



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:39 PM GMT

PDB ID : 4MB2  
Title : Crystal structure of TON1374 in complex with ATP  
Authors : Kim, M.-K.; An, Y.J.; Cha, S.-S.  
Deposited on : 2013-08-19  
Resolution : 2.19 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

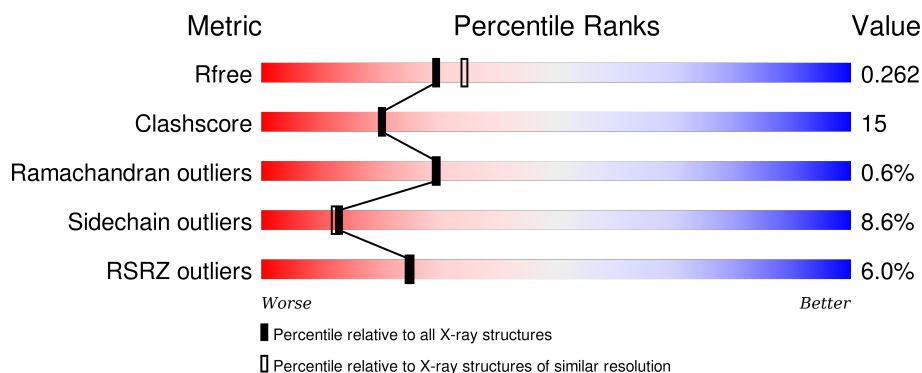
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	261	<div> <div>2%</div> <div>75% 19% . .</div> </div>
1	B	261	<div> <div>6%</div> <div>72% 22% . .</div> </div>
1	C	261	<div> <div>7%</div> <div>70% 21% . 6%</div> </div>
1	D	261	<div> <div>8%</div> <div>66% 28% . . .</div> </div>

## 2 Entry composition [i](#)

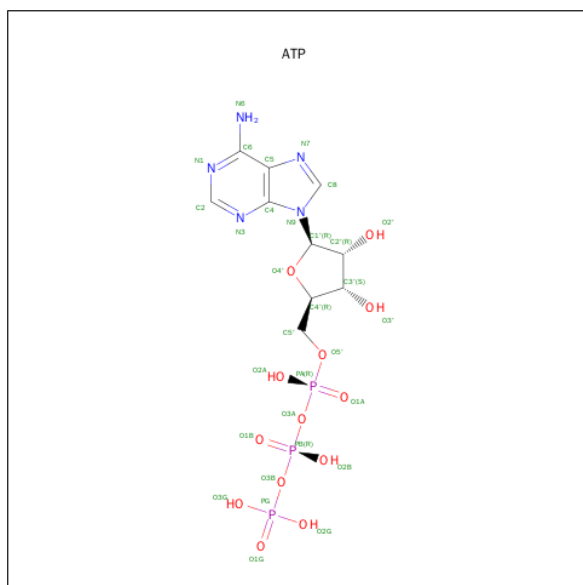
There are 4 unique types of molecules in this entry. The entry contains 8325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphopantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2008	1271	359	371	7			
1	B	257	Total	C	N	O	S	0	0	0
			2038	1292	365	374	7			
1	C	246	Total	C	N	O	S	0	0	0
			1959	1240	351	361	7			
1	D	254	Total	C	N	O	S	0	0	0
			2016	1275	359	375	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		

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

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

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

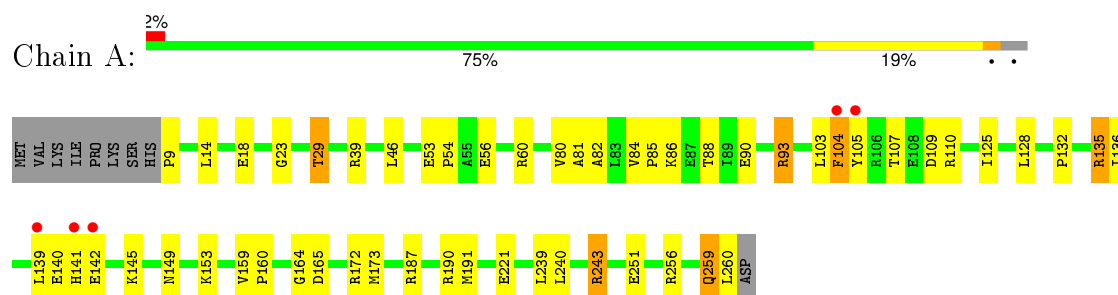
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	57	Total	O	0	0
			57	57		
4	C	39	Total	O	0	0
			39	39		
4	D	31	Total	O	0	0
			31	31		

