



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:23 AM GMT

PDB ID : 1Z0S
Title : Crystal structure of an NAD kinase from *Archaeoglobus fulgidus* in complex with ATP
Authors : Liu, J.; Lou, Y.; Yokota, H.; Adams, P.D.; Kim, R.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2005-03-02
Resolution : 1.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

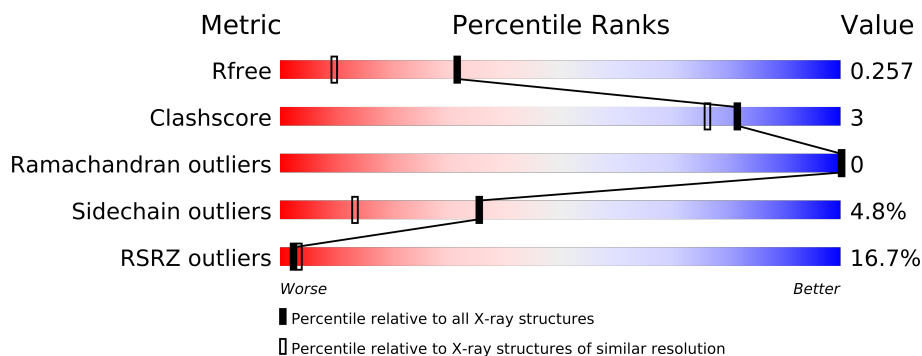
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.70 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}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	278	
1	B	278	
1	C	278	
1	D	278	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	C	5003	-	X
2	MG	D	5004	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8423 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Probable inorganic polyphosphate/ATP-NADkinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1963	1266	334	355	8			
1	B	249	Total	C	N	O	S	0	0	0
			1963	1266	334	355	8			
1	C	249	Total	C	N	O	S	0	0	0
			1963	1266	334	355	8			
1	D	249	Total	C	N	O	S	0	0	0
			1963	1266	334	355	8			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	cloning artifact	UNP O30297
A	-27	GLY	-	cloning artifact	UNP O30297
A	-26	SER	-	cloning artifact	UNP O30297
A	-25	SER	-	cloning artifact	UNP O30297
A	-24	HIS	-	cloning artifact	UNP O30297
A	-23	HIS	-	cloning artifact	UNP O30297
A	-22	HIS	-	cloning artifact	UNP O30297
A	-21	HIS	-	cloning artifact	UNP O30297
A	-20	HIS	-	cloning artifact	UNP O30297
A	-19	HIS	-	cloning artifact	UNP O30297
A	-18	ASP	-	cloning artifact	UNP O30297
A	-17	TYR	-	cloning artifact	UNP O30297
A	-16	ASP	-	cloning artifact	UNP O30297
A	-15	ILE	-	cloning artifact	UNP O30297
A	-14	PRO	-	cloning artifact	UNP O30297
A	-13	THR	-	cloning artifact	UNP O30297
A	-12	THR	-	cloning artifact	UNP O30297
A	-11	GLU	-	cloning artifact	UNP O30297
A	-10	ASN	-	cloning artifact	UNP O30297
A	-9	LEU	-	cloning artifact	UNP O30297
A	-8	TYR	-	cloning artifact	UNP O30297

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	PHE	-	cloning artifact	UNP O30297
A	-6	GLN	-	cloning artifact	UNP O30297
A	-5	GLY	-	cloning artifact	UNP O30297
A	-4	GLY	-	cloning artifact	UNP O30297
A	-3	GLY	-	cloning artifact	UNP O30297
A	-2	GLY	-	cloning artifact	UNP O30297
A	-1	GLY	-	cloning artifact	UNP O30297
A	0	GLY	-	cloning artifact	UNP O30297
B	-28	MET	-	cloning artifact	UNP O30297
B	-27	GLY	-	cloning artifact	UNP O30297
B	-26	SER	-	cloning artifact	UNP O30297
B	-25	SER	-	cloning artifact	UNP O30297
B	-24	HIS	-	cloning artifact	UNP O30297
B	-23	HIS	-	cloning artifact	UNP O30297
B	-22	HIS	-	cloning artifact	UNP O30297
B	-21	HIS	-	cloning artifact	UNP O30297
B	-20	HIS	-	cloning artifact	UNP O30297
B	-19	HIS	-	cloning artifact	UNP O30297
B	-18	ASP	-	cloning artifact	UNP O30297
B	-17	TYR	-	cloning artifact	UNP O30297
B	-16	ASP	-	cloning artifact	UNP O30297
B	-15	ILE	-	cloning artifact	UNP O30297
B	-14	PRO	-	cloning artifact	UNP O30297
B	-13	THR	-	cloning artifact	UNP O30297
B	-12	THR	-	cloning artifact	UNP O30297
B	-11	GLU	-	cloning artifact	UNP O30297
B	-10	ASN	-	cloning artifact	UNP O30297
B	-9	LEU	-	cloning artifact	UNP O30297
B	-8	TYR	-	cloning artifact	UNP O30297
B	-7	PHE	-	cloning artifact	UNP O30297
B	-6	GLN	-	cloning artifact	UNP O30297
B	-5	GLY	-	cloning artifact	UNP O30297
B	-4	GLY	-	cloning artifact	UNP O30297
B	-3	GLY	-	cloning artifact	UNP O30297
B	-2	GLY	-	cloning artifact	UNP O30297
B	-1	GLY	-	cloning artifact	UNP O30297
B	0	GLY	-	cloning artifact	UNP O30297
C	-28	MET	-	cloning artifact	UNP O30297
C	-27	GLY	-	cloning artifact	UNP O30297
C	-26	SER	-	cloning artifact	UNP O30297
C	-25	SER	-	cloning artifact	UNP O30297
C	-24	HIS	-	cloning artifact	UNP O30297

