



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:58 AM GMT

PDB ID : 2JJX  
Title : THE CRYSTAL STRUCTURE OF UMP KINASE FROM BACILLUS ANTHRACIS (BA1797)  
Authors : Meier, C.; Carter, L.G.; Mancini, E.J.; Owens, R.J.; Stuart, D.I.; Esnouf, R.M.; Oxford Protein Production Facility (Oppf); Structural Proteomics in Europe (Spine)  
Deposited on : 2008-04-23  
Resolution : 2.82 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](mailto: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.

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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

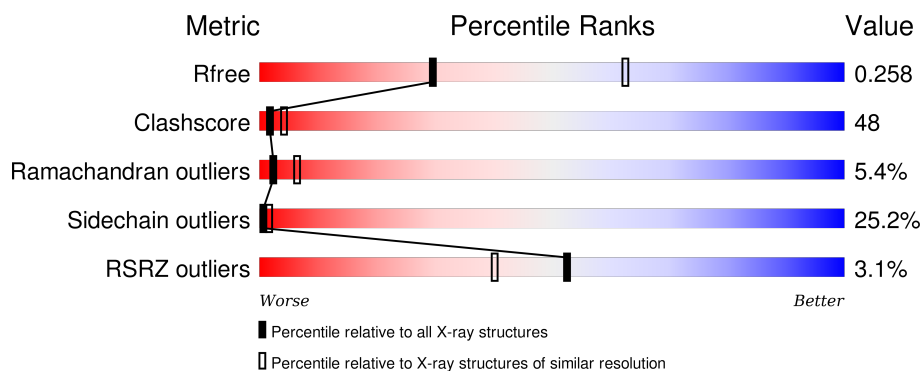
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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  $\geq 3$ , 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	255	<div> <div>4%</div> <div>37% 43% 15% .</div> </div>
1	B	255	<div> <div>2%</div> <div>35% 42% 17% . .</div> </div>
1	C	255	<div> <div>3%</div> <div>37% 43% 15% . .</div> </div>

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
2	ATP	A	1246	X	-	-	-
2	ATP	B	1246	X	-	-	X
2	ATP	C	1246	X	-	-	X

## 2 Entry composition [i](#)

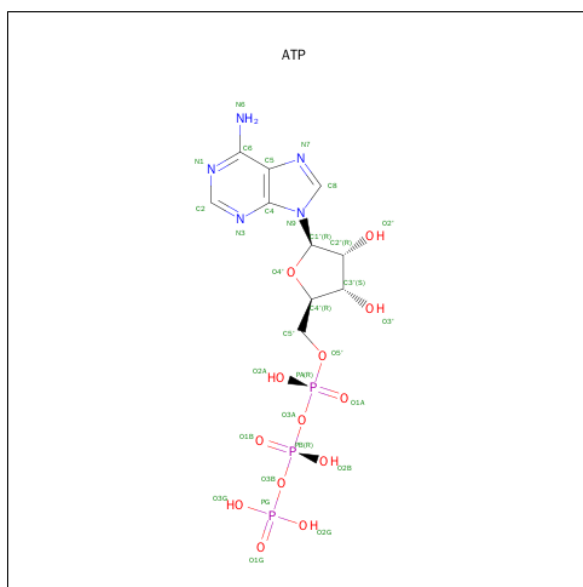
There are 4 unique types of molecules in this entry. The entry contains 5909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 URIDYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1891	1192	341	351	7			
1	B	244	Total	C	N	O	S	0	0	0
			1891	1192	341	351	7			
1	C	244	Total	C	N	O	S	0	0	0
			1891	1192	341	351	7			

- 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	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		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Mg 1	0	0

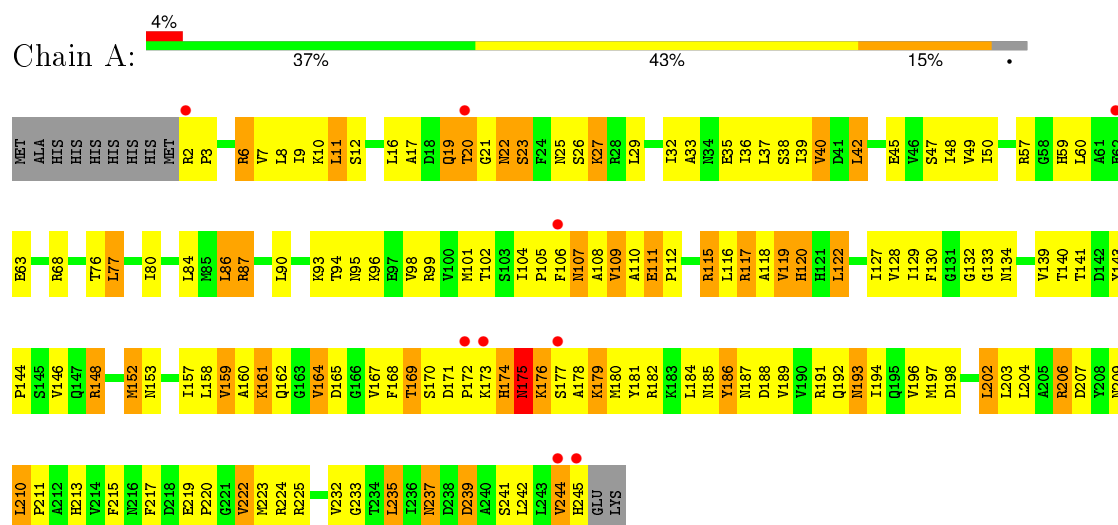
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total 48	O 48	0	0
4	B	47	Total 47	O 47	0	0
4	C	47	Total 47	O 47	0	0