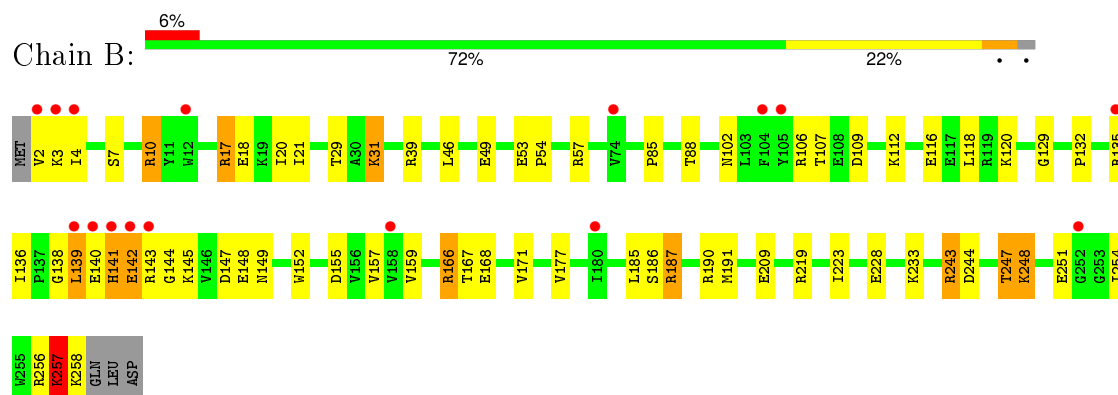
### 3 Residue-property plots

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.

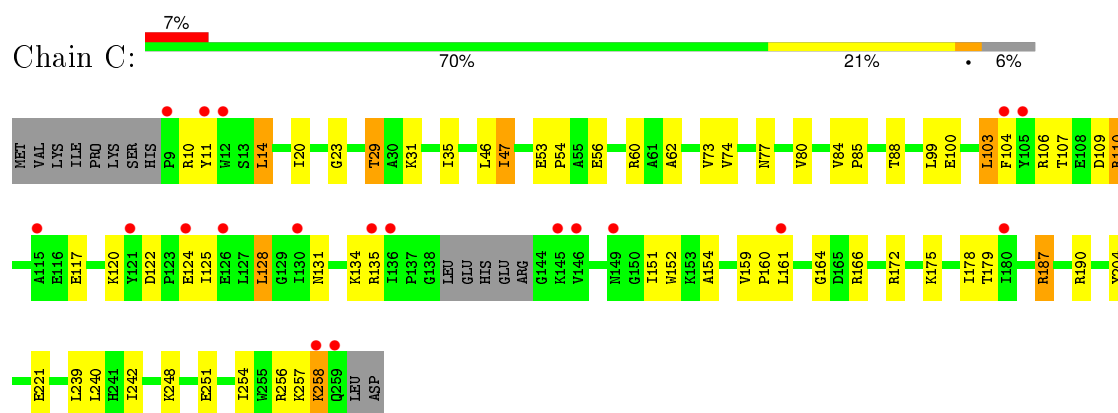
#### • Molecule 1: Phosphopantothenate synthetase



