42
1:O:58:ASP:OD2	1:O:250:ARG:HG2	2.20	0.42
1:P:114:VAL:HB	1:P:157:ALA:HA	2.01	0.42
1:N:206:CYS:HB3	1:N:211:LEU:O	2.20	0.42
1:N:7:PHE:HD1	1:N:8:HIS:CE1	2.38	0.42
1:F:196:GLU:HA	4:F:2062:THM:O2	2.20	0.42
1:C:58:ASP:OD2	1:C:250:ARG:HG2	2.20	0.41
1:I:157:ALA:O	1:I:195:TYR:HA	2.20	0.41
1:I:166:GLN:HG2	1:I:195:TYR:CD1	2.55	0.41
1:B:114:VAL:HB	1:B:157:ALA:HA	2.01	0.41
1:E:60:LYS:HA	1:E:61:PRO:HD3	1.91	0.41
1:F:60:LYS:HA	1:F:61:PRO:HD3	1.94	0.41
1:D:159:SER:O	1:D:197:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:ASN:HB3	1:H:225:GLN:HE21	1.85	0.41
1:J:26:GLY:H	1:J:30:ARG:NH2	2.18	0.41
1:I:15:ASP:HB3	1:I:44:LEU:HD13	2.02	0.41
1:N:219:VAL:O	1:N:237:THR:HG21	2.20	0.41
1:G:206:CYS:HB3	1:G:211:LEU:O	2.20	0.41
1:G:60:LYS:HA	1:G:61:PRO:HD3	1.92	0.41
1:N:220:ILE:HD11	4:N:2142:THM:HM51	2.03	0.41
1:B:116:LEU:HB2	1:B:159:SER:HA	2.01	0.41
1:A:240:HIS:O	1:A:244:ILE:HD12	2.20	0.41
1:K:116:LEU:HB2	1:K:159:SER:HA	2.01	0.41
1:R:48:ARG:NH1	5:R:1728:HOH:O	2.49	0.41
1:N:15:ASP:HB3	1:N:44:LEU:HD13	2.01	0.41
1:I:60:LYS:HA	1:I:61:PRO:HD3	1.91	0.41
1:H:116:LEU:HB2	1:H:159:SER:HA	2.02	0.41
1:H:240:HIS:O	1:H:244:ILE:HD12	2.20	0.41
1:C:116:LEU:HB2	1:C:159:SER:HA	2.01	0.41
1:A:114:VAL:HB	1:A:157:ALA:HA	2.01	0.41
1:N:228:ILE:HA	1:N:229:PRO:HD3	1.92	0.41
1:D:7:PHE:HD1	1:D:8:HIS:CE1	2.38	0.41
1:A:181:LYS:O	1:E:178:ARG:NH2	2.49	0.41
1:M:89:PHE:O	1:M:213:ALA:HA	2.21	0.41
1:A:228:ILE:HA	1:A:229:PRO:HD3	1.96	0.41
1:C:7:PHE:HD1	1:C:8:HIS:CE1	2.38	0.41
1:F:159:SER:O	1:F:197:MET:HG2	2.21	0.41
1:G:114:VAL:HB	1:G:157:ALA:HA	2.02	0.41
1:B:24:VAL:HG23	1:B:24:VAL:O	2.21	0.41
1:J:89:PHE:O	1:J:213:ALA:HA	2.20	0.41
1:I:48:ARG:NH1	5:I:828:HOH:O	2.48	0.41
1:M:219:VAL:O	1:M:237:THR:HG21	2.21	0.41
1:F:30:ARG:HH22	2:F:2061:PO4:P	2.43	0.41
1:M:58:ASP:OD2	1:M:250:ARG:HG2	2.21	0.41
1:O:15:ASP:HB3	1:O:44:LEU:HD13	2.02	0.41
1:A:15:ASP:HB3	1:A:44:LEU:HD13	2.02	0.41
1:N:240:HIS:O	1:N:244:ILE:HD12	2.21	0.40
1:R:206:CYS:HB3	1:R:211:LEU:O	2.21	0.40
1:R:114:VAL:HB	1:R:157:ALA:HA	2.03	0.40
1:G:166:GLN:HG2	1:G:195:TYR:CD1	2.56	0.40
1:K:30:ARG:HH22	2:K:2111:PO4:P	2.44	0.40
1:Q:7:PHE:HD1	1:Q:8:HIS:CE1	2.39	0.40
1:K:229:PRO:HG2	1:L:7:PHE:CZ	2.56	0.40
1:P:15:ASP:HB3	1:P:44:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:15:ASP:HB3	1:Q:44:LEU:HD13	2.03	0.40
1:A:158:SER:HA	1:A:196:GLU:O	2.22	0.40
1:R:38:MET:SD	1:R:57:LEU:HD13	2.61	0.40
1:F:7:PHE:HD1	1:F:8:HIS:CE1	2.38	0.40
1:R:89:PHE:O	1:R:213:ALA:HA	2.22	0.40
1:B:15:ASP:HB3	1:B:44:LEU:HD13	2.04	0.40
1:L:89:PHE:O	1:L:213:ALA:HA	2.21	0.40
1:L:166:GLN:HG2	1:L:195:TYR:CD1	2.56	0.40
1:C:25:PRO:O	1:C:66:SER:HA	2.21	0.40
1:M:15:ASP:HB3	1:M:44:LEU:HD13	2.02	0.40
1:F:220:ILE:HD11	4:F:2062:THM:HM51	2.03	0.40