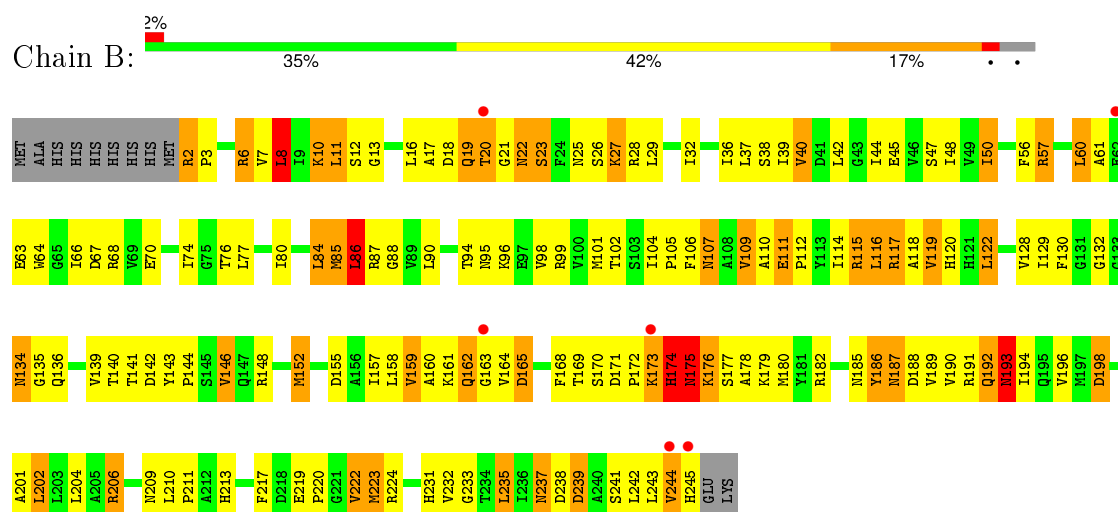
### 3 Residue-property plots

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: URIDYLATE KINASE

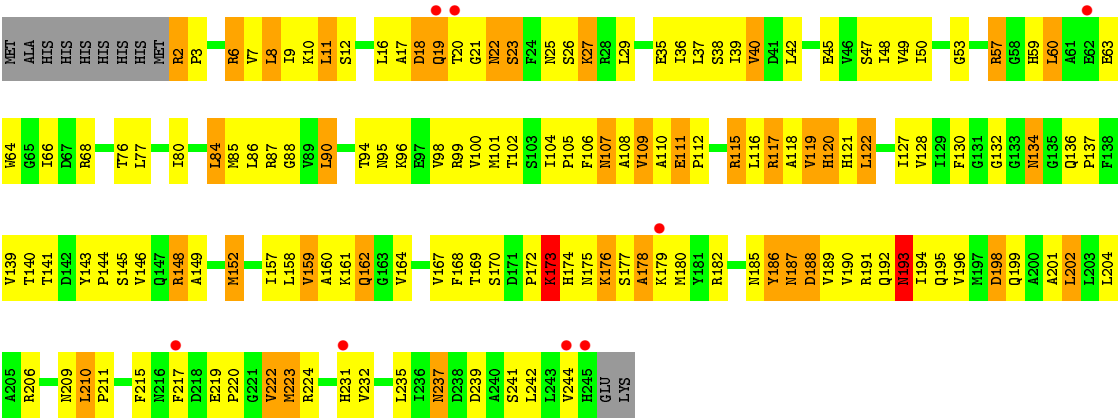


#### • Molecule 1: URIDYLATE KINASE



#### • Molecule 1: URIDYLATE KINASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.30 Å 87.30 Å 383.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.82 35.17 – 2.72	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.82) 95.9 (35.17-2.72)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.72 Å)	Xtriage
Refinement program	BUSTER	Depositor
R, $R_{free}$	0.200 , 0.252 0.216 , 0.258	Depositor DCC
$R_{free}$ test set	1069 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 79.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	6 of 23460 reflections (0.026%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.59	0/1923	0.83	1/2604 (0.0%)
1	B	0.55	0/1923	0.83	1/2604 (0.0%)
1	C	0.58	0/1923	0.81	1/2604 (0.0%)
All	All	0.57	0/5769	0.82	3/7812 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASN	N-CA-C	5.26	125.21	111.00
1	C	178	ALA	N-CA-C	-5.03	97.42	111.00
1	B	8	LEU	CB-CG-CD2	5.00	119.50	111.00

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	1891	0	1907	175	0
1	B	1891	0	1907	194	0
1	C	1891	0	1907	187	0
2	A	31	0	12	8	0
2	B	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	12	3	0
3	C	1	0	0	0	0
4	A	48	0	0	10	0
4	B	47	0	0	15	0
4	C	47	0	0	11	0
All	All	5909	0	5757	556	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 48.

