



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:52 AM GMT

PDB ID : 3JZM
Title : Crystal structure of the phosphorylation-site mutant T432A of the KaiC circadian clock protein
Authors : Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on : 2009-09-23
Resolution : 2.90 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) : 1.9-1692
EDS : trunk26765
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

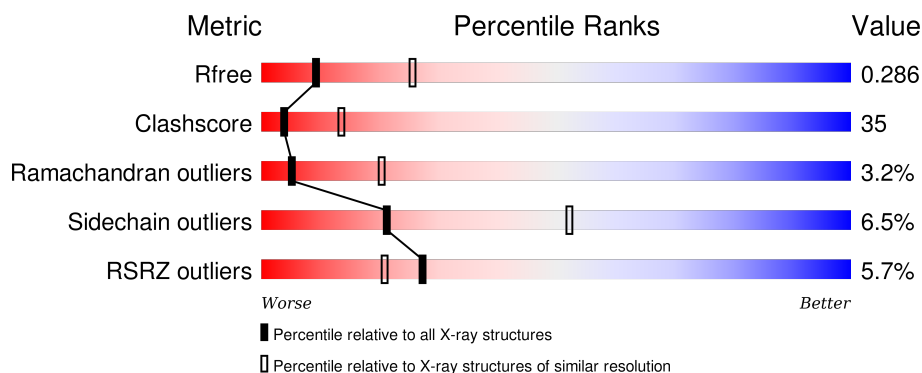
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>6%</div> <div>45%</div> <div>43%</div> <div>5%</div> <div>7%</div> </div>
1	B	519	<div> <div>7%</div> <div>44%</div> <div>45%</div> <div>•</div> <div>7%</div> </div>
1	C	519	<div> <div>6%</div> <div>42%</div> <div>45%</div> <div>6%</div> <div>7%</div> </div>
1	D	519	<div> <div>4%</div> <div>47%</div> <div>40%</div> <div>6%</div> <div>•</div> <div>7%</div> </div>
1	E	519	<div> <div>5%</div> <div>41%</div> <div>47%</div> <div>6%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	

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	MG	B	527	-	-	-	X
3	MG	B	701	-	-	-	X
3	MG	D	701	-	-	-	X
3	MG	E	701	-	-	-	X
3	MG	F	702	-	-	-	X
3	MG	F	801	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23355 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 Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	P	S	0	0	0
			3817	2406	670	725	1	15			
1	B	484	Total	C	N	O	P	S	0	0	0
			3817	2406	670	725	1	15			
1	C	484	Total	C	N	O	P	S	0	0	0
			3817	2406	670	725	1	15			
1	D	484	Total	C	N	O	P	S	0	0	0
			3817	2406	670	725	1	15			
1	E	484	Total	C	N	O	P	S	0	0	0
			3817	2406	670	725	1	15			
1	F	484	Total	C	N	O	P	S	0	0	0
			3817	2406	670	725	1	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	ALA	THR	ENGINEERED	UNP Q79PF4
B	432	ALA	THR	ENGINEERED	UNP Q79PF4
C	432	ALA	THR	ENGINEERED	UNP Q79PF4
D	432	ALA	THR	ENGINEERED	UNP Q79PF4
E	432	ALA	THR	ENGINEERED	UNP Q79PF4
F	432	ALA	THR	ENGINEERED	UNP Q79PF4

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	3	Total 3 Mg 3	0	0
3	E	3	Total 3 Mg 3	0	0
3	B	3	Total 3 Mg 3	0	0
3	C	2	Total 2 Mg 2	0	0
3	A	3	Total 3 Mg 3	0	0
3	F	4	Total 4 Mg 4	0	0