All (14) 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:H:232:GLU:CG	1:L:13:LYS:CE[2_657]	1.02	1.18
1:H:232:GLU:CG	1:L:13:LYS:NZ[2_657]	1.34	0.86
1:H:232:GLU:CB	1:L:13:LYS:CD[2_657]	1.35	0.85
1:H:232:GLU:CG	1:L:13:LYS:CD[2_657]	1.47	0.73
1:H:232:GLU:CB	1:L:13:LYS:CE[2_657]	1.68	0.52
1:H:232:GLU:CD	1:L:13:LYS:NZ[2_657]	1.85	0.35
1:M:232:GLU:OE1	5:F:3035:HOH:O[2_646]	2.06	0.14
1:A:101:HIS:N	5:N:1338:HOH:O[2_646]	2.08	0.12
1:H:232:GLU:OE2	1:L:13:LYS:NZ[2_657]	2.09	0.11
1:C:146:SER:OG	1:L:32:GLU:OE2[1_454]	2.10	0.10
1:D:232:GLU:CB	5:C:3051:HOH:O[2_555]	2.11	0.09
1:H:232:GLU:OE1	1:L:84:LEU:O[2_657]	2.13	0.07
1:G:103:ASN:OD1	1:H:181:LYS:NZ[2_647]	2.17	0.03
1:A:101:HIS:CB	5:N:1338:HOH:O[2_646]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	39	75
1	B	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	39	75
1	C	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	39	75
1	D	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	39	75
1	E	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	39	75
1	F	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	39	75
1	G	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	39	75
1	H	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	39	75
1	I	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	39	75
1	J	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	39	75
1	K	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	39	75
1	L	248/253 (98%)	242 (98%)	5 (2%)	1 (0%)	39	75
1	M	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	39	75
1	N	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	39	75
1	O	248/253 (98%)	244 (98%)	3 (1%)	1 (0%)	39	75
1	P	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	39	75
1	Q	248/253 (98%)	244 (98%)	3 (1%)	1 (0%)	39	75
1	R	248/253 (98%)	243 (98%)	4 (2%)	1 (0%)	39	75
All	All	4464/4554 (98%)	4364 (98%)	82 (2%)	18 (0%)	39	75

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	TYR
1	L	163	TYR
1	A	163	TYR
1	C	163	TYR
1	D	163	TYR
1	E	163	TYR
1	F	163	TYR
1	G	163	TYR
1	H	163	TYR
1	I	163	TYR
1	J	163	TYR
1	K	163	TYR

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Mol	Chain	Res	Type
1	M	163	TYR
1	N	163	TYR
1	O	163	TYR
1	P	163	TYR
1	Q	163	TYR
1	R	163	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	B	201/204 (98%)	190 (94%)	11 (6%)	27	63
1	C	201/204 (98%)	190 (94%)	11 (6%)	27	63
1	D	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	E	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	F	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	G	201/204 (98%)	191 (95%)	10 (5%)	30	67
1	H	201/204 (98%)	188 (94%)	13 (6%)	21	57
1	I	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	J	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	K	201/204 (98%)	190 (94%)	11 (6%)	27	63
1	L	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	M	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	N	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	O	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	P	201/204 (98%)	190 (94%)	11 (6%)	27	63
1	Q	201/204 (98%)	189 (94%)	12 (6%)	24	60
1	R	201/204 (98%)	189 (94%)	12 (6%)	24	60
All	All	3618/3672 (98%)	3407 (94%)	211 (6%)	25	61

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	37	LEU
1	A	84	LEU
1	A	92	ILE
1	A	147	ILE
1	A	150	THR
1	A	175	ARG
1	A	186	GLU
1	A	196	GLU
1	A	232	GLU
1	A	240	HIS
1	A	243	LYS
1	B	33	LYS
1	B	37	LEU
1	B	84	LEU
1	B	92	ILE
1	B	147	ILE
1	B	150	THR
1	B	196	GLU
1	B	232	GLU
1	B	240	HIS
1	B	243	LYS
1	B	245	VAL
1	C	33	LYS
1	C	37	LEU
1	C	84	LEU
1	C	92	ILE
1	C	147	ILE
1	C	150	THR
1	C	175	ARG
1	C	196	GLU
1	C	232	GLU
1	C	240	HIS
1	C	243	LYS
1	D	33	LYS
1	D	37	LEU
1	D	84	LEU
1	D	92	ILE
1	D	147	ILE
1	D	150	THR
1	D	175	ARG
1	D	196	GLU

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Mol	Chain	Res	Type
1	D	232	GLU
1	D	240	HIS
1	D	243	LYS
1	D	245	VAL
1	E	33	LYS
1	E	37	LEU
1	E	84	LEU
1	E	92	ILE
1	E	147	ILE
1	E	150	THR
1	E	175	ARG
1	E	186	GLU
1	E	196	GLU
1	E	232	GLU
1	E	240	HIS
1	E	243	LYS
1	F	33	LYS
1	F	37	LEU
1	F	84	LEU
1	F	92	ILE
1	F	147	ILE
1	F	150	THR
1	F	181	LYS
1	F	186	GLU
1	F	196	GLU
1	F	232	GLU
1	F	240	HIS
1	F	243	LYS
1	G	33	LYS
1	G	37	LEU
1	G	84	LEU
1	G	92	ILE
1	G	147	ILE
1	G	150	THR
1	G	196	GLU
1	G	232	GLU
1	G	240	HIS
1	G	243	LYS
1	H	33	LYS
1	H	37	LEU
1	H	84	LEU
1	H	92	ILE

