



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:54 PM 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 X-ray Structure 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/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 : rb-20026688
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

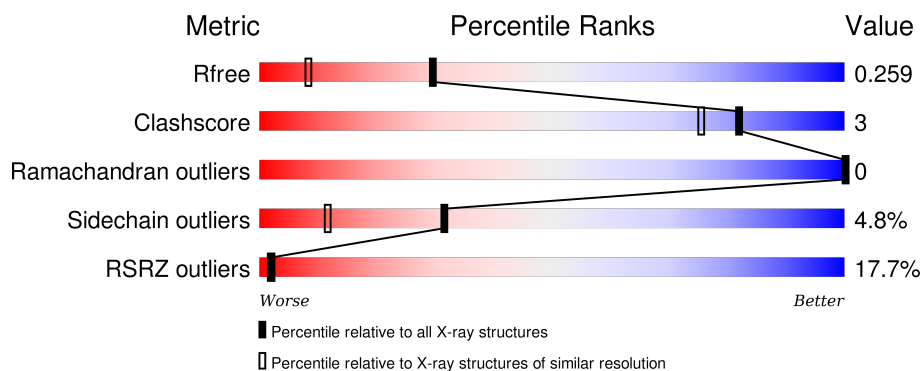
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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. 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	278	<div> <div>15%</div> <div>77%</div> <div>11%</div> <div>•</div> <div>10%</div> </div>
1	B	278	<div> <div>17%</div> <div>79%</div> <div>10%</div> <div></div> <div>10%</div> </div>
1	C	278	<div> <div>18%</div> <div>80%</div> <div>9%</div> <div></div> <div>10%</div> </div>
1	D	278	<div> <div>13%</div> <div>79%</div> <div>10%</div> <div></div> <div>10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8423 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 Probable inorganic polyphosphate/ATP-NAD kinase.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

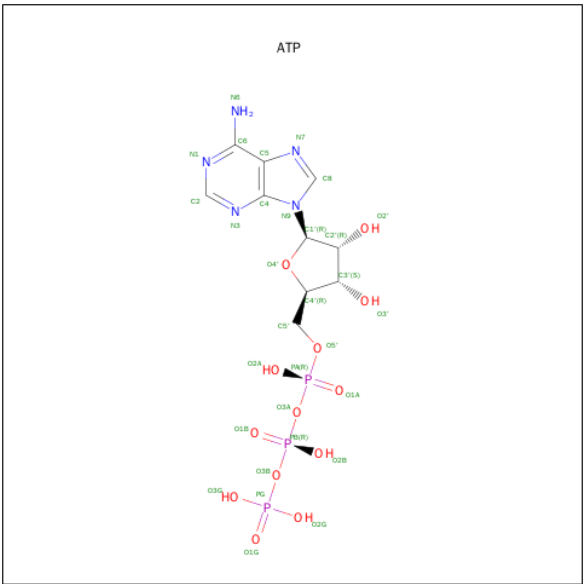
Continued from previous page...

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).

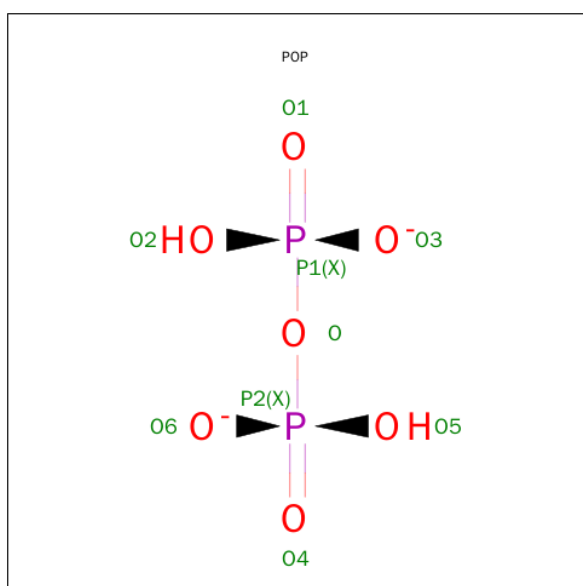
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- 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		

Continued on next page...