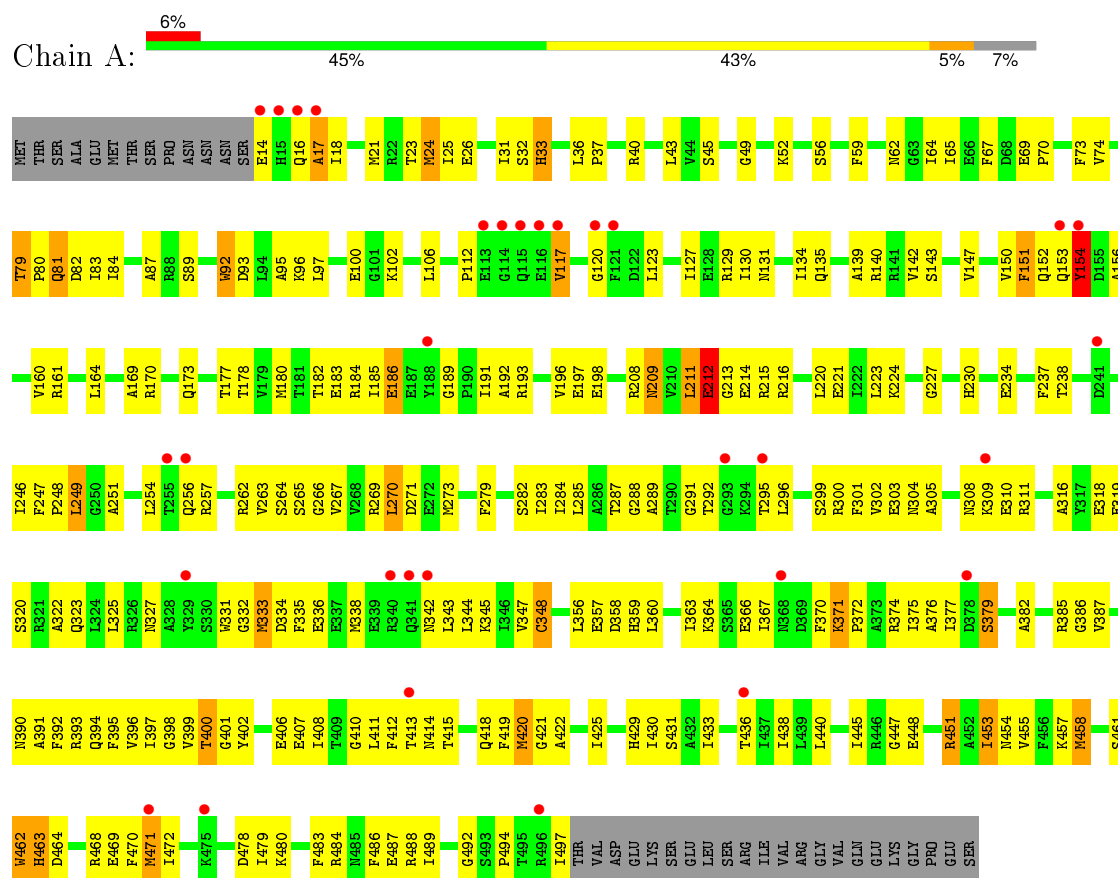
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total 7 O 7	0	0
4	B	5	Total 5 O 5	0	0
4	C	7	Total 7 O 7	0	0
4	D	12	Total 12 O 12	0	0
4	E	13	Total 13 O 13	0	0
4	F	19	Total 19 O 19	0	0