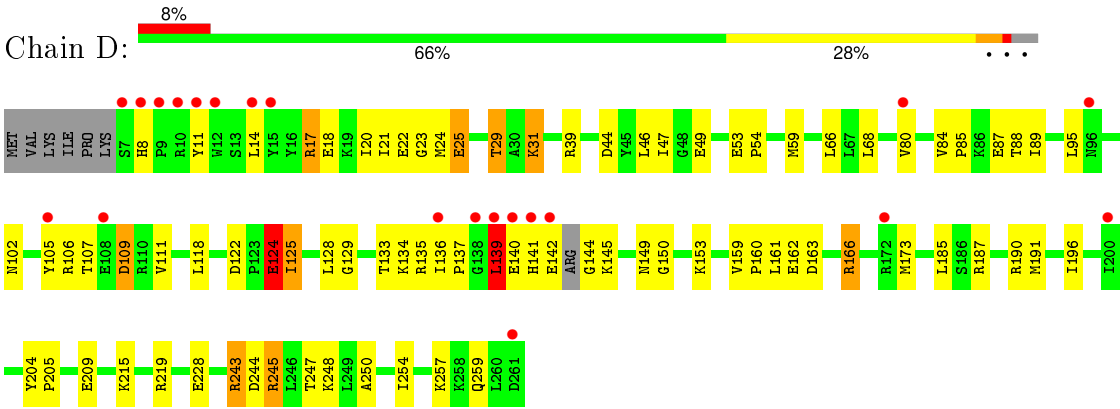
#### • Molecule 1: Phosphopantothenate synthetase



#### • Molecule 1: Phosphopantothenate synthetase



#### • Molecule 1: Phosphopantothenate synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	266.43Å 60.91Å 75.24Å 90.00° 92.38° 90.00°	Depositor
Resolution (Å)	37.62 – 2.19 37.59 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.62-2.19) 97.8 (37.59-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.201 , 0.260 0.209 , 0.262	Depositor DCC
$R_{free}$ test set	3084 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.8	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 60918 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

### 5.1 Standard geometry

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	0.41	0/2038	0.54	0/2749
1	B	0.43	0/2069	0.56	0/2792
1	C	0.40	0/1987	0.54	0/2678
1	D	0.40	0/2044	0.52	0/2757
All	All	0.41	0/8138	0.54	0/10976

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	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	9	PRO	Peptide
1	C	103	LEU	Peptide
1	D	129	GLY	Peptide



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2008	0	2071	63	1
1	B	2038	0	2107	72	0
1	C	1959	0	2027	64	0
1	D	2016	0	2070	81	0
2	A	31	0	12	4	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
2	D	31	0	12	5	0
3	A	1	0	0	0	0
4	A	52	0	0	6	1
4	B	57	0	0	3	3
4	C	39	0	0	0	2
4	D	31	0	0	0	0
All	All	8325	0	8323	240	4

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 15.