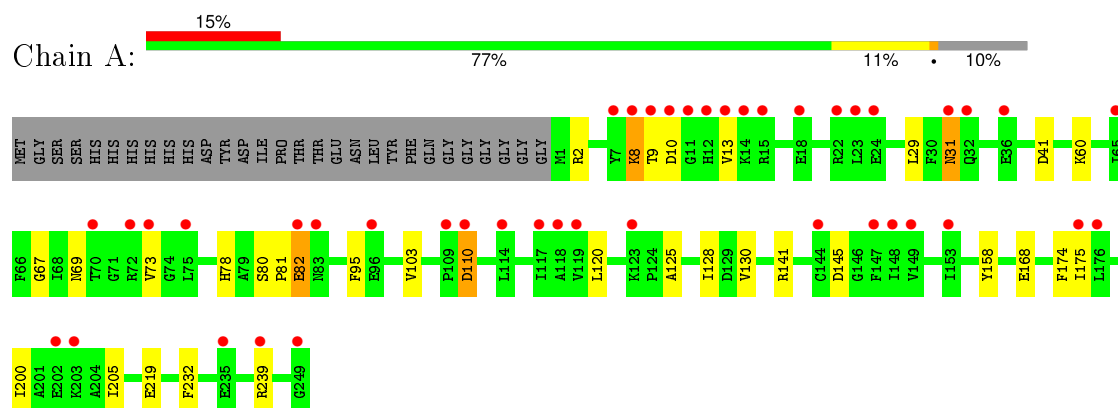
Continued from previous page...

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

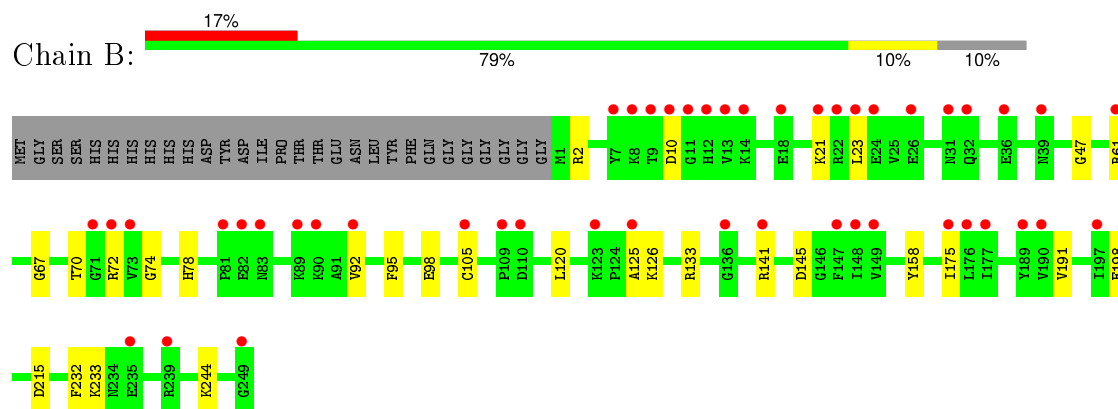
3 Residue-property plots

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.

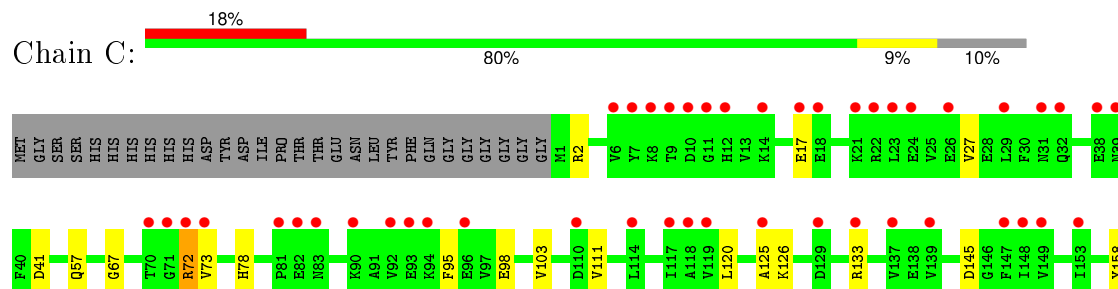
- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