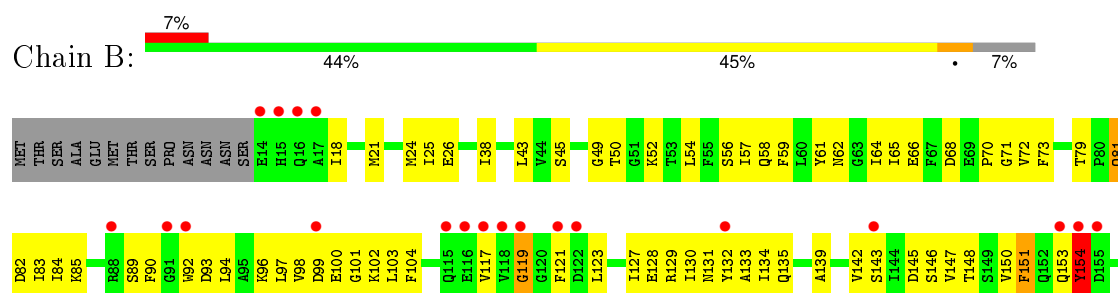
3 Residue-property plots

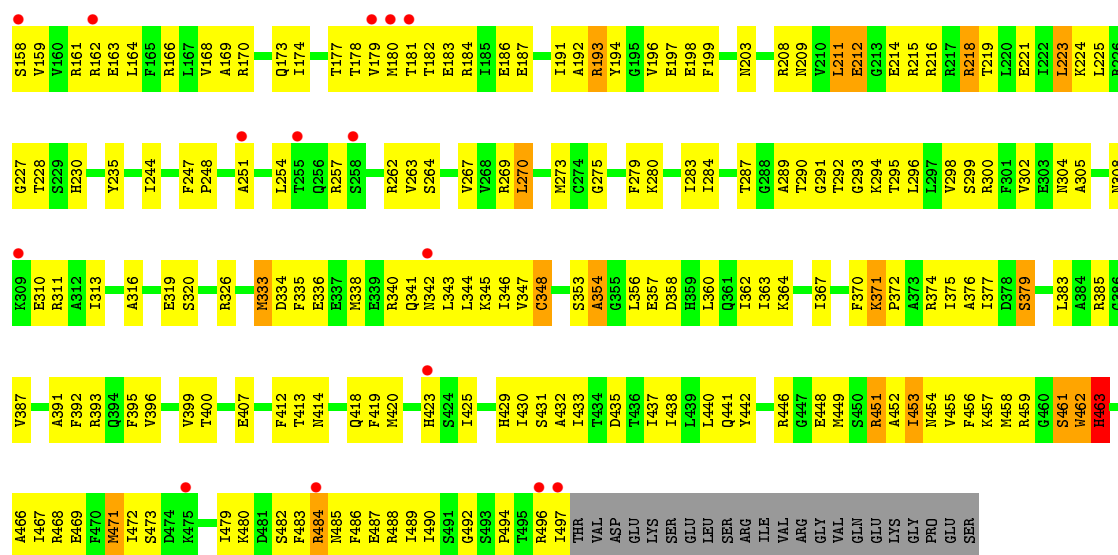
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Circadian clock protein kinase kaiC