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	HIS	-	cloning artifact	UNP O30297
C	-22	HIS	-	cloning artifact	UNP O30297
C	-21	HIS	-	cloning artifact	UNP O30297
C	-20	HIS	-	cloning artifact	UNP O30297
C	-19	HIS	-	cloning artifact	UNP O30297
C	-18	ASP	-	cloning artifact	UNP O30297
C	-17	TYR	-	cloning artifact	UNP O30297
C	-16	ASP	-	cloning artifact	UNP O30297
C	-15	ILE	-	cloning artifact	UNP O30297
C	-14	PRO	-	cloning artifact	UNP O30297
C	-13	THR	-	cloning artifact	UNP O30297
C	-12	THR	-	cloning artifact	UNP O30297
C	-11	GLU	-	cloning artifact	UNP O30297
C	-10	ASN	-	cloning artifact	UNP O30297
C	-9	LEU	-	cloning artifact	UNP O30297
C	-8	TYR	-	cloning artifact	UNP O30297
C	-7	PHE	-	cloning artifact	UNP O30297
C	-6	GLN	-	cloning artifact	UNP O30297
C	-5	GLY	-	cloning artifact	UNP O30297
C	-4	GLY	-	cloning artifact	UNP O30297
C	-3	GLY	-	cloning artifact	UNP O30297
C	-2	GLY	-	cloning artifact	UNP O30297
C	-1	GLY	-	cloning artifact	UNP O30297
C	0	GLY	-	cloning artifact	UNP O30297
D	-28	MET	-	cloning artifact	UNP O30297
D	-27	GLY	-	cloning artifact	UNP O30297
D	-26	SER	-	cloning artifact	UNP O30297
D	-25	SER	-	cloning artifact	UNP O30297
D	-24	HIS	-	cloning artifact	UNP O30297
D	-23	HIS	-	cloning artifact	UNP O30297
D	-22	HIS	-	cloning artifact	UNP O30297
D	-21	HIS	-	cloning artifact	UNP O30297
D	-20	HIS	-	cloning artifact	UNP O30297
D	-19	HIS	-	cloning artifact	UNP O30297
D	-18	ASP	-	cloning artifact	UNP O30297
D	-17	TYR	-	cloning artifact	UNP O30297
D	-16	ASP	-	cloning artifact	UNP O30297
D	-15	ILE	-	cloning artifact	UNP O30297
D	-14	PRO	-	cloning artifact	UNP O30297
D	-13	THR	-	cloning artifact	UNP O30297
D	-12	THR	-	cloning artifact	UNP O30297
D	-11	GLU	-	cloning artifact	UNP O30297

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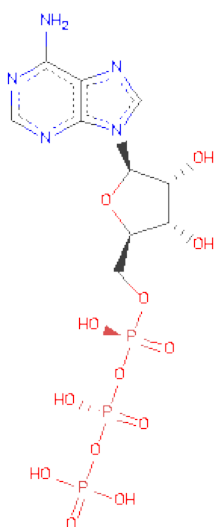
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	ASN	-	cloning artifact	UNP O30297
D	-9	LEU	-	cloning artifact	UNP O30297
D	-8	TYR	-	cloning artifact	UNP O30297
D	-7	PHE	-	cloning artifact	UNP O30297
D	-6	GLN	-	cloning artifact	UNP O30297
D	-5	GLY	-	cloning artifact	UNP O30297
D	-4	GLY	-	cloning artifact	UNP O30297
D	-3	GLY	-	cloning artifact	UNP O30297
D	-2	GLY	-	cloning artifact	UNP O30297
D	-1	GLY	-	cloning artifact	UNP O30297
D	0	GLY	-	cloning artifact	UNP O30297

