



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:12 am 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

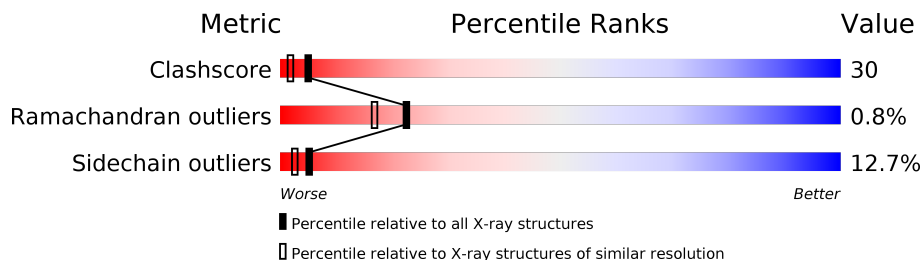
1 Overall quality at a glance

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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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	 54% 36% 7%

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).

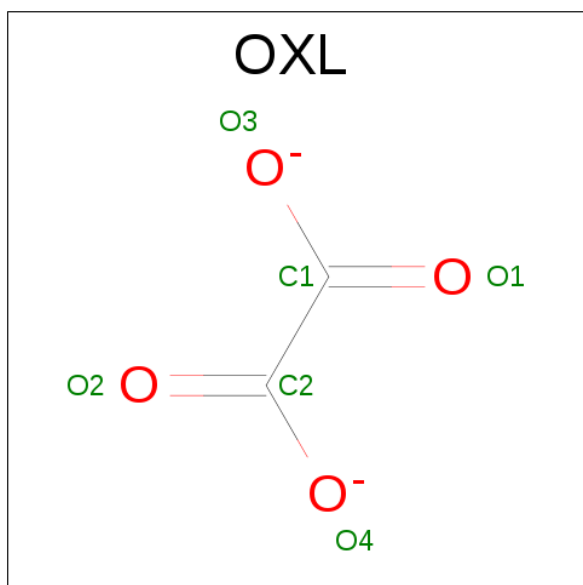
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		
2	H	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		

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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).

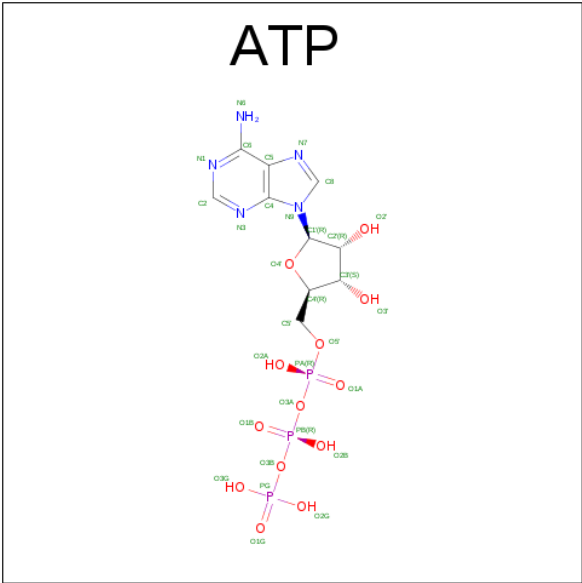


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

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

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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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.