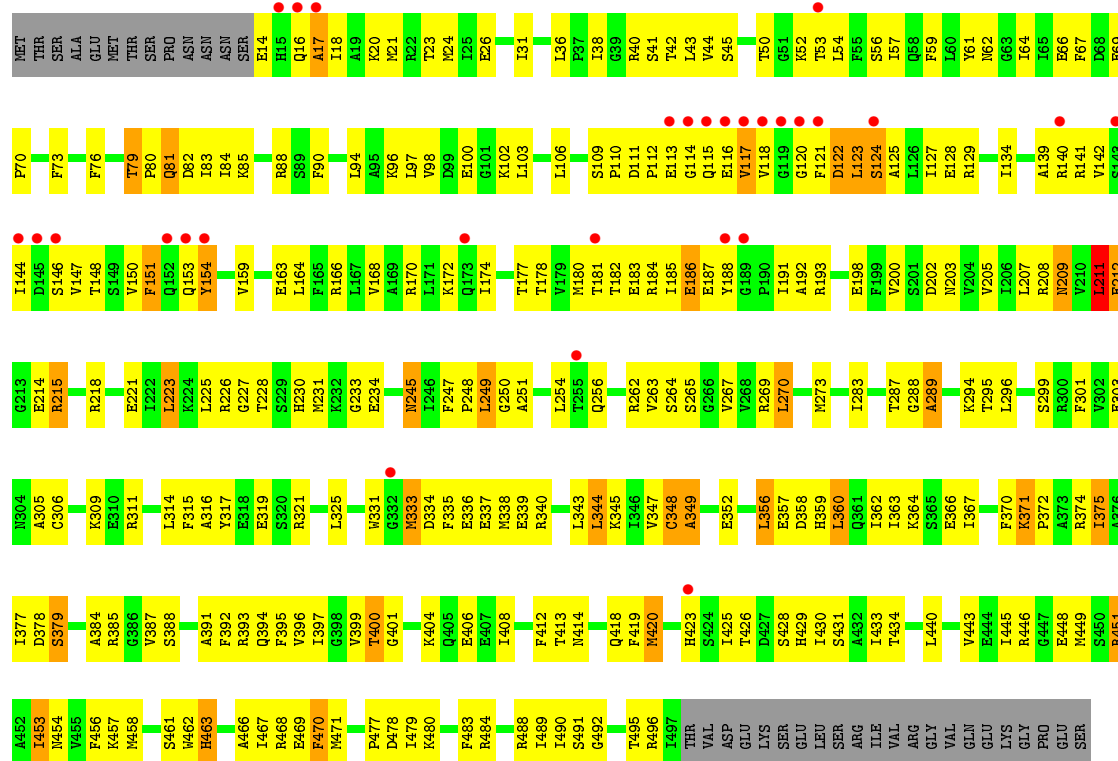


• Molecule 1: Circadian clock protein kinase kaiC



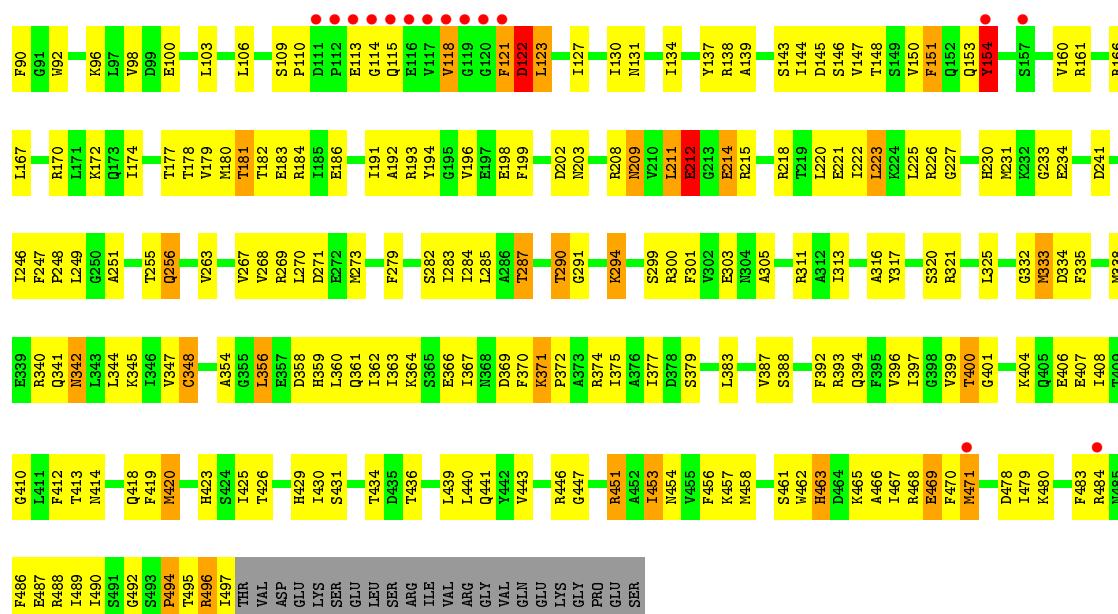


• Molecule 1: Circadian clock protein kinase kaiC

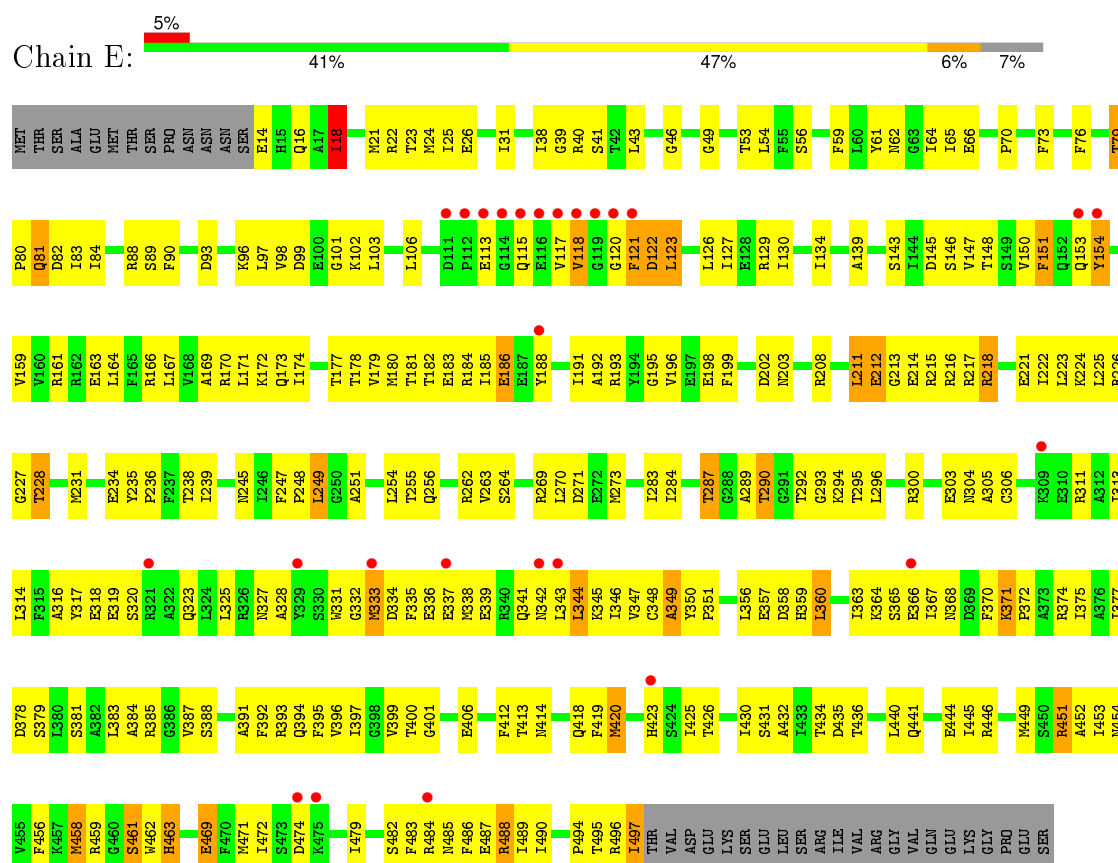


• Molecule 1: Circadian clock protein kinase kaiC





• Molecule 1: Circadian clock protein kinase kaiC



• Molecule 1: Circadian clock protein kinase kaiC



ILE VAL ARG GLY VAL GLN GLU LYS GLY PRO GLU SER	I433	I434	D435	T436	I437	I438	I439	I440	I441	Q441	Y442	V443	E444	I445	R451	A452	I453	M454	V455	F456	R457	M458	R459	G460	S461	M462	H463	I467	R468	E469	F470	M471	D478	I479	F483	R484	D485	F486	E487	R488	I489	I490	P494	T495	R496	I497	THR	VAL	ASP	GLU	LYS	SER	GLU	LEU	SER	ARG
	H359	L360	Q361	I362	I363	I367	F370	K371	P372	A373	R374	I375	A376	I377	D378	S379	L380	S381	A382	L383	R459	G460	S461	M462	H463	I467	R468	E469	F470	M471	D478	I479	F483	R484	D485	F486	E487	R488	I489	I490	P494	T495	R496	I497	THR	VAL	ASP	GLU	LYS	SER	GLU	LEU	SER	ARG		
	T290	G291	T292	G293	K294	T295	L296	L297	V298	S299	R300	F301	A305	C306	R311	A312	I313	A316	E319	S320	R321	A322	Q323	L324	L325	Y329	S330	W331	G332	M333	D334	F335	E336	F337	M338	E339	R340	M342	L343	L344	K345	I346	V347	C348	A349	Y350	F351	E352	S353	A354	G355	L356	E357	D358		
	R218	E221	I222	K223	K224	L225	R226	G227	T228	S229	H230	M231	E234	F237	T238	L239	T240	D241	H242	I246	F247	P248	L249	A251	M252	R253	L254	T255	Q256	R257	M260	V263	S264	S265	R269	L270	D271	E272	M273	C274	F278	F279	S282	I283	L284	L285	A286	G288	A289							