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

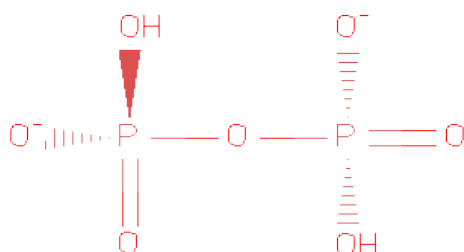
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total 1 Mg 1	0	0
2	A	1	Total 1 Mg 1	0	0
2	D	1	Total 1 Mg 1	0	0
2	C	1	Total 1 Mg 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O P	0	0
			9 7 2			
4	B	1	Total	O P	0	0
			9 7 2			
4	C	1	Total	O P	0	0
			9 7 2			
4	D	1	Total	O P	0	0
			9 7 2			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	0	0
			103 103			
5	B	90	Total	O	0	0
			90 90			

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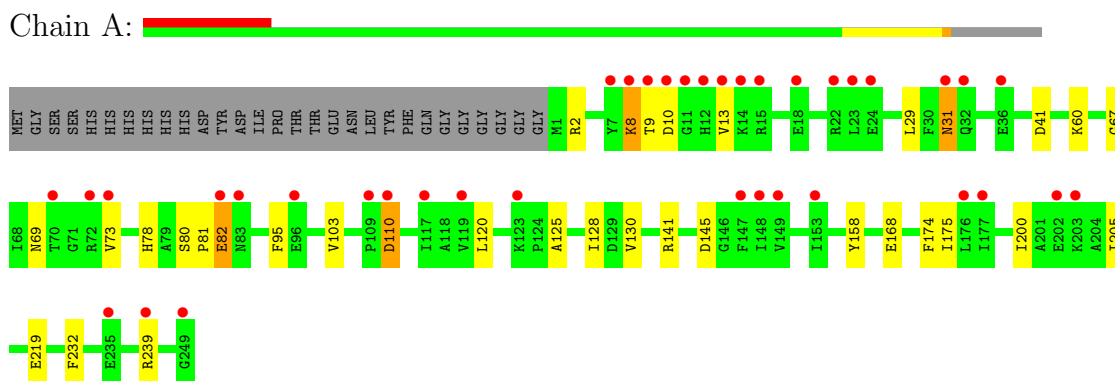
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	103	Total 103	O 103	0	0
5	D	111	Total 111	O 111	0	0

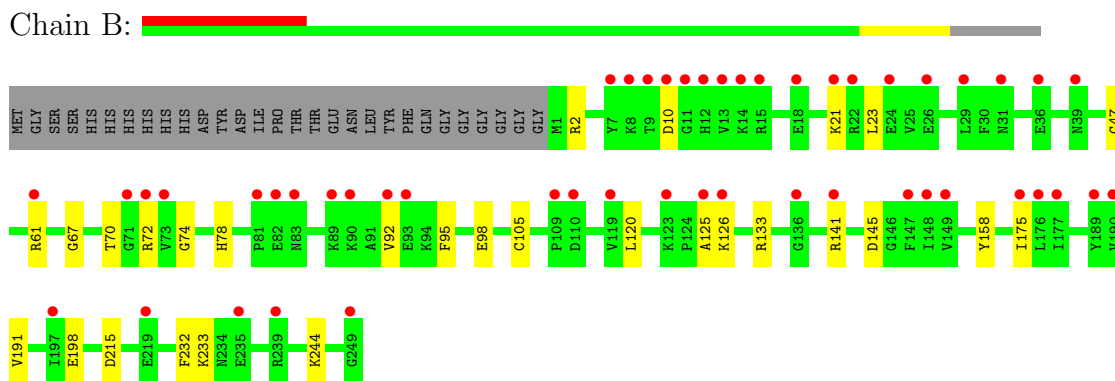
3 Residue-property plots

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.