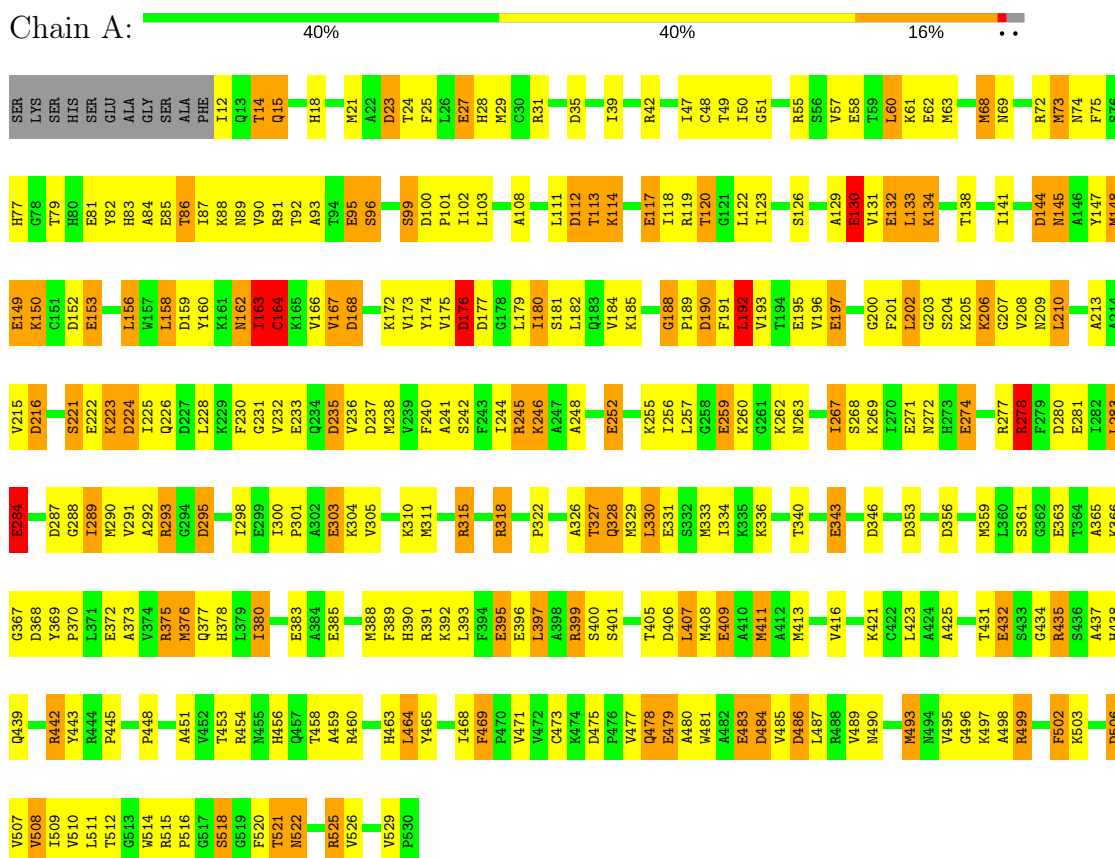
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	270	Total	O	0	0
			270	270		
6	C	178	Total	O	0	0
			178	178		
6	D	272	Total	O	0	0
			272	272		
6	E	279	Total	O	0	0
			279	279		
6	F	197	Total	O	0	0
			197	197		
6	G	228	Total	O	0	0
