



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 04:09 pm BST

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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

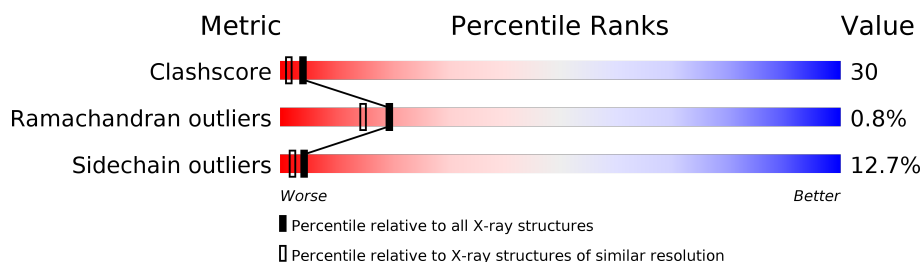
1 Overall quality at a glance

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	
1	H	530	

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).

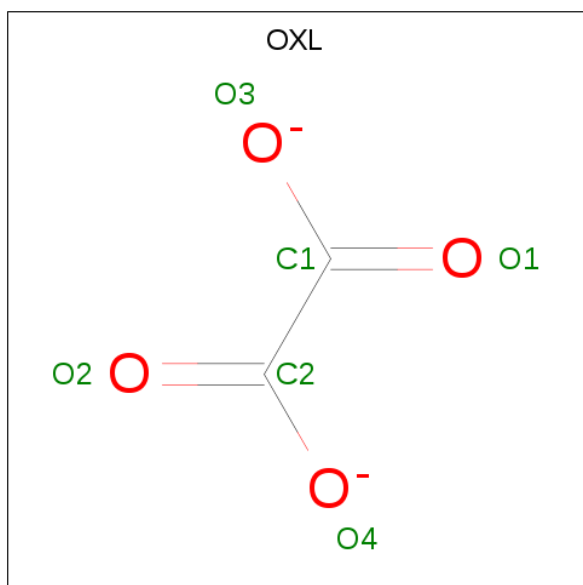
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		
2	E	1	Total	K	0	0
			1	1		
2	H	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		

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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).

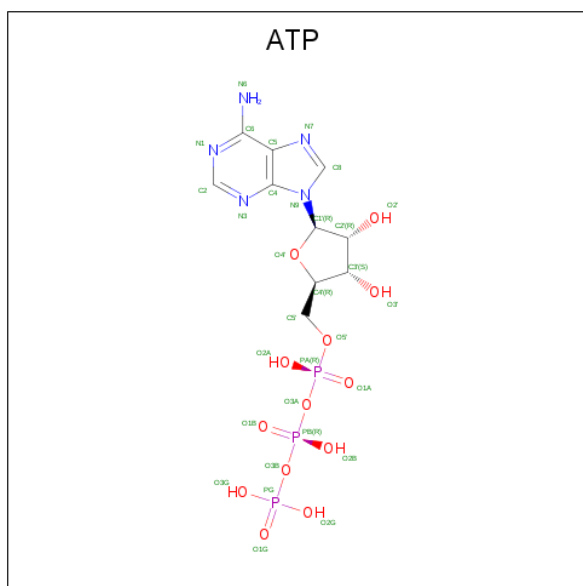


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

- 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.

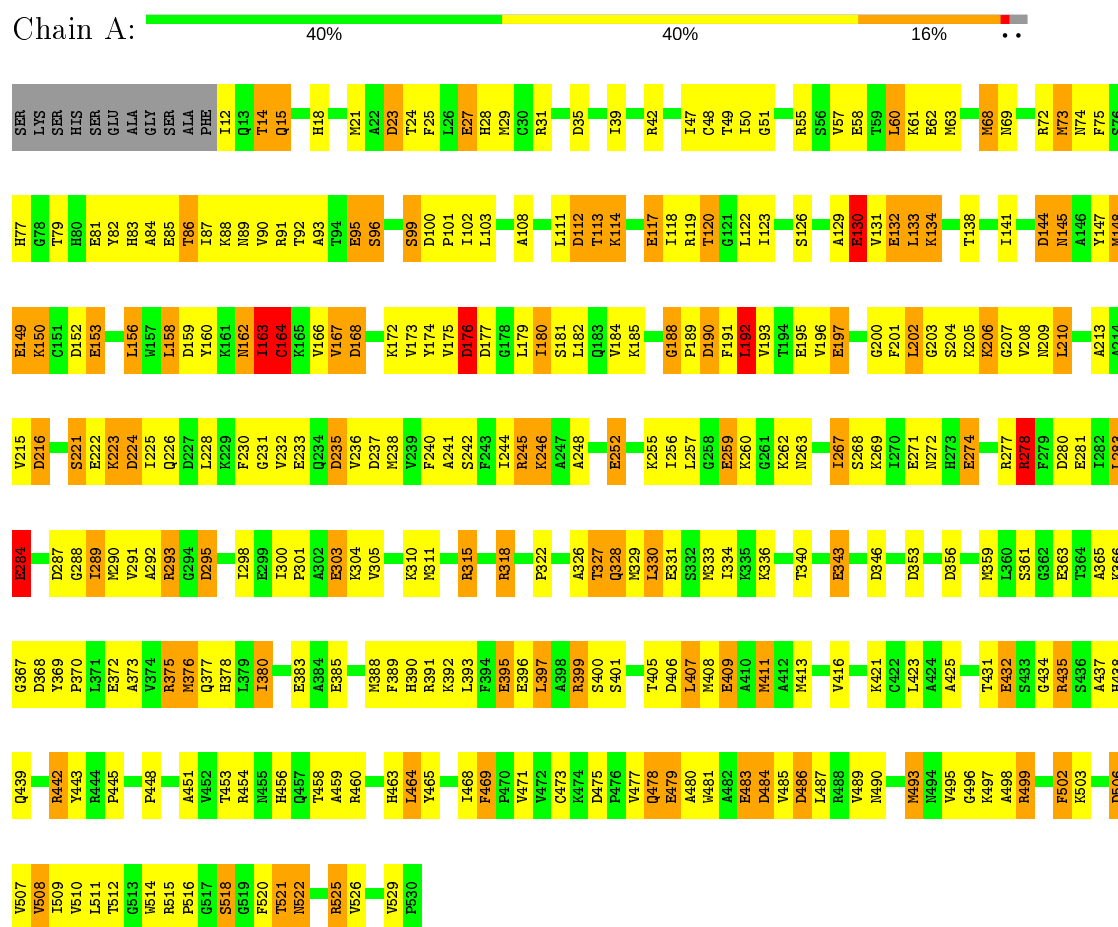
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	270	Total	O	0	0
			270	270		
6	C	178	Total	O	0	0
			178	178		
6	D	272	Total	O	0	0
			272	272		
6	E	279	Total	O	0	0
			279	279		
6	F	197	Total	O	0	0
			197	197		
6	G	228	Total	O	0	0
			228	228		
6	H	302	Total	O	0	0
			302	302		