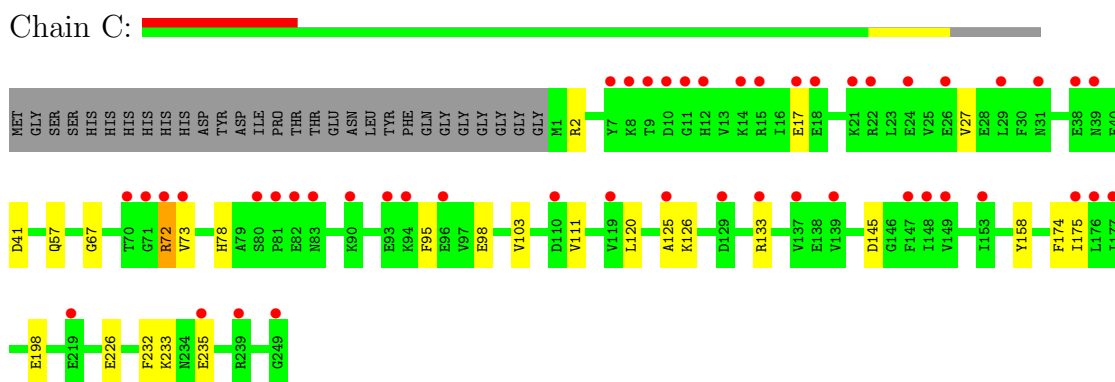
- Molecule 1: Probable inorganic polyphosphate/ATP-NADkinase



- Molecule 1: Probable inorganic polyphosphate/ATP-NADkinase

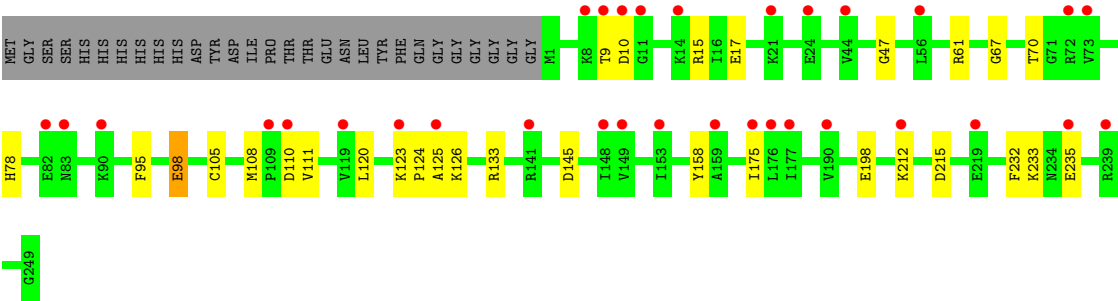


- Molecule 1: Probable inorganic polyphosphate/ATP-NADkinase



● Molecule 1: Probable inorganic polyphosphate/ATP-NADkinase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.25Å 69.73Å 76.29Å 106.35° 111.32° 101.30°	Depositor
Resolution (Å)	20.00 – 1.70 20.04 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.70) 92.0 (20.04-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.200 , 0.231 0.234 , 0.257	Depositor DCC
R_{free} test set	4882 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 100973 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8423	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, POP, 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	0.42	0/2001	0.70	4/2698 (0.1%)
1	B	0.41	0/2001	0.69	3/2698 (0.1%)
1	C	0.44	0/2001	0.72	4/2698 (0.1%)
1	D	0.44	0/2001	0.70	2/2698 (0.1%)
All	All	0.43	0/8004	0.70	13/10792 (0.1%)