All (556) 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:B:94:THR:HG22	1:B:96:LYS:H	1.09	1.11
1:A:94:THR:HG22	1:A:96:LYS:H	1.07	1.10
1:C:94:THR:HG22	1:C:96:LYS:H	1.08	1.10
1:C:80:ILE:HD13	1:C:106:PHE:HE2	1.01	1.10
1:A:80:ILE:HD13	1:A:106:PHE:HE2	1.05	1.10
1:A:39:ILE:HD11	1:A:223:MET:HG2	1.34	1.09
1:C:80:ILE:HD13	1:C:106:PHE:CE2	1.88	1.08
1:A:80:ILE:HD13	1:A:106:PHE:CE2	1.89	1.07
1:B:80:ILE:HD13	1:B:106:PHE:HE2	1.18	1.04
1:B:101:MET:HE1	1:B:118:ALA:HA	1.38	1.02
1:C:101:MET:HE1	1:C:118:ALA:HA	1.42	0.99
1:A:101:MET:HE1	1:A:118:ALA:HA	1.42	0.99
1:A:194:ILE:HG22	1:A:196:VAL:HG23	1.48	0.95
1:C:185:ASN:HB3	1:C:188:ASP:HB2	1.49	0.94
1:B:80:ILE:HD13	1:B:106:PHE:CE2	2.02	0.93
1:B:116:LEU:H	1:B:116:LEU:HD12	1.31	0.93
1:B:39:ILE:HD11	1:B:223:MET:HG2	1.48	0.92
1:A:115:ARG:HH11	1:A:115:ARG:HG2	1.33	0.91
1:C:116:LEU:H	1:C:116:LEU:HD12	1.37	0.90
1:A:94:THR:HG22	1:A:96:LYS:N	1.86	0.89
1:B:94:THR:HG22	1:B:96:LYS:N	1.89	0.87
1:C:173:LYS:HE3	1:C:174:HIS:CE1	2.10	0.86
1:C:189:VAL:CG1	1:C:202:LEU:HD11	2.06	0.86
1:A:116:LEU:HD12	1:A:116:LEU:H	1.41	0.86
1:A:39:ILE:HD11	1:A:223:MET:CG	2.06	0.85
1:B:194:ILE:HG22	1:B:196:VAL:HG23	1.58	0.84
1:B:186:TYR:O	1:B:189:VAL:HG12	1.77	0.84
1:B:122:LEU:HD13	1:B:128:VAL:HG13	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:HG21	1:B:158:LEU:HD11	1.60	0.83
1:A:160:ALA:HB1	1:A:217:PHE:HB2	1.57	0.83
1:C:39:ILE:HD11	1:C:223:MET:HG2	1.58	0.83
1:B:160:ALA:HB1	1:B:217:PHE:HB2	1.61	0.82
1:A:186:TYR:O	1:A:189:VAL:HG12	1.79	0.82
1:A:122:LEU:HD13	1:A:128:VAL:HG13	1.59	0.82
1:B:60:LEU:HB2	4:B:2016:HOH:O	1.79	0.82
1:C:94:THR:HG22	1:C:96:LYS:N	1.93	0.82
1:B:2:ARG:HG2	1:B:3:PRO:N	1.94	0.82
1:C:87:ARG:HG3	1:C:98:VAL:HG22	1.63	0.81
1:C:186:TYR:O	1:C:189:VAL:HG12	1.80	0.81
1:B:7:VAL:HG21	1:B:158:LEU:CD1	2.10	0.81
1:B:6:ARG:NH1	1:B:45:GLU:OE1	2.14	0.80
1:A:189:VAL:HG23	1:A:194:ILE:HB	1.63	0.80
1:A:80:ILE:CD1	1:A:106:PHE:HE2	1.92	0.79
1:C:36:ILE:HD13	1:C:48:ILE:HD13	1.65	0.79
1:B:189:VAL:CG1	1:B:202:LEU:HD11	2.13	0.79
1:B:39:ILE:HD11	1:B:223:MET:CG	2.12	0.79
1:B:168:PHE:CE2	1:B:180:MET:HB2	2.18	0.79
1:C:160:ALA:HB1	1:C:217:PHE:HB2	1.63	0.79
1:C:194:ILE:HD13	4:C:2031:HOH:O	1.82	0.78
1:A:189:VAL:CG1	1:A:202:LEU:HD11	2.12	0.78
1:C:101:MET:HE1	1:C:118:ALA:CA	2.13	0.78
1:B:101:MET:HE1	1:B:118:ALA:CA	2.12	0.78
1:C:188:ASP:O	1:C:192:GLN:HG3	1.84	0.77
1:C:122:LEU:CD1	1:C:128:VAL:HG13	2.14	0.77
1:C:36:ILE:HD13	1:C:48:ILE:CD1	2.14	0.77
2:B:1246:ATP:H5'1	1:C:117:ARG:HH12	1.47	0.77
1:B:185:ASN:OD1	1:B:239:ASP:O	2.02	0.77
1:A:107:ASN:HA	2:A:1246:ATP:N6	1.99	0.77
1:C:19:GLN:H	1:C:19:GLN:NE2	1.81	0.77
1:B:146:VAL:HG11	1:B:201:ALA:HB1	1.66	0.76
1:A:99:ARG:HD2	1:A:111:GLU:OE2	1.85	0.76
1:A:87:ARG:HG2	1:A:98:VAL:HG22	1.67	0.76
1:C:122:LEU:HD13	1:C:128:VAL:HG13	1.66	0.76
1:A:19:GLN:H	1:A:19:GLN:NE2	1.82	0.76
1:A:6:ARG:NH1	1:A:45:GLU:OE1	2.18	0.76
1:C:87:ARG:HG3	1:C:98:VAL:CG2	2.14	0.76
1:C:6:ARG:HH11	1:C:6:ARG:HG3	1.51	0.76
1:A:175:ASN:O	1:A:177:SER:N	2.18	0.76
1:A:101:MET:HE1	1:A:118:ALA:CA	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ARG:HG2	1:C:115:ARG:HH11	1.51	0.75
1:B:19:GLN:H	1:B:19:GLN:NE2	1.83	0.75
1:C:2:ARG:HG2	1:C:3:PRO:N	2.01	0.75
1:A:108:ALA:HA	4:B:2024:HOH:O	1.85	0.75
1:C:193:ASN:OD1	1:C:195:GLN:NE2	2.18	0.75
1:A:115:ARG:NH1	1:A:115:ARG:HG2	2.00	0.74
1:A:6:ARG:HH11	1:A:6:ARG:HG3	1.49	0.74
1:C:194:ILE:HG22	1:C:196:VAL:HG23	1.68	0.74
1:C:168:PHE:CE2	1:C:180:MET:HB2	2.22	0.74
1:B:115:ARG:HG2	1:B:115:ARG:HH11	1.50	0.73
1:B:80:ILE:CD1	1:B:106:PHE:HE2	2.00	0.73
1:C:6:ARG:NH1	1:C:45:GLU:OE1	2.22	0.73
1:A:152:MET:HA	1:A:152:MET:HE2	1.70	0.73
1:A:105:PRO:HB3	1:A:112:PRO:HB3	1.70	0.73
1:C:189:VAL:HG23	1:C:194:ILE:HB	1.70	0.73
1:B:99:ARG:HD2	1:B:111:GLU:OE2	1.87	0.73
1:B:2:ARG:HG2	1:B:3:PRO:CD	2.18	0.73
1:A:19:GLN:H	1:A:19:GLN:CD	1.92	0.72
1:C:19:GLN:H	1:C:19:GLN:CD	1.93	0.72
1:B:217:PHE:HE1	1:B:223:MET:HE1	1.54	0.72
1:C:122:LEU:HD13	1:C:128:VAL:CG1	2.19	0.72
1:A:87:ARG:HG2	1:A:98:VAL:CG2	2.19	0.72
1:B:105:PRO:HB3	1:B:112:PRO:HB3	1.70	0.72
1:B:140:THR:HG22	1:B:141:THR:N	2.05	0.72
1:C:172:PRO:C	1:C:174:HIS:H	1.93	0.71
1:A:168:PHE:CE2	1:A:180:MET:HB2	2.24	0.71
1:C:76:THR:HG23	1:C:132:GLY:HA2	1.72	0.71
1:B:19:GLN:H	1:B:19:GLN:CD	1.93	0.71
1:B:36:ILE:HD13	1:B:48:ILE:CD1	2.22	0.70
1:C:117:ARG:NH2	2:C:1246:ATP:O1A	2.24	0.70
1:B:117:ARG:HH11	1:B:117:ARG:CG	2.03	0.70
1:B:39:ILE:HG22	4:B:2014:HOH:O	1.90	0.70
1:B:148:ARG:NH1	4:B:2032:HOH:O	2.23	0.70
1:A:185:ASN:OD1	1:A:239:ASP:O	2.09	0.70
1:A:217:PHE:CE1	1:A:223:MET:HE1	2.27	0.70
1:C:104:ILE:HB	1:C:106:PHE:CZ	2.27	0.70
1:A:219:GLU:O	1:A:222:VAL:HG13	1.92	0.70
1:B:44:ILE:HB	4:B:2014:HOH:O	1.91	0.69
1:C:185:ASN:ND2	1:C:239:ASP:O	2.25	0.69
1:C:224:ARG:NH1	4:C:2041:HOH:O	2.26	0.69
2:B:1246:ATP:H5'1	1:C:117:ARG:NH1	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ARG:HG2	1:C:3:PRO:CD	2.22	0.69
1:B:188:ASP:O	1:B:192:GLN:HG3	1.92	0.68
1:A:140:THR:HG22	1:A:141:THR:N	2.08	0.68
1:C:237:ASN:HB3	1:C:239:ASP:H	1.58	0.68
1:C:6:ARG:NH1	1:C:6:ARG:HG3	2.08	0.68
1:B:8:LEU:HD12	1:B:157:ILE:HG13	1.75	0.68
1:B:61:ALA:HA	4:B:2017:HOH:O	1.94	0.68
1:A:188:ASP:O	1:A:192:GLN:HG3	1.94	0.68
1:C:189:VAL:HG11	1:C:202:LEU:HD11	1.75	0.67
1:B:104:ILE:HB	1:B:106:PHE:CZ	2.29	0.67
1:C:80:ILE:CD1	1:C:106:PHE:HE2	1.94	0.67
1:B:94:THR:HG22	1:B:95:ASN:N	2.09	0.67
1:A:60:LEU:O	1:A:63:GLU:N	2.28	0.67
1:B:120:HIS:HD2	4:B:2025:HOH:O	1.77	0.67
1:C:105:PRO:HB3	1:C:112:PRO:HB3	1.75	0.66
1:B:189:VAL:HG23	1:B:194:ILE:HB	1.77	0.66
1:B:60:LEU:HD12	1:B:64:TRP:CD1	2.31	0.66
1:A:76:THR:HG23	1:A:132:GLY:HA2	1.75	0.66
1:B:16:LEU:HD12	1:B:16:LEU:N	2.10	0.66
1:C:122:LEU:CD2	1:C:152:MET:HG2	2.25	0.66
1:C:217:PHE:HE1	1:C:223:MET:HE1	1.59	0.66
1:C:99:ARG:HD2	1:C:111:GLU:OE2	1.96	0.66
1:B:42:LEU:HD11	1:B:224:ARG:NH1	2.11	0.66
1:B:80:ILE:HG12	1:B:102:THR:HG22	1.78	0.65
1:C:60:LEU:HD12	1:C:64:TRP:CD1	2.31	0.65
1:A:6:ARG:NH1	1:A:6:ARG:HG3	2.06	0.65
1:C:152:MET:HA	1:C:152:MET:HE2	1.79	0.65
