



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:21 PM GMT

PDB ID : 1A49
Title : BIS MG-ATP-K-OXALATE COMPLEX OF PYRUVATE KINASE
Authors : Larsen, T.M.; Benning, M.M.; Rayment, I.; Reed, G.H.
Deposited on : 1998-02-12
Resolution : 2.10 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

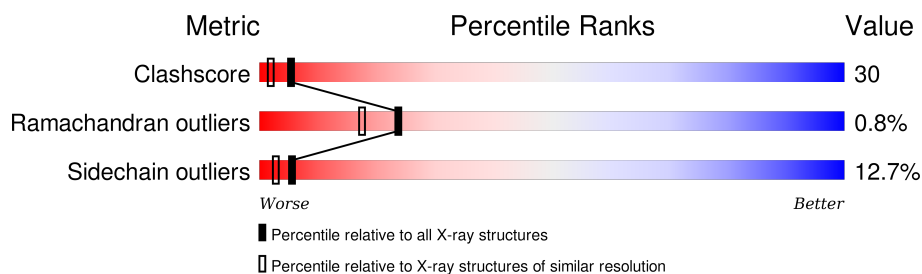
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)


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 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	
1	B	530	
1	C	530	
1	D	530	
1	E	530	
1	F	530	
1	G	530	

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Mol	Chain	Length	Quality of chain
1	H	530	 A horizontal bar chart showing the quality of chain 1. The bar is divided into three segments: green (54%), yellow (36%), and red (7%). The red segment is the smallest and is followed by two small black dots.

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
3	OXL	A	533	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34001 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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	B	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	C	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	D	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	E	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	F	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	G	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	H	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			

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

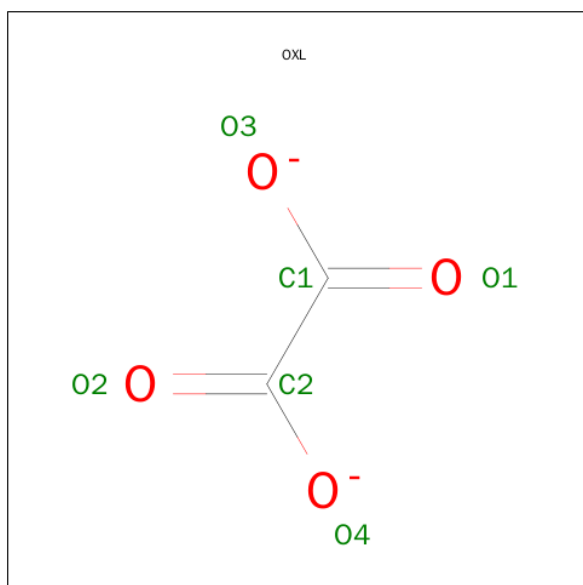
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		
2	H	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	F	1	Total	K	0	0
			1	1		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).

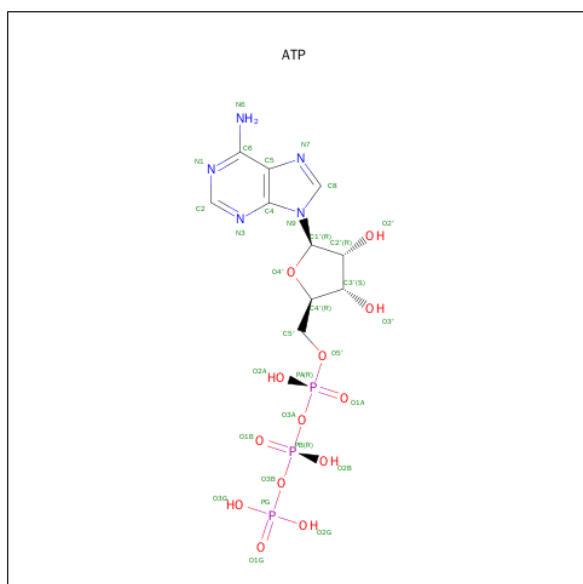


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	H	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	2	Total Mg 2 2	0	0
4	A	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
5	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is water.