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	C	1	0

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ASP	CB-CG-OD2	7.10	124.69	118.30
1	C	145	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	215	ASP	CB-CG-OD2	6.08	123.77	118.30
1	D	215	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	145	ASP	CB-CG-OD2	5.85	123.57	118.30
1	C	72	ARG	N-CA-C	5.84	126.78	111.00
1	A	41	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	145	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	110	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	41	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	72	ARG	CB-CA-C	5.10	120.61	110.40
1	B	10	ASP	CB-CG-OD2	5.06	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	72	ARG	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1963	0	2015	19	0
1	B	1963	0	2015	13	0
1	C	1963	0	2015	12	0
1	D	1963	0	2015	16	0
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
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	9	0	0	1	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
5	A	103	0	0	2	0
5	B	90	0	0	0	1
5	C	103	0	0	0	1
5	D	111	0	0	0	0
All	All	8423	0	8108	52	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 3.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:111:VAL:HG21	1:D:212:LYS:HZ2	0.98	1.06
1:D:111:VAL:HG21	1:D:212:LYS:NZ	1.78	0.97
1:A:128:ILE:O	5:A:5098:HOH:O	1.92	0.87
1:A:125:ALA:HB2	1:D:120:LEU:HD11	1.71	0.71
1:A:120:LEU:HD11	1:D:125:ALA:HB2	1.74	0.69
1:B:120:LEU:HD11	1:C:125:ALA:HB2	1.75	0.68
1:C:78:HIS:HE1	1:C:232:PHE:O	1.77	0.67
1:D:108:MET:SD	1:D:212:LYS:NZ	2.63	0.66
1:B:125:ALA:HB2	1:C:120:LEU:HD11	1.79	0.65
1:B:78:HIS:HE1	1:B:232:PHE:O	1.79	0.64
1:D:78:HIS:HE1	1:D:232:PHE:O	1.81	0.63
1:A:78:HIS:HE1	1:A:232:PHE:O	1.82	0.63
1:B:120:LEU:CD1	1:C:125:ALA:HB2	2.31	0.60
1:C:57:GLN:HE22	1:C:111:VAL:HG13	1.68	0.57
1:A:8:LYS:HD2	1:A:9:THR:HG23	1.87	0.57
1:B:23:LEU:HD13	1:B:92:VAL:HG11	1.86	0.56
1:D:111:VAL:CG2	1:D:212:LYS:HZ2	1.93	0.56
1:B:175:ILE:HD12	1:B:175:ILE:N	2.22	0.54
1:A:200:ILE:HG13	1:A:219:GLU:HG2	1.89	0.53
1:B:125:ALA:HB2	1:C:120:LEU:CD1	2.40	0.52
1:A:67:GLY:H	1:A:78:HIS:CD2	2.29	0.51
1:D:67:GLY:H	1:D:78:HIS:CD2	2.29	0.51
1:B:133:ARG:HB2	1:B:198:GLU:HB2	1.93	0.50
1:C:175:ILE:N	1:C:175:ILE:HD12	2.27	0.50
1:A:130:VAL:HG23	5:A:5098:HOH:O	2.14	0.48
1:A:31:ASN:N	1:A:31:ASN:OD1	2.47	0.47
1:C:133:ARG:HB2	1:C:198:GLU:HB2	1.96	0.47
1:A:8:LYS:NZ	4:A:3953:POP:P1	2.88	0.47
1:A:80:SER:OG	1:A:82:GLU:CD	2.53	0.47
1:D:175:ILE:N	1:D:175:ILE:HD12	2.30	0.47
1:B:47:GLY:HA2	1:B:70:THR:OG1	2.15	0.47
1:D:133:ARG:HB2	1:D:198:GLU:HB2	1.98	0.46
1:C:17:GLU:HG3	1:C:27:VAL:HG11	1.99	0.44
1:A:67:GLY:H	1:A:78:HIS:HD2	1.66	0.44
1:B:98:GLU:HG3	1:B:233:LYS:HA	1.99	0.44
1:C:67:GLY:H	1:C:78:HIS:CD2	2.37	0.43
1:D:108:MET:CG	1:D:212:LYS:HZ3	2.30	0.42
1:D:47:GLY:HA2	1:D:70:THR:OG1	2.18	0.42
1:B:67:GLY:H	1:B:78:HIS:CD2	2.37	0.42
1:C:98:GLU:HG3	1:C:233:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:175:ILE:N	1:A:175:ILE:HD12	2.35	0.42
1:D:108:MET:HB3	1:D:212:LYS:NZ	2.35	0.41
1:D:67:GLY:H	1:D:78:HIS:HD2	1.67	0.41
1:A:168:GLU:HG2	1:B:191:VAL:HA	2.01	0.41
1:B:74:GLY:O	1:B:244:LYS:NZ	2.40	0.41
1:A:200:ILE:CG1	1:A:219:GLU:HG2	2.49	0.41
1:A:205:ILE:HD11	1:D:124:PRO:HB2	2.03	0.41
1:D:98:GLU:CG	1:D:233:LYS:HA	2.51	0.40
1:A:69:ASN:O	1:A:81:PRO:HD3	2.21	0.40
1:C:103:VAL:HG11	1:C:174:PHE:HE2	1.86	0.40
1:A:103:VAL:HG11	1:A:174:PHE:HE2	1.87	0.40
1:A:13:VAL:CG1	1:A:29:LEU:HD22	2.50	0.40

All (1) 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	Distance(Å)	Clash(Å)
5:B:5085:HOH:O	5:C:5096:HOH:O[1_554]	2.05	0.15

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	247/278 (89%)	243 (98%)	4 (2%)	0	100	100
1	B	247/278 (89%)	242 (98%)	5 (2%)	0	100	100
1	C	247/278 (89%)	243 (98%)	4 (2%)	0	100	100
1	D	247/278 (89%)	243 (98%)	4 (2%)	0	100	100
All	All	988/1112 (89%)	971 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	213/235 (91%)	202 (95%)	11 (5%)	32	11
1	B	213/235 (91%)	204 (96%)	9 (4%)	40	16
1	C	213/235 (91%)	205 (96%)	8 (4%)	44	19
1	D	213/235 (91%)	200 (94%)	13 (6%)	26	8
All	All	852/940 (91%)	811 (95%)	41 (5%)	35	13