1:A:117:ARG:CG	1:A:117:ARG:HH11	2.09	0.64
1:A:17:ALA:HB2	1:A:23:SER:O	1.96	0.64
1:B:115:ARG:NH1	1:B:115:ARG:HG2	2.13	0.64
1:A:209:ASN:O	1:A:211:PRO:HD3	1.97	0.64
1:C:137:PRO:HD3	4:C:2024:HOH:O	1.97	0.64
1:C:6:ARG:HH11	1:C:6:ARG:CG	2.11	0.64
1:C:21:GLY:O	1:C:22:ASN:HB2	1.97	0.64
1:B:101:MET:CE	1:B:118:ALA:HA	2.22	0.64
1:B:60:LEU:HD12	1:B:64:TRP:HD1	1.62	0.64
1:A:94:THR:HG22	1:A:95:ASN:N	2.12	0.64
1:A:217:PHE:HE1	1:A:223:MET:HE1	1.61	0.63
1:B:94:THR:HG21	1:B:96:LYS:HB2	1.81	0.63
1:B:119:VAL:HG12	1:B:120:HIS:N	2.11	0.63
1:C:94:THR:HG21	1:C:96:LYS:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:O	1:C:107:ASN:O	2.16	0.63
1:A:99:ARG:NH2	2:A:1246:ATP:O1A	2.29	0.63
1:B:175:ASN:O	1:B:177:SER:N	2.31	0.63
1:A:36:ILE:HD13	1:A:48:ILE:CD1	2.29	0.63
1:B:2:ARG:CG	1:B:3:PRO:HD2	2.29	0.62
1:A:37:LEU:HA	1:A:40:VAL:HG13	1.80	0.62
1:C:94:THR:HG22	1:C:95:ASN:N	2.14	0.62
1:C:108:ALA:H	2:C:1246:ATP:N6	1.97	0.62
1:B:122:LEU:HD13	1:B:128:VAL:CG1	2.29	0.62
1:A:143:TYR:HB3	1:A:144:PRO:CD	2.29	0.62
1:C:16:LEU:HD12	1:C:16:LEU:N	2.14	0.62
1:A:6:ARG:HH11	1:A:6:ARG:CG	2.12	0.62
1:C:2:ARG:HG2	1:C:3:PRO:HD2	1.80	0.62
1:A:21:GLY:O	1:A:22:ASN:HB2	1.99	0.62
1:C:57:ARG:HH11	1:C:57:ARG:HG3	1.64	0.62
1:B:85:MET:O	1:B:88:GLY:N	2.33	0.62
1:B:217:PHE:CE1	1:B:223:MET:HE1	2.34	0.62
1:C:8:LEU:HD22	1:C:47:SER:HB2	1.81	0.62
1:B:2:ARG:HG2	1:B:3:PRO:HD2	1.81	0.61
1:A:32:ILE:HG12	1:A:217:PHE:HE2	1.65	0.61
1:C:186:TYR:O	1:C:189:VAL:N	2.30	0.61
1:B:189:VAL:HG11	1:B:202:LEU:HD11	1.82	0.61
1:B:95:ASN:HB2	4:B:2021:HOH:O	2.00	0.61
1:B:6:ARG:HG3	1:B:6:ARG:HH11	1.64	0.61
1:C:63:GLU:HB3	4:C:2013:HOH:O	1.99	0.61
1:C:49:VAL:HG11	1:C:145:SER:HB3	1.83	0.61
1:B:114:ILE:HG23	4:B:2024:HOH:O	2.00	0.60
1:A:38:SER:O	1:A:42:LEU:HD13	2.01	0.60
1:B:106:PHE:O	1:B:107:ASN:O	2.19	0.60
1:C:19:GLN:N	1:C:19:GLN:NE2	2.48	0.60
1:C:195:GLN:OE1	1:C:195:GLN:HA	2.01	0.60
1:A:189:VAL:HG13	1:A:202:LEU:HD11	1.83	0.60
1:B:87:ARG:HG2	1:B:98:VAL:HG22	1.83	0.60
1:B:19:GLN:N	1:B:19:GLN:NE2	2.49	0.60
1:A:86:LEU:HD12	1:A:129:ILE:HD13	1.83	0.60
1:B:6:ARG:NH1	1:B:6:ARG:HG3	2.17	0.59
1:B:101:MET:HE3	1:B:118:ALA:CB	2.33	0.59
1:A:207:ASP:OD2	4:A:2036:HOH:O	2.17	0.59
1:B:76:THR:HG23	1:B:132:GLY:HA2	1.83	0.59
1:B:64:TRP:HB2	4:B:2017:HOH:O	2.02	0.59
1:B:117:ARG:NH1	1:B:117:ARG:HG2	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ASN:O	1:C:23:SER:OG	2.18	0.58
1:C:117:ARG:HH11	1:C:117:ARG:CG	2.15	0.58
2:A:1246:ATP:H5'1	1:B:117:ARG:NH1	2.18	0.58
1:C:39:ILE:HD11	1:C:223:MET:CG	2.29	0.58
1:B:140:THR:HG22	1:B:141:THR:H	1.68	0.58
1:C:115:ARG:NH1	1:C:115:ARG:HG2	2.18	0.58
1:B:171:ASP:C	1:B:173:LYS:H	2.06	0.58
1:B:186:TYR:O	1:B:189:VAL:N	2.35	0.58
1:A:170:SER:OG	1:A:175:ASN:ND2	2.36	0.58
1:C:162:GLN:N	1:C:162:GLN:CD	2.55	0.58
1:C:36:ILE:CD1	1:C:48:ILE:HD13	2.32	0.58
1:B:104:ILE:HG12	4:B:2022:HOH:O	2.04	0.58
1:B:101:MET:HE3	1:B:118:ALA:HB2	1.85	0.57
1:A:107:ASN:HA	2:A:1246:ATP:HN62	1.68	0.57
1:C:101:MET:CE	1:C:118:ALA:HA	2.25	0.57
1:C:167:VAL:HG21	1:C:196:VAL:HG11	1.86	0.57
1:B:36:ILE:HD13	1:B:48:ILE:HD13	1.84	0.57
1:B:6:ARG:CG	1:B:6:ARG:HH11	2.16	0.57
1:A:117:ARG:NH1	1:A:117:ARG:HG2	2.18	0.57
1:C:189:VAL:HG13	1:C:202:LEU:HD11	1.82	0.57
1:B:21:GLY:O	1:B:22:ASN:HB2	2.02	0.57
1:A:217:PHE:CE1	1:A:223:MET:CE	2.87	0.57
1:C:101:MET:HE3	1:C:118:ALA:HB2	1.86	0.57
1:A:19:GLN:N	1:A:19:GLN:NE2	2.51	0.57
1:C:42:LEU:HD11	1:C:224:ARG:NH1	2.20	0.57
1:A:167:VAL:HG21	1:A:196:VAL:HG11	1.86	0.57
1:C:140:THR:HG22	1:C:141:THR:N	2.20	0.56
1:C:107:ASN:HA	2:C:1246:ATP:HN62	1.69	0.56
1:C:140:THR:O	1:C:144:PRO:HD2	2.05	0.56
1:B:116:LEU:O	1:B:120:HIS:HB2	2.05	0.56
1:C:2:ARG:CG	1:C:3:PRO:HD2	2.35	0.56
1:B:117:ARG:NH1	1:B:117:ARG:CG	2.64	0.56
1:B:140:THR:CG2	1:B:141:THR:N	2.68	0.56
1:B:122:LEU:CD1	1:B:128:VAL:HG13	2.32	0.56
1:B:36:ILE:O	1:B:40:VAL:HG12	2.05	0.56
1:A:87:ARG:CG	1:A:98:VAL:HG22	2.35	0.56
1:A:140:THR:HG22	1:A:141:THR:H	1.71	0.56
1:A:94:THR:HG21	1:A:96:LYS:HB2	1.87	0.56
1:C:8:LEU:HD12	1:C:157:ILE:HG13	1.87	0.56
1:C:162:GLN:H	1:C:162:GLN:CD	2.09	0.55
1:A:157:ILE:HB	1:A:210:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASN:CG	2:A:1246:ATP:HN62	2.09	0.55
1:C:87:ARG:CG	1:C:98:VAL:HG22	2.35	0.55
1:A:119:VAL:HG12	1:A:120:HIS:N	2.19	0.55
1:A:16:LEU:N	1:A:16:LEU:HD12	2.21	0.55
1:C:175:ASN:HB2	4:C:2033:HOH:O	2.05	0.55
1:C:38:SER:O	1:C:42:LEU:HD13	2.07	0.55
1:A:117:ARG:HG2	1:A:117:ARG:HH11	1.70	0.55
1:A:36:ILE:HD13	1:A:48:ILE:HD13	1.88	0.55
1:B:87:ARG:CG	1:B:98:VAL:CG2	2.85	0.55
1:A:194:ILE:CG2	1:A:196:VAL:HG23	2.30	0.55
1:B:86:LEU:HD12	1:B:129:ILE:HD13	1.88	0.55
1:A:106:PHE:O	1:A:107:ASN:O	2.24	0.55
1:C:122:LEU:CD2	1:C:152:MET:CG	2.85	0.55
1:A:104:ILE:HG22	1:A:106:PHE:CE1	2.42	0.54
1:B:87:ARG:CG	1:B:98:VAL:HG22	2.37	0.54
1:B:174:HIS:O	1:B:176:LYS:N	2.33	0.54
1:C:101:MET:HE3	1:C:118:ALA:CB	2.38	0.54
1:B:60:LEU:O	1:B:63:GLU:N	2.41	0.54
1:C:47:SER:HB3	1:C:130:PHE:HE1	1.73	0.54
1:A:167:VAL:CG2	1:A:196:VAL:HG11	2.37	0.54
1:B:94:THR:CG2	1:B:96:LYS:H	2.01	0.54
1:A:101:MET:CE	1:A:118:ALA:CB	2.85	0.54
1:A:152:MET:HA	1:A:152:MET:CE	2.38	0.54
1:B:217:PHE:HE1	1:B:223:MET:CE	2.21	0.54
1:B:57:ARG:HH11	1:B:57:ARG:HG3	1.72	0.54
1:C:37:LEU:HA	1:C:40:VAL:HG13	1.88	0.54
1:A:122:LEU:CD2	1:A:152:MET:HG2	2.38	0.53
1:B:29:LEU:N	1:B:29:LEU:HD12	2.23	0.53
1:B:80:ILE:HG12	1:B:102:THR:CG2	2.38	0.53
1:C:60:LEU:HD12	1:C:64:TRP:HD1	1.72	0.53
1:A:8:LEU:HD22	1:A:47:SER:HB2	1.89	0.53
1:B:37:LEU:HA	1:B:40:VAL:HG13	1.91	0.53
1:C:57:ARG:HH11	1:C:57:ARG:CG	2.21	0.53
1:B:94:THR:HG22	1:B:95:ASN:H	1.72	0.53
1:B:101:MET:CE	1:B:118:ALA:CB	2.86	0.53
1:B:66:ILE:HG13	4:B:2017:HOH:O	2.08	0.53
1:A:98:VAL:HA	1:A:127:ILE:O	2.09	0.53
1:B:109:VAL:HG12	1:B:110:ALA:N	2.24	0.53
1:C:172:PRO:C	1:C:174:HIS:N	2.61	0.53
1:A:122:LEU:HD13	1:A:128:VAL:CG1	2.34	0.53
1:B:42:LEU:HD12	1:B:42:LEU:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:THR:CG2	1:B:132:GLY:HA2	2.39	0.53
1:A:107:ASN:OD1	2:A:1246:ATP:N6	2.39	0.52