All (240) 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:243:ARG:HH11	1:B:243:ARG:HG2	1.06	1.20
1:A:93:ARG:HG2	1:A:93:ARG:HH11	1.00	1.12
1:B:106:ARG:NH2	1:B:129:GLY:O	1.81	1.11
1:B:256:ARG:HA	1:B:257:LYS:HB3	1.18	1.09
1:D:124:GLU:O	1:D:125:ILE:HG22	1.51	1.07
1:A:239:LEU:CD1	1:B:254:ILE:HD11	1.88	1.03
1:A:256:ARG:NH1	1:B:191:MET:O	1.93	1.02
1:D:243:ARG:HH11	1:D:243:ARG:HG2	1.25	1.00
1:B:243:ARG:NH1	1:B:244:ASP:OD1	2.00	0.94
1:A:93:ARG:HG2	1:A:93:ARG:NH1	1.77	0.94
1:A:191:MET:HE3	1:B:257:LYS:HB2	1.50	0.94
1:B:102:ASN:OD1	1:B:166:ARG:NH1	2.03	0.91
1:A:259:GLN:OE1	1:C:31:LYS:NZ	2.03	0.91
1:C:256:ARG:NH1	1:D:191:MET:O	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:NH1	1:B:243:ARG:HG2	1.81	0.90
1:A:243:ARG:CD	1:B:247:THR:HG22	2.04	0.87
1:A:239:LEU:HD12	1:B:254:ILE:HD11	1.54	0.87
1:B:256:ARG:HA	1:B:257:LYS:CB	2.01	0.85
1:B:140:GLU:O	1:B:142:GLU:N	2.10	0.85
1:A:191:MET:CE	1:B:257:LYS:HB2	2.07	0.84
1:A:191:MET:CE	1:B:257:LYS:CB	2.55	0.83
1:D:17:ARG:O	1:D:20:ILE:HG22	1.77	0.83
1:A:239:LEU:HD11	1:B:254:ILE:HD11	1.58	0.83
1:A:191:MET:HE1	1:B:257:LYS:CB	2.10	0.82
1:D:243:ARG:HG2	1:D:243:ARG:NH1	1.94	0.81
1:A:93:ARG:CG	1:A:93:ARG:HH11	1.87	0.80
1:C:85:PRO:O	1:C:88:THR:HG22	1.81	0.80
1:C:85:PRO:O	1:C:88:THR:CG2	2.30	0.79
1:B:107:THR:HG22	1:B:109:ASP:H	1.47	0.79
1:A:191:MET:HE1	1:B:257:LYS:HB3	1.63	0.78
1:C:239:LEU:HD12	1:D:254:ILE:HD11	1.67	0.77
1:D:243:ARG:CG	1:D:243:ARG:HH11	1.97	0.76
1:C:187:ARG:HH22	1:D:259:GLN:CB	1.99	0.76
1:C:239:LEU:CD1	1:D:254:ILE:HD11	2.16	0.76
1:A:39:ARG:HH21	2:A:301:ATP:PA	2.08	0.75
1:D:139:LEU:HD12	1:D:144:GLY:HA2	1.70	0.73
1:A:135:ARG:HD2	1:A:141:HIS:CD2	2.24	0.73
1:B:159:VAL:HG23	1:B:159:VAL:O	1.88	0.73
1:C:187:ARG:HA	1:C:187:ARG:HE	1.53	0.72
1:B:256:ARG:CA	1:B:257:LYS:HB3	2.08	0.71
1:A:191:MET:CE	1:B:257:LYS:HB3	2.20	0.70
1:C:74:VAL:HG23	1:C:99:LEU:HD12	1.72	0.70
1:A:93:ARG:NH1	1:A:93:ARG:CG	2.51	0.70
1:D:23:GLY:C	1:D:29:THR:HG23	2.11	0.70
1:C:84:VAL:O	1:C:88:THR:HG22	1.92	0.69
1:D:102:ASN:HD21	1:D:166:ARG:NE	1.92	0.68
1:A:243:ARG:HD3	1:B:247:THR:HG22	1.74	0.68
1:A:23:GLY:C	1:A:29:THR:HG23	2.14	0.68
1:C:239:LEU:HD13	1:D:250:ALA:HB2	1.77	0.67