	T179	F80	Q81	D82	V150	I83	I84	R88	S89	F90	G91	W92	D93	L94	A95	R96	V98	D99	E100	L103	L106	D111	F112	E113	G114	Q115	E116	V117	V118	G119	G120	F121	D122	L123	S124	A125	L126	I127	E128	R129	I130	M131	Y132	A133	I134	Q135	K136	Y137	R138	A139	L140	R141	V142	S143	I144	D145
	S146	V147	T148	S149	V150	F151	Q152	Q153	Y154	D155	A156	S157	V158	V159	V160	R161	E163	L164	F165	R166	A169	R170	Q173	T177	T178	V179	M180	T181	T182	E183	R184	I185	E186	G189	P190	I191	A192	R193	Y194	G195	V196	E197	E198	N203	R208	N209	V210	A139	L211	E212	R215	R216	I144	R217		
	R218	E221	I222	K223	K224	L225	R226	G227	T228	S229	H230	M231	E234	F237	T238	L239	T240	D241	H242	I246	F247	P248	L249	A251	M252	R253	L254	T255	Q256	R257	M260	V263	S264	S265	R269	L270	D271	E272	M273	C274	F278	F279	S282	I283	L284	L285	A286	G288	A289							
	T290	G291	T292	G293	K294	T295	L296	L297	V298	S299	R300	F301	A305	C306	R311	A312	I313	A316	E319	S320	R321	A322	Q323	L324	L325	Y329	S330	W331	G332	M333	D334	F335	E336	F337	M338	E339	R340	M342	L343	L344	K345	I346	V347	C348	A349	Y350	F351	E352	S353	A354	G355	L356	E357	D358		
	H359	L360	Q361	I362	I363	I367	F370	K371	P372	A373	R374	I375	A376	I377	D378	S379	L380	S381	A382	L383	R459	G460	S461	M462	H463	I467	R468	E469	F470	M471	D478	I479	F483	R484	D485	F486	E487	R488	I489	I490	P494	T495	R496	I497	THR	VAL	ASP	GLU	LYS	SER	GLU	LEU	SER	ARG		
	H359	L360	Q361	I362	I363	I367	F370	K371	P372	A373	R374	I375	A376	I377	D378	S379	L380	S381	A382	L383	R459	G460	S461	M462	H463	I467	R468	E469	F470	M471	D478	I479	F483	R484	D485	F486	E487	R488	I489	I490	P494	T495	R496	I497	THR	VAL	ASP	GLU	LYS	SER	GLU	LEU	SER	ARG		