1:B:140:THR:CG2	1:B:141:THR:H	2.22	0.52
1:A:115:ARG:CG	1:A:115:ARG:NH1	2.69	0.52
1:B:40:VAL:HA	4:B:2014:HOH:O	2.10	0.52
1:B:42:LEU:N	1:B:42:LEU:CD1	2.72	0.52
1:C:17:ALA:HB2	1:C:23:SER:O	2.10	0.52
1:B:217:PHE:CE1	1:B:223:MET:CE	2.92	0.52
1:A:225:ARG:NH2	4:A:2039:HOH:O	2.42	0.52
1:B:135:GLY:HA2	4:B:2028:HOH:O	2.09	0.52
1:A:159:VAL:O	1:A:159:VAL:HG22	2.09	0.52
1:A:237:ASN:HB3	1:A:239:ASP:H	1.75	0.52
1:A:140:THR:HB	4:A:2035:HOH:O	2.09	0.52
1:B:22:ASN:O	1:B:23:SER:OG	2.22	0.52
1:C:29:LEU:HD12	1:C:29:LEU:N	2.25	0.52
1:B:94:THR:CG2	1:B:95:ASN:N	2.74	0.51
1:A:213:HIS:CE1	1:A:235:LEU:HG	2.45	0.51
1:C:35:GLU:O	1:C:38:SER:OG	2.27	0.51
1:C:47:SER:HB3	1:C:130:PHE:CE1	2.45	0.51
1:C:101:MET:CE	1:C:118:ALA:CB	2.89	0.51
1:B:60:LEU:CD1	1:B:64:TRP:CD1	2.93	0.51
1:B:6:ARG:HG2	1:B:45:GLU:HB2	1.93	0.51
1:A:175:ASN:O	1:A:178:ALA:N	2.43	0.51
1:C:109:VAL:HG12	1:C:110:ALA:N	2.23	0.51
1:C:172:PRO:O	1:C:174:HIS:N	2.43	0.51
1:A:36:ILE:O	1:A:40:VAL:HG12	2.11	0.51
1:A:42:LEU:CD1	1:A:42:LEU:N	2.73	0.51
1:B:60:LEU:HD13	1:B:63:GLU:HB2	1.91	0.51
1:A:140:THR:CG2	1:A:141:THR:N	2.74	0.51
1:B:11:LEU:O	1:B:50:ILE:HA	2.11	0.51
1:B:38:SER:O	1:B:42:LEU:HD13	2.11	0.51
1:B:87:ARG:HG2	1:B:98:VAL:CG2	2.41	0.51
1:A:165:ASP:O	1:A:233:GLY:HA2	2.10	0.51
1:A:186:TYR:O	1:A:189:VAL:N	2.42	0.51
1:A:189:VAL:HG11	1:A:202:LEU:HD11	1.88	0.51
1:B:87:ARG:HG3	1:B:98:VAL:CG2	2.40	0.51
1:A:94:THR:CG2	1:A:96:LYS:H	1.99	0.51
1:A:217:PHE:HE1	1:A:223:MET:CE	2.24	0.51
1:A:143:TYR:HB3	1:A:144:PRO:HD2	1.93	0.51
1:C:80:ILE:HG12	1:C:102:THR:HG22	1.92	0.50
1:C:117:ARG:CG	1:C:117:ARG:NH1	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HD11	1:C:64:TRP:HE1	1.76	0.50
1:B:190:VAL:HA	4:B:2040:HOH:O	2.11	0.50
1:A:94:THR:CG2	1:A:95:ASN:N	2.75	0.50
1:B:237:ASN:HB3	1:B:239:ASP:H	1.75	0.50
1:A:105:PRO:HA	4:A:2020:HOH:O	2.10	0.50
1:A:106:PHE:HB2	1:A:109:VAL:HG12	1.92	0.50
1:B:101:MET:CE	1:B:118:ALA:HB2	2.41	0.50
1:C:217:PHE:CE1	1:C:223:MET:HE1	2.42	0.50
1:C:162:GLN:N	1:C:162:GLN:OE1	2.45	0.50
1:A:181:TYR:HE2	4:A:2032:HOH:O	1.95	0.50
1:A:174:HIS:HB2	1:A:175:ASN:OD1	2.12	0.50
1:B:7:VAL:CG2	1:B:158:LEU:CD1	2.85	0.50
1:C:152:MET:HA	1:C:152:MET:CE	2.42	0.50
1:C:98:VAL:HA	1:C:127:ILE:O	2.12	0.49
1:A:101:MET:HE3	1:A:118:ALA:CB	2.43	0.49
1:C:167:VAL:CG2	1:C:196:VAL:HG11	2.42	0.49
1:B:7:VAL:HG21	1:B:158:LEU:HD12	1.91	0.49
1:B:235:LEU:HD13	1:B:237:ASN:ND2	2.27	0.49
1:B:187:ASN:O	1:B:190:VAL:HG13	2.13	0.49
1:C:9:ILE:HG22	1:C:11:LEU:HD22	1.94	0.49
1:B:244:VAL:HG12	1:B:245:HIS:N	2.27	0.49
1:A:101:MET:CE	1:A:118:ALA:HB2	2.42	0.49
1:B:7:VAL:HG22	1:B:8:LEU:N	2.28	0.49
1:A:148:ARG:NH1	4:A:2027:HOH:O	2.46	0.49
1:B:39:ILE:HD11	1:B:223:MET:SD	2.52	0.49
1:C:173:LYS:CE	1:C:174:HIS:CE1	2.91	0.48
1:C:85:MET:O	1:C:88:GLY:N	2.46	0.48
1:C:94:THR:HG22	1:C:95:ASN:H	1.75	0.48
1:B:146:VAL:CG1	1:B:201:ALA:HB1	2.38	0.48
1:A:117:ARG:NH1	1:A:117:ARG:CG	2.71	0.48
1:C:209:ASN:O	1:C:211:PRO:HD3	2.13	0.48
1:B:122:LEU:CD2	1:B:152:MET:CG	2.92	0.48
1:B:28:ARG:O	1:B:32:ILE:HG13	2.13	0.48
1:A:86:LEU:CD1	1:A:129:ILE:HD13	2.43	0.48
1:A:32:ILE:HG12	1:A:217:PHE:CE2	2.48	0.48
1:A:87:ARG:CG	1:A:98:VAL:CG2	2.89	0.48
1:A:35:GLU:HB3	1:A:223:MET:CE	2.43	0.48
1:A:80:ILE:CD1	1:A:106:PHE:CE2	2.79	0.48
1:C:148:ARG:NH1	4:C:2027:HOH:O	2.46	0.48
1:C:59:HIS:O	1:C:63:GLU:HG3	2.13	0.48
1:C:115:ARG:CG	1:C:115:ARG:HH11	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HB3	1:A:215:PHE:HE1	1.78	0.48
1:C:101:MET:CE	1:C:118:ALA:HB2	2.43	0.47
1:A:101:MET:HE1	1:A:118:ALA:CB	2.44	0.47
1:A:175:ASN:HB3	4:A:2033:HOH:O	2.14	0.47
1:C:175:ASN:OD1	1:C:175:ASN:N	2.47	0.47
1:C:104:ILE:HG22	1:C:106:PHE:CE1	2.49	0.47
1:B:213:HIS:CE1	1:B:235:LEU:HG	2.49	0.47
1:C:76:THR:CG2	1:C:132:GLY:HA2	2.42	0.47
1:B:175:ASN:O	1:B:176:LYS:C	2.52	0.47
1:C:42:LEU:N	1:C:42:LEU:CD1	2.78	0.47
1:B:209:ASN:O	1:B:211:PRO:HD3	2.14	0.47
1:B:84:LEU:HA	1:B:84:LEU:HD12	1.71	0.47
1:B:189:VAL:HG13	1:B:202:LEU:HD11	1.92	0.47
1:B:152:MET:HA	1:B:152:MET:HE2	1.97	0.47
1:C:39:ILE:HD11	1:C:223:MET:SD	2.54	0.47
1:A:122:LEU:HD23	1:A:152:MET:CG	2.44	0.47
1:B:16:LEU:N	1:B:16:LEU:CD1	2.76	0.47
1:A:140:THR:O	1:A:144:PRO:HD2	2.14	0.47
1:B:94:THR:CG2	1:B:96:LYS:HB2	2.44	0.47
1:A:152:MET:O	1:A:153:ASN:HB2	2.15	0.47
1:A:174:HIS:O	1:A:176:LYS:HG3	2.15	0.47
1:A:175:ASN:N	1:A:175:ASN:OD1	2.48	0.47
1:A:165:ASP:HB2	4:A:2031:HOH:O	2.15	0.47
1:C:94:THR:CG2	1:C:96:LYS:HB2	2.43	0.47
1:A:104:ILE:CG2	1:A:106:PHE:CE1	2.98	0.46
1:C:157:ILE:HB	1:C:210:LEU:HD11	1.97	0.46
1:C:242:LEU:HA	1:C:242:LEU:HD12	1.67	0.46
1:C:186:TYR:O	1:C:188:ASP:N	2.47	0.46
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.78	0.46
1:C:222:VAL:HG21	4:C:2030:HOH:O	2.15	0.46
1:C:173:LYS:HG3	1:C:174:HIS:CD2	2.51	0.46
1:C:98:VAL:HB	1:C:127:ILE:HB	1.98	0.46
1:C:146:VAL:HG11	1:C:201:ALA:HB1	1.97	0.46
1:A:104:ILE:HB	1:A:106:PHE:CZ	2.50	0.46
1:B:80:ILE:CD1	1:B:106:PHE:CE2	2.87	0.46
1:A:192:GLN:O	1:A:193:ASN:C	2.54	0.46
1:B:244:VAL:CG1	1:B:245:HIS:N	2.79	0.46
1:A:170:SER:CB	1:A:175:ASN:ND2	2.79	0.46
1:C:178:ALA:HB2	4:C:2033:HOH:O	2.15	0.46
1:C:176:LYS:HG3	1:C:177:SER:OG	2.16	0.46
1:A:21:GLY:O	1:A:22:ASN:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:SER:HB3	1:B:130:PHE:CE1	2.51	0.46
1:A:219:GLU:HA	1:A:220:PRO:HD2	1.85	0.46
1:C:136:GLN:HB3	1:C:137:PRO:HD2	1.98	0.46
1:B:171:ASP:O	1:B:173:LYS:N	2.49	0.46
1:B:57:ARG:CG	1:B:57:ARG:HH11	2.29	0.46
1:B:159:VAL:HG22	1:B:159:VAL:O	2.16	0.46
1:C:104:ILE:CG2	1:C:106:PHE:CE1	2.99	0.45
1:A:107:ASN:HA	2:A:1246:ATP:HN61	1.79	0.45
1:C:21:GLY:O	1:C:22:ASN:CB	2.63	0.45
1:B:25:ASN:O	1:B:29:LEU:HD13	2.15	0.45
1:B:47:SER:HB3	1:B:130:PHE:HE1	1.81	0.45
1:C:116:LEU:O	1:C:120:HIS:HB2	2.16	0.45
1:A:122:LEU:CD1	1:A:128:VAL:HG13	2.39	0.45
1:A:6:ARG:HG2	1:A:45:GLU:HB2	1.97	0.45
1:B:165:ASP:O	1:B:233:GLY:HA2	2.15	0.45
1:B:242:LEU:O	1:B:243:LEU:HB2	2.17	0.45
1:A:109:VAL:HG12	1:A:110:ALA:N	2.31	0.45
1:B:29:LEU:HD23	1:B:85:MET:CE	2.47	0.45