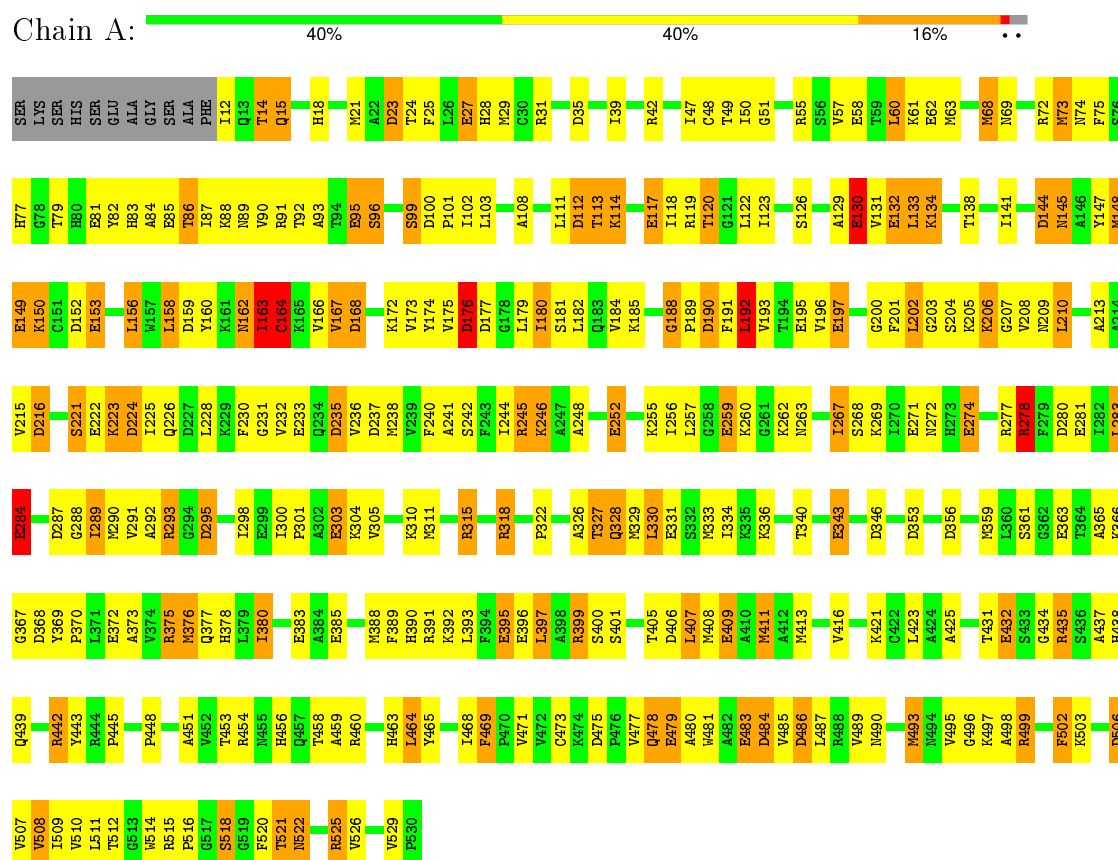
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	270	Total	O	0	0
			270	270		
6	C	178	Total	O	0	0
			178	178		
6	D	272	Total	O	0	0
			272	272		
6	E	279	Total	O	0	0
			279	279		
6	F	197	Total	O	0	0
			197	197		
6	G	228	Total	O	0	0
			228	228		
6	H	302	Total	O	0	0
			302	302		

3 Residue-property plots

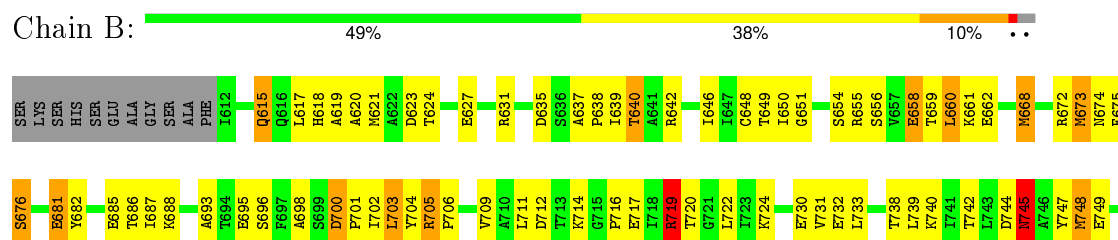
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

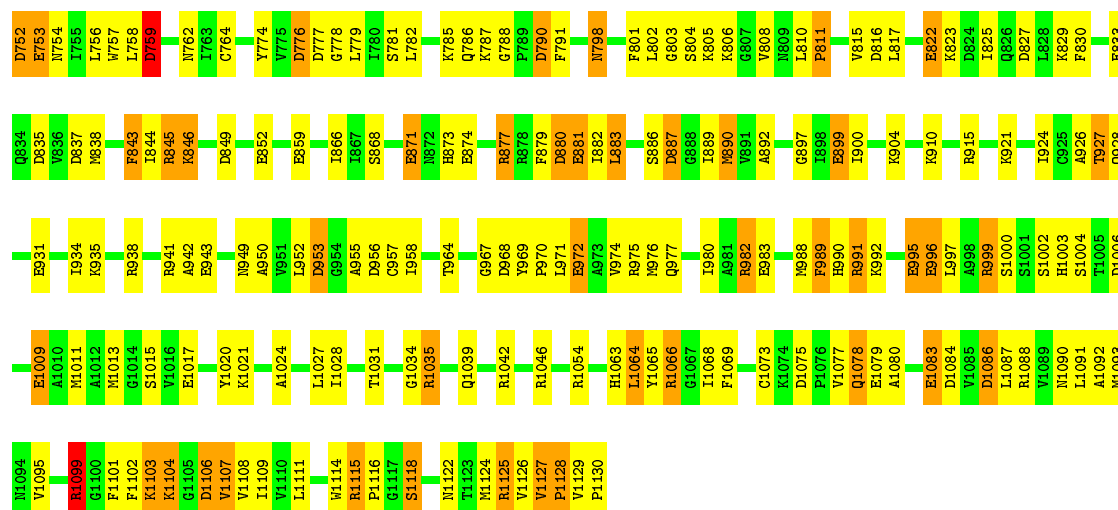
Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE



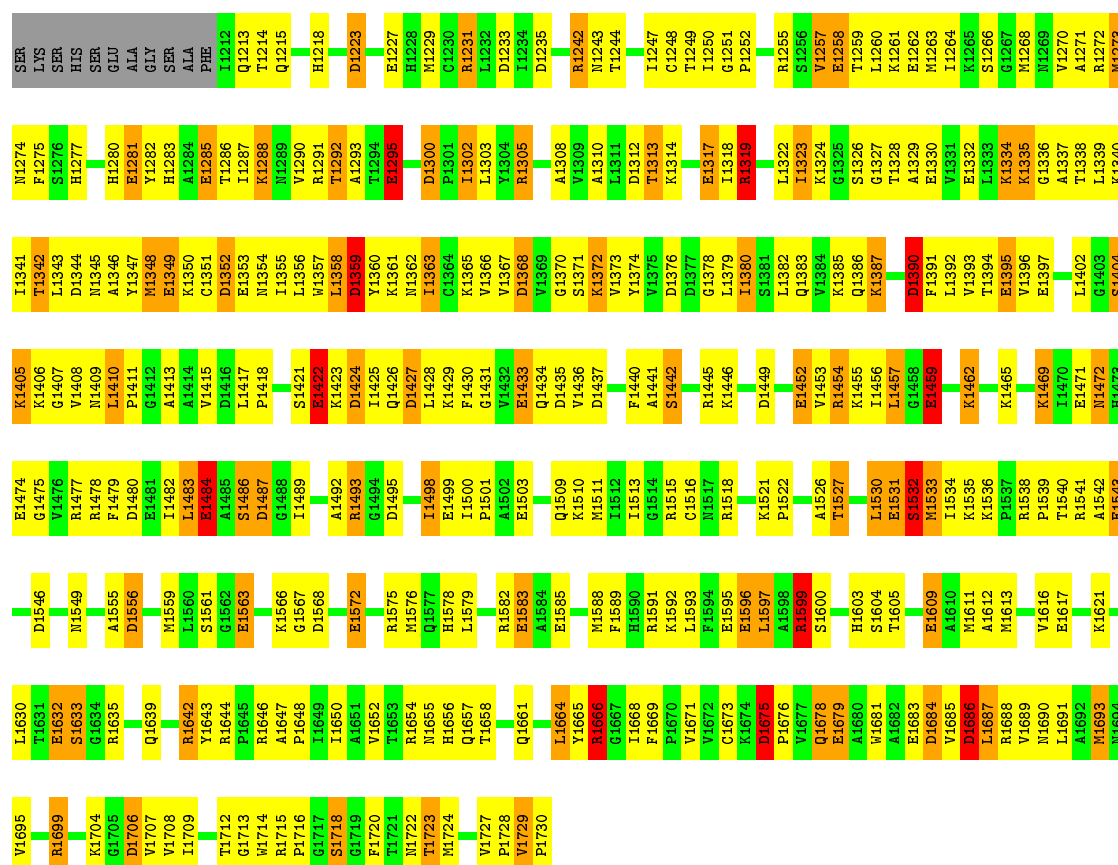
• Molecule 1: PYRUVATE KINASE





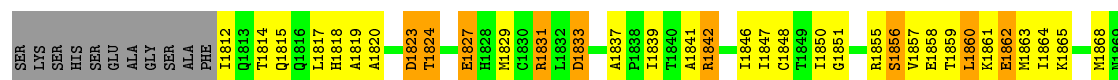
• Molecule 1: PYRUVATE KINASE

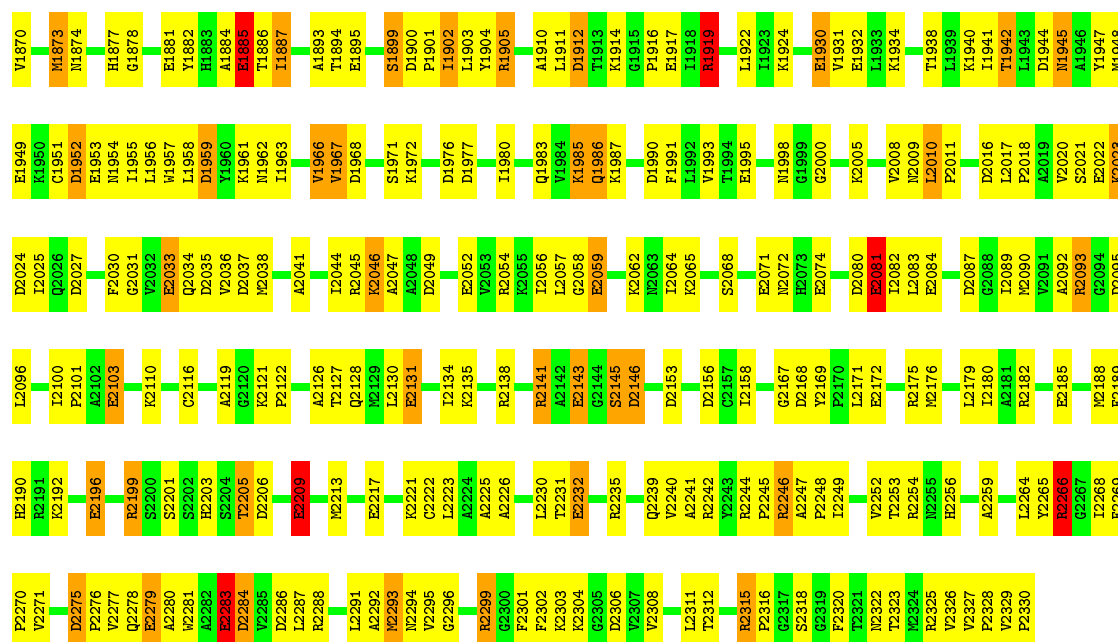
Chain C: 38% 44% 14%



• Molecule 1: PYRUVATE KINASE

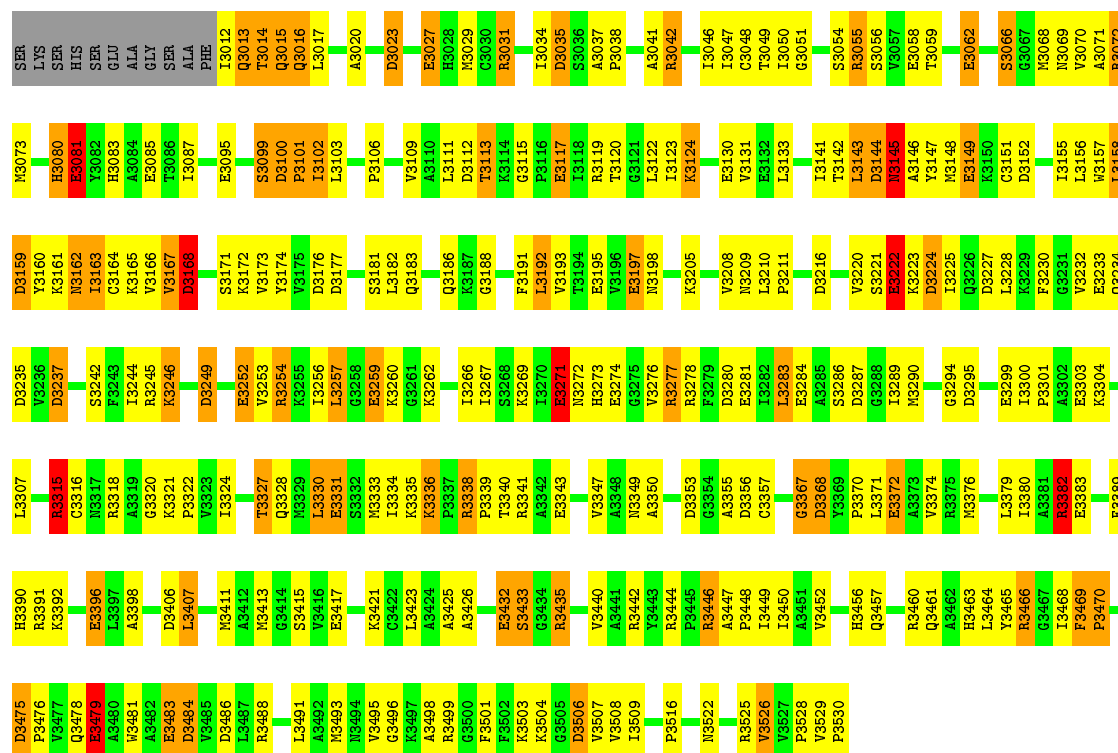
Chain D: 45% 42% 9%





• Molecule 1: PYRUVATE KINASE

Chain E: 47% 37% 12% ••



• Molecule 1: PYRUVATE KINASE

Chain F: 44% 41% 11% ••

SER	H660	R4575	G4494	P4411	E4349	M4274	K3966	I3882	L3810	A3746	H680	SER
LYS	R4660	M4576	D4495	G4412	K4350	F4275	G3967	L3883	P3811	Y3747	E681	LYS
SER			L4496	A4413	G4352	S4276	Y3969	E3884	G3812	M3748	Y3682	SER
HIS		E4585	G4497		D4352		Y3969	A3884	A3813	G3749	H3683	HIS
SER		F4589	I4498	D4416	E4353	H4280	Y3971	S3886	A3814	K3750	A3684	SER
GLU		L4664	E4499	L4417	E4353	H4281	G3972	G3887	G3815	C3751	E3685	GLU
ALA		Y4665	L4500	P4418	M4354	Y4282		G3888	D3816	D3752	T3686	ALA
GLY		R4666			M4357			G3889	L3817	E3753	T3687	GLY
SER		K4592	E4503	E4422	L4358	E4285	R3975	M3890		N3754	K3688	SER
ALA		F4592	F4506	K4423	T4286	T4287	M3976	V3891	V3820	L3755	N3689	ALA