MET	THR	SER	ALA	GLU	MET	THR	SER	PRO	ASN	ASN	ASN	SER	E14	H15	Q16	I17	I18	M21	R22	T23	M24	G27	T31	S32	R33	G34	G35	T42	S45	S48	G49	R52	T53	L54	P55	S56	F59	L60	V61	I65	B66	F67	D68	B69	P70	F73	V74	V75
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.37Å 135.11Å 204.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.24 – 2.90 29.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (6.24-2.90) 91.2 (29.66-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.282 0.233 , 0.286	Depositor DCC
R_{free} test set	6717 reflections (9.95%)	DCC
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.6	EDS
Estimated twinning fraction	0.018 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 86773 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23355	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/3871	0.66	0/5215
1	B	0.38	0/3871	0.63	0/5215
1	C	0.42	0/3871	0.64	0/5215
1	D	0.47	0/3871	0.68	0/5215
1	E	0.47	0/3871	0.69	2/5215 (0.0%)
1	F	0.44	0/3871	0.67	0/5215
All	All	0.43	0/23226	0.66	2/31290 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	213	GLY	N-CA-C	-5.79	98.62	113.10
1	E	218	ARG	NE-CZ-NH2	-5.28	117.66	120.30

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	3817	0	3811	269	0
1	B	3817	0	3810	283	0
1	C	3817	0	3810	287	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3817	0	3811	273	0
1	E	3817	0	3809	288	0
1	F	3817	0	3809	300	0
2	A	62	0	24	5	0
2	B	62	0	24	6	0
2	C	62	0	24	2	0
2	D	62	0	24	6	0
2	E	62	0	24	9	0
2	F	62	0	23	11	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
4	A	7	0	0	2	0
4	B	5	0	0	0	0
4	C	7	0	0	2	0
4	D	12	0	0	0	0
4	E	13	0	0	4	0
4	F	19	0	0	6	0
All	All	23355	0	23003	1609	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 1609 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:E:263:VAL:HG12	1:E:374:ARG:HH21	0.99	1.13
1:B:311:ARG:HD2	1:B:371:LYS:HD2	1.29	1.12
1:F:191:ILE:HD12	1:F:198:GLU:HG2	1.35	1.08
1:A:311:ARG:HD2	1:A:371:LYS:HD2	1.34	1.07
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.37	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/519 (93%)	427 (89%)	36 (8%)	18 (4%)	4	17
1	B	481/519 (93%)	414 (86%)	52 (11%)	15 (3%)	5	21
1	C	481/519 (93%)	428 (89%)	37 (8%)	16 (3%)	5	20
1	D	481/519 (93%)	431 (90%)	38 (8%)	12 (2%)	7	27
1	E	481/519 (93%)	423 (88%)	43 (9%)	15 (3%)	5	21
1	F	481/519 (93%)	429 (89%)	37 (8%)	15 (3%)	5	21
All	All	2886/3114 (93%)	2552 (88%)	243 (8%)	91 (3%)	5	20

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	117	VAL
1	A	154	TYR
1	A	211	LEU
1	A	463	HIS

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	410/442 (93%)	386 (94%)	24 (6%)	24	58
1	B	410/442 (93%)	393 (96%)	17 (4%)	37	73
1	C	410/442 (93%)	384 (94%)	26 (6%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	410/442 (93%)	378 (92%)	32 (8%)	16	41
1	E	410/442 (93%)	379 (92%)	31 (8%)	16	43
1	F	410/442 (93%)	381 (93%)	29 (7%)	18	47
All	All	2460/2652 (93%)	2301 (94%)	159 (6%)	21	52

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	122	ASP
1	D	369	ASP
1	F	282	SER
1	D	151	PHE
1	D	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	323	GLN
1	D	33	HIS
1	F	209	ASN
1	C	368	ASN
1	C	414	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	A	431	1	8,9,10	1.53	1 (12%)	8,12,14	1.68	2 (25%)
1	SEP	B	431	1	8,9,10	1.54	1 (12%)	8,12,14	1.50	2 (25%)
1	SEP	C	431	1	8,9,10	1.61	2 (25%)	8,12,14	3.17	2 (25%)
1	SEP	D	431	1	8,9,10	1.50	1 (12%)	8,12,14	1.30	1 (12%)
1	SEP	E	431	1	8,9,10	1.50	1 (12%)	8,12,14	1.01	0
1	SEP	F	431	1	8,9,10	1.56	1 (12%)	8,12,14	1.52	2 (25%)