1:B:17:ARG:O	1:B:21:ILE:HG12	1.95	0.67
1:D:85:PRO:O	1:D:88:THR:HG22	1.95	0.66
1:A:149:ASN:HA	1:A:153:LYS:HD3	1.77	0.65
1:D:185:LEU:O	1:D:190:ARG:NH1	2.30	0.65
1:C:100:GLU:HG3	1:C:128:LEU:HB3	1.78	0.64
1:C:74:VAL:HG23	1:C:99:LEU:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:VAL:O	1:D:159:VAL:HG23	1.98	0.64
1:A:239:LEU:HD11	1:B:254:ILE:CD1	2.29	0.63
1:D:135:ARG:HA	1:D:144:GLY:O	1.99	0.63
1:A:39:ARG:NH2	2:A:301:ATP:O1A	2.20	0.63
1:A:39:ARG:NH2	2:A:301:ATP:PA	2.72	0.62
1:C:56:GLU:O	1:C:60:ARG:HG3	2.00	0.62
1:D:53:GLU:HB3	1:D:54:PRO:HD3	1.81	0.62
1:B:136:ILE:HB	1:B:139:LEU:HD12	1.80	0.62
1:C:187:ARG:HH22	1:D:259:GLN:HB2	1.65	0.62
1:D:124:GLU:O	1:D:125:ILE:CG2	2.37	0.61
1:C:161:LEU:N	1:C:161:LEU:HD12	2.15	0.61
1:D:243:ARG:NH1	1:D:244:ASP:OD1	2.33	0.61
1:B:39:ARG:NH2	2:B:301:ATP:O1A	2.33	0.61
1:B:53:GLU:HB3	1:B:54:PRO:HD3	1.80	0.61
1:A:135:ARG:CD	1:A:141:HIS:CD2	2.83	0.60
1:A:107:THR:HG22	1:A:109:ASP:H	1.66	0.60
1:A:107:THR:HG22	1:A:109:ASP:N	2.16	0.60
1:C:85:PRO:C	1:C:88:THR:HG22	2.21	0.60
1:B:107:THR:HG22	1:B:109:ASP:N	2.16	0.60
1:B:139:LEU:CD1	1:B:144:GLY:HA3	2.31	0.60
1:D:106:ARG:NH2	1:D:111:VAL:HG21	2.17	0.60
1:B:243:ARG:HH11	1:B:243:ARG:CG	1.94	0.59
1:B:135:ARG:NH1	1:B:142:GLU:OE1	2.34	0.59
1:D:80:VAL:HG21	1:D:160:PRO:HG2	1.84	0.59
1:B:219:ARG:HG2	1:B:223:ILE:HD12	1.84	0.59
1:B:257:LYS:O	1:B:258:LYS:HB2	2.02	0.59
1:C:46:LEU:HD11	1:D:46:LEU:CD1	2.34	0.58
1:A:46:LEU:HD11	1:B:46:LEU:HD13	1.86	0.58
1:A:46:LEU:HD11	1:B:46:LEU:CD1	2.34	0.57
1:C:47:ILE:HD11	1:C:242:ILE:HD11	1.87	0.57
1:A:260:LEU:HD12	4:B:426:HOH:O	2.03	0.57
1:C:85:PRO:O	1:C:88:THR:HG23	2.05	0.56
1:A:136:ILE:HG23	1:A:173:MET:SD	2.45	0.56
1:C:159:VAL:O	1:C:179:THR:OG1	2.19	0.56
1:A:239:LEU:O	1:A:243:ARG:HG3	2.05	0.56
1:D:135:ARG:NH1	1:D:141:HIS:CB	2.68	0.56
1:D:39:ARG:NH2	2:D:301:ATP:O2B	2.38	0.56
1:C:258:LYS:HG2	1:D:187:ARG:HH22	1.71	0.56
1:C:23:GLY:C	1:C:29:THR:HG23	2.26	0.56
1:C:239:LEU:HD13	1:D:250:ALA:CB	2.37	0.55
1:C:239:LEU:CD1	1:D:250:ALA:HB2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LEU:HD12	1:D:144:GLY:CA	2.36	0.55
1:A:243:ARG:HD2	1:B:247:THR:HG22	1.86	0.55
1:C:187:ARG:HE	1:C:187:ARG:CA	2.17	0.55