PHE		L4668	F4506	K4423	Y4360	L4287	K3980	A3892	S3821	L3756	V3690	PHE
		E4595		I4425	K4361	K4288	I3980	R3893	E3822	K3757	R3691	
		L4597	Q4509	Q4426	M4362	M4289	A3981	G3894	K3823	L3758	T3614	
		L4597	K4510	D4427	I4363		R3982	D3895	D3824	E3759	E3695	
		A4598	M4511	L4428	K4364	A4293	E3983	L3896	K3826	Y3760	S3696	
		S4600	I4513	F4430	G4366	E4295	E3983	G3897	K3826	K3761	F3697	
			G4514	F4430	V4367	S4296	E3985	I3898	D3827	N3762	A3698	
			G4514	P4301	V4367	F4297		I3898	K3828	I3763	S3699	
			K4521	K4372	I4302	F4225		E3989	K3829	C3764	R3700	
			V4522	V4373	I4303	L4226	M3988	E3903	F3830	K3765	P3701	
			V4523	Y4374	L4303	E4227	F3989	K3904	G3831	V3766	I3702	
			A4526	Y4375	Y4304		E3990	V3905	V3832	V3767	L3703	
			K4527	D4376	R4305		R3999	F3906	E3833	K3768	Y3704	
			Q4528	D4377			L3993		K3834	V3769	R3705	
			L4529	G4378	D4312		E3996	K3910	D3835			
			L4530	D4378	I4234			C3916	V3836	K3772	V3709	
				D4379	D4235		R3999	K3921	D3837	Y3773	D3712	
				L4379	D4235				N3838	Y3774	I3639	
				V4380	D4235		S4002	A3926	S3842	D3775	K3714	
				E4381	T4240		H4003	T3927	F3843	D3777	G3715	
				L4382	A4241		S4004	T3927	I3844	G3778	P3716	