			228	228		
6	H	302	Total	O	0	0
			302	302		

3 Residue-property plots

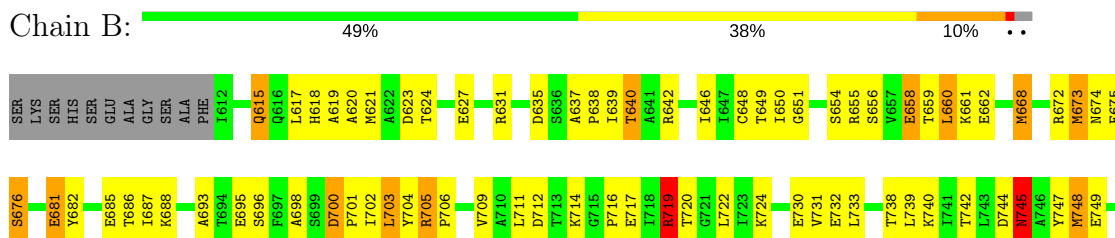
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

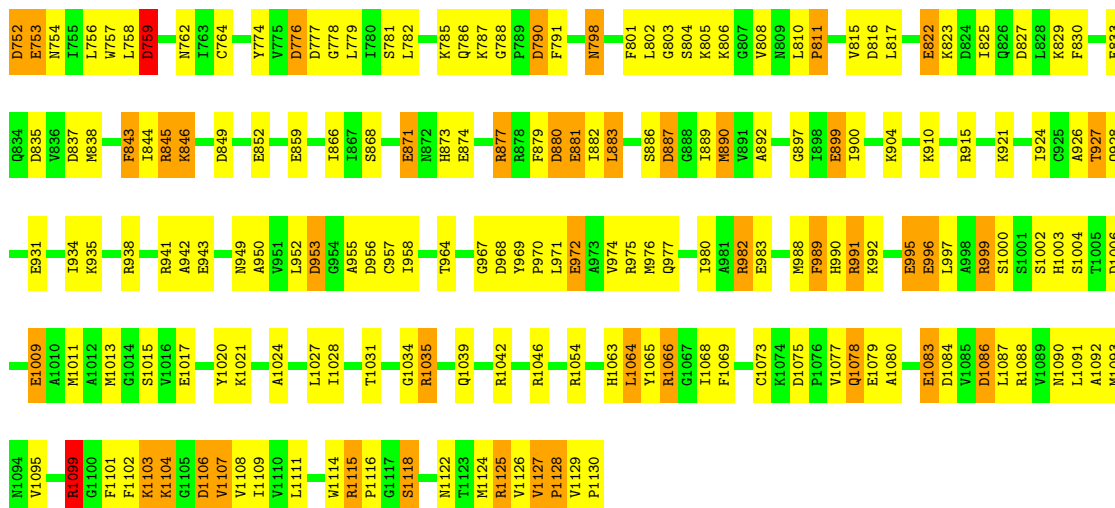
Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE



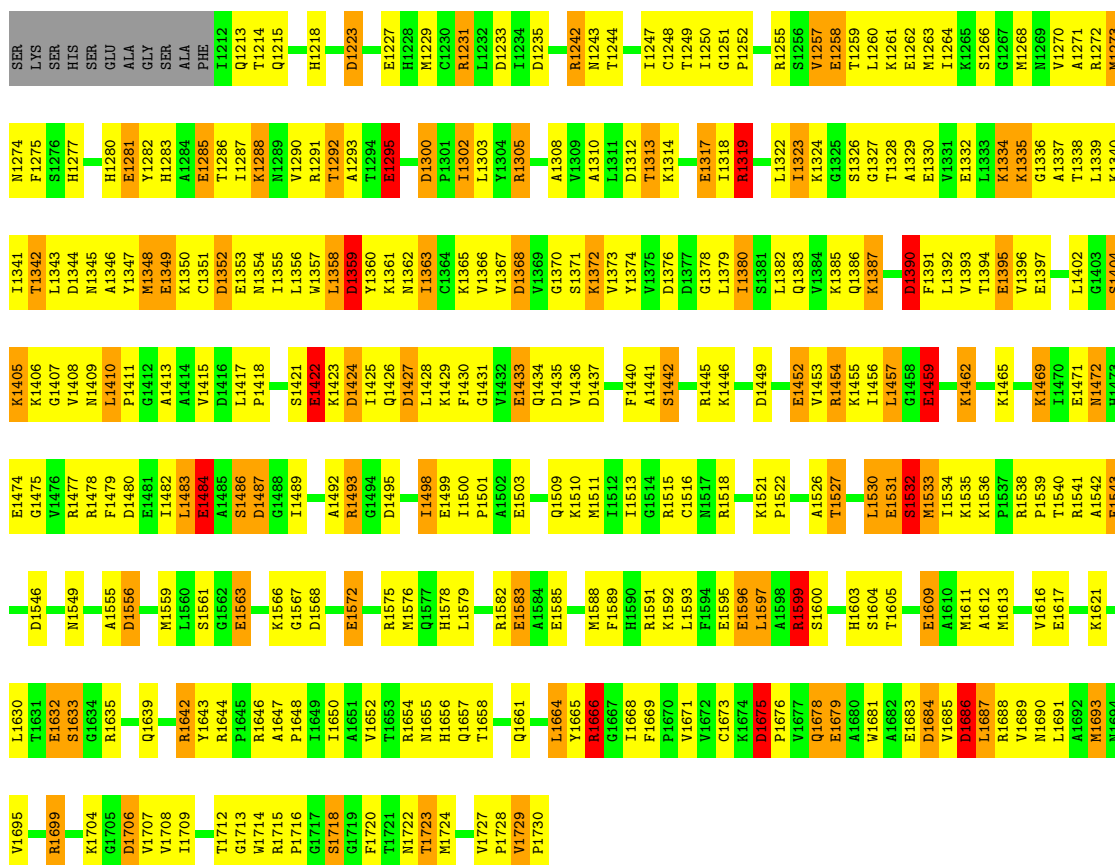
• Molecule 1: PYRUVATE KINASE





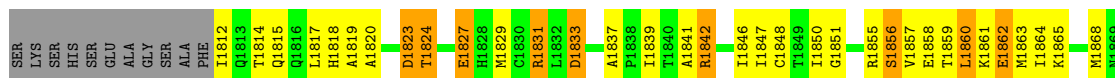
• Molecule 1: PYRUVATE KINASE

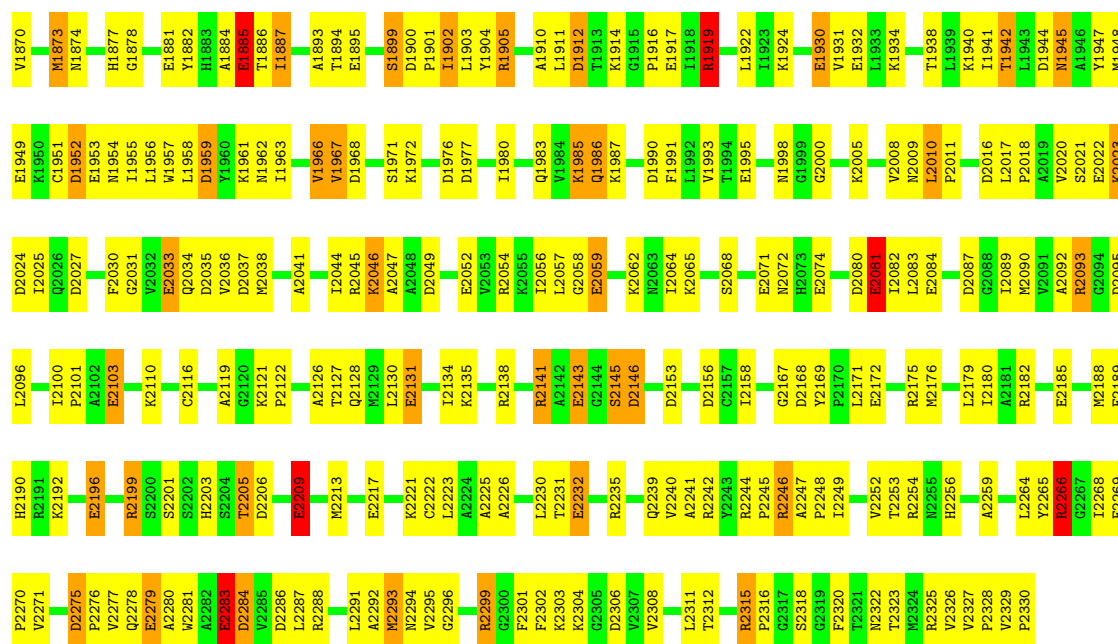
Chain C: 38% 44% 14% ••



• Molecule 1: PYRUVATE KINASE

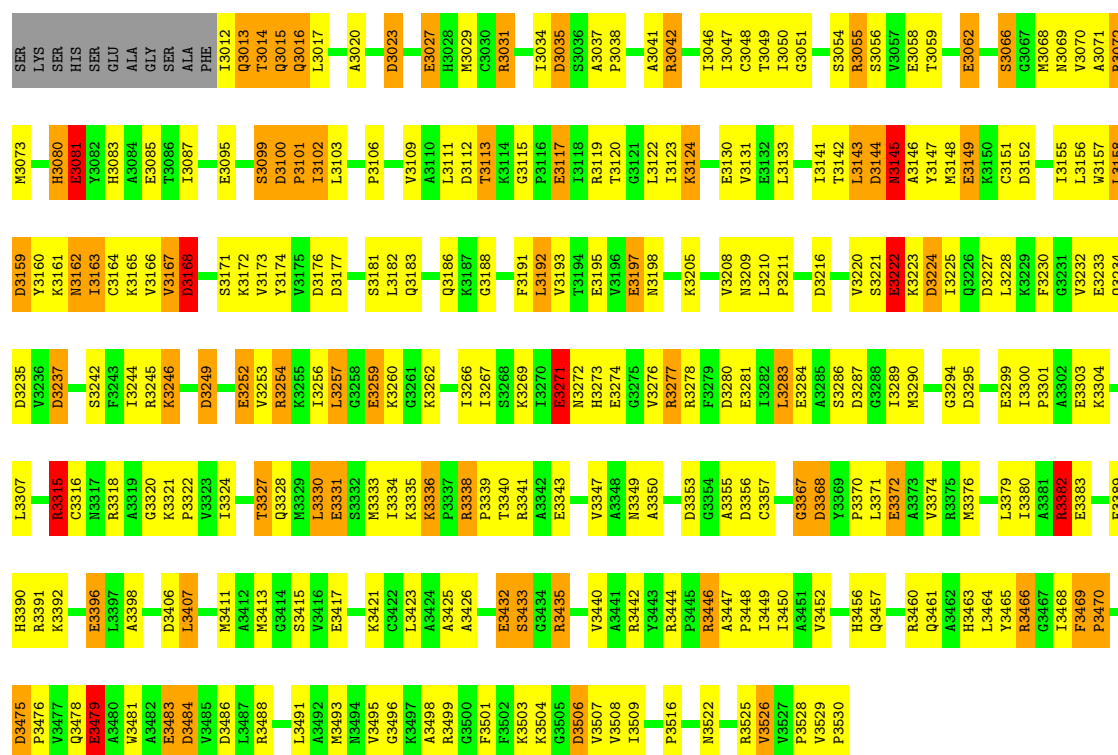
Chain D: 45% 42% 9% ••





• Molecule 1: PYRUVATE KINASE

Chain E: 47% 37% 12% ••



• Molecule 1: PYRUVATE KINASE

Chain F: 44% 41% 11% ••

SER	H3680	L3810	I3882	K3966	T4058	K3966	I3882	L3810	A3746	H3680	SER
LYS	E3681	P3811	L3883	G3967	Q4061	G3967	L3883	P3811	Y3747	E3681	LYS
SER	Y3682	G3812	E3884	Y3969	Q4062	Y3969	E3884	G3812	M3749	Y3682	SER
HIS	H3683	A3813	A3885	Y3969	A4062	Y3969	A3885	A3813	A3749	H3683	HIS
GLU	A3684	A3814	S3886	P3970	H4063	P3970	S3886	A3814	K3750	A3684	GLU
ALA	E3685	V3815	D3887	L3971	R4066	L3971	D3887	V3815	C3751	E3685	ALA
GLY	T3686	D3816	G3888	E3972	G4067	E3972	G3888	D3816	D3752	T3686	GLY
SER	I3687	L3817	I3889	R3975	C4073	R3975	I3889	L3817	E3753	I3687	SER
ALA	K3688	V3820	M3890	M3976	K4074	M3976	M3890	V3820	N3754	K3688	ALA
PHE	V3690	S3821	A3892	M3976	D4075	M3976	A3892	S3821	L3755	V3690	PHE
I3612	R3691	E3822	R3893	I3980	D4075	I3980	R3893	E3822	K3757	I3612	I3612
Q3613	E3695	K3823	G3894	E3981	P4076	E3981	G3894	K3823	L3758	Q3613	Q3613