1:B:139:LEU:HD13	1:B:144:GLY:HA3	1.89	0.55
2:D:301:ATP:O2B	2:D:301:ATP:O1A	2.26	0.54
1:A:191:MET:HA	1:A:191:MET:HE2	1.89	0.54
1:A:39:ARG:HD2	4:A:451:HOH:O	2.07	0.54
1:B:7:SER:N	4:B:447:HOH:O	2.35	0.54
1:C:100:GLU:OE1	1:C:151:ILE:HG13	2.08	0.54
1:B:159:VAL:CG2	1:B:159:VAL:O	2.56	0.54
1:C:74:VAL:CG2	1:C:99:LEU:CD1	2.85	0.53
1:A:153:LYS:HA	4:A:443:HOH:O	2.08	0.53
1:C:239:LEU:CD1	1:D:250:ALA:CB	2.87	0.53
1:A:159:VAL:HG23	1:A:159:VAL:O	2.08	0.53
1:A:190:ARG:HD3	1:B:257:LYS:O	2.08	0.53
1:A:141:HIS:HE1	4:A:417:HOH:O	1.91	0.52
1:D:137:PRO:HG2	1:D:173:MET:HG2	1.90	0.52
1:D:125:ILE:HG23	1:D:125:ILE:O	2.08	0.52
1:D:46:LEU:O	1:D:245:ARG:HD3	2.08	0.52
1:C:134:LYS:HB3	1:C:152:TRP:CE3	2.45	0.52
1:C:187:ARG:HA	1:C:187:ARG:NE	2.24	0.52
2:C:301:ATP:O1B	2:C:301:ATP:O5'	2.27	0.52
1:C:117:GLU:O	1:C:120:LYS:HB3	2.09	0.52
1:C:190:ARG:HD3	1:D:257:LYS:O	2.09	0.52
1:D:163:ASP:HB2	2:D:301:ATP:O2A	2.10	0.52
1:A:259:GLN:HG3	4:A:450:HOH:O	2.10	0.51
1:B:17:ARG:O	1:B:20:ILE:HG22	2.10	0.51
1:B:186:SER:O	1:B:190:ARG:HG3	2.10	0.51
1:D:122:ASP:O	1:D:124:GLU:O	2.28	0.51
1:C:187:ARG:NH2	1:D:259:GLN:H	2.07	0.51
1:B:167:THR:O	1:B:171:VAL:HG23	2.10	0.51
1:A:81:ALA:O	1:A:85:PRO:HD3	2.11	0.51
1:C:239:LEU:HD11	1:D:254:ILE:HD11	1.91	0.51
1:A:53:GLU:N	1:A:54:PRO:CD	2.74	0.51
1:D:84:VAL:HB	1:D:87:GLU:HB2	1.92	0.51
1:A:53:GLU:HB3	1:A:54:PRO:HD3	1.92	0.51
1:D:107:THR:HG22	1:D:109:ASP:H	1.77	0.50
1:C:107:THR:O	1:C:110:ARG:N	2.44	0.50
1:C:161:LEU:CD1	1:C:161:LEU:N	2.74	0.50
1:D:107:THR:HG22	1:D:109:ASP:N	2.25	0.50
1:C:187:ARG:NH2	1:D:259:GLN:HB2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:CE	1:B:18:GLU:OE2	2.59	0.50
1:B:138:GLY:O	1:B:139:LEU:HB2	2.12	0.49
1:D:162:GLU:OE2	1:D:163:ASP:N	2.45	0.49
1:C:107:THR:HG22	1:C:110:ARG:H	1.77	0.49
1:A:104:PHE:N	1:A:104:PHE:CD1	2.80	0.49
1:D:128:LEU:HD23	1:D:150:GLY:CA	2.43	0.49
1:B:3:LYS:HE3	1:B:18:GLU:OE2	2.13	0.49
1:B:157:VAL:O	1:B:157:VAL:HG23	2.12	0.48
1:D:17:ARG:O	1:D:21:ILE:HG12	2.12	0.48
1:A:165:ASP:OD1	1:A:165:ASP:N	2.46	0.48
1:A:239:LEU:CD1	1:B:254:ILE:CD1	2.77	0.48
1:C:187:ARG:HH22	1:D:259:GLN:HB3	1.74	0.48
1:C:74:VAL:CG2	1:C:99:LEU:HD12	2.42	0.48