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	8	LYS
1	A	31	ASN
1	A	60	LYS
1	A	73	VAL
1	A	82	GLU
1	A	95	PHE
1	A	110	ASP
1	A	141	ARG
1	A	158	TYR
1	A	239	ARG
1	B	2	ARG
1	B	21	LYS
1	B	61	ARG
1	B	72	ARG
1	B	95	PHE
1	B	105	CYS
1	B	126	LYS
1	B	141	ARG
1	B	158	TYR
1	C	2	ARG
1	C	72	ARG
1	C	73	VAL
1	C	95	PHE
1	C	126	LYS
1	C	158	TYR

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Mol	Chain	Res	Type
1	C	226	GLU
1	C	235	GLU
1	D	9	THR
1	D	10	ASP
1	D	15	ARG
1	D	17	GLU
1	D	61	ARG
1	D	95	PHE
1	D	98	GLU
1	D	105	CYS
1	D	110	ASP
1	D	123	LYS
1	D	126	LYS
1	D	158	TYR
1	D	235	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	B	78	HIS
1	C	57	GLN
1	C	78	HIS
1	D	78	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	POP	A	3953	2	8,8,8	0.61	0	13,13,13	1.24	1 (7%)
3	ATP	A	737	2	33,33,33	0.87	1 (3%)	52,52,52	2.14	10 (19%)
4	POP	B	3954	2	8,8,8	0.65	0	13,13,13	1.30	2 (15%)
3	ATP	B	738	2	33,33,33	0.93	2 (6%)	52,52,52	2.12	9 (17%)
4	POP	C	3955	2	8,8,8	0.70	0	13,13,13	1.30	1 (7%)
3	ATP	C	739	2	33,33,33	0.94	2 (6%)	52,52,52	2.11	8 (15%)
4	POP	D	3956	2	8,8,8	0.58	0	13,13,13	1.30	2 (15%)
3	ATP	D	740	2	33,33,33	0.84	1 (3%)	52,52,52	2.10	8 (15%)