1:C:157:ILE:HG22	1:C:210:LEU:HD13	1.97	0.45
1:A:182:ARG:NH2	1:A:244:VAL:HG22	2.31	0.45
1:C:109:VAL:CG1	1:C:110:ALA:N	2.79	0.45
1:C:57:ARG:NH1	1:C:57:ARG:CG	2.80	0.45
1:B:117:ARG:HG2	1:B:117:ARG:HH11	1.72	0.45
1:B:235:LEU:HD13	1:B:237:ASN:HD22	1.80	0.45
1:A:101:MET:HE3	1:A:118:ALA:HB2	1.98	0.45
1:B:60:LEU:HD13	1:B:60:LEU:HA	1.51	0.45
1:B:94:THR:CG2	1:B:95:ASN:H	2.28	0.45
1:A:106:PHE:HB2	1:A:109:VAL:CG1	2.47	0.45
1:A:169:THR:HG1	1:A:179:LYS:H	1.61	0.45
1:A:191:ARG:C	1:A:193:ASN:H	2.20	0.45
1:B:21:GLY:O	1:B:22:ASN:CB	2.65	0.45
1:C:159:VAL:HG22	1:C:159:VAL:O	2.16	0.45
1:C:191:ARG:C	1:C:193:ASN:H	2.21	0.45
1:C:94:THR:CG2	1:C:95:ASN:N	2.79	0.44
1:C:122:LEU:HA	1:C:122:LEU:HD12	1.84	0.44
1:A:143:TYR:CB	1:A:144:PRO:CD	2.94	0.44
1:C:158:LEU:HB3	1:C:215:PHE:HE1	1.82	0.44
1:C:182:ARG:NH2	1:C:244:VAL:HG22	2.32	0.44
1:A:2:ARG:N	4:A:2001:HOH:O	2.50	0.44
1:A:39:ILE:CD1	1:A:223:MET:SD	3.05	0.44
1:B:122:LEU:HD23	1:B:152:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:C	1:B:8:LEU:HD13	2.38	0.44
1:C:217:PHE:HE1	1:C:223:MET:CE	2.29	0.44
1:A:134:ASN:HB2	1:A:144:PRO:HG3	1.98	0.44
1:B:219:GLU:O	1:B:222:VAL:HG13	2.16	0.44
1:B:186:TYR:CE2	1:B:206:ARG:HA	2.53	0.44
1:B:191:ARG:C	1:B:193:ASN:H	2.21	0.44
1:A:2:ARG:HB3	1:A:2:ARG:HE	1.59	0.44
1:A:9:ILE:HG22	1:A:11:LEU:HD22	2.00	0.44
1:B:10:LYS:O	1:B:10:LYS:HG3	2.14	0.44
1:B:192:GLN:O	1:B:193:ASN:C	2.55	0.44
1:A:98:VAL:HB	1:A:127:ILE:HB	1.99	0.44
1:B:106:PHE:HB2	1:B:109:VAL:CG1	2.47	0.44
1:C:60:LEU:HD13	1:C:60:LEU:HA	1.70	0.44
1:C:17:ALA:C	1:C:18:ASP:O	2.55	0.44
1:C:182:ARG:HD2	1:C:231:HIS:HB3	1.99	0.44
1:C:130:PHE:HB3	4:C:2027:HOH:O	2.18	0.44
1:B:60:LEU:CD1	1:B:63:GLU:HB2	2.48	0.44
1:A:2:ARG:HB3	1:A:3:PRO:HD2	1.99	0.44
1:B:13:GLY:HA2	1:B:16:LEU:HD13	2.00	0.43
1:C:29:LEU:N	1:C:29:LEU:CD1	2.81	0.43
1:C:192:GLN:O	1:C:193:ASN:C	2.57	0.43
1:A:122:LEU:CD2	1:A:152:MET:CG	2.96	0.43
1:A:159:VAL:O	1:A:159:VAL:CG2	2.65	0.43
1:B:122:LEU:CD2	1:B:152:MET:HG2	2.48	0.43
1:B:6:ARG:O	1:B:155:ASP:HB2	2.19	0.43
1:C:27:LYS:HD3	1:C:27:LYS:HA	1.84	0.43
1:C:66:ILE:HA	4:C:2015:HOH:O	2.18	0.43
1:A:39:ILE:HD11	1:A:223:MET:SD	2.58	0.43
1:A:186:TYR:CE2	1:A:206:ARG:HA	2.53	0.43
1:B:17:ALA:HB2	1:B:23:SER:O	2.18	0.43
1:C:187:ASN:HA	1:C:190:VAL:CG1	2.48	0.43
1:B:116:LEU:CD1	1:B:116:LEU:H	2.06	0.43
1:B:101:MET:CE	1:B:118:ALA:CA	2.89	0.43
1:B:36:ILE:CD1	1:B:48:ILE:HD13	2.48	0.43
1:B:193:ASN:CG	1:B:193:ASN:O	2.56	0.43
1:A:60:LEU:O	1:A:63:GLU:HB2	2.19	0.43
1:C:16:LEU:N	1:C:16:LEU:CD1	2.79	0.43
1:A:161:LYS:HD2	1:A:161:LYS:HA	1.61	0.43
1:C:84:LEU:HD13	1:C:100:VAL:HG11	1.99	0.43
1:C:115:ARG:CG	1:C:115:ARG:NH1	2.78	0.43
1:A:33:ALA:HB3	1:A:93:LYS:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ASN:O	1:C:190:VAL:HG13	2.18	0.43
1:A:94:THR:CG2	1:A:96:LYS:CG	2.97	0.43
1:C:80:ILE:CD1	1:C:106:PHE:CE2	2.80	0.43
1:B:109:VAL:CG1	1:B:110:ALA:N	2.79	0.43
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.79	0.43
1:A:140:THR:CG2	1:A:141:THR:H	2.30	0.43
1:A:168:PHE:HA	1:A:179:LYS:O	2.18	0.43
1:B:219:GLU:HA	1:B:220:PRO:HD2	1.89	0.43
1:A:25:ASN:OD1	1:A:27:LYS:HB2	2.19	0.43
1:C:173:LYS:HE3	1:C:174:HIS:NE2	2.32	0.42
1:C:161:LYS:HD2	1:C:161:LYS:HA	1.69	0.42
1:A:49:VAL:HG22	1:A:130:PHE:HB2	2.01	0.42
1:A:94:THR:HG22	1:A:95:ASN:H	1.81	0.42
1:C:116:LEU:H	1:C:116:LEU:CD1	2.08	0.42
1:A:59:HIS:O	1:A:63:GLU:HG3	2.18	0.42
1:C:57:ARG:HA	1:C:57:ARG:HD3	1.58	0.42
1:A:244:VAL:HG12	1:A:245:HIS:N	2.34	0.42
1:C:217:PHE:CE1	1:C:223:MET:CE	3.02	0.42
1:C:170:SER:O	1:C:178:ALA:HB1	2.20	0.42
1:C:117:ARG:HH11	1:C:117:ARG:HG3	1.82	0.42
1:C:193:ASN:CG	1:C:193:ASN:O	2.58	0.42
1:C:99:ARG:NH1	1:C:121:HIS:CE1	2.87	0.42
1:C:143:TYR:HB3	1:C:144:PRO:CD	2.49	0.42
1:B:182:ARG:HD2	1:B:231:HIS:HB3	2.01	0.42
1:B:67:ASP:O	1:B:70:GLU:N	2.52	0.42
1:A:77:LEU:HA	1:A:77:LEU:HD12	1.83	0.42
1:A:35:GLU:HB3	1:A:223:MET:HE1	2.02	0.42
1:B:17:ALA:C	1:B:18:ASP:O	2.57	0.42
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.80	0.42
1:A:22:ASN:O	1:A:23:SER:OG	2.26	0.42
1:C:8:LEU:C	1:C:8:LEU:HD13	2.40	0.42
1:C:140:THR:CG2	1:C:141:THR:N	2.82	0.42
1:A:157:ILE:HB	1:A:210:LEU:CD1	2.50	0.42
1:B:162:GLN:O	1:B:164:VAL:N	2.49	0.42
1:A:80:ILE:HG12	1:A:102:THR:HG22	2.01	0.41
1:A:94:THR:CG2	1:A:95:ASN:H	2.33	0.41
1:C:219:GLU:HA	1:C:220:PRO:HD2	1.88	0.41
1:B:170:SER:O	1:B:178:ALA:CB	2.68	0.41
1:B:171:ASP:C	1:B:173:LYS:N	2.72	0.41
1:C:84:LEU:HD12	1:C:84:LEU:HA	1.82	0.41
1:B:134:ASN:HB3	1:B:136:GLN:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:CG2	1:B:158:LEU:HD12	2.51	0.41
1:A:122:LEU:HD23	1:A:152:MET:HG3	2.03	0.41
1:B:143:TYR:HB3	1:B:144:PRO:CD	2.51	0.41
1:B:29:LEU:N	1:B:29:LEU:CD1	2.82	0.41
1:B:238:ASP:C	1:B:239:ASP:O	2.59	0.41
1:B:140:THR:O	1:B:144:PRO:HD2	2.21	0.41
1:C:8:LEU:HG	1:C:149:ALA:HB2	2.02	0.41
1:A:235:LEU:HD13	1:A:237:ASN:OD1	2.20	0.41
1:C:42:LEU:HD12	1:C:42:LEU:N	2.35	0.41
1:C:134:ASN:HB3	1:C:136:GLN:H	1.86	0.41
1:A:171:ASP:HA	1:A:172:PRO:HD2	1.69	0.41
1:A:94:THR:CG2	1:A:96:LYS:HB2	2.50	0.41
1:A:160:ALA:HB1	1:A:217:PHE:CB	2.41	0.41
1:C:22:ASN:O	1:C:23:SER:CB	2.69	0.41
1:A:164:VAL:HG12	4:A:2030:HOH:O	2.19	0.41
1:A:167:VAL:HG11	1:A:184:LEU:CD2	2.51	0.41
1:B:56:PHE:CD2	1:B:74:ILE:HG22	2.56	0.41
1:C:186:TYR:CE2	1:C:206:ARG:HA	2.56	0.41
1:B:8:LEU:C	1:B:8:LEU:CD1	2.89	0.41
1:B:7:VAL:CG2	1:B:8:LEU:N	2.84	0.41
1:A:33:ALA:O	1:A:37:LEU:HG	2.21	0.41
1:C:25:ASN:O	1:C:29:LEU:HD13	2.20	0.41
1:B:27:LYS:HD3	1:B:27:LYS:HA	1.80	0.41
1:B:37:LEU:HA	1:B:37:LEU:HD23	1.82	0.41
1:C:53:GLY:HA3	1:C:57:ARG:HH21	1.86	0.41
2:A:1246:ATP:O2G	1:B:120:HIS:CE1	2.75	0.40
1:B:104:ILE:CG2	1:B:106:PHE:CE1	3.04	0.40
1:C:194:ILE:HG21	4:C:2031:HOH:O	2.20	0.40
1:B:122:LEU:CD2	1:B:152:MET:HG3	2.51	0.40
1:C:119:VAL:HG23	1:C:152:MET:HE2	2.03	0.40
1:B:39:ILE:CD1	1:B:223:MET:SD	3.09	0.40
1:A:22:ASN:O	1:A:23:SER:CB	2.68	0.40
1:C:186:TYR:CG	1:C:206:ARG:HB2	2.56	0.40
1:B:186:TYR:O	1:B:188:ASP:N	2.54	0.40
1:C:6:ARG:HG2	1:C:45:GLU:HB2	2.02	0.40
1:C:90:LEU:HA	1:C:90:LEU:HD12	1.96	0.40