3 Residue-property plots

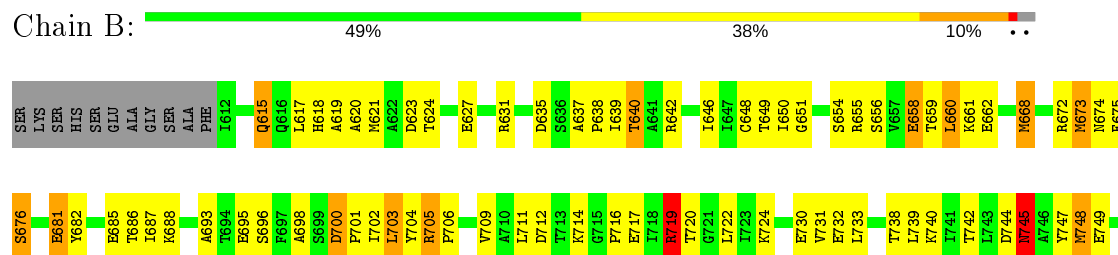
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

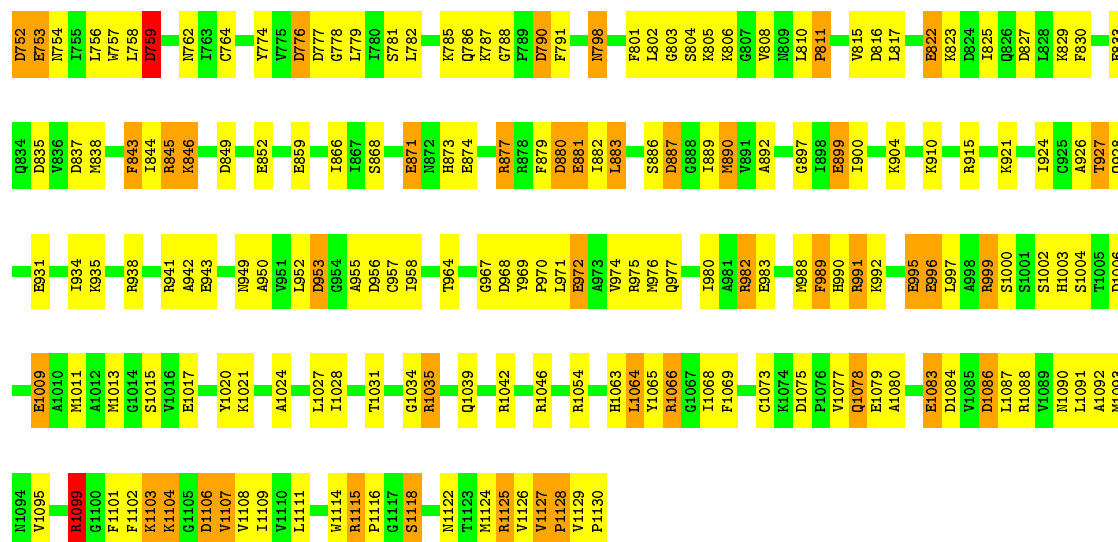
Note EDS was not executed.

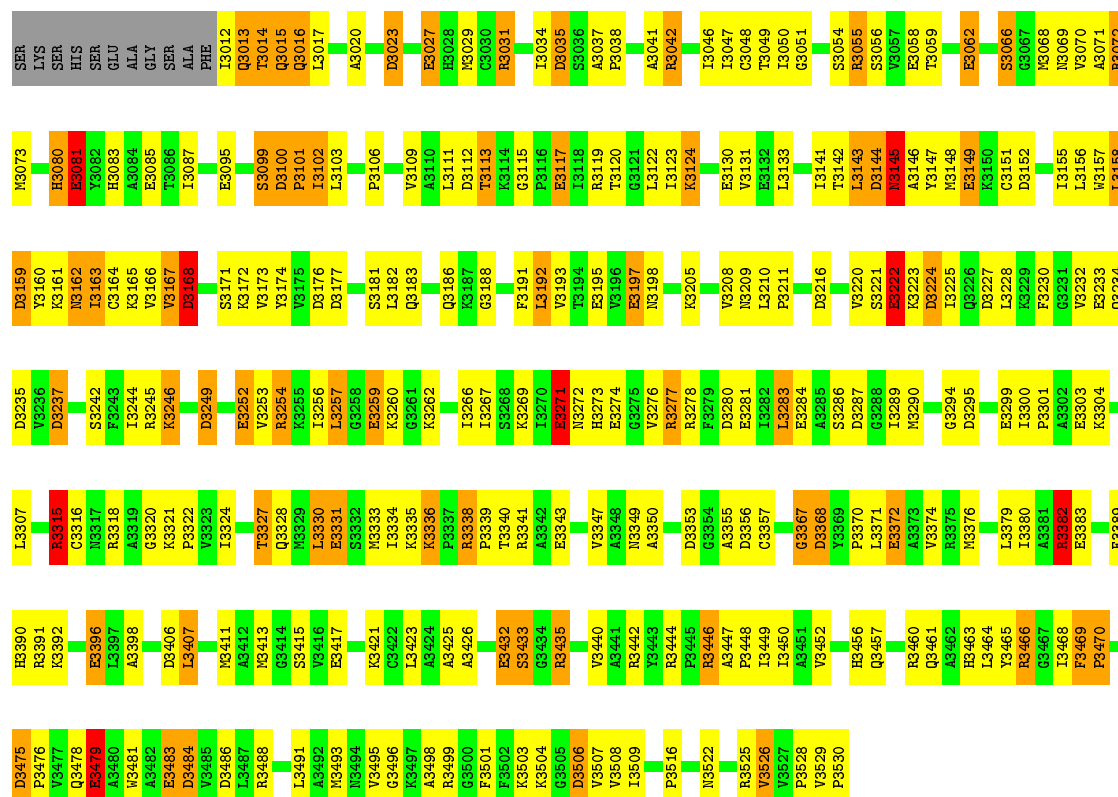
• Molecule 1: PYRUVATE KINASE



• Molecule 1: PYRUVATE KINASE







● Molecule 1: PYRUVATE KINASE

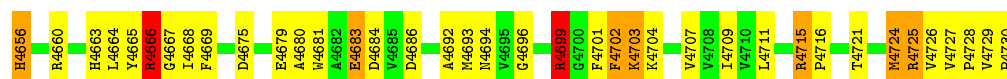
Chain F: 