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
4	POP	A	3953	2	-	0/6/6/6	0/0/0/0
3	ATP	A	737	2	-	0/22/38/38	0/1/3/3
4	POP	B	3954	2	-	0/6/6/6	0/0/0/0
3	ATP	B	738	2	-	0/22/38/38	0/1/3/3
4	POP	C	3955	2	-	0/6/6/6	0/0/0/0
3	ATP	C	739	2	-	0/22/38/38	0/1/3/3
4	POP	D	3956	2	-	0/6/6/6	0/0/0/0
3	ATP	D	740	2	-	0/22/38/38	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	739	ATP	C2-N3	3.41	1.38	1.32
3	D	740	ATP	C2-N3	3.27	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	737	ATP	C2-N3	3.17	1.38	1.32
3	B	738	ATP	C2-N3	3.05	1.38	1.32
3	B	738	ATP	C2-N1	2.37	1.38	1.33
3	C	739	ATP	C2-N1	2.22	1.38	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	740	ATP	N3-C2-N1	-11.43	119.16	128.71
3	A	737	ATP	N3-C2-N1	-11.06	119.47	128.71
3	B	738	ATP	N3-C2-N1	-10.53	119.91	128.71
3	C	739	ATP	N3-C2-N1	-10.34	120.06	128.71
3	A	737	ATP	O4'-C1'-N9	6.36	114.36	108.44
3	C	739	ATP	O4'-C1'-N9	5.63	113.68	108.44
3	D	740	ATP	O4'-C1'-N9	5.36	113.42	108.44
3	B	738	ATP	O4'-C1'-N9	5.35	113.41	108.44
3	B	738	ATP	O3A-PB-O3B	4.53	110.88	101.66
3	C	739	ATP	O3A-PB-O3B	4.27	110.35	101.66
3	C	739	ATP	N3-C4-N9	3.35	131.47	125.43
3	B	738	ATP	N3-C4-N9	3.27	131.34	125.43
3	A	737	ATP	N3-C4-N9	3.26	131.33	125.43
4	C	3955	POP	P2-O-P1	-3.18	122.18	131.74
3	C	739	ATP	C4'-O4'-C1'	-3.13	106.34	109.75
3	B	738	ATP	C3'-C2'-C1'	3.05	105.68	100.91
3	D	740	ATP	PA-O3A-PB	-3.04	122.76	131.68
3	B	738	ATP	PA-O3A-PB	-2.98	122.93	131.68
3	C	739	ATP	C3'-C2'-C1'	2.96	105.54	100.91
4	D	3956	POP	P2-O-P1	-2.95	122.87	131.74
3	D	740	ATP	N3-C4-N9	2.92	130.70	125.43
4	A	3953	POP	P2-O-P1	-2.91	123.00	131.74
4	B	3954	POP	P2-O-P1	-2.85	123.19	131.74
3	A	737	ATP	PB-O3B-PG	-2.84	123.36	131.68
3	A	737	ATP	C3'-C2'-C1'	2.82	105.33	100.91
3	D	740	ATP	C4'-O4'-C1'	-2.82	106.69	109.75
3	D	740	ATP	C3'-C2'-C1'	2.60	104.98	100.91
3	A	737	ATP	C4'-O4'-C1'	-2.60	106.93	109.75
3	B	738	ATP	C4'-O4'-C1'	-2.55	106.97	109.75
3	B	738	ATP	PB-O3B-PG	-2.53	124.27	131.68
3	D	740	ATP	C4-C5-N7	-2.48	107.39	109.52
3	C	739	ATP	PA-O3A-PB	-2.45	124.49	131.68
3	A	737	ATP	C4-C5-N7	-2.42	107.45	109.52
3	C	739	ATP	PB-O3B-PG	-2.38	124.70	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3954	POP	O2-P1-O	2.28	111.56	104.29
3	A	737	ATP	C2-N3-C4	2.20	120.28	114.01
3	D	740	ATP	C2-N3-C4	2.18	120.21	114.01
3	A	737	ATP	C5-C4-N3	-2.17	120.97	125.70
3	A	737	ATP	PA-O3A-PB	-2.13	125.44	131.68
3	B	738	ATP	C5-C4-N3	-2.05	121.23	125.70
4	D	3956	POP	O5-P2-O	2.05	110.81	104.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	249/278 (89%)	1.12	38 (15%) 3 4	4, 12, 19, 25	0
1	B	249/278 (89%)	1.17	50 (20%) 2 2	5, 12, 19, 25	0
1	C	249/278 (89%)	1.21	48 (19%) 2 2	5, 12, 19, 25	0
1	D	249/278 (89%)	1.03	32 (12%) 4 6	4, 12, 19, 26	0
All	All	996/1112 (89%)	1.13	168 (16%) 2 3	4, 12, 19, 26	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72	ARG	7.9
1	B	72	ARG	7.3
1	C	11	GLY	6.9
1	B	9	THR	6.8
1	C	73	VAL	6.8
1	D	72	ARG	6.7
1	A	9	THR	6.6
1	B	8	LYS	6.3
1	B	73	VAL	6.0
1	C	9	THR	5.6
1	B	10	ASP	5.4
1	A	73	VAL	5.3
1	D	73	VAL	5.2
1	A	72	ARG	5.2
1	B	11	GLY	5.1
1	A	11	GLY	5.1
1	C	249	GLY	5.0
1	A	10	ASP	4.9
1	C	8	LYS	4.8
1	A	8	LYS	4.7