There are no symmetry-related clashes.

## 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	242/255 (95%)	210 (87%)	20 (8%)	12 (5%)	3	7
1	B	242/255 (95%)	209 (86%)	16 (7%)	17 (7%)	1	3
1	C	242/255 (95%)	212 (88%)	20 (8%)	10 (4%)	3	11
All	All	726/765 (95%)	631 (87%)	56 (8%)	39 (5%)	2	6

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	23	SER
1	A	107	ASN
1	A	175	ASN
1	A	176	LYS
1	B	20	THR
1	B	23	SER
1	B	107	ASN
1	B	175	ASN
1	B	176	LYS
1	C	20	THR
1	C	22	ASN
1	C	23	SER
1	C	107	ASN
1	A	22	ASN
1	A	174	HIS
1	B	22	ASN
1	B	172	PRO
1	C	173	LYS
1	C	187	ASN
1	A	187	ASN
1	A	239	ASP
1	B	85	MET
1	B	86	LEU

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Mol	Chain	Res	Type
1	B	187	ASN
1	B	198	ASP
1	C	186	TYR
1	A	133	GLY
1	B	186	TYR
1	B	239	ASP
1	A	186	TYR
1	B	163	GLY
1	B	193	ASN
1	C	18	ASP
1	C	193	ASN
1	C	198	ASP
1	B	174	HIS
1	A	244	VAL
1	B	244	VAL