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Mol	Chain	Res	Type
1	H	147	ILE
1	H	150	THR
1	H	175	ARG
1	H	186	GLU
1	H	196	GLU
1	H	232	GLU
1	H	239	SER
1	H	240	HIS
1	H	243	LYS
1	I	33	LYS
1	I	37	LEU
1	I	84	LEU
1	I	92	ILE
1	I	147	ILE
1	I	150	THR
1	I	175	ARG
1	I	186	GLU
1	I	196	GLU
1	I	232	GLU
1	I	240	HIS
1	I	243	LYS
1	J	33	LYS
1	J	37	LEU
1	J	84	LEU
1	J	92	ILE
1	J	147	ILE
1	J	150	THR
1	J	175	ARG
1	J	181	LYS
1	J	196	GLU
1	J	232	GLU
1	J	240	HIS
1	J	243	LYS
1	K	33	LYS
1	K	37	LEU
1	K	84	LEU
1	K	92	ILE
1	K	147	ILE
1	K	150	THR
1	K	175	ARG
1	K	196	GLU
1	K	232	GLU

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Mol	Chain	Res	Type
1	K	240	HIS
1	K	243	LYS
1	L	33	LYS
1	L	37	LEU
1	L	84	LEU
1	L	92	ILE
1	L	147	ILE
1	L	150	THR
1	L	181	LYS
1	L	196	GLU
1	L	232	GLU
1	L	240	HIS
1	L	243	LYS
1	L	245	VAL
1	M	33	LYS
1	M	37	LEU
1	M	84	LEU
1	M	92	ILE
1	M	147	ILE
1	M	150	THR
1	M	175	ARG
1	M	186	GLU
1	M	196	GLU
1	M	232	GLU
1	M	240	HIS
1	M	243	LYS
1	N	33	LYS
1	N	37	LEU
1	N	84	LEU
1	N	92	ILE
1	N	147	ILE
1	N	150	THR
1	N	175	ARG
1	N	186	GLU
1	N	196	GLU
1	N	232	GLU
1	N	240	HIS
1	N	243	LYS
1	O	33	LYS
1	O	37	LEU
1	O	84	LEU
1	O	92	ILE

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Mol	Chain	Res	Type
1	O	147	ILE
1	O	150	THR
1	O	175	ARG
1	O	186	GLU
1	O	196	GLU
1	O	232	GLU
1	O	240	HIS
1	O	243	LYS
1	P	33	LYS
1	P	37	LEU
1	P	84	LEU
1	P	92	ILE
1	P	147	ILE
1	P	150	THR
1	P	175	ARG
1	P	196	GLU
1	P	232	GLU
1	P	240	HIS
1	P	243	LYS
1	Q	33	LYS
1	Q	37	LEU
1	Q	84	LEU
1	Q	92	ILE
1	Q	147	ILE
1	Q	150	THR
1	Q	175	ARG
1	Q	181	LYS
1	Q	196	GLU
1	Q	232	GLU
1	Q	240	HIS
1	Q	243	LYS
1	R	33	LYS
1	R	37	LEU
1	R	84	LEU
1	R	92	ILE
1	R	147	ILE
1	R	150	THR
1	R	175	ARG
1	R	181	LYS
1	R	196	GLU
1	R	232	GLU
1	R	240	HIS

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Mol	Chain	Res	Type
1	R	243	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	226	GLN
1	A	230	ASN
1	B	225	GLN
1	B	226	GLN
1	B	230	ASN
1	C	225	GLN
1	C	226	GLN
1	C	230	ASN
1	D	225	GLN
1	D	226	GLN
1	D	230	ASN
1	E	225	GLN
1	E	226	GLN
1	E	230	ASN
1	F	225	GLN
1	F	226	GLN
1	F	230	ASN
1	G	225	GLN
1	G	226	GLN
1	G	230	ASN
1	H	225	GLN
1	H	226	GLN
1	H	230	ASN
1	I	225	GLN
1	I	226	GLN
1	I	230	ASN
1	J	225	GLN
1	J	226	GLN
1	J	230	ASN
1	K	225	GLN
1	K	226	GLN
1	K	230	ASN
1	L	225	GLN
1	L	226	GLN
1	L	230	ASN
1	M	225	GLN