1	C	10	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	7	TYR	4.6
1	D	9	THR	4.4
1	C	235	GLU	4.3
1	A	249	GLY	4.3
1	A	110	ASP	4.3
1	D	110	ASP	4.2
1	C	21	LYS	4.1
1	C	24	GLU	4.1
1	B	125	ALA	4.0
1	A	13	VAL	4.0
1	A	31	ASN	3.9
1	A	82	GLU	3.8
1	C	7	TYR	3.8
1	D	11	GLY	3.8
1	C	71	GLY	3.8
1	B	109	PRO	3.8
1	B	21	LYS	3.7
1	D	235	GLU	3.7
1	A	123	LYS	3.7
1	C	83	ASN	3.6
1	C	70	THR	3.6
1	B	110	ASP	3.6
1	B	82	GLU	3.5
1	A	235	GLU	3.5
1	B	24	GLU	3.5
1	D	239	ARG	3.4
1	D	176	LEU	3.4
1	B	36	GLU	3.3
1	C	14	LYS	3.3
1	B	14	LYS	3.2
1	A	14	LYS	3.2
1	A	7	TYR	3.2
1	D	14	LYS	3.2
1	C	18	GLU	3.2
1	D	123	LYS	3.1
1	C	12	HIS	3.1
1	C	82	GLU	3.1
1	A	109	PRO	3.1
1	B	71	GLY	3.1
1	C	110	ASP	3.1
1	C	81	PRO	3.0
1	A	119	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	39	ASN	3.0
1	C	94	LYS	3.0
1	C	239	ARG	3.0
1	A	239	ARG	3.0
1	B	83	ASN	3.0
1	D	109	PRO	2.9
1	C	90	LYS	2.9
1	C	39	ASN	2.9
1	A	12	HIS	2.9
1	B	239	ARG	2.9
1	A	23	LEU	2.9
1	B	176	LEU	2.9
1	D	21	LYS	2.9
1	B	12	HIS	2.9
1	C	22	ARG	2.9
1	B	177	ILE	2.9
1	B	235	GLU	2.8
1	B	175	ILE	2.8
1	B	123	LYS	2.7
1	D	90	LYS	2.7
1	C	139	VAL	2.7
1	A	18	GLU	2.7
1	A	83	ASN	2.7
1	B	61	ARG	2.7
1	B	190	VAL	2.7
1	D	44	VAL	2.7
1	D	83	ASN	2.7
1	C	125	ALA	2.7
1	C	148	ILE	2.6
1	D	125	ALA	2.6
1	B	90	LYS	2.6
1	B	31	ASN	2.6
1	A	36	GLU	2.6
1	C	137	VAL	2.6
1	B	18	GLU	2.6
1	D	148	ILE	2.6
1	B	249	GLY	2.6
1	B	13	VAL	2.6
1	D	149	VAL	2.6
1	A	176	LEU	2.6
1	B	148	ILE	2.5
1	A	70	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	15	ARG	2.5
1	A	149	VAL	2.5
1	C	176	LEU	2.5
1	C	93	GLU	2.5
1	A	22	ARG	2.4
1	D	24	GLU	2.4
1	A	117	ILE	2.4
1	B	136	GLY	2.4
1	B	26	GLU	2.4
1	A	203	LYS	2.4
1	D	8	LYS	2.4
1	A	32	GLN	2.4
1	D	10	ASP	2.4
1	D	177	ILE	2.4
1	C	38	GLU	2.4
1	C	31	ASN	2.4
1	D	119	VAL	2.4
1	D	56	LEU	2.3
1	C	175	ILE	2.3
1	D	212	LYS	2.3
1	A	24	GLU	2.3
1	A	96	GLU	2.3
1	D	153	ILE	2.3
1	B	92	VAL	2.3
1	D	190	VAL	2.3
1	B	147	PHE	2.3
1	C	129	ASP	2.3
1	B	197	ILE	2.3
1	D	82	GLU	2.2
1	A	153	ILE	2.2
1	C	153	ILE	2.2
1	B	149	VAL	2.2
1	C	17	GLU	2.2
1	C	26	GLU	2.2
1	C	96	GLU	2.2
1	B	22	ARG	2.2
1	C	119	VAL	2.2
1	B	126	LYS	2.1
1	D	175	ILE	2.1
1	D	159	ALA	2.1
1	B	189	TYR	2.1
1	B	119	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	219	GLU	2.1
1	D	141	ARG	2.1
1	C	80	SER	2.1
1	A	202	GLU	2.1
1	C	15	ARG	2.1
1	A	148	ILE	2.1
1	A	147	PHE	2.1
1	B	29	LEU	2.1
1	B	93	GLU	2.1
1	C	147	PHE	2.1
1	C	149	VAL	2.1
1	C	177	ILE	2.1
1	B	89	LYS	2.1
1	C	133	ARG	2.0
1	B	81	PRO	2.0
1	A	177	ILE	2.0
1	B	15	ARG	2.0
1	B	141	ARG	2.0
1	B	219	GLU	2.0
1	D	219	GLU	2.0
1	C	29	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	C	5003	1/1	0.16	3.35	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	D	5004	1/1	0.12	2.36	29,29,29,29	0
3	ATP	D	740	31/31	0.14	0.38	15,16,36,37	0
3	ATP	C	739	31/31	0.15	0.21	16,21,48,48	0
3	ATP	B	738	31/31	0.16	0.17	18,20,47,47	0
4	POP	C	3955	9/9	0.19	-0.18	62,63,63,64	0
4	POP	D	3956	9/9	0.15	-0.24	29,34,36,37	0
3	ATP	A	737	31/31	0.13	-0.28	14,17,35,37	0
4	POP	A	3953	9/9	0.15	-0.30	34,37,39,39	0
4	POP	B	3954	9/9	0.18	-0.31	38,41,43,43	0
2	MG	B	5002	1/1	0.08	-0.73	42,42,42,42	0
2	MG	A	5001	1/1	0.09	-0.79	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.