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
1	SEP	A	431	1	-	0/6/8/10	0/0/0/0
1	SEP	B	431	1	-	0/6/8/10	0/0/0/0
1	SEP	C	431	1	-	0/6/8/10	0/0/0/0
1	SEP	D	431	1	-	0/6/8/10	0/0/0/0
1	SEP	E	431	1	-	0/6/8/10	0/0/0/0
1	SEP	F	431	1	-	0/6/8/10	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	431	SEP	P-O3P	2.01	1.61	1.54
1	E	431	SEP	P-O1P	3.09	1.61	1.51
1	A	431	SEP	P-O1P	3.10	1.61	1.51
1	F	431	SEP	P-O1P	3.12	1.61	1.51
1	D	431	SEP	P-O1P	3.12	1.61	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	431	SEP	O-C-CA	-2.30	119.49	125.49
1	C	431	SEP	O-C-CA	-2.21	119.74	125.49
1	A	431	SEP	O-C-CA	-2.18	119.82	125.49
1	B	431	SEP	O-C-CA	-2.14	119.93	125.49
1	D	431	SEP	OG-CB-CA	2.49	110.40	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	431	SEP	1	0
1	B	431	SEP	1	0
1	C	431	SEP	2	0
1	D	431	SEP	2	0
1	E	431	SEP	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 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	ATP	A	901	3	24,33,33	1.35	3 (12%)	31,52,52	2.59	6 (19%)
2	ATP	A	903	3	24,33,33	1.25	3 (12%)	31,52,52	2.53	7 (22%)
2	ATP	B	901	3	24,33,33	1.22	2 (8%)	31,52,52	2.61	6 (19%)
2	ATP	B	903	3	24,33,33	1.34	3 (12%)	31,52,52	2.59	6 (19%)
2	ATP	C	901	3	24,33,33	1.37	3 (12%)	31,52,52	2.48	7 (22%)
2	ATP	C	903	3	24,33,33	1.16	1 (4%)	31,52,52	2.58	5 (16%)
2	ATP	D	901	3	24,33,33	1.26	3 (12%)	31,52,52	2.60	8 (25%)
2	ATP	D	903	3	24,33,33	1.18	2 (8%)	31,52,52	2.72	5 (16%)
2	ATP	E	901	3	24,33,33	1.41	4 (16%)	31,52,52	2.57	6 (19%)
2	ATP	E	903	3	24,33,33	1.33	2 (8%)	31,52,52	2.65	6 (19%)
2	ATP	F	901	3	24,33,33	1.35	4 (16%)	31,52,52	2.61	9 (29%)
2	ATP	F	903	3	24,33,33	1.55	5 (20%)	31,52,52	2.59	5 (16%)

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	ATP	A	901	3	-	0/18/38/38	0/3/3/3
2	ATP	A	903	3	-	0/18/38/38	0/3/3/3
2	ATP	B	901	3	-	0/18/38/38	0/3/3/3
2	ATP	B	903	3	-	0/18/38/38	0/3/3/3
2	ATP	C	901	3	-	0/18/38/38	0/3/3/3
2	ATP	C	903	3	-	0/18/38/38	0/3/3/3
2	ATP	D	901	3	-	0/18/38/38	0/3/3/3
2	ATP	D	903	3	-	0/18/38/38	0/3/3/3
2	ATP	E	901	3	-	0/18/38/38	0/3/3/3
2	ATP	E	903	3	-	0/18/38/38	0/3/3/3
2	ATP	F	901	3	-	0/18/38/38	0/3/3/3
2	ATP	F	903	3	-	0/18/38/38	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	903	ATP	O2'-C2'	-2.82	1.36	1.43
2	D	903	ATP	O2'-C2'	-2.40	1.37	1.43
2	E	903	ATP	O4'-C4'	-2.16	1.40	1.45
2	F	903	ATP	PB-O1B	-2.16	1.43	1.51
2	A	903	ATP	C2-N1	2.01	1.37	1.33