				Q4383	R4242		T4005	Q3928	R3845	K3779	E3717	
				V4384	I4243		D4006	M3929	I3718	I3780	T3649	
				K4385	T4244		L4007		D3849	S3781	R3719	
				Q4386	L4222		M4008	M3933		L3782	T3720	
				K4387			E4009	I3934	E3852	K3783	G3721	
				G4388	I4247			K3935	I3856	Q3786	G3722	
				P4389	C4248		M4013	K3936	K3787	K3787	I3723	
				D4390	T4249		G4014	P3937	G3788	G3725	R3654	
				F4391	I4250		S4015	R3938	E3859	P3789	G3726	
				V4392	G4251		V4016	P3939	K3862	D3790	G3727	
				L4393	P4252		E4017	T3940	I3863	F3791	T3728	
				T4394	A4253		L4030	K3941	I3864	L3792	A3729	
				V4396	S4254		E3943	A3942		V3793	E3662	
				E4397	S4256		T4031	G3944	I3867	T3794	V3731	
				N4398	V4257		R4035	S3945	S3868	E3795	I3664	
				F4401	E4259		Q4039	K3869	K3869	V3796	K3665	
				L4402	L4260			I3870	E3797	E3797	S3666	
				G4403	K4261			E3871	K3735	G3800	G3667	
				S4404	E4262			N3872	F3801	N3668	N3669	
				K4405	N4263			E3873	L3739	L3739	N3673	
				K4406	I4264			G3875	K3740	L3802	I3674	
				D4407	K4265			S3804	I3741	G3803	N3674	
				V4408	M4268			K3806	T3742	K3606	F3675	
				L4410				E3881	L3743	S3676	S3676	
										N3809	T3679	