1:A:56:GLU:HG2	4:A:410:HOH:O	2.13	0.48
1:C:47:ILE:CD1	1:C:242:ILE:HD11	2.42	0.48
1:B:2:VAL:O	1:B:2:VAL:HG13	2.12	0.48
1:B:168:GLU:OE1	1:B:187:ARG:NE	2.42	0.48
1:C:80:VAL:HG21	1:C:160:PRO:HG2	1.95	0.48
1:B:140:GLU:HG2	1:B:141:HIS:H	1.79	0.48
1:C:46:LEU:HD11	1:D:46:LEU:HD11	1.95	0.48
1:D:133:THR:O	1:D:134:LYS:HD2	2.14	0.47
1:C:46:LEU:HD11	1:D:46:LEU:HD13	1.95	0.47
1:C:11:TYR:HA	1:C:14:LEU:HD12	1.96	0.47
1:C:159:VAL:HG23	1:C:159:VAL:O	2.15	0.47
1:D:24:MET:N	1:D:29:THR:HG23	2.29	0.47
1:A:164:GLY:HA3	1:A:187:ARG:HB3	1.95	0.47
1:A:14:LEU:O	1:A:18:GLU:HG2	2.15	0.47
1:C:77:ASN:OD1	1:C:80:VAL:HG23	2.16	0.46
1:B:139:LEU:HD12	1:B:144:GLY:HA3	1.97	0.46
1:C:122:ASP:OD1	1:C:122:ASP:C	2.54	0.46
1:D:125:ILE:CG2	1:D:125:ILE:O	2.64	0.46
1:D:128:LEU:HD23	1:D:150:GLY:HA3	1.97	0.46
1:B:31:LYS:HB2	1:B:31:LYS:HE2	1.74	0.46
1:C:85:PRO:HA	1:C:88:THR:CG2	2.45	0.45
1:A:23:GLY:CA	1:A:29:THR:HG23	2.46	0.45
1:D:59:MET:HG2	1:D:196:ILE:HD13	1.98	0.45
1:A:23:GLY:HA3	1:A:29:THR:CG2	2.47	0.45
1:A:39:ARG:NH2	2:A:301:ATP:O2A	2.50	0.45
1:C:164:GLY:HA3	1:C:187:ARG:HB3	1.99	0.45
1:A:86:LYS:NZ	1:A:90:GLU:OE2	2.50	0.45
1:D:87:GLU:OE1	1:D:87:GLU:N	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASP:OD1	1:D:49:GLU:HA	2.16	0.44
1:C:62:ALA:HB1	1:C:178:ILE:HD13	1.99	0.44
1:C:258:LYS:HG2	1:D:187:ARG:NH2	2.32	0.44
1:A:29:THR:HG21	1:A:82:ALA:HB2	1.98	0.44
1:B:132:PRO:HG2	1:B:145:LYS:HD2	2.00	0.44
1:C:187:ARG:CZ	1:D:259:GLN:H	2.31	0.44
1:C:122:ASP:O	1:C:125:ILE:HG22	2.18	0.44
1:C:53:GLU:HB3	1:C:54:PRO:HD3	1.99	0.44
1:B:209:GLU:HB3	4:B:436:HOH:O	2.17	0.44
1:B:141:HIS:O	1:B:143:ARG:N	2.51	0.44
1:B:112:LYS:HE2	1:B:116:GLU:OE2	2.18	0.44
1:A:142:GLU:OE2	1:A:145:LYS:HE3	2.18	0.44
1:B:31:LYS:CE	1:B:31:LYS:H	2.31	0.43
1:A:85:PRO:O	1:A:88:THR:HG22	2.17	0.43
1:C:85:PRO:CA	1:C:88:THR:HG22	2.49	0.43
1:D:102:ASN:ND2	1:D:166:ARG:NE	2.63	0.43
1:C:73:VAL:HG23	1:C:154:ALA:HB2	2.01	0.43
1:A:56:GLU:CG	4:A:410:HOH:O	2.65	0.43
1:C:35:ILE:HG21	1:D:17:ARG:NH1	2.34	0.43
1:D:141:HIS:C	1:D:142:GLU:OE2	2.57	0.43
1:A:132:PRO:CG	1:A:145:LYS:HB3	2.48	0.43
1:A:80:VAL:HG21	1:A:160:PRO:HG2	1.99	0.43
1:D:8:HIS:O	1:D:11:TYR:CB	2.66	0.43