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	903	ATP	N3-C2-N1	-12.48	119.34	128.89
2	F	903	ATP	N3-C2-N1	-12.11	119.62	128.89
2	B	901	ATP	N3-C2-N1	-11.99	119.72	128.89
2	E	903	ATP	N3-C2-N1	-11.59	120.02	128.89
2	F	901	ATP	N3-C2-N1	-11.52	120.08	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ATP	3	0
2	A	903	ATP	2	0
2	B	901	ATP	4	0
2	B	903	ATP	2	0
2	C	901	ATP	1	0
2	C	903	ATP	1	0
2	D	901	ATP	4	0
2	D	903	ATP	2	0
2	E	901	ATP	5	0
2	E	903	ATP	4	0
2	F	901	ATP	5	0
2	F	903	ATP	6	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](#)

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, 95th 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	483/519 (93%)	0.28	31 (6%) 23 16	34, 74, 118, 149	0
1	B	483/519 (93%)	0.38	35 (7%) 18 12	46, 78, 120, 159	0
1	C	483/519 (93%)	0.17	29 (6%) 25 18	33, 67, 116, 160	0
1	D	483/519 (93%)	-0.07	19 (3%) 43 36	25, 54, 101, 148	0
1	E	483/519 (93%)	0.03	26 (5%) 29 23	18, 57, 97, 147	0
1	F	483/519 (93%)	0.07	24 (4%) 32 26	24, 65, 106, 143	0
All	All	2898/3114 (93%)	0.14	164 (5%) 27 21	18, 66, 114, 160	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120	GLY	11.6
1	C	118	VAL	9.0
1	B	116	GLU	8.7
1	F	154	TYR	8.1
1	B	117	VAL	7.8

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
1	SEP	C	431	10/11	0.74	0.30	-	79,84,100,100	0
1	SEP	D	431	10/11	0.84	0.24	-	69,77,94,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SEP	E	431	10/11	0.83	0.23	-	57,65,81,82	0
1	SEP	F	431	10/11	0.86	0.22	-	74,79,89,90	0
1	SEP	A	431	10/11	0.89	0.18	-	78,83,94,95	0
1	SEP	B	431	10/11	0.85	0.23	-	81,88,100,102	0

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, 95th 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(\AA^2)	Q<0.9
3	MG	D	701	1/1	0.80	0.85	28.68	61,61,61,61	0
3	MG	E	701	1/1	0.92	0.47	6.76	49,49,49,49	0
3	MG	B	701	1/1	0.70	0.52	6.08	84,84,84,84	0
3	MG	F	801	1/1	0.50	0.38	5.15	31,31,31,31	0
3	MG	B	527	1/1	0.28	0.33	4.80	29,29,29,29	0
3	MG	F	702	1/1	0.93	0.30	2.51	80,80,80,80	0
2	ATP	F	901	31/31	0.89	0.25	1.20	70,79,84,85	0
2	ATP	D	901	31/31	0.95	0.21	0.86	50,59,61,63	0
2	ATP	B	901	31/31	0.92	0.23	0.56	69,73,77,78	0
2	ATP	A	901	31/31	0.88	0.28	0.43	70,82,84,85	0
2	ATP	E	901	31/31	0.91	0.23	0.05	63,70,77,77	0
2	ATP	A	903	31/31	0.90	0.19	-0.24	28,47,55,55	0
2	ATP	D	903	31/31	0.91	0.16	-0.24	10,17,27,30	0
2	ATP	C	903	31/31	0.87	0.20	-0.32	32,33,49,53	0
2	ATP	C	901	31/31	0.94	0.17	-0.34	41,44,53,56	0
2	ATP	B	903	31/31	0.90	0.17	-0.35	57,66,69,69	0
3	MG	A	802	1/1	0.90	0.25	-0.39	75,75,75,75	0
2	ATP	F	903	31/31	0.94	0.15	-0.57	10,12,19,19	0
2	ATP	E	903	31/31	0.95	0.14	-0.59	9,13,21,25	0
3	MG	D	702	1/1	0.87	0.29	-	75,75,75,75	0
3	MG	C	801	1/1	0.56	0.51	-	56,56,56,56	0
3	MG	E	702	1/1	0.94	0.36	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	F	701	1/1	0.87	0.60	-	54,54,54,54	0
3	MG	B	801	1/1	0.61	0.51	-	69,69,69,69	0
3	MG	C	520	1/1	0.67	0.42	-	99,99,99,99	0
3	MG	A	701	1/1	0.84	0.38	-	85,85,85,85	0
3	MG	A	801	1/1	0.58	0.56	-	64,64,64,64	0
3	MG	F	802	1/1	0.86	0.56	-	91,91,91,91	0
3	MG	D	802	1/1	0.77	0.37	-	35,35,35,35	0
3	MG	E	801	1/1	0.87	0.45	-	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.