• Molecule 1: PYRUVATE KINASE

Chain G:  43% 43% 12%

SER	H4656	R4575	G4494	P4411	E4349	M4274	K3966	I3882	L3810	A3746	H680	SER
LYS	R4660	M4576	D4495	G4412	K4350	F4275	G3967	L3883	P3811	Y3747	E681	LYS
SER			L4496	A4413	G4352	S4276	Y3969	E3884	G3812	M3748	Y3682	SER
HIS		E4585	G4497		D4352		Y3969	A3884	A3813	G3749	H3683	HIS
SER		F4589	I4498	D4416	E4353	H4280	Y3971	S3886	A3814	K3750	A3684	SER
GLU		L4664	E4499	L4417	E4353	H4281	G3972	G3887	G3815	C3751	E3685	GLU
ALA		Y4665	L4500	P4418	M4354	Y4282		G3888	D3816	D3752	T3686	ALA
GLY		R4666			M4357			G3889	L3817	E3753	T3687	GLY
SER		K4592	E4503	E4422	L4358	E4285	R3975	M3890		N3754	K3688	SER
ALA		F4592	F4506	K4423	T4286	T4287	M3976	V3891	V3820	L3755	N3689	ALA
PHE		L4668	F4506	K4423	Y4360	L4287	K3980	A3892	S3821	L3756	V3690	PHE
		E4595		I4425	K4361	K4288	I3980	R3893	E3822	K3757	R3691	
		L4597	Q4509	Q4426	M4362	M4289	A3981	G3894	K3823	L3758	T3614	
		L4597	K4510	D4427	I4363		R3982	D3895	D3824	E3759	E3695	
		A4598	M4511	L4428	K4364	A4293	E3983	L3896	K3826	Y3760	S3696	
		S4600	I4513	F4430	G4366	E4295	E3983	G3897	K3826	K3761	F3697	
			G4514	F4430	V4367	S4296	E3985	I3898	D3827	N3762	A3698	
			G4514	P4301	V4367	F4297		I3898	K3828	I3763	S3699	
			K4521	K4372	I4302	F4225		E3989	K3829	C3764	R3700	
			V4522	V4373	I4303	L4226	M3988	E3903	F3830	K3765	P3701	
			V4523	Y4374	L4303	E4227	F3989	K3904	G3831	V3766	I3702	
			A4526	Y4375	Y4304		E3990	V3905	V3832	V3767	L3703	
			K4527	D4376	R4305		R3999	F3906	E3833	K3768	Y3704	
			Q4528	D4377			L3993		K3834	V3769	R3705	
			L4529	G4378	D4312		E3996	K3910	D3835			
			L4530	D4378	I4234			C3916	V3836	K3772	V3709	
				D4379	D4235		R3999	K3921	D3837	Y3773	D3712	
				V4380	D4235				N3838	Y3774	I3639	
				L4379	D4235		S4002	A3926	S3842	D3775	K3714	
				V4381	T4240		H4003	T3927	F3843	D3777	G3715	
				L4382	A4241		S4004	T3927	I3844	G3778	P3716	
				Q4383	R4242		T4005	Q3928	R3845	K3779	E3717	
				V4384	I4243		D4006	M3929	I3718	I3780	T3649	
				K4385	T4244		L4007		D3849	S3781	R3719	
				Q4386	L4222		M4008	M3933		L3782	T3720	
				K4387			E4009	I3934	E3852	K3783	G3721	
				G4388	I4247			K3935	I3856	Q3786	G3722	
				P4389	C4248		M4013	K3936	K3787	K3787	I3723	
				D4390	T4249		G4014	P3937	G3788	G3725	R3654	
				F4391	I4250		S4015	R3938	E3859	P3789	G3726	
				V4392	G4251		V4016	P3939	K3862	D3790	G3727	
				L4393	P4252		E4017	T3940	I3863	F3791	T3728	
				T4394	A4253		L4030	K3941	I3864	L3792	A3729	
				V4396	S4254		E3943	A3942		V3793	E3662	
				E4397	S4256		T4031	G3944	I3867	T3794	V3731	
				N4398	V4257		R4035	S3945	S3868	E3795	I3664	
				F4401	E4259		Q4039	K3869	K3869	V3796	K3665	
				L4402	L4260			I3870	E3797	E3797	S3666	
				G4403	K4261			E3871	K3735	G3800	G3667	
				S4404	E4262			N3872	F3801	N3668	N3669	
				K4405	N4263			E3873	L3739	L3739	N3673	
				K4406	I4264			G3875	K3740	L3802	I3674	
				D4407	K4265			S3804	I3741	G3803	N3674	
				V4408	M4268			K3806	T3742	K3606	F3675	
				L4410				E3881	L3743	S3676	S3676	
										N3809	T3679	

• Molecule 1: PYRUVATE KINASE

Chain H:

54%

36%

7%

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SER	R4891	D4877	K5060	A5142	A5237	V5327
LYS	E4895	G4878	M5063	E5143	R5238	P5328
SER		L4879	I5067	D5146	Q5239	V5329
HIS					R5242	P5330
SER	D4900	Q4886	E5071	M5149	R5246	
GLU	P4901	K4887	M5072	D5156	A5247	
ALA	I4902	K4888	H5073	G5157		
GLY	L4903	P4889	E5074	I5158	H5256	
SER	Y4904	D4990	G5075	M5159		
ALA	R4905	F4991	V5076	E5163	R5260	
PHE	A4908	L4992	V5077	T5164	Q5261	
	Q4812	V4993		A5165		
	Q4813	T4994	D5080	R5166	L5264	
	T4814	E4995	E5081	G5167	Y5265	
	Q4815	V4996	E5084	D5168	R5266	
	D4823	E4997			G5267	
		F5001	E5087	E5172	I5268	
	E4827	R5005	G5088		F5269	
	D4833	K5006	I5089	R5175	D5275	
	T4834	D5009	M5090	M5176	P5276	
	D4835	N5009	V5091	Q5177	V5277	
	S4836	L5010	A5092	R5182	Q5278	
		P5011	R5093	E5183	E5279	
	T4839		G5094	A5184	A5280	
		V4931	D5095	E5185	W5281	
	R4842	L4933	L5096		A5282	
	N4843	K4934			E5283	
		K4935	E5099	M5188	E5284	
	T4847		I5100	F5189	V5285	
	C4848	T4942	E5103	H5190	D5286	
	T4849	L4943		R5191	L5287	
	T4850	D4944	A5108	E5195	R5288	
	G4851	N4945	I5025	E5196		
	P4852		Q5026	S5202	G5296	
			D5027		K5297	
	R4855	N4948	F5030	T5205	A5298	
		E4949	E5033	D5206	R5299	
	E4858	K4950	E5034	L5207		
	T4859	C4951	Q5035	M5208	F5302	
	L4860	D4952	D5036	E5209	K5303	
	K4861	N4954	F5037	A5210	K5304	
	E4862	T4955	I5112	G5212	G5305	
	N4863	L4956	I5113	M5213	D5306	
			G5114		V5307	
	N4868		R5115		V5308	
		D4959	R5118	T5127		
	R4872	M5038		Q5128	L5311	
		Y4960	T5129	M5129	T5312	
			L5130	E5131	G5313	
	R4873	I4963	E5040	S5132	W5314	
		C4964	R5046	M5133	R5315	
	R4877	V4965	D5049	I5134	P5316	
	E4881	V4966		K5135	G5317	
	Y4882	V4967	E5052		S5318	
	H4883	D4968	T5053	R5138		
			R5054	P5139		
		R4972	R5140	T5231		
	T4886	V4973	R5141	E5232	T5321	
	T4887	Y4974				