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Mol	Chain	Res	Type
1	M	226	GLN
1	M	230	ASN
1	N	225	GLN
1	N	226	GLN
1	N	230	ASN
1	O	225	GLN
1	O	226	GLN
1	O	230	ASN
1	P	225	GLN
1	P	226	GLN
1	P	230	ASN
1	Q	225	GLN
1	Q	226	GLN
1	Q	230	ASN
1	R	225	GLN
1	R	226	GLN
1	R	230	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 45 ligands modelled in this entry, 9 are monoatomic - leaving 36 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	$\#\|Z\|>2$
2	PO4	A	2011	-	4,4,4	0.50	0	6,6,6	0.27	0
4	THM	A	2012	-	13,18,18	2.30	2 (15%)	16,26,26	4.99	5 (31%)
2	PO4	B	2021	-	4,4,4	0.60	0	6,6,6	0.27	0
4	THM	B	2022	-	13,18,18	2.14	2 (15%)	16,26,26	5.16	6 (37%)
2	PO4	C	2031	-	4,4,4	0.39	0	6,6,6	0.28	0
4	THM	C	2032	-	13,18,18	2.33	2 (15%)	16,26,26	5.21	7 (43%)
2	PO4	D	2041	-	4,4,4	0.59	0	6,6,6	0.27	0
4	THM	D	2042	-	13,18,18	2.34	2 (15%)	16,26,26	4.90	5 (31%)
2	PO4	E	2051	-	4,4,4	0.37	0	6,6,6	0.27	0
4	THM	E	2052	-	13,18,18	2.33	2 (15%)	16,26,26	4.80	5 (31%)
2	PO4	F	2061	-	4,4,4	0.56	0	6,6,6	0.29	0
4	THM	F	2062	-	13,18,18	2.18	2 (15%)	16,26,26	4.97	5 (31%)
2	PO4	G	2071	-	4,4,4	0.41	0	6,6,6	0.28	0
4	THM	G	2072	-	13,18,18	2.39	2 (15%)	16,26,26	4.85	5 (31%)
2	PO4	H	2081	-	4,4,4	0.44	0	6,6,6	0.29	0
4	THM	H	2082	-	13,18,18	2.24	2 (15%)	16,26,26	4.97	5 (31%)
2	PO4	I	2091	-	4,4,4	0.55	0	6,6,6	0.28	0
4	THM	I	2092	-	13,18,18	2.33	2 (15%)	16,26,26	4.83	5 (31%)
2	PO4	J	2101	-	4,4,4	0.55	0	6,6,6	0.26	0
4	THM	J	2102	-	13,18,18	2.34	2 (15%)	16,26,26	5.17	7 (43%)
2	PO4	K	2111	-	4,4,4	0.56	0	6,6,6	0.28	0
4	THM	K	2112	-	13,18,18	2.19	2 (15%)	16,26,26	4.80	5 (31%)
2	PO4	L	2121	-	4,4,4	0.44	0	6,6,6	0.28	0
4	THM	L	2122	-	13,18,18	2.18	3 (23%)	16,26,26	4.94	7 (43%)
2	PO4	M	2131	-	4,4,4	0.59	0	6,6,6	0.28	0
4	THM	M	2132	-	13,18,18	2.32	2 (15%)	16,26,26	4.97	6 (37%)
2	PO4	N	2141	-	4,4,4	0.35	0	6,6,6	0.28	0
4	THM	N	2142	-	13,18,18	2.31	2 (15%)	16,26,26	4.81	5 (31%)
2	PO4	O	2151	-	4,4,4	0.55	0	6,6,6	0.27	0
4	THM	O	2152	-	13,18,18	2.22	2 (15%)	16,26,26	4.78	5 (31%)
2	PO4	P	2161	-	4,4,4	0.38	0	6,6,6	0.27	0
4	THM	P	2162	-	13,18,18	2.21	2 (15%)	16,26,26	4.84	5 (31%)
2	PO4	Q	2171	-	4,4,4	0.49	0	6,6,6	0.27	0
4	THM	Q	2172	-	13,18,18	2.22	3 (23%)	16,26,26	5.10	6 (37%)
2	PO4	R	2181	-	4,4,4	0.48	0	6,6,6	0.28	0
4	THM	R	2182	-	13,18,18	2.28	2 (15%)	16,26,26	5.19	5 (31%)