T4058	R3966	T3882	L3810	A3746	E3680	SER
Q4061	G3967	L3883	P3811	T3747	E3681	LYS
A4062	D3968	E3884	G3812	M3748	E3682	SER
H4063	Y3969	A3885	A3813	E3749	H3683	HIS
R4066	P3970	S3886	L3814	K3750	A3884	SER
	L3971	D3887	V3815	C3751	E3685	GLU
G4067	E3972	G3888	D3816	D3752	ALA	ALA
Q4066	R3975	I3889	L3817	E3753	K3687	GLY
Q4073	K3976	V3890	V3820	N3754	K3688	SER
L4074	S3976	V3891	S3821	I3755	K3689	ALA
D4075	I3980	A3892	E3822	L3756	V3690	PHE
P4076	A3981	K3893	E3823	K3757	R3691	I3612
E4079	R3982	D3895	D3824	L3758	R3695	
A4080	E3983	L3896	I3825	Y3760	S3696	T3614
E4083	A3984	G3897	Q3826	K3761	F3697	T3615
	E3985	L3898	D3827	N3762	S3698	R3623
D4084	M3988	E3899	L3828	I3763	S3699	T3624
V4085	F3989	E3903	K3829	C3764	D3700	E3627
D4086	K3990	K3904	F3830	K3765	P3701	
L4087	R3991	V3905	G3831	V3766	I3702	R3631
R4088	K3992	F3906	V3832	V3767	L3703	
M4093	L3993	K3910	E3834	D3768	X3704	I3634
	D3835		V3769	R3705	D3635	
N4094	E3996	I3934	V3836	K3772	V3709	P3638
V4095	R3999	C3916	D3837	V3773	D3712	I3639
R4099	S4002	K3921	M3838	Y3774	T3713	T3640
		A3926	S3842	D3776	K3714	I3643
F4102	H4003	I3926	F3843	D3777	G3715	
K4103	S4004	T3927	I3844	G3778	P3716	T3649
K4104	T4005	Q3928	R3845	L3779	E3717	I3650
G4105	D4006	N3929	D3849	I3780	T3649	
D4106	L4007	E3933		E3851	S3781	R3719
V4107	M4008	M3933	E3852	L3782	T3720	P3652
	E4009	I3934	I3935	Q3783	G3721	A3653
V4110	M4013	K3936	L3856	Q3786	I3723	S3654
L4111	G4014	P3937	E3859	K3787	K3724	R3655
T4112	S4015	R3938	I3862	G3788	G3725	E3658
Q4113	V4016	P3939		P3789	S3726	T3659
M4115	E4017	T3940	K3862	D3790	L3660	L3661
	L4030	A3942	L3864	F3791	A3729	R3661
S4118	E4032	E3943	I3867	V3793	E3730	R3662
M4122	R4035	S3945	G3944	T3794	V3731	K3663
	Q4039	D3946	I3870	E3795	E3732	I3664
V4123	R4042	N3949	E3871	V3796	L3733	K3665
L4125	Y4043	D3953	R3872	G3801	K3734	G3667
V4127	R4044	G3954	E3874	L3802	R3735	K3668
E4128	R4054	D3956	G3875	G3803	I3740	I3669
V4129	N4055	E3963	R3878	S3804	K3741	M3673
P4130	H4056	F3879	R3880	E3805	T3742	
T4133	Q4057	I3955	E3881	K3806	L3743	S3676
					D3744	T3679

● Molecule 1: PYRUVATE KINASE

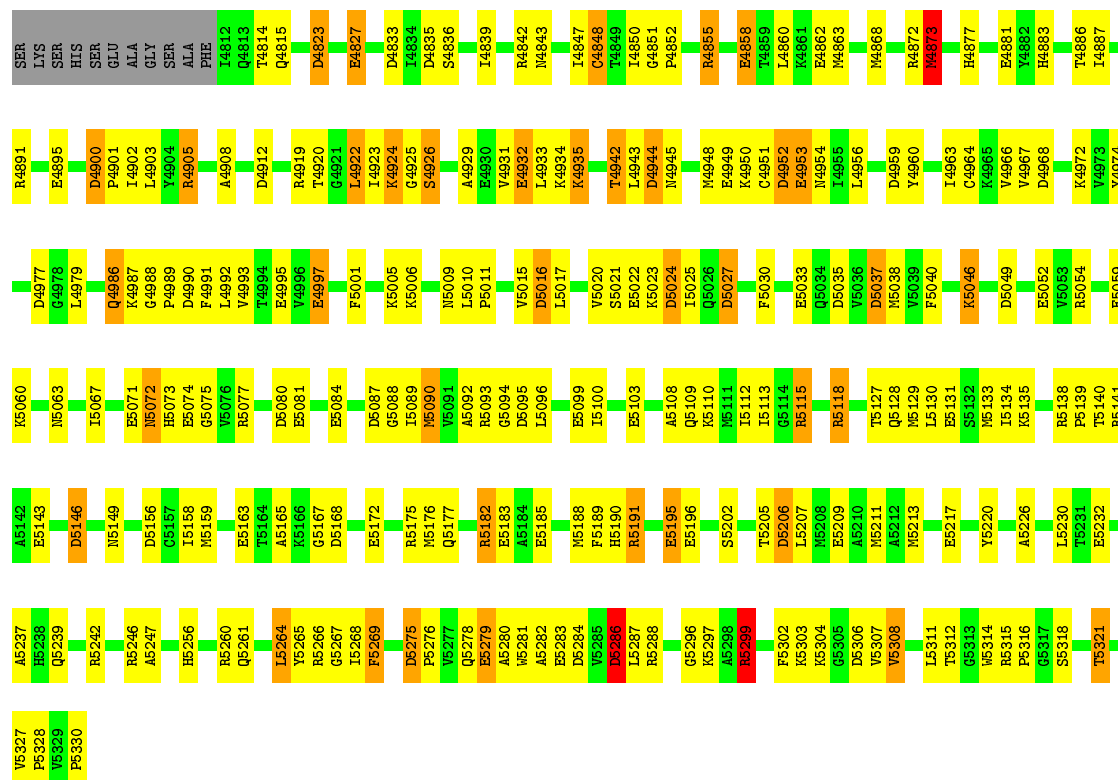
Chain G: 