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.30 Å 216.50 Å 258.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	87.0 (30.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34001	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, MG, K, ATP

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	1.36	35/4041 (0.9%)	1.29	48/5452 (0.9%)
1	B	1.38	29/4041 (0.7%)	1.31	58/5452 (1.1%)
1	C	1.30	36/4041 (0.9%)	1.34	63/5452 (1.2%)
1	D	1.38	35/4041 (0.9%)	1.30	57/5452 (1.0%)
1	E	1.37	32/4041 (0.8%)	1.32	52/5452 (1.0%)
1	F	1.31	31/4041 (0.8%)	1.32	64/5452 (1.2%)
1	G	1.34	30/4041 (0.7%)	1.30	50/5452 (0.9%)
1	H	1.36	27/4041 (0.7%)	1.31	63/5452 (1.2%)
All	All	1.35	255/32328 (0.8%)	1.31	455/43616 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	H	1	0
All	All	1	2

The worst 5 of 255 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4595	GLU	CD-OE1	11.92	1.38	1.25
1	B	681	GLU	CD-OE2	11.16	1.38	1.25
1	B	627	GLU	CD-OE2	10.56	1.37	1.25
1	A	27	GLU	CD-OE2	10.12	1.36	1.25
1	F	3797	GLU	CD-OE1	10.11	1.36	1.25

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1919	ARG	NE-CZ-NH1	13.83	127.21	120.30
1	C	1666	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	F	4066	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	B	1127	VAL	C-N-CD	-11.65	94.97	120.60
1	D	1919	ARG	NE-CZ-NH2	-11.52	114.54	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	5205	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	759	ASP	Mainchain
1	C	1599	ARG	Mainchain

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	3978	0	4055	326	2
1	B	3978	0	4056	216	1
1	C	3978	0	4055	321	3
1	D	3978	0	4055	251	5
1	E	3978	0	4056	221	14
1	F	3978	0	4055	240	2
1	G	3978	0	4055	276	2
1	H	3978	0	4055	187	18
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	1	0
3	G	6	0	0	1	0
3	H	6	0	0	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	A	31	0	12	3	0
5	C	31	0	12	3	0
5	D	31	0	12	1	0
5	E	31	0	12	0	0
5	F	31	0	12	0	0
5	G	31	0	12	1	0
6	A	195	0	0	11	0
6	B	270	0	0	17	0
6	C	178	0	0	11	0
6	D	272	0	0	21	0
6	E	279	0	0	15	0
6	F	197	0	0	9	0
6	G	228	0	0	7	0
6	H	302	0	0	12	3
All	All	34001	0	32514	1940	25

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 30.

The worst 5 of 1940 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:A:499:ARG:NH2	6:A:6596:HOH:O	1.57	1.36
1:C:1248:CYS:HB2	1:C:1268:MET:HE3	1.25	1.19
1:E:3142:THR:HG22	1:E:3144:ASP:H	1.05	1.10
1:H:5130:LEU:HD13	1:H:5133:MET:HE3	1.20	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4665:TYR:HB2	1:G:4668:ILE:HD12	1.36	1.07

The worst 5 of 25 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:E:3149:GLU:OE1	1:H:4934:LYS:CE[3_655]	0.65	1.55
1:E:3149:GLU:CD	1:H:4934:LYS:NZ[3_655]	1.12	1.08
1:E:3081:GLU:OE1	1:H:4924:LYS:NZ[3_655]	1.15	1.05
1:E:3149:GLU:CD	1:H:4934:LYS:CE[3_655]	1.22	0.98
1:D:1924:LYS:NZ	1:H:4858:GLU:OE1[1_455]	1.29	0.91