### 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	205/215 (95%)	153 (75%)	52 (25%)	1	1
1	B	205/215 (95%)	152 (74%)	53 (26%)	0	1
1	C	205/215 (95%)	155 (76%)	50 (24%)	1	2
All	All	615/645 (95%)	460 (75%)	155 (25%)	1	2

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	7	VAL
1	A	10	LYS
1	A	11	LEU
1	A	12	SER
1	A	19	GLN
1	A	20	THR

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Mol	Chain	Res	Type
1	A	26	SER
1	A	27	LYS
1	A	29	LEU
1	A	40	VAL
1	A	42	LEU
1	A	50	ILE
1	A	57	ARG
1	A	68	ARG
1	A	77	LEU
1	A	84	LEU
1	A	86	LEU
1	A	87	ARG
1	A	90	LEU
1	A	109	VAL
1	A	111	GLU
1	A	115	ARG
1	A	117	ARG
1	A	119	VAL
1	A	120	HIS
1	A	122	LEU
1	A	139	VAL
1	A	146	VAL
1	A	148	ARG
1	A	152	MET
1	A	159	VAL
1	A	161	LYS
1	A	162	GLN
1	A	164	VAL
1	A	169	THR
1	A	173	LYS
1	A	179	LYS
1	A	193	ASN
1	A	197	MET
1	A	198	ASP
1	A	202	LEU
1	A	203	LEU
1	A	204	LEU
1	A	206	ARG
1	A	210	LEU
1	A	222	VAL
1	A	224	ARG
1	A	232	VAL

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Mol	Chain	Res	Type
1	A	235	LEU
1	A	237	ASN
1	A	241	SER
1	B	2	ARG
1	B	6	ARG
1	B	8	LEU
1	B	10	LYS
1	B	11	LEU
1	B	12	SER
1	B	19	GLN
1	B	20	THR
1	B	26	SER
1	B	27	LYS
1	B	40	VAL
1	B	50	ILE
1	B	57	ARG
1	B	60	LEU
1	B	68	ARG
1	B	77	LEU
1	B	84	LEU
1	B	86	LEU
1	B	90	LEU
1	B	109	VAL
1	B	111	GLU
1	B	115	ARG
1	B	116	LEU
1	B	117	ARG
1	B	119	VAL
1	B	122	LEU
1	B	134	ASN
1	B	139	VAL
1	B	142	ASP
1	B	146	VAL
1	B	152	MET
1	B	159	VAL
1	B	161	LYS
1	B	162	GLN
1	B	165	ASP
1	B	169	THR
1	B	173	LYS
1	B	174	HIS
1	B	175	ASN

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Mol	Chain	Res	Type
1	B	179	LYS
1	B	192	GLN
1	B	193	ASN
1	B	198	ASP
1	B	202	LEU
1	B	204	LEU
1	B	206	ARG
1	B	210	LEU
1	B	222	VAL
1	B	223	MET
1	B	232	VAL
1	B	235	LEU
1	B	237	ASN
1	B	241	SER
1	C	2	ARG
1	C	6	ARG
1	C	7	VAL
1	C	8	LEU
1	C	10	LYS
1	C	11	LEU
1	C	12	SER
1	C	19	GLN
1	C	26	SER
1	C	27	LYS
1	C	40	VAL
1	C	50	ILE
1	C	57	ARG
1	C	60	LEU
1	C	68	ARG
1	C	77	LEU
1	C	84	LEU
1	C	86	LEU
1	C	90	LEU
1	C	109	VAL
1	C	111	GLU
1	C	115	ARG
1	C	117	ARG
1	C	119	VAL
1	C	120	HIS
1	C	122	LEU
1	C	134	ASN
1	C	139	VAL

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Mol	Chain	Res	Type
1	C	148	ARG
1	C	152	MET
1	C	159	VAL
1	C	162	GLN
1	C	164	VAL
1	C	169	THR
1	C	173	LYS
1	C	176	LYS
1	C	179	LYS
1	C	188	ASP
1	C	193	ASN
1	C	198	ASP
1	C	199	GLN
1	C	202	LEU
1	C	204	LEU
1	C	210	LEU
1	C	222	VAL
1	C	223	MET
1	C	232	VAL
1	C	235	LEU
1	C	237	ASN
1	C	241	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	1246	-	24,33,33	1.29	2 (8%)	31,52,52	1.51	3 (9%)
2	ATP	B	1246	-	24,33,33	1.20	2 (8%)	31,52,52	1.33	3 (9%)
2	ATP	C	1246	3	24,33,33	1.09	1 (4%)	31,52,52	1.44	4 (12%)

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	1246	-	1/1/7/7	0/18/38/38	0/3/3/3
2	ATP	B	1246	-	1/1/7/7	0/18/38/38	0/3/3/3
2	ATP	C	1246	3	1/1/7/7	0/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1246	ATP	C2-N3	2.07	1.35	1.32
2	A	1246	ATP	C2-N3	2.11	1.35	1.32
2	C	1246	ATP	O4'-C1'	4.14	1.46	1.41
2	B	1246	ATP	O4'-C1'	4.46	1.46	1.41
2	A	1246	ATP	O4'-C1'	4.92	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1246	ATP	N3-C2-N1	-2.75	126.79	128.89
2	C	1246	ATP	PA-O3A-PB	-2.02	127.06	132.73
2	C	1246	ATP	O4'-C4'-C5'	2.02	116.56	109.32
2	B	1246	ATP	C2'-C3'-C4'	2.05	106.83	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1246	ATP	C2'-C1'-N9	2.84	118.64	114.29
2	A	1246	ATP	C4-C5-N7	3.38	112.59	109.48
2	C	1246	ATP	O4'-C1'-N9	3.59	115.61	108.10
2	C	1246	ATP	C2'-C1'-N9	3.69	119.94	114.29
2	B	1246	ATP	O4'-C1'-N9	3.85	116.16	108.10
2	A	1246	ATP	O4'-C1'-N9	4.81	118.17	108.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1246	ATP	C1'
2	C	1246	ATP	C1'
2	A	1246	ATP	C1'

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1246	ATP	8	0
2	B	1246	ATP	2	0
2	C	1246	ATP	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	244/255 (95%)	-0.02	9 (3%)	45 33	29, 55, 103, 115	0
1	B	244/255 (95%)	-0.25	6 (2%)	61 48	25, 53, 102, 121	0
1	C	244/255 (95%)	-0.08	8 (3%)	50 38	27, 55, 105, 121	0
All	All	732/765 (95%)	-0.11	23 (3%)	52 40	25, 55, 104, 121	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	GLU	5.9
1	B	62	GLU	5.9
1	C	20	THR	5.2
1	A	20	THR	4.0
1	C	62	GLU	3.3
1	A	245	HIS	3.2
1	A	172	PRO	3.1
1	A	173	LYS	3.0
1	C	19	GLN	2.9
1	C	245	HIS	2.7
1	B	163	GLY	2.7
1	B	20	THR	2.7
1	A	2	ARG	2.7
1	C	244	VAL	2.6
1	B	245	HIS	2.6
1	B	173	LYS	2.4
1	A	106	PHE	2.3
1	A	177	SER	2.3
1	B	244	VAL	2.2
1	C	217	PHE	2.1
1	A	244	VAL	2.1
1	C	179	LYS	2.1
1	C	231	HIS	2.0



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

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

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	ATP	B	1246	31/31	0.57	0.48	8.02	154,160,204,206	0
2	ATP	C	1246	31/31	0.66	0.53	6.52	166,174,220,221	0
2	ATP	A	1246	31/31	0.74	0.31	1.98	126,137,176,178	0
3	MG	C	1247	1/1	0.82	0.11	-	82,82,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.