SER	LYS	SER	HIS	SER	GLU	ALA	GLY	SER	ALA	PHE	I4212	Q4215	Q4216	L4217	M4221	A4222	D4223	T4224	E4225	L4226	E4227	C4230	D4233	I4234	D4235	T4240	A4241	R4242	N4243	T4244	I4247	C4248	T4249	I4250	G4251	P4252	A4253	S4254	R4255	S4256	E4257	V4258	T4259	L4260	K4261	E4262	N4263	I4264	K4265	M4268	N4273						
M4274	F4275	S4276			H4280	E4281	Y4282		E4285	E4286	I4287	K4288	N4289	A4293	T4294	E4295	S4296	F4297	A4298	S4299	D4300	P4301	L4302	I4303	Y4304	R4305	D4312	T4313		E4317	I4318	Q4319	T4320	G4321	L4322	S4326	G4327	E4330	V4331	E4332	L4333	K4334	G4335	E4336	E4337	T4338	L4339	K4340	I4341	T4342	D4343	N4345	I4346	N4348	Y4347	N4349	
E4349	K4350	C4351	D4352	E4353	M4354			M4357	L4358	D4359	Y4360	K4361	M4362	C4364	V4366	V4367	D4368	V4369	G4370	S4371	K4372	V4373	V4374	V4375	D4376	G4377	G4378	L4379	I4380	S4381	L4382	Q4383	V4384	K4385	Q4386	K4387	G4388	P4389	D4390	F4391	L4392	V4393	T4394	V4395	E4397	N4398	F4401	L4402	G4403	S4404	L4405	K4406	G4407	N4408	Y4437	N4438	
P4411	G4412	A4413			D4416	L4417	P4418		E4422	K4423	D4424	I4425	Q4426	D4427	L4428	K4429	F4430		E4433	D4437	N4438	S4442	F4443	V4444	R4445	D4449		I4456	L4457	Q4458	E4459			M4463	I4464			I4467	S4468	K4469	L4470	E4471		R4477	L4478	D4480	E4481	I4482	L4483	E4484	D4487	G4488	Y4489	N4490	Y4491	L4492	R4493
G4494	D4495	L4496	G4497	T4498	E4499	I4500	E4503	F4506	Q4509	K4510	M4511	I4512	L4513	G4514	R4515	C4516	N4517	K4521	P4522	V4523	A4526	T4527	Q4528	M4529	V4530	R4538	P4539	T4540		E4543	G4544	D4546	L4552	D4553	A4554	A4555	D4556	M4559	E4560	E4563	K4566	G4567	P4568	Y4569	P4570	L4571	E4572	R4573	N4574								
R4575	M4576	E4585	F4589	H4590	K4591	L4592	L4593	F4594	E4595	L4597	A4598	R4599	S4600	S4604	T4605	D4606	L4607	M4608	E4609	M4613	E4617	A4618	S4619	V4620	K4621	A4625	A4626	L4627	E4632	S4633	G4634	R4635	S4636	H4637	Q4638	V4640	A4641	R4642	R4644	P4645	R4646	A4647	P4648	I4649	V4652	T4653	R4654	N4655									



● Molecule 1: PYRUVATE KINASE

Chain H: 54% 36% 7% ..



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	95.30 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 5D	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($^{\circ}$)	Ideal($^{\circ}$)
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 [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	517/530 (98%)	480 (93%)	33 (6%)	4 (1%)	19	15
1	B	517/530 (98%)	492 (95%)	20 (4%)	5 (1%)	15	11
1	C	517/530 (98%)	471 (91%)	41 (8%)	5 (1%)	15	11
1	D	517/530 (98%)	493 (95%)	21 (4%)	3 (1%)	25	21
1	E	517/530 (98%)	488 (94%)	24 (5%)	5 (1%)	15	11
1	F	517/530 (98%)	490 (95%)	23 (4%)	4 (1%)	19	15
1	G	517/530 (98%)	488 (94%)	25 (5%)	4 (1%)	19	15
1	H	517/530 (98%)	490 (95%)	24 (5%)	3 (1%)	25	21
All	All	4136/4240 (98%)	3892 (94%)	211 (5%)	33 (1%)	19	15

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

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 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	H	5333	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	F	4133	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	A	535	2,4	26,33,33	1.52	5 (19%)	31,52,52	1.27	2 (6%)
3	OXL	E	3533	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	A	533	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	G	4733	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	D	2335	2,4	26,33,33	1.73	6 (23%)	31,52,52	1.16	3 (9%)
5	ATP	C	1735	2,4	26,33,33	1.58	5 (19%)	31,52,52	1.21	3 (9%)
5	ATP	E	3535	2,4	26,33,33	1.58	4 (15%)	31,52,52	1.05	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	B	1133	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	F	4135	2,4	26,33,33	1.62	4 (15%)	31,52,52	1.04	3 (9%)
3	OXL	D	2333	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	G	4735	2,4	26,33,33	1.59	4 (15%)	31,52,52	1.32	3 (9%)
3	OXL	C	1733	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	H	5333	4	-	0/0/4/4	-
3	OXL	F	4133	4	-	0/0/4/4	-
5	ATP	A	535	2,4	-	0/18/38/38	0/3/3/3
3	OXL	E	3533	4	-	0/0/4/4	-
3	OXL	A	533	4	-	0/0/4/4	-
3	OXL	G	4733	4	-	0/0/4/4	-
5	ATP	D	2335	2,4	-	3/18/38/38	0/3/3/3
5	ATP	C	1735	2,4	-	5/18/38/38	0/3/3/3
5	ATP	E	3535	2,4	-	3/18/38/38	0/3/3/3
3	OXL	B	1133	4	-	0/0/4/4	-
5	ATP	F	4135	2,4	-	0/18/38/38	0/3/3/3
3	OXL	D	2333	4	-	0/0/4/4	-
5	ATP	G	4735	2,4	-	3/18/38/38	0/3/3/3
3	OXL	C	1733	4	-	0/0/4/4	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3535	ATP	PG-O3G	-4.88	1.36	1.54
5	D	2335	ATP	C2'-C1'	-4.81	1.46	1.53
5	D	2335	ATP	PG-O3G	-4.13	1.38	1.54
5	G	4735	ATP	PG-O3G	-4.06	1.39	1.54
5	F	4135	ATP	C2-N1	4.02	1.41	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4735	ATP	C5-C6-N6	5.13	128.15	120.35
5	A	535	ATP	C5-C6-N6	4.13	126.62	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1735	ATP	C5-C6-N6	3.71	125.98	120.35
5	D	2335	ATP	O3G-PG-O3B	3.26	115.58	104.64
5	E	3535	ATP	C5-C6-N6	2.87	124.71	120.35