T3614	E3695	D3824	D3895	R3982	E4079	R3982	D3895	D3824	D3759	T3614	T3614
Q3615	S3696	I3825	L3896	E3983	A4080	E3983	L3896	I3825	K3760	Q3615	Q3615
T3623	G3697	G3826	G3897	E3984	E4080	E3984	G3897	G3826	K3761	T3623	T3623
D3624	A3698	I3898	E3985	E3985	E4083	E3985	I3898	I3898	N3762	D3624	D3624
E3627	S3699	K3827	E3989	M3988	E4084	M3988	K3827	K3827	I3763	E3627	E3627
R3631	D3700	L3828	E3903	F3989	E4085	F3989	L3828	L3828	C3764	R3631	R3631
I3634	P3701	F3830	K3904	H3990	D4086	H3990	F3830	F3830	K3765	I3634	I3634
D3635	I3702	V3832	K3904	R3991	L4087	R3991	V3832	V3832	V3766	D3635	D3635
P3638	L3703	E3833	F3906	K3992	R4088	K3992	E3833	E3833	V3767	P3638	P3638
I3639	Y3704	K3834	L3993	L3993	M4093	L3993	K3834	K3834	V3769	I3639	I3639
T3640	R3705	D3835	C3910	E3996	M4094	E3996	D3835	D3835	K3772	T3640	T3640
N3643	V3709	V3837	C3916	R3999	E4095	R3999	V3837	V3837	Y3774	N3643	N3643
C3648	G3715	M3842	K3921	S4002	R4099	S4002	M3842	M3842	D3776	C3648	C3648
T3649	P3716	F3843	A3926	H4003	F4102	H4003	F3843	F3843	D3777	T3649	T3649
I3650	E3717	I3844	T3927	T4005	R4103	T4005	I3844	I3844	G3778	I3650	I3650
G3651	L3718	D3849	M3929	K4104	G4105	K4104	D3849	D3849	L3779	G3651	G3651
P3652	T3720	L3782	M3933	L4007	D4106	L4007	L3782	L3782	I3780	P3652	P3652
A3653	G3721	Q3783	E3934	E4009	V4107	E4009	Q3783	Q3783	K3781	A3653	A3653