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	PO4	A	2011	-	-	0/0/0/0	0/0/0/0
4	THM	A	2012	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	B	2021	-	-	0/0/0/0	0/0/0/0
4	THM	B	2022	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	C	2031	-	-	0/0/0/0	0/0/0/0
4	THM	C	2032	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	D	2041	-	-	0/0/0/0	0/0/0/0
4	THM	D	2042	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	E	2051	-	-	0/0/0/0	0/0/0/0
4	THM	E	2052	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	F	2061	-	-	0/0/0/0	0/0/0/0
4	THM	F	2062	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	G	2071	-	-	0/0/0/0	0/0/0/0
4	THM	G	2072	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	H	2081	-	-	0/0/0/0	0/0/0/0
4	THM	H	2082	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	I	2091	-	-	0/0/0/0	0/0/0/0
4	THM	I	2092	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	J	2101	-	-	0/0/0/0	0/0/0/0
4	THM	J	2102	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	K	2111	-	-	0/0/0/0	0/0/0/0
4	THM	K	2112	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	L	2121	-	-	0/0/0/0	0/0/0/0
4	THM	L	2122	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	M	2131	-	-	0/0/0/0	0/0/0/0
4	THM	M	2132	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	N	2141	-	-	0/0/0/0	0/0/0/0
4	THM	N	2142	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	O	2151	-	-	0/0/0/0	0/0/0/0
4	THM	O	2152	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	P	2161	-	-	0/0/0/0	0/0/0/0
4	THM	P	2162	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	Q	2171	-	-	0/0/0/0	0/0/0/0
4	THM	Q	2172	-	1/1/3/3	0/2/18/18	0/2/2/2
2	PO4	R	2181	-	-	0/0/0/0	0/0/0/0
4	THM	R	2182	-	1/1/3/3	0/2/18/18	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2052	THM	C6-N1	-5.65	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2072	THM	C6-N1	-5.28	1.27	1.35
4	Q	2172	THM	C6-N1	-5.25	1.27	1.35
4	A	2012	THM	C6-N1	-5.22	1.27	1.35
4	O	2152	THM	C6-N1	-4.96	1.27	1.35
4	D	2042	THM	C6-N1	-4.93	1.27	1.35
4	M	2132	THM	C6-N1	-4.90	1.27	1.35
4	C	2032	THM	C6-N1	-4.89	1.27	1.35
4	N	2142	THM	C6-N1	-4.83	1.27	1.35
4	F	2062	THM	C6-N1	-4.78	1.27	1.35
4	B	2022	THM	C6-N1	-4.61	1.28	1.35
4	R	2182	THM	C6-N1	-4.56	1.28	1.35
4	P	2162	THM	C6-N1	-4.48	1.28	1.35
4	L	2122	THM	C6-N1	-4.48	1.28	1.35
4	K	2112	THM	C6-N1	-4.46	1.28	1.35
4	H	2082	THM	C6-N1	-4.37	1.28	1.35
4	I	2092	THM	C6-N1	-4.29	1.28	1.35
4	J	2102	THM	C6-N1	-3.97	1.29	1.35
4	L	2122	THM	C6-C5	-2.05	1.34	1.40
4	Q	2172	THM	C6-C5	-2.00	1.34	1.40
4	Q	2172	THM	C4-N3	5.54	1.43	1.33
4	E	2052	THM	C4-N3	5.76	1.43	1.33
4	B	2022	THM	C4-N3	5.76	1.43	1.33
4	F	2062	THM	C4-N3	5.79	1.43	1.33
4	O	2152	THM	C4-N3	5.83	1.43	1.33
4	L	2122	THM	C4-N3	5.88	1.44	1.33
4	A	2012	THM	C4-N3	6.04	1.44	1.33
4	K	2112	THM	C4-N3	6.05	1.44	1.33
4	P	2162	THM	C4-N3	6.06	1.44	1.33
4	M	2132	THM	C4-N3	6.28	1.44	1.33
4	N	2142	THM	C4-N3	6.29	1.44	1.33
4	G	2072	THM	C4-N3	6.31	1.44	1.33
4	H	2082	THM	C4-N3	6.37	1.44	1.33
4	C	2032	THM	C4-N3	6.41	1.45	1.33
4	R	2182	THM	C4-N3	6.46	1.45	1.33
4	D	2042	THM	C4-N3	6.49	1.45	1.33
4	I	2092	THM	C4-N3	6.87	1.45	1.33
4	J	2102	THM	C4-N3	7.08	1.46	1.33