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

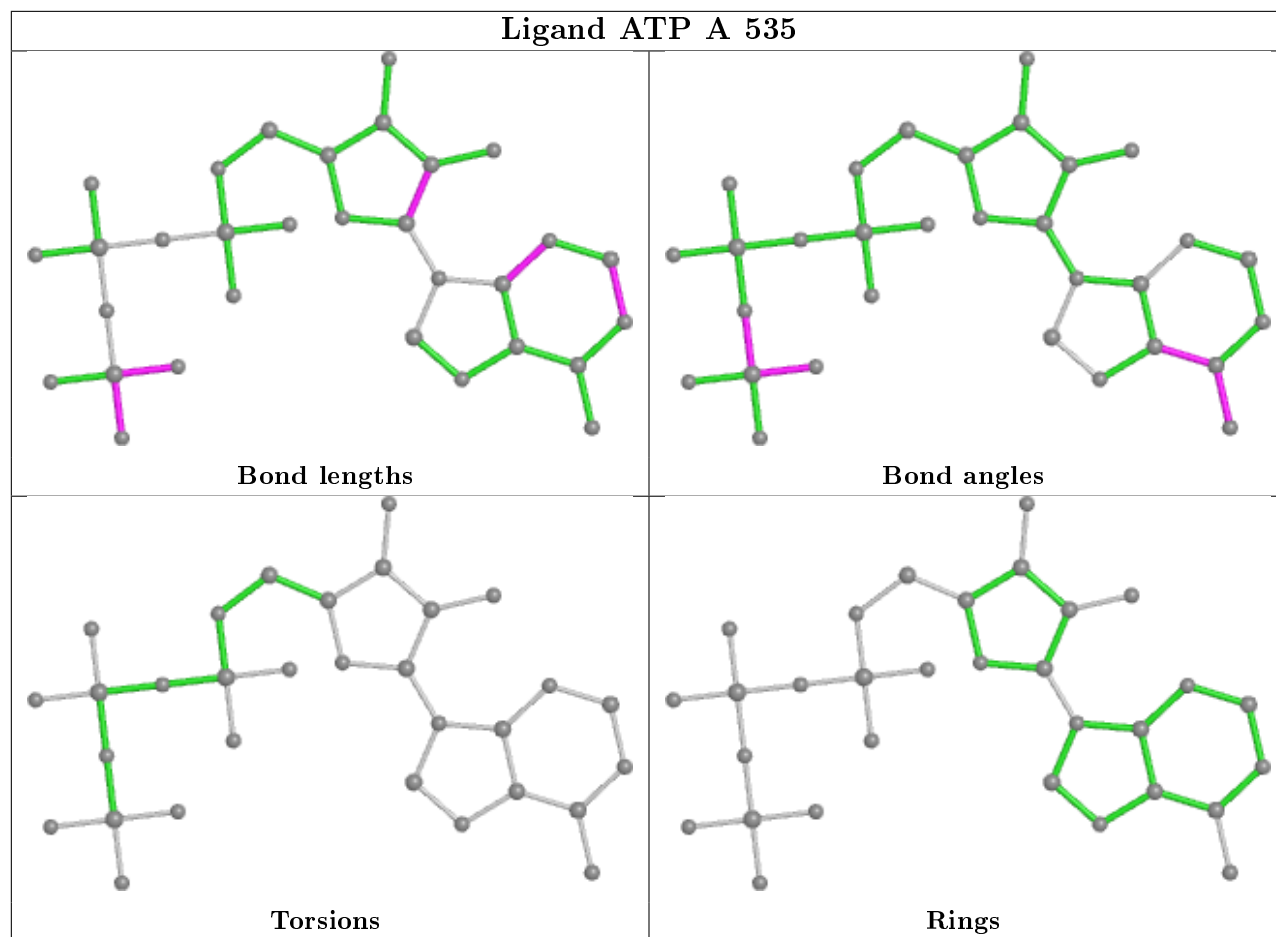
Mol	Chain	Res	Type	Atoms
5	E	3535	ATP	PB-O3B-PG-O3G
5	C	1735	ATP	PB-O3B-PG-O1G
5	E	3535	ATP	PB-O3A-PA-O1A
5	D	2335	ATP	PB-O3B-PG-O1G
5	G	4735	ATP	PA-O3A-PB-O1B