S3654	L3722	Q3786	K3935	M4013	V4110	M4013	L3722	L3722	K3782	S3654	S3654
E3658	K3724	K3787	K3936	G4014	L4111	G4014	K3724	K3724	Q3787	E3658	E3658
T3659	G3726	G3788	P3937	S4015	T4112	S4015	G3726	G3726	G3789	T3659	T3659
L3660	G3727	P3789	P3939	V4016	G4113	V4016	L3660	L3660	D3790	L3660	L3660
K3661	T3728	K3862	T3940	E4017	V4114	E4017	K3862	K3862	F3791	K3661	K3661
M3663	A3729	I3864	A3941	L4030	R4115	L4030	A3941	A3941	L3792	M3663	M3663
I3664	E3730	V3793	E3943	T4031	S4118	T4031	E3943	E3943	V3793	I3664	I3664
K3665	V3731	T3794	G3944	E4032	N4122	E4032	T3794	T3794	T3794	K3665	K3665
S3666	L3732	K3869	S3945	R4035	T4123	R4035	K3869	K3869	V3796	S3666	S3666
G3667	K3734	I3870	D3946	Q4039	M4124	Q4039	I3870	I3870	E3797	G3667	G3667
M3668	K3735	E3871	N3949	R4125	R4126	R4125	E3871	E3871	G3800	M3668	M3668
N3669	G3736	N3872	D3953	V4127	P4128	V4127	N3872	N3872	F3801	N3669	N3669
M3673	L3739	H3873	G3953	Y4042	R4044	Y4042	H3873	H3873	L3802	M3673	M3673
N3674	K3740	E3874	A3955	R4044	P4130	R4044	E3874	E3874	G3803	N3674	N3674
F3675	I3741	G3875	D3956	R4054	M4055	R4054	G3875	G3875	S3804	F3675	F3675
S3676	T3742	K3876	E3963	H4056	M4055	H4056	K3876	K3876	K3806	S3676	S3676
T3679	L3743	F3879	T3964	Q4057	M4057	Q4057	F3879	F3879	K3806	T3679	T3679
	N3745	E3881	A3965				E3881	E3881	N3809		