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2032	THM	C5-C4-N3	-11.44	112.40	125.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	2172	THM	C5-C4-N3	-11.38	112.47	125.14
4	D	2042	THM	C5-C4-N3	-11.37	112.48	125.14
4	F	2062	THM	C5-C4-N3	-11.26	112.60	125.14
4	J	2102	THM	C5-C4-N3	-11.23	112.64	125.14
4	B	2022	THM	C5-C4-N3	-11.21	112.65	125.14
4	E	2052	THM	C5-C4-N3	-11.17	112.70	125.14
4	H	2082	THM	C5-C4-N3	-11.15	112.73	125.14
4	R	2182	THM	C5-C4-N3	-11.14	112.73	125.14
4	A	2012	THM	C5-C4-N3	-11.07	112.81	125.14
4	I	2092	THM	C5-C4-N3	-10.88	113.02	125.14
4	G	2072	THM	C5-C4-N3	-10.70	113.22	125.14
4	N	2142	THM	C5-C4-N3	-10.64	113.29	125.14
4	M	2132	THM	C5-C4-N3	-10.53	113.42	125.14
4	O	2152	THM	C5-C4-N3	-10.47	113.48	125.14
4	P	2162	THM	C5-C4-N3	-10.34	113.63	125.14
4	K	2112	THM	C5-C4-N3	-10.31	113.65	125.14
4	L	2122	THM	C5-C4-N3	-10.27	113.71	125.14
4	R	2182	THM	O4'-C1'-C2'	-4.83	96.64	106.27
4	G	2072	THM	O4'-C1'-C2'	-4.56	97.19	106.27
4	B	2022	THM	O4'-C1'-C2'	-4.46	97.38	106.27
4	M	2132	THM	O4'-C1'-C2'	-4.40	97.50	106.27
4	A	2012	THM	O4'-C1'-C2'	-4.25	97.79	106.27
4	Q	2172	THM	O4'-C1'-C2'	-4.13	98.04	106.27
4	K	2112	THM	O4'-C1'-C2'	-3.82	98.65	106.27
4	C	2032	THM	O4'-C1'-C2'	-3.81	98.69	106.27
4	J	2102	THM	O4'-C1'-C2'	-3.75	98.79	106.27
4	O	2152	THM	O4'-C1'-C2'	-3.68	98.93	106.27
4	P	2162	THM	O4'-C1'-C2'	-3.65	98.99	106.27
4	L	2122	THM	O4'-C1'-C2'	-3.56	99.18	106.27
4	I	2092	THM	O4'-C1'-C2'	-3.53	99.24	106.27
4	L	2122	THM	O4'-C4'-C5'	-3.52	101.55	109.17
4	D	2042	THM	O4'-C1'-C2'	-3.27	99.76	106.27
4	H	2082	THM	O4'-C1'-C2'	-3.22	99.85	106.27
4	F	2062	THM	O4'-C1'-C2'	-2.92	100.44	106.27
4	N	2142	THM	O4'-C1'-C2'	-2.86	100.58	106.27
4	C	2032	THM	O4'-C4'-C5'	-2.58	103.57	109.17
4	E	2052	THM	O4'-C1'-C2'	-2.56	101.17	106.27
4	M	2132	THM	C5M-C5-C4	-2.18	117.24	120.05
4	J	2102	THM	C5'-C4'-C3'	2.04	120.22	114.80
4	J	2102	THM	O3'-C3'-C2'	2.04	117.50	110.74
4	C	2032	THM	C5'-C4'-C3'	2.22	120.72	114.80
4	B	2022	THM	O3'-C3'-C2'	2.37	118.60	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	2172	THM	O3'-C3'-C2'	2.47	118.92	110.74
4	E	2052	THM	O4'-C1'-N1	2.58	112.18	107.72
4	J	2102	THM	O4'-C1'-N1	2.58	112.19	107.72
4	C	2032	THM	O4'-C1'-N1	2.86	112.67	107.72
4	L	2122	THM	C5'-C4'-C3'	2.88	122.47	114.80
4	L	2122	THM	O4'-C1'-N1	2.96	112.84	107.72
4	N	2142	THM	O4'-C1'-N1	3.01	112.93	107.72
4	F	2062	THM	O4'-C1'-N1	3.08	113.05	107.72
4	R	2182	THM	O4'-C1'-N1	3.18	113.23	107.72
4	Q	2172	THM	O4'-C1'-N1	3.19	113.25	107.72
4	A	2012	THM	O4'-C1'-N1	3.28	113.39	107.72
4	K	2112	THM	O4'-C1'-N1	3.42	113.64	107.72
4	H	2082	THM	O4'-C1'-N1	3.45	113.69	107.72
4	P	2162	THM	O4'-C1'-N1	3.72	114.15	107.72
4	B	2022	THM	O4'-C1'-N1	3.74	114.20	107.72
4	O	2152	THM	O4'-C1'-N1	3.83	114.34	107.72
4	I	2092	THM	O4'-C1'-N1	3.95	114.55	107.72
4	M	2132	THM	O4'-C1'-N1	3.96	114.57	107.72
4	D	2042	THM	O4'-C1'-N1	4.03	114.70	107.72
4	G	2072	THM	O4'-C1'-N1	4.15	114.90	107.72
4	G	2072	THM	C4-N3-C2	5.11	119.67	115.25
4	A	2012	THM	C4-N3-C2	6.33	120.72	115.25
4	K	2112	THM	C4-N3-C2	6.36	120.74	115.25
4	O	2152	THM	C4-N3-C2	6.39	120.77	115.25
4	M	2132	THM	C4-N3-C2	6.48	120.85	115.25
4	E	2052	THM	C4-N3-C2	6.50	120.87	115.25
4	L	2122	THM	C4-N3-C2	6.51	120.87	115.25
4	N	2142	THM	C4-N3-C2	6.89	121.20	115.25
4	R	2182	THM	C4-N3-C2	6.98	121.28	115.25
4	P	2162	THM	C4-N3-C2	7.20	121.47	115.25
4	D	2042	THM	C4-N3-C2	7.21	121.48	115.25
4	I	2092	THM	C4-N3-C2	7.29	121.55	115.25
4	Q	2172	THM	C4-N3-C2	7.42	121.66	115.25
4	F	2062	THM	C4-N3-C2	7.64	121.85	115.25
4	B	2022	THM	C4-N3-C2	7.70	121.91	115.25
4	H	2082	THM	C4-N3-C2	7.83	122.01	115.25
4	J	2102	THM	C4-N3-C2	8.01	122.17	115.25
4	C	2032	THM	C4-N3-C2	8.38	122.49	115.25
4	D	2042	THM	C2'-C1'-N1	12.84	145.39	114.16
4	I	2092	THM	C2'-C1'-N1	12.93	145.60	114.16
4	H	2082	THM	C2'-C1'-N1	13.25	146.38	114.16
4	O	2152	THM	C2'-C1'-N1	13.27	146.42	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	2142	THM	C2'-C1'-N1	13.29	146.49	114.16
4	F	2062	THM	C2'-C1'-N1	13.30	146.50	114.16
4	P	2162	THM	C2'-C1'-N1	13.31	146.52	114.16
4	E	2052	THM	C2'-C1'-N1	13.36	146.63	114.16
4	G	2072	THM	C2'-C1'-N1	13.49	146.95	114.16
4	K	2112	THM	C2'-C1'-N1	13.53	147.07	114.16
4	Q	2172	THM	C2'-C1'-N1	13.81	147.74	114.16
4	M	2132	THM	C2'-C1'-N1	13.84	147.82	114.16
4	C	2032	THM	C2'-C1'-N1	13.86	147.86	114.16
4	B	2022	THM	C2'-C1'-N1	13.89	147.94	114.16
4	L	2122	THM	C2'-C1'-N1	13.90	147.95	114.16
4	A	2012	THM	C2'-C1'-N1	13.99	148.19	114.16
4	J	2102	THM	C2'-C1'-N1	14.25	148.80	114.16
4	R	2182	THM	C2'-C1'-N1	14.44	149.27	114.16

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2022	THM	C1'
4	L	2122	THM	C1'
4	C	2032	THM	C1'
4	A	2012	THM	C1'
4	J	2102	THM	C1'
4	D	2042	THM	C1'
4	G	2072	THM	C1'
4	N	2142	THM	C1'
4	H	2082	THM	C1'
4	O	2152	THM	C1'
4	P	2162	THM	C1'
4	Q	2172	THM	C1'
4	R	2182	THM	C1'
4	I	2092	THM	C1'
4	M	2132	THM	C1'
4	E	2052	THM	C1'
4	F	2062	THM	C1'
4	K	2112	THM	C1'