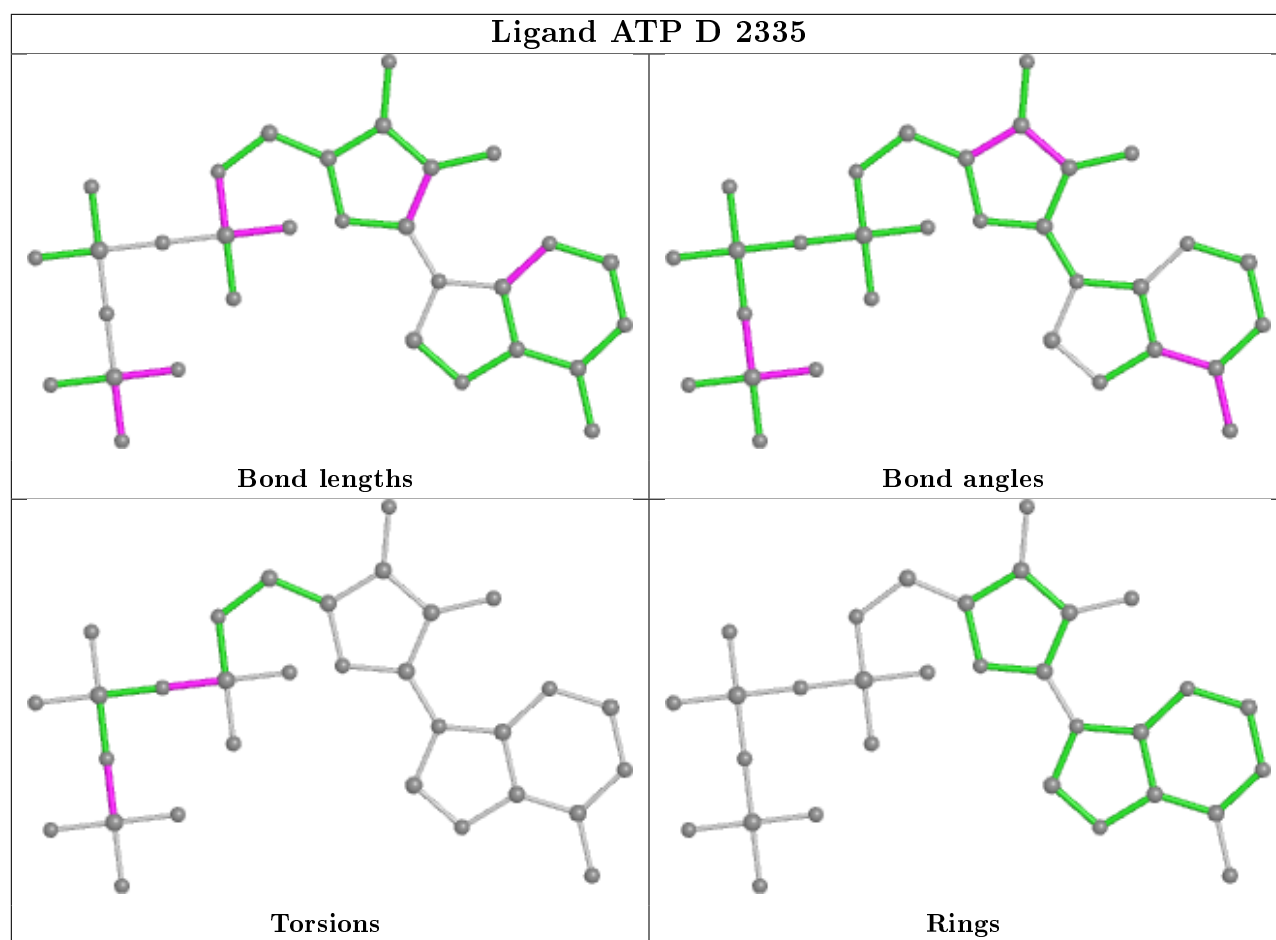
There are no ring outliers.

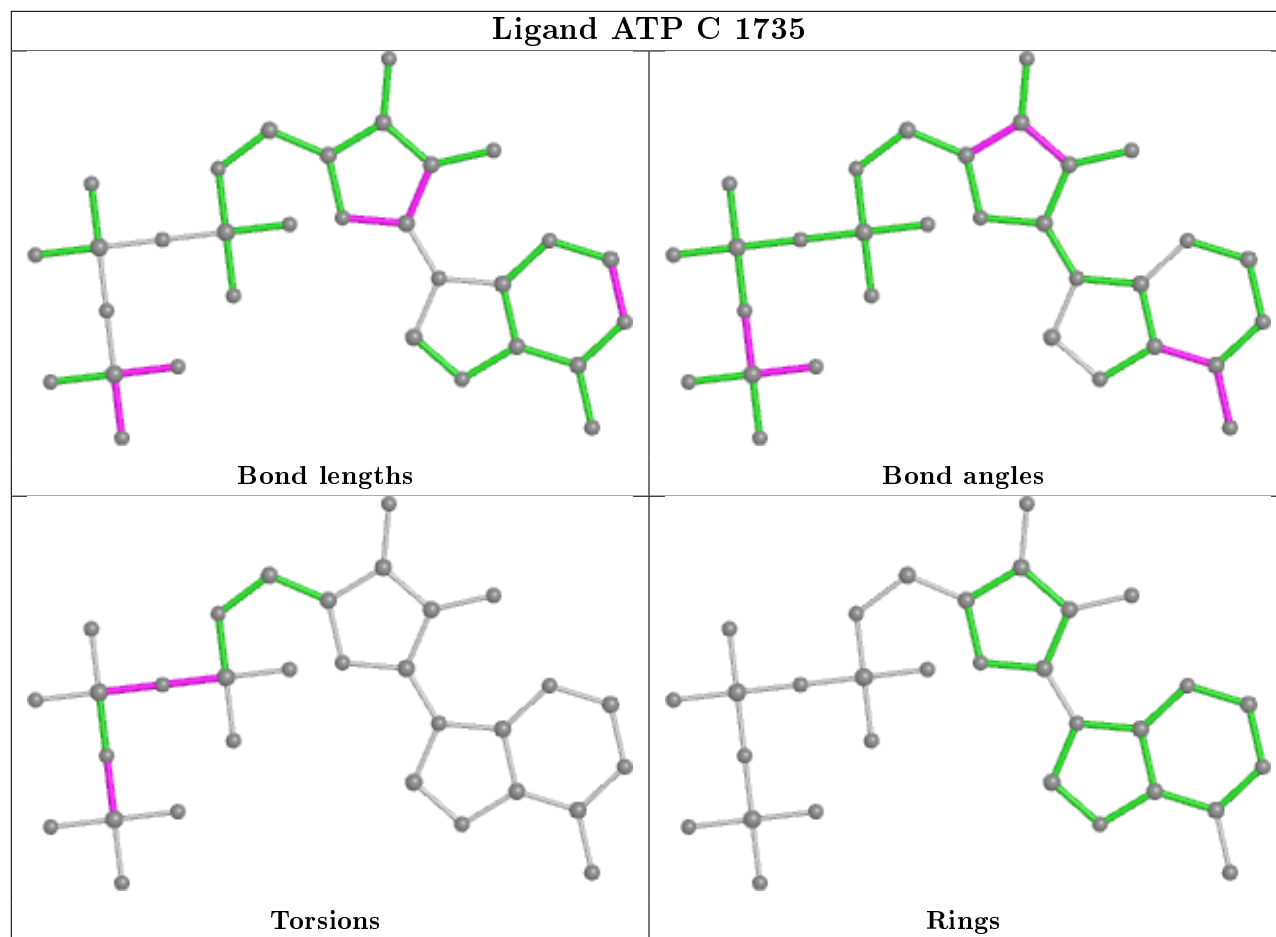
9 monomers are involved in 14 short contacts:

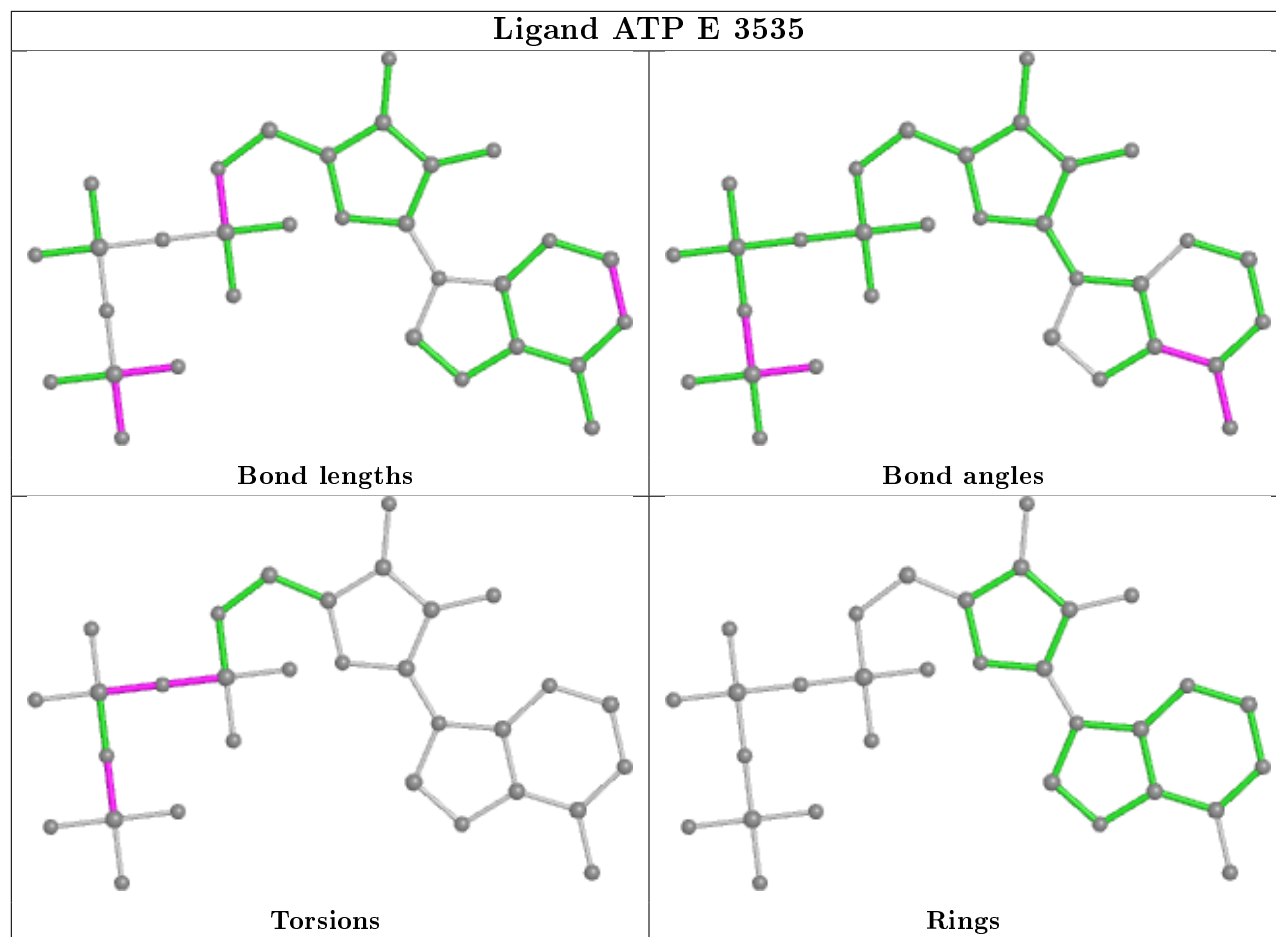
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	5333	OXL	1	0
3	F	4133	OXL	1	0
5	A	535	ATP	3	0
3	A	533	OXL	2	0
3	G	4733	OXL	1	0
5	D	2335	ATP	1	0
5	C	1735	ATP	3	0
5	G	4735	ATP	1	0
3	C	1733	OXL	1	0