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/530 (98%)	480 (93%)	33 (6%)	4 (1%)	24	17
1	B	517/530 (98%)	492 (95%)	20 (4%)	5 (1%)	19	13
1	C	517/530 (98%)	471 (91%)	41 (8%)	5 (1%)	19	13
1	D	517/530 (98%)	493 (95%)	21 (4%)	3 (1%)	30	24
1	E	517/530 (98%)	488 (94%)	24 (5%)	5 (1%)	19	13
1	F	517/530 (98%)	490 (95%)	23 (4%)	4 (1%)	24	17
1	G	517/530 (98%)	488 (94%)	25 (5%)	4 (1%)	24	17
1	H	517/530 (98%)	490 (95%)	24 (5%)	3 (1%)	30	24
All	All	4136/4240 (98%)	3892 (94%)	211 (5%)	33 (1%)	24	17

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	PRO
1	C	1533	MET
1	E	3506	ASP
1	F	3729	ALA
1	F	3789	PRO

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	426/434 (98%)	349 (82%)	77 (18%)	2	1
1	B	426/434 (98%)	379 (89%)	47 (11%)	8	4
1	C	426/434 (98%)	358 (84%)	68 (16%)	3	1
1	D	426/434 (98%)	384 (90%)	42 (10%)	10	6
1	E	426/434 (98%)	372 (87%)	54 (13%)	5	3
1	F	426/434 (98%)	373 (88%)	53 (12%)	6	3
1	G	426/434 (98%)	368 (86%)	58 (14%)	5	2
1	H	426/434 (98%)	391 (92%)	35 (8%)	14	10
All	All	3408/3472 (98%)	2974 (87%)	434 (13%)	5	3

5 of 434 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1873	MET
1	E	3066	SER
1	H	4848	CYS
1	D	1930	GLU
1	D	2141	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1998	ASN

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Mol	Chain	Res	Type
1	E	3080	HIS
1	H	4986	GLN
1	D	2073	HIS
1	D	2238	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 22 are monoatomic - leaving 14 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	$\# Z > 2$
3	OXL	A	533	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	A	535	2,4	24,33,33	1.49	5 (20%)	31,52,52	1.49	4 (12%)
3	OXL	B	1133	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	C	1733	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	C	1735	2,4	24,33,33	1.63	4 (16%)	31,52,52	1.17	4 (12%)
3	OXL	D	2333	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	D	2335	2,4	24,33,33	1.55	5 (20%)	31,52,52	1.29	6 (19%)
3	OXL	E	3533	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	E	3535	2,4	24,33,33	1.65	4 (16%)	31,52,52	1.18	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	F	4133	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	F	4135	2,4	24,33,33	1.62	4 (16%)	31,52,52	1.05	1 (3%)
3	OXL	G	4733	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	G	4735	2,4	24,33,33	1.65	4 (16%)	31,52,52	1.25	3 (9%)
3	OXL	H	5333	4	0,5,5	0.00	-	0,6,6	0.00	-

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
3	OXL	A	533	4	-	0/0/4/4	0/0/0/0
5	ATP	A	535	2,4	-	0/18/38/38	0/3/3/3
3	OXL	B	1133	4	-	0/0/4/4	0/0/0/0
3	OXL	C	1733	4	-	0/0/4/4	0/0/0/0
5	ATP	C	1735	2,4	-	0/18/38/38	0/3/3/3
3	OXL	D	2333	4	-	0/0/4/4	0/0/0/0
5	ATP	D	2335	2,4	-	0/18/38/38	0/3/3/3
3	OXL	E	3533	4	-	0/0/4/4	0/0/0/0
5	ATP	E	3535	2,4	-	0/18/38/38	0/3/3/3
3	OXL	F	4133	4	-	0/0/4/4	0/0/0/0
5	ATP	F	4135	2,4	-	0/18/38/38	0/3/3/3
3	OXL	G	4733	4	-	0/0/4/4	0/0/0/0
5	ATP	G	4735	2,4	-	0/18/38/38	0/3/3/3
3	OXL	H	5333	4	-	0/0/4/4	0/0/0/0

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3535	ATP	PG-O3G	-5.19	1.36	1.54
5	D	2335	ATP	PG-O3G	-4.40	1.38	1.54
5	G	4735	ATP	PG-O3G	-4.32	1.39	1.54
5	C	1735	ATP	PG-O3G	-3.99	1.40	1.54
5	C	1735	ATP	O4'-C1'	-3.94	1.36	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3535	ATP	C2'-C1'-N9	-2.93	109.81	114.29
5	A	535	ATP	O3A-PA-O5'	-2.92	95.19	102.94
5	G	4735	ATP	C1'-N9-C4	-2.78	122.75	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2335	ATP	O3A-PA-O5'	-2.63	95.96	102.94
5	C	1735	ATP	C2'-C1'-N9	-2.57	110.37	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	533	OXL	2	0
5	A	535	ATP	3	0
3	C	1733	OXL	1	0
5	C	1735	ATP	3	0
5	D	2335	ATP	1	0
3	F	4133	OXL	1	0
3	G	4733	OXL	1	0
5	G	4735	ATP	1	0
3	H	5333	OXL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.