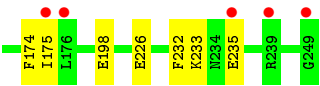


- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

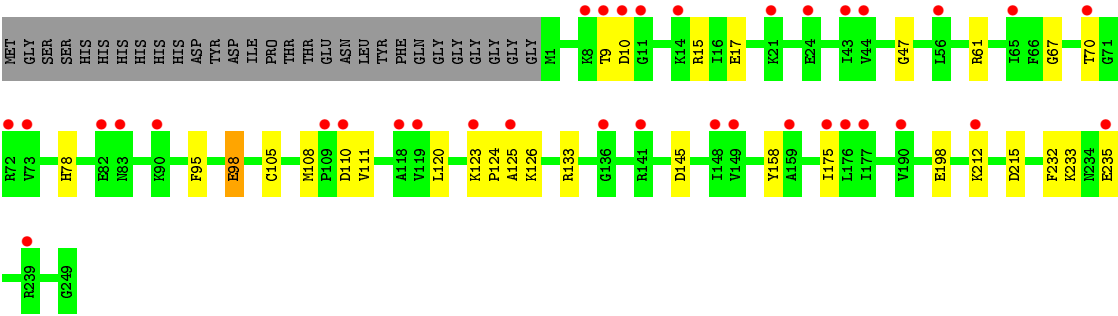
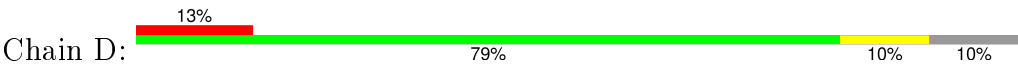


- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase





● Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase



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) 80.8 (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 0.232 , 0.259	Depositor DCC
R_{free} test set	5111 reflections (5.58%)	DCC
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.

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

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($^{\circ}$)	Ideal($^{\circ}$)
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

Continued on next page...

Continued from previous page...

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 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	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

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 3.

All (52) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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	Interatomic distance (Å)	Clash overlap (Å)
5:B:5085:HOH:O	5:C:5096:HOH:O[1_554]	2.05	0.15

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	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%)	29	10
1	B	213/235 (91%)	204 (96%)	9 (4%)	36	14
1	C	213/235 (91%)	205 (96%)	8 (4%)	40	17
1	D	213/235 (91%)	200 (94%)	13 (6%)	23	7
All	All	852/940 (91%)	811 (95%)	41 (5%)	31	12

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	126	LYS
1	C	158	TYR
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 [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

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	0.62	0	13,13,13	1.22	1 (7%)
3	ATP	A	737	2	24,33,33	1.02	1 (4%)	31,52,52	2.54	6 (19%)
4	POP	B	3954	2	8,8,8	0.66	0	13,13,13	1.26	1 (7%)
3	ATP	B	738	2	24,33,33	1.03	2 (8%)	31,52,52	2.44	5 (16%)
4	POP	C	3955	2	8,8,8	0.70	0	13,13,13	1.29	1 (7%)
3	ATP	C	739	2	24,33,33	1.07	2 (8%)	31,52,52	2.41	5 (16%)
4	POP	D	3956	2	8,8,8	0.60	0	13,13,13	1.27	1 (7%)
3	ATP	D	740	2	24,33,33	1.00	1 (4%)	31,52,52	2.59	6 (19%)

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	-	0/18/38/38	0/3/3/3
4	POP	B	3954	2	-	0/6/6/6	0/0/0/0
3	ATP	B	738	2	-	0/18/38/38	0/3/3/3
4	POP	C	3955	2	-	0/6/6/6	0/0/0/0
3	ATP	C	739	2	-	0/18/38/38	0/3/3/3
4	POP	D	3956	2	-	0/6/6/6	0/0/0/0
3	ATP	D	740	2	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	739	ATP	C2-N1	2.31	1.38	1.33
3	B	738	ATP	C2-N1	2.47	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	738	ATP	C2-N3	3.40	1.38	1.32
3	A	737	ATP	C2-N3	3.54	1.38	1.32
3	D	740	ATP	C2-N3	3.65	1.38	1.32
3	C	739	ATP	C2-N3	3.81	1.38	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	740	ATP	N3-C2-N1	-12.72	119.16	128.89
3	A	737	ATP	N3-C2-N1	-12.31	119.47	128.89
3	B	738	ATP	N3-C2-N1	-11.74	119.91	128.89
3	C	739	ATP	N3-C2-N1	-11.54	120.06	128.89
4	C	3955	POP	P2-O-P1	-3.76	122.18	132.73
3	D	740	ATP	PA-O3A-PB	-3.55	122.76	132.73
4	D	3956	POP	P2-O-P1	-3.51	122.87	132.73
3	B	738	ATP	PA-O3A-PB	-3.49	122.93	132.73
4	A	3953	POP	P2-O-P1	-3.46	123.00	132.73
4	B	3954	POP	P2-O-P1	-3.40	123.19	132.73
3	C	739	ATP	C4'-O4'-C1'	-3.07	106.34	109.72
3	C	739	ATP	PA-O3A-PB	-2.94	124.49	132.73
3	A	737	ATP	PB-O3B-PG	-2.78	123.36	132.67
3	D	740	ATP	C4'-O4'-C1'	-2.76	106.69	109.72
3	A	737	ATP	PA-O3A-PB	-2.60	125.44	132.73
3	A	737	ATP	C4'-O4'-C1'	-2.54	106.93	109.72
3	B	738	ATP	PB-O3B-PG	-2.50	124.27	132.67
3	B	738	ATP	C4'-O4'-C1'	-2.50	106.97	109.72
3	C	739	ATP	PB-O3B-PG	-2.38	124.70	132.67
3	D	740	ATP	C4-C5-N7	-2.27	107.39	109.48
3	A	737	ATP	C4-C5-N7	-2.21	107.45	109.48
3	D	740	ATP	PB-O3B-PG	-2.03	125.86	132.67
3	B	738	ATP	O4'-C1'-N9	2.54	113.41	108.10
3	D	740	ATP	O4'-C1'-N9	2.54	113.42	108.10
3	C	739	ATP	O4'-C1'-N9	2.67	113.68	108.10
3	A	737	ATP	O4'-C1'-N9	2.99	114.36	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3953	POP	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 ⓘ