• Molecule 1: PYRUVATE KINASE

Chain G:  43%  43%  12% ..

SER	E4349	P4411	G4494	R4575	H4656	E4349	P4411	G4494	R4575	H4656	SER
LYS	K4350	G4412	D4495	M4576	R4660	K4350	G4412	D4495	M4576	R4660	LYS
SER	D4352	A4413	L4496	E4585	A4664	D4352	A4413	L4496	E4585	A4664	SER
HIS	C4352	D4416	I4498	F4589	L4664	C4352	D4416	I4498	F4589	L4664	HIS
GLU	M4354	L4417	E4499	H4690	Y4665	M4354	L4417	E4499	H4690	Y4665	GLU
ALA	N4357	P4418	T4500	R4591	R4666	N4357	P4418	T4500	R4591	R4666	ALA
GLY	L4358	E4422	E4503	K4592	G4667	L4358	E4422	E4503	K4592	G4667	GLY
PHE	D4359	K4423	F4506	F4593	F4668	D4359	K4423	F4506	F4593	F4668	PHE
I4212	T4287	D4424	I4512	F4594	D4669	T4287	D4424	I4512	F4594	D4669	I4212
Q4215	K4288	I4425	Q4509	E4595	D4675	K4288	I4425	Q4509	E4595	D4675	Q4215
L4216	M4289	D4427	K4510	L4597		L4216	M4289	D4427	K4510		L4216
L4217	I4363	K4428	G4511	A4598		L4217	I4363	K4428	G4511		L4217
Q4221	A4293	L4429	T4513	S4600		Q4221	A4293	L4429	T4513		Q4221
A4222	E4296	F4430	G4514			A4222	E4296	F4430	G4514		A4222
D4223	F4297	D4298	R4515			D4223	F4297	D4298	R4515		D4223
T4224	A4298	S4299	C4516			T4224	A4298	S4299	C4516		T4224
F4225	D4300	P4301	M4517			F4225	D4300	P4301	M4517		F4225
L4226	E4302	I4303	K4521			L4226	E4302	I4303	K4521		L4226
E4227	Y4304	Y4304	P4522			E4227	Y4304	Y4304	P4522		E4227
C4230	R4305	R4305	V4523			C4230	R4305	R4305	V4523		C4230
D4233	D4312	D4312	A4526			D4233	D4312	D4312	A4526		D4233
I4234	T4313	T4313	T4527			I4234	T4313	T4313	T4527		I4234
D4235	E4317	E4317	G4544			D4235	E4317	E4317	G4544		D4235
T4240	I4318	L4362	S4545			T4240	I4318	L4362	S4545		T4240
A4241	R4319	Q4382	S4546			A4241	R4319	Q4382	S4546		A4241
R4242	T4320	Q4383	G4634			R4242	T4320	Q4383	G4634		R4242
N4243	G4321	K4385	L4635			N4243	G4321	K4385	L4635		N4243
T4244	L4322	Q4386	D4636			T4244	L4322	Q4386	D4636		T4244
I4247	S4326	K4387	E4637			I4247	S4326	K4387	E4637		I4247
C4248	G4327	G4388	S4633			C4248	G4327	G4388	S4633		C4248
T4249	E4327	P4389	D4634			T4249	E4327	P4389	D4634		T4249
G4251	E4330	F4391	R4635			G4251	E4330	F4391	R4635		G4251
P4252	V4331	L4392	L4636			P4252	V4331	L4392	L4636		P4252
A4253	E4332	V4393	S4637			A4253	E4332	V4393	S4637		A4253
S4254	L4333	T4394	Q4638			S4254	L4333	T4394	Q4638		S4254
R4255	K4334	V4396	H4639			R4255	K4334	V4396	H4639		R4255
V4257	G4336	E4397	L4640			V4257	G4336	E4397	L4640		V4257
O4258	A4337	N4398	R4641			O4258	A4337	N4398	R4641		O4258
T4259	T4338	F4401	F4642			T4259	T4338	F4401	F4642		T4259
L4260	L4339	L4402	R4643			L4260	L4339	L4402	R4643		L4260
K4261	F4340	G4403	Y4644			K4261	F4340	G4403	Y4644		K4261
E4262	T4341	S4404	P4645			E4262	T4341	S4404	P4645		E4262
M4263	T4342	K4405	I4646			M4263	T4342	K4405	I4646		M4263
I4264	L4343	K4406	T4647			I4264	L4343	K4406	T4647		I4264
K4265	D4344	M4345	A4648			K4265	D4344	M4345	A4648		K4265
M4268	M4346	G4407	P4649			M4268	M4346	G4407	P4649		M4268
M4273	A4346	V4408	R4650			M4273	A4346	V4408	R4650		M4273
	Y4347	M4409	R4651				Y4347	M4409	R4651		
	M4348	L4410					M4348	L4410			