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2011	PO4	1	0
2	B	2021	PO4	1	0
2	C	2031	PO4	1	0
4	C	2032	THM	2	0
2	D	2041	PO4	3	0
2	E	2051	PO4	2	0
4	E	2052	THM	1	0
2	F	2061	PO4	2	0
4	F	2062	THM	2	0
2	G	2071	PO4	1	0
2	H	2081	PO4	1	0
2	J	2101	PO4	1	0
4	J	2102	THM	1	0
2	K	2111	PO4	3	0
4	L	2122	THM	1	0
2	M	2131	PO4	1	0
4	M	2132	THM	1	0
2	N	2141	PO4	1	0
4	N	2142	THM	1	0
2	O	2151	PO4	3	0
4	O	2152	THM	1	0
4	Q	2172	THM	1	0
2	R	2181	PO4	1	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

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^{th} 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%)	-0.39	7 (2%) 56 32	7, 22, 47, 73	0
1	B	250/253 (98%)	-0.52	5 (2%) 68 46	7, 22, 47, 73	0
1	C	250/253 (98%)	-0.45	4 (1%) 74 55	7, 22, 47, 73	0
1	D	250/253 (98%)	-0.45	7 (2%) 56 32	7, 22, 47, 73	0
1	E	250/253 (98%)	-0.37	8 (3%) 51 27	7, 22, 47, 73	0
1	F	250/253 (98%)	-0.30	9 (3%) 46 23	7, 22, 47, 73	0
1	G	250/253 (98%)	-0.45	7 (2%) 56 32	7, 22, 47, 73	0
1	H	250/253 (98%)	-0.46	7 (2%) 56 32	7, 22, 47, 73	0
1	I	250/253 (98%)	-0.40	4 (1%) 74 55	7, 22, 47, 73	0
1	J	250/253 (98%)	-0.31	6 (2%) 62 39	7, 22, 47, 73	0
1	K	250/253 (98%)	-0.55	5 (2%) 68 46	7, 22, 47, 73	0
1	L	250/253 (98%)	-0.48	5 (2%) 68 46	7, 22, 47, 73	0
1	M	250/253 (98%)	-0.33	8 (3%) 51 27	7, 22, 47, 73	0
1	N	250/253 (98%)	-0.33	6 (2%) 62 39	7, 22, 47, 73	0
1	O	250/253 (98%)	-0.27	7 (2%) 56 32	7, 22, 47, 73	0
1	P	250/253 (98%)	-0.20	11 (4%) 38 17	7, 22, 47, 73	0
1	Q	250/253 (98%)	-0.39	1 (0%) 93 85	7, 22, 47, 73	0
1	R	250/253 (98%)	-0.40	3 (1%) 81 64	7, 22, 47, 73	0
All	All	4500/4554 (98%)	-0.39	110 (2%) 62 39	7, 22, 48, 73	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	229	PRO	7.6
1	M	238	GLU	5.7
1	H	236	GLN	5.4