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%)	1.16	43 (17%) 2 2	4, 12, 19, 25	0
1	B	249/278 (89%)	1.20	47 (18%) 2 1	5, 12, 19, 25	0
1	C	249/278 (89%)	1.26	51 (20%) 1 1	5, 12, 19, 25	0
1	D	249/278 (89%)	1.07	35 (14%) 4 4	4, 12, 19, 26	0
All	All	996/1112 (89%)	1.17	176 (17%) 2 2	4, 12, 19, 26	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72	ARG	8.5
1	C	11	GLY	7.4
1	A	9	THR	7.3
1	C	73	VAL	7.3
1	B	72	ARG	7.1
1	B	9	THR	7.1
1	D	72	ARG	7.0
1	B	8	LYS	7.0
1	C	9	THR	6.4
1	B	73	VAL	6.1
1	A	72	ARG	5.7
1	B	11	GLY	5.6
1	D	73	VAL	5.6
1	C	249	GLY	5.4
1	A	10	ASP	5.4
1	D	9	THR	5.4
1	A	73	VAL	5.2
1	A	11	GLY	5.1
1	A	8	LYS	5.1
1	B	7	TYR	4.9
1	B	10	ASP	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	8	LYS	4.7
1	C	10	ASP	4.7
1	D	11	GLY	4.5
1	A	13	VAL	4.4
1	C	21	LYS	4.3
1	C	235	GLU	4.3
1	A	110	ASP	4.3
1	C	24	GLU	4.2
1	A	31	ASN	4.2
1	D	110	ASP	4.1
1	A	249	GLY	4.1
1	B	109	PRO	4.1
1	A	82	GLU	4.0
1	C	7	TYR	3.9
1	C	70	THR	3.9
1	C	71	GLY	3.9
1	B	24	GLU	3.8
1	D	235	GLU	3.7
1	A	123	LYS	3.7
1	C	12	HIS	3.7
1	B	125	ALA	3.7
1	B	12	HIS	3.6
1	B	110	ASP	3.6
1	B	21	LYS	3.6
1	A	14	LYS	3.6
1	A	7	TYR	3.5
1	A	12	HIS	3.4
1	C	14	LYS	3.4
1	D	239	ARG	3.4
1	C	39	ASN	3.4
1	A	235	GLU	3.4
1	B	14	LYS	3.4
1	C	83	ASN	3.4
1	B	82	GLU	3.4
1	B	36	GLU	3.3
1	B	39	ASN	3.3
1	D	176	LEU	3.3
1	B	123	LYS	3.2
1	C	110	ASP	3.2
1	B	71	GLY	3.2
1	C	82	GLU	3.2
1	C	125	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	14	LYS	3.1
1	C	18	GLU	3.1
1	D	8	LYS	3.1
1	B	175	ILE	3.1
1	A	119	VAL	3.1
1	B	83	ASN	3.1
1	C	94	LYS	3.1
1	D	123	LYS	3.1
1	D	109	PRO	3.0
1	C	148	ILE	3.0
1	C	90	LYS	3.0
1	D	149	VAL	3.0
1	B	90	LYS	3.0
1	A	23	LEU	2.9
1	B	31	ASN	2.9
1	D	44	VAL	2.9
1	B	235	GLU	2.9
1	B	148	ILE	2.9
1	B	13	VAL	2.9
1	B	239	ARG	2.9
1	B	92	VAL	2.9
1	C	239	ARG	2.9
1	D	90	LYS	2.8
1	C	22	ARG	2.8
1	A	18	GLU	2.8
1	B	190	VAL	2.8
1	A	109	PRO	2.8
1	A	22	ARG	2.8
1	A	83	ASN	2.8
1	A	149	VAL	2.8
1	A	239	ARG	2.7
1	B	149	VAL	2.7
1	C	81	PRO	2.7
1	C	139	VAL	2.7
1	D	148	ILE	2.7
1	D	21	LYS	2.7
1	A	203	LYS	2.7