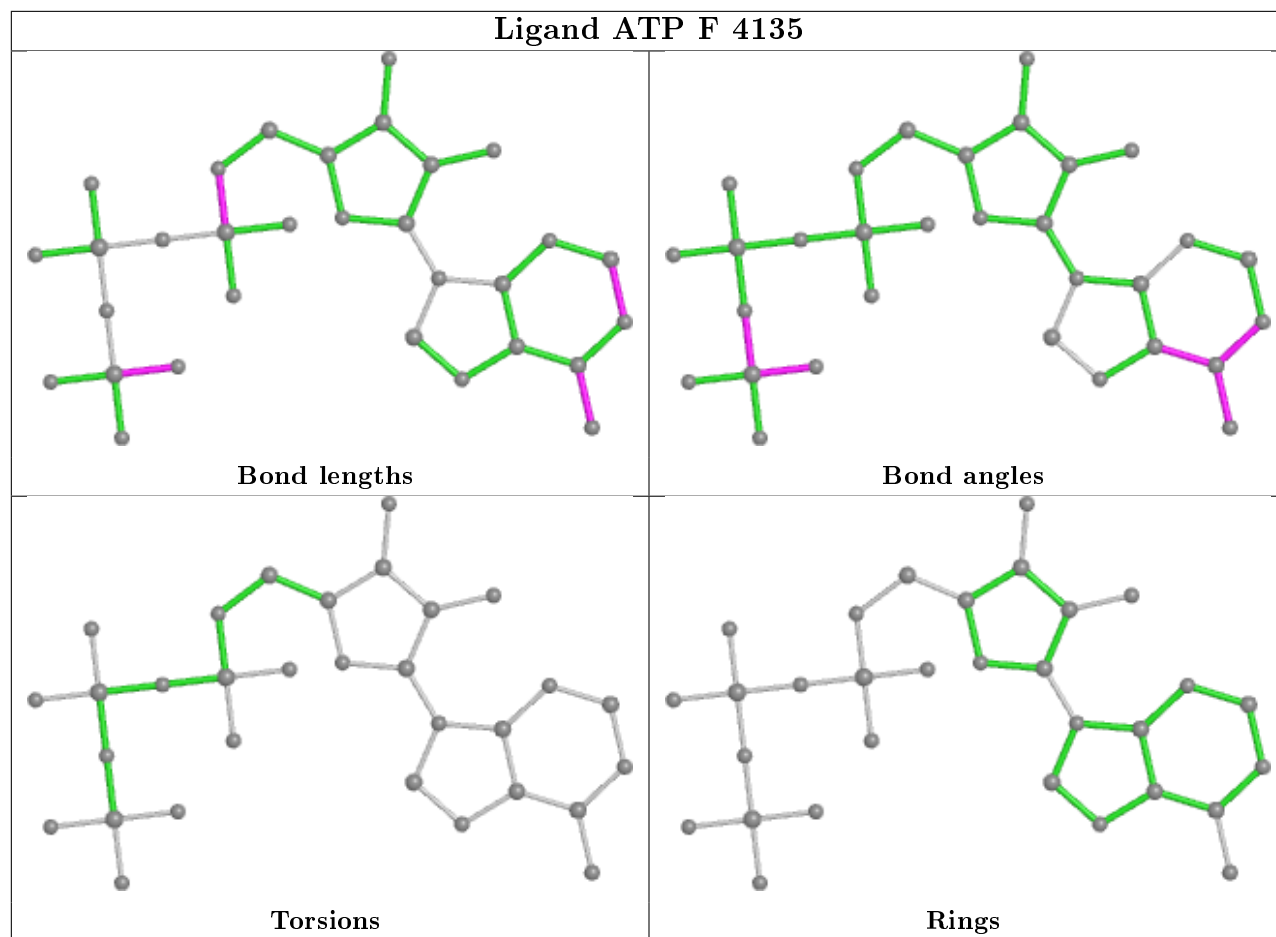
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

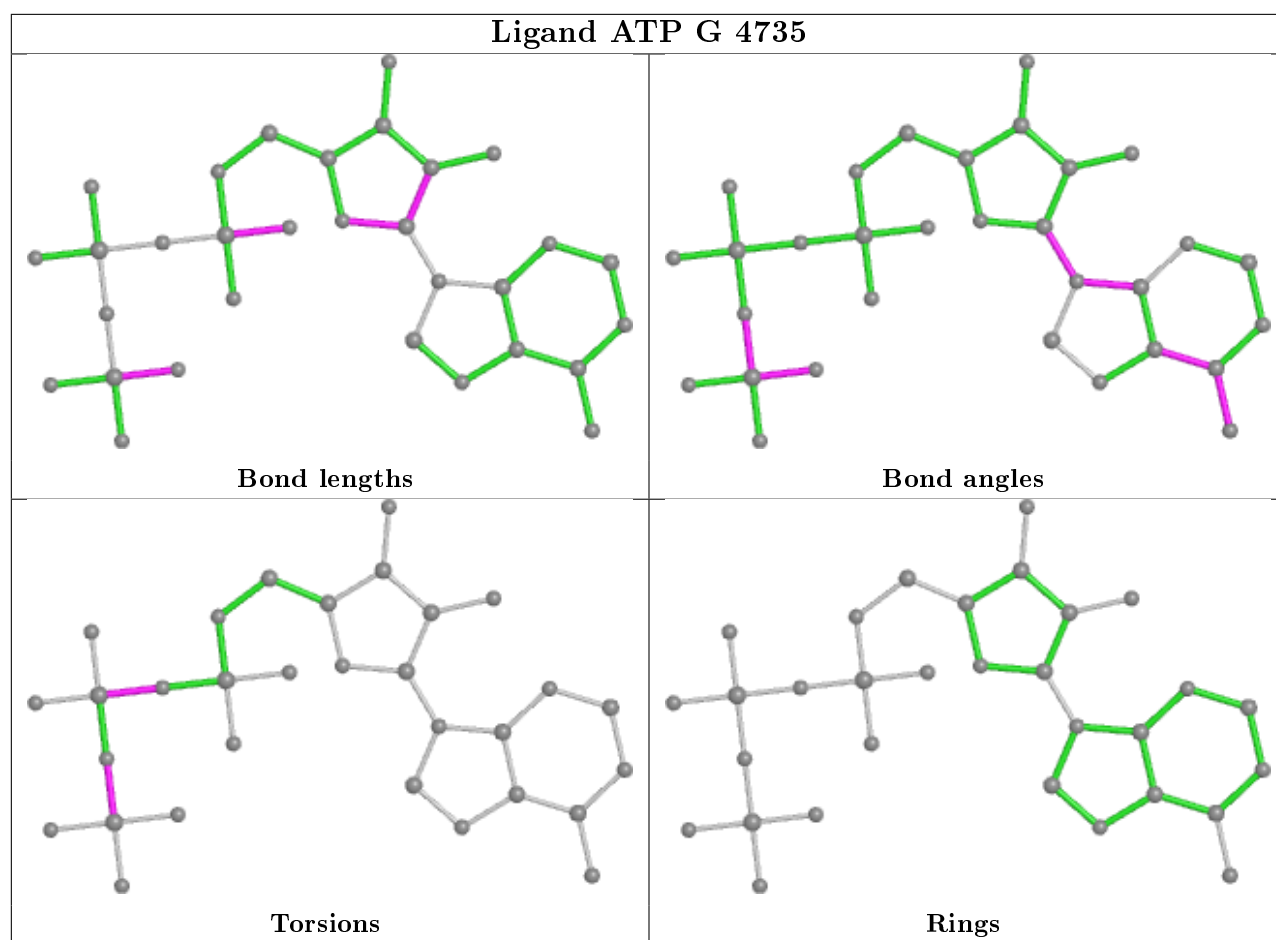












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.