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Mol	Chain	Res	Type	RSRZ
1	M	239	SER	5.4
1	N	231	ALA	5.3
1	M	235	LYS	5.1
1	D	236	GLN	5.0
1	A	239	SER	5.0
1	H	233	THR	4.9
1	E	231	ALA	4.9
1	M	234	MET	4.6
1	M	233	THR	4.5
1	G	237	THR	4.5
1	P	237	THR	4.4
1	L	231	ALA	4.2
1	D	234	MET	4.2
1	D	233	THR	4.2
1	O	230	ASN	4.1
1	P	234	MET	4.0
1	C	230	ASN	4.0
1	P	231	ALA	4.0
1	H	235	LYS	3.9
1	F	229	PRO	3.9
1	H	232	GLU	3.8
1	G	235	LYS	3.8
1	B	234	MET	3.7
1	H	237	THR	3.6
1	A	235	LYS	3.6
1	M	237	THR	3.6
1	E	234	MET	3.5
1	O	231	ALA	3.5
1	A	238	GLU	3.4
1	G	236	GLN	3.4
1	A	237	THR	3.4
1	I	230	ASN	3.4
1	L	229	PRO	3.4
1	M	236	GLN	3.4
1	B	233	THR	3.4
1	J	230	ASN	3.3
1	I	229	PRO	3.3
1	O	229	PRO	3.3
1	G	234	MET	3.3
1	H	238	GLU	3.3
1	I	233	THR	3.2
1	H	234	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	237	THR	3.2
1	A	234	MET	3.2
1	N	228	ILE	3.2
1	E	232	GLU	3.1
1	B	235	LYS	3.1
1	F	231	ALA	3.1
1	Q	233	THR	3.1
1	K	231	ALA	3.1
1	N	234	MET	3.1
1	A	233	THR	3.0
1	C	235	LYS	3.0
1	F	230	ASN	3.0
1	P	226	GLN	2.9
1	O	235	LYS	2.9
1	L	232	GLU	2.9
1	P	233	THR	2.9
1	C	231	ALA	2.8
1	N	226	GLN	2.8
1	F	235	LYS	2.8
1	R	235	LYS	2.8
1	F	238	GLU	2.7
1	P	235	LYS	2.7
1	G	238	GLU	2.7
1	J	225	GLN	2.7
1	J	233	THR	2.6
1	O	234	MET	2.6
1	E	230	ASN	2.6
1	L	237	THR	2.6
1	K	235	LYS	2.5
1	N	230	ASN	2.5
1	I	232	GLU	2.5
1	F	237	THR	2.4
1	J	235	LYS	2.4
1	E	239	SER	2.4
1	B	231	ALA	2.4
1	P	232	GLU	2.4
1	P	229	PRO	2.4
1	F	233	THR	2.4
1	F	236	GLN	2.4
1	G	231	ALA	2.3
1	F	234	MET	2.3
1	D	238	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	236	GLN	2.3
1	R	237	THR	2.3
1	P	230	ASN	2.3
1	E	236	GLN	2.3
1	J	226	GLN	2.3
1	C	234	MET	2.3
1	O	236	GLN	2.3
1	M	230	ASN	2.3
1	K	148	GLY	2.3
1	L	230	ASN	2.2
1	K	39	ASP	2.2
1	P	4	SER	2.2
1	R	234	MET	2.2
1	A	236	GLN	2.2
1	E	233	THR	2.2
1	E	237	THR	2.2
1	D	235	LYS	2.1
1	K	233	THR	2.1
1	G	239	SER	2.0
1	P	145	LYS	2.0
1	O	233	THR	2.0
1	D	231	ALA	2.0
1	B	237	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	H	2081	5/5	0.82	0.33	2.58	76,76,77,77	0
2	PO4	C	2031	5/5	0.91	0.27	1.99	74,74,74,75	0
2	PO4	P	2161	5/5	0.80	0.34	1.88	72,73,73,73	0
2	PO4	G	2071	5/5	0.92	0.26	1.61	77,77,77,77	0
4	THM	C	2032	17/17	0.90	0.24	1.57	45,47,48,48	0
4	THM	K	2112	17/17	0.95	0.21	1.39	36,43,44,45	0
2	PO4	M	2131	5/5	0.93	0.29	1.38	77,77,77,78	0
4	THM	A	2012	17/17	0.95	0.22	1.31	41,42,43,45	0
2	PO4	E	2051	5/5	0.87	0.26	1.03	73,73,75,75	0
4	THM	G	2072	17/17	0.95	0.19	0.94	44,47,51,53	0
4	THM	Q	2172	17/17	0.92	0.26	0.91	42,45,46,46	0
2	PO4	R	2181	5/5	0.90	0.24	0.91	69,70,70,71	0
4	THM	H	2082	17/17	0.94	0.20	0.87	40,42,44,45	0
4	THM	M	2132	17/17	0.93	0.21	0.86	37,39,40,42	0
4	THM	E	2052	17/17	0.95	0.23	0.83	38,40,44,45	0
2	PO4	J	2101	5/5	0.92	0.26	0.80	59,59,60,60	0
4	THM	J	2102	17/17	0.91	0.24	0.73	37,43,44,45	0
4	THM	R	2182	17/17	0.96	0.23	0.63	37,40,41,42	0
4	THM	O	2152	17/17	0.93	0.26	0.55	44,47,48,50	0
4	THM	P	2162	17/17	0.90	0.25	0.39	43,45,46,46	0
2	PO4	Q	2171	5/5	0.93	0.23	0.38	67,67,67,68	0
2	PO4	N	2141	5/5	0.91	0.22	0.30	63,63,64,64	0
4	THM	L	2122	17/17	0.94	0.22	0.28	35,41,42,43	0
4	THM	I	2092	17/17	0.92	0.21	0.25	45,46,48,48	0
3	K	Q	3008	1/1	0.83	0.14	0.22	70,70,70,70	0
4	THM	F	2062	17/17	0.94	0.22	0.17	43,44,45,45	0
4	THM	D	2042	17/17	0.95	0.16	0.13	44,46,49,51	0
4	THM	B	2022	17/17	0.96	0.16	0.04	42,44,45,45	0
4	THM	N	2142	17/17	0.93	0.22	0.00	53,54,54,55	0
2	PO4	L	2121	5/5	0.96	0.14	-0.48	61,61,61,61	0
2	PO4	K	2111	5/5	0.97	0.15	-0.55	65,65,65,65	0
2	PO4	B	2021	5/5	0.97	0.13	-0.56	58,59,59,59	0
2	PO4	O	2151	5/5	0.93	0.16	-0.86	61,62,62,62	0
2	PO4	I	2091	5/5	0.95	0.15	-0.87	48,48,48,48	0
2	PO4	D	2041	5/5	0.97	0.12	-0.99	55,55,56,56	0
2	PO4	A	2011	5/5	0.97	0.13	-1.04	69,69,69,70	0
2	PO4	F	2061	5/5	0.96	0.14	-1.16	51,51,51,51	0
3	K	C	3002	1/1	0.93	0.10	-1.43	37,37,37,37	0
3	K	I	3005	1/1	0.95	0.08	-2.02	49,49,49,49	0
3	K	G	3004	1/1	0.95	0.07	-2.08	45,45,45,45	0
3	K	M	3007	1/1	0.94	0.08	-2.11	50,50,50,50	0
3	K	O	3009	1/1	0.89	0.09	-2.51	66,66,66,66	0
3	K	F	3003	1/1	0.89	0.07	-2.54	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	K	A	3001	1/1	0.97	0.05	-3.18	40,40,40,40	0
3	K	K	3006	1/1	0.93	0.05	-3.54	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.