• Molecule 1: PYRUVATE KINASE

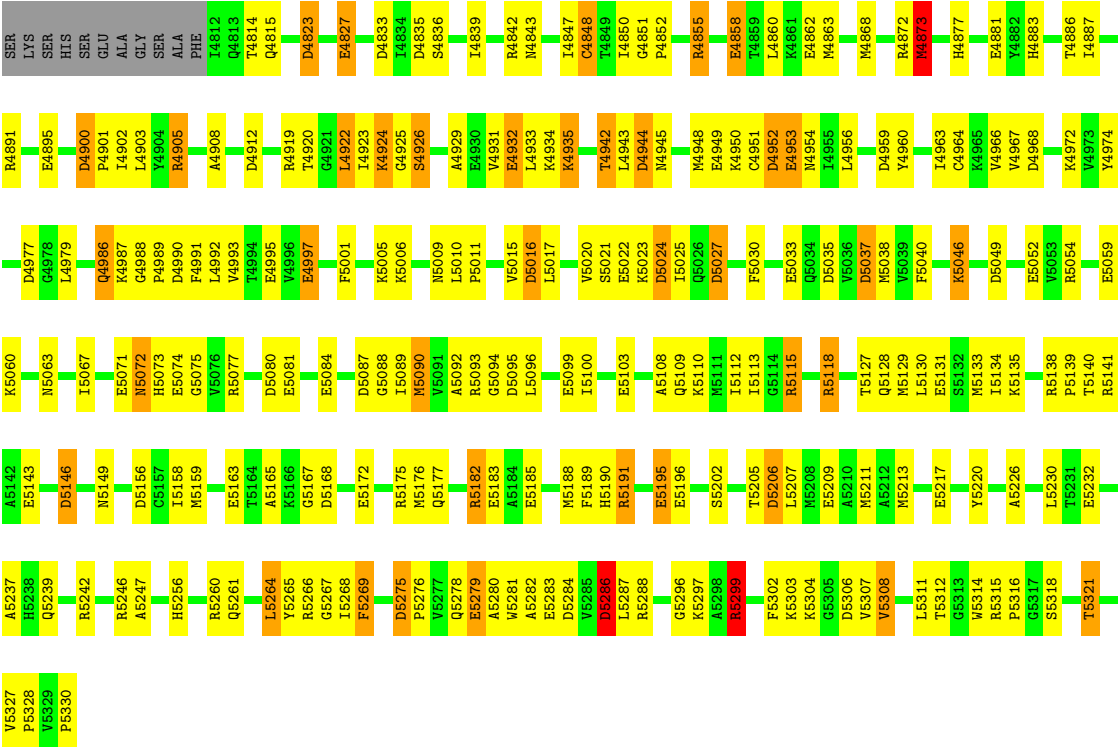
Chain H:

54%

36%

7%

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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.30Å 216.50Å 258.60Å 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 [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	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%)	22	17
1	B	517/530 (98%)	492 (95%)	20 (4%)	5 (1%)	18	12
1	C	517/530 (98%)	471 (91%)	41 (8%)	5 (1%)	18	12
1	D	517/530 (98%)	493 (95%)	21 (4%)	3 (1%)	28	24
1	E	517/530 (98%)	488 (94%)	24 (5%)	5 (1%)	18	12
1	F	517/530 (98%)	490 (95%)	23 (4%)	4 (1%)	22	17
1	G	517/530 (98%)	488 (94%)	25 (5%)	4 (1%)	22	17
1	H	517/530 (98%)	490 (95%)	24 (5%)	3 (1%)	28	24
All	All	4136/4240 (98%)	3892 (94%)	211 (5%)	33 (1%)	22	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%)	7	4
1	C	426/434 (98%)	358 (84%)	68 (16%)	3	1
1	D	426/434 (98%)	384 (90%)	42 (10%)	9	5
1	E	426/434 (98%)	372 (87%)	54 (13%)	5	2
1	F	426/434 (98%)	373 (88%)	53 (12%)	5	3
1	G	426/434 (98%)	368 (86%)	58 (14%)	4	2
1	H	426/434 (98%)	391 (92%)	35 (8%)	13	9
All	All	3408/3472 (98%)	2974 (87%)	434 (13%)	5	2

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	27,33,33	1.43	4 (14%)	25,52,52	1.15	1 (4%)
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	27,33,33	1.82	5 (18%)	25,52,52	1.13	2 (8%)
3	OXL	D	2333	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	D	2335	2,4	27,33,33	1.93	6 (22%)	25,52,52	1.00	3 (12%)
3	OXL	E	3533	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	E	3535	2,4	27,33,33	1.85	5 (18%)	25,52,52	0.99	1 (4%)

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	27,33,33	1.96	4 (14%)	25,52,52	0.87	1 (4%)
3	OXL	G	4733	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	G	4735	2,4	27,33,33	1.52	3 (11%)	25,52,52	1.13	2 (8%)
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 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3535	ATP	PG-O3G	-4.56	1.36	1.54
5	D	2335	ATP	C2'-C1'	-4.52	1.46	1.53
5	D	2335	ATP	PG-O3G	-3.87	1.38	1.54
5	G	4735	ATP	PG-O3G	-3.80	1.39	1.54
5	C	1735	ATP	O4'-C1'	-3.64	1.36	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4735	ATP	C1'-N9-C4	-2.25	122.75	126.64
5	C	1735	ATP	C2'-C3'-C4'	-2.17	98.39	102.62
5	D	2335	ATP	C2'-C3'-C4'	-2.07	98.59	102.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2335	ATP	C4-C5-N7	2.04	111.38	109.41
5	D	2335	ATP	C5-C6-N6	2.08	124.70	120.47

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.