1	B	18	GLU	2.6
1	A	148	ILE	2.6
1	C	175	ILE	2.6
1	A	176	LEU	2.6
1	C	137	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	176	LEU	2.6
1	C	38	GLU	2.6
1	D	83	ASN	2.6
1	A	70	THR	2.6
1	D	24	GLU	2.6
1	A	117	ILE	2.6
1	C	31	ASN	2.5
1	A	32	GLN	2.5
1	D	190	VAL	2.5
1	D	212	LYS	2.5
1	C	93	GLU	2.5
1	B	136	GLY	2.5
1	C	149	VAL	2.4
1	A	24	GLU	2.4
1	D	82	GLU	2.4
1	D	175	ILE	2.4
1	A	36	GLU	2.4
1	D	10	ASP	2.4
1	D	118	ALA	2.4
1	A	15	ARG	2.4
1	C	129	ASP	2.4
1	C	119	VAL	2.4
1	B	81	PRO	2.4
1	B	197	ILE	2.3
1	B	22	ARG	2.3
1	C	23	LEU	2.3
1	D	65	ILE	2.3
1	B	61	ARG	2.3
1	D	56	LEU	2.3
1	B	177	ILE	2.3
1	A	96	GLU	2.3
1	B	147	PHE	2.3
1	D	125	ALA	2.3
1	D	43	ILE	2.3
1	B	189	TYR	2.3
1	C	176	LEU	2.2
1	A	153	ILE	2.2
1	D	159	ALA	2.2
1	C	117	ILE	2.2
1	A	147	PHE	2.2
1	D	70	THR	2.2
1	D	136	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	144	CYS	2.2
1	C	29	LEU	2.2
1	C	6	VAL	2.2
1	B	26	GLU	2.2
1	B	89	LYS	2.2
1	C	118	ALA	2.2
1	C	147	PHE	2.1
1	B	141	ARG	2.1
1	C	92	VAL	2.1
1	D	119	VAL	2.1
1	D	141	ARG	2.1
1	B	32	GLN	2.1
1	C	32	GLN	2.1
1	A	202	GLU	2.1
1	C	96	GLU	2.1
1	A	114	LEU	2.1
1	A	65	ILE	2.1
1	A	175	ILE	2.1
1	B	249	GLY	2.1
1	B	23	LEU	2.1
1	C	17	GLU	2.1
1	C	153	ILE	2.1
1	B	105	CYS	2.1
1	C	114	LEU	2.1
1	C	133	ARG	2.0
1	A	75	LEU	2.0
1	C	26	GLU	2.0
1	D	177	ILE	2.0
1	A	118	ALA	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 [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
3	ATP	D	740	31/31	0.92	0.14	0.31	15,16,36,37	0
3	ATP	B	738	31/31	0.85	0.16	0.12	18,20,47,47	0
3	ATP	C	739	31/31	0.89	0.15	0.08	16,21,48,48	0
4	POP	C	3955	9/9	0.79	0.20	-0.15	62,63,63,64	0
3	ATP	A	737	31/31	0.91	0.13	-0.25	14,17,35,37	0
4	POP	A	3953	9/9	0.84	0.15	-0.25	34,37,39,39	0
4	POP	D	3956	9/9	0.89	0.15	-0.27	29,34,36,37	0
4	POP	B	3954	9/9	0.86	0.17	-0.31	38,41,43,43	0
2	MG	D	5004	1/1	0.92	0.10	-	29,29,29,29	0
2	MG	A	5001	1/1	0.89	0.09	-	32,32,32,32	0
2	MG	C	5003	1/1	0.89	0.14	-	37,37,37,37	0
2	MG	B	5002	1/1	0.87	0.07	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.