1:A:125:ILE:O	1:A:125:ILE:HG23	2.18	0.43
1:D:31:LYS:HD3	1:D:31:LYS:H	1.83	0.43
1:D:135:ARG:HH12	1:D:141:HIS:CB	2.31	0.43
1:C:258:LYS:CG	1:D:187:ARG:HH22	2.31	0.43
1:C:254:ILE:O	1:D:190:ARG:HD2	2.19	0.42
1:C:154:ALA:O	1:C:175:LYS:HD2	2.19	0.42
1:D:134:LYS:HD2	1:D:134:LYS:HA	1.90	0.42
1:B:148:GLU:HA	1:B:152:TRP:HB3	2.02	0.42
1:B:147:ASP:OD1	1:B:149:ASN:N	2.51	0.42
1:B:147:ASP:OD1	1:B:148:GLU:N	2.53	0.42
1:B:142:GLU:HB3	1:B:145:LYS:HE3	2.01	0.42
1:D:142:GLU:CB	1:D:145:LYS:HG3	2.50	0.42
2:D:301:ATP:O2G	2:D:301:ATP:O1B	2.37	0.42
1:A:149:ASN:HA	1:A:153:LYS:CD	2.48	0.42
1:D:14:LEU:O	1:D:18:GLU:HG3	2.19	0.42
1:D:25:GLU:H	1:D:25:GLU:HG2	1.57	0.42
1:D:161:LEU:HG	2:D:301:ATP:C4	2.55	0.41
1:D:85:PRO:O	1:D:89:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:O	1:B:190:ARG:NH1	2.53	0.41
1:B:248:LYS:O	1:B:248:LYS:HD2	2.20	0.41
1:B:142:GLU:OE2	1:B:145:LYS:HE2	2.20	0.41
1:B:157:VAL:HG23	1:B:159:VAL:HG13	2.02	0.41
1:B:10:ARG:NH1	1:B:49:GLU:OE2	2.52	0.41
1:B:85:PRO:O	1:B:88:THR:HG22	2.20	0.41
1:D:142:GLU:HB2	1:D:145:LYS:HG3	2.01	0.41
1:A:105:TYR:HB3	1:A:110:ARG:HH12	1.86	0.41
1:A:84:VAL:N	1:A:85:PRO:CD	2.84	0.41
1:B:167:THR:HG23	1:B:177:VAL:HG11	2.03	0.41
1:D:66:LEU:HB3	1:D:95:LEU:HD22	2.03	0.41
1:B:155:ASP:OD1	1:B:155:ASP:N	2.53	0.41
1:D:136:ILE:N	1:D:144:GLY:O	2.48	0.40
1:D:68:LEU:HD22	1:D:219:ARG:NH1	2.36	0.40
1:D:205:PRO:O	1:D:209:GLU:HG3	2.21	0.40
1:D:149:ASN:HA	1:D:153:LYS:HD2	2.03	0.40
1:D:22:GLU:HA	1:D:25:GLU:CG	2.52	0.40
1:B:57:ARG:NH1	1:B:233:LYS:HE3	2.37	0.40
1:C:187:ARG:HH22	1:D:259:GLN:H	1.69	0.40
1:D:122:ASP:OD1	1:D:125:ILE:HB	2.22	0.40
1:C:172:ARG:HB2	1:C:172:ARG:NH1	2.37	0.40

All (4) 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)
4:B:450:HOH:O	4:C:435:HOH:O[4_545]	1.74	0.46
4:B:444:HOH:O	4:C:403:HOH:O[4_545]	1.81	0.39
4:A:443:HOH:O	4:B:447:HOH:O[2_555]	1.86	0.34
1:A:139:LEU:O	1:A:139:LEU:O[2_555]	2.08	0.12

## 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	250/261 (96%)	243 (97%)	7 (3%)	0	100	100
1	B	255/261 (98%)	244 (96%)	8 (3%)	3 (1%)	16	12
1	C	242/261 (93%)	236 (98%)	6 (2%)	0	100	100
1	D	250/261 (96%)	242 (97%)	5 (2%)	3 (1%)	16	12
All	All	997/1044 (96%)	965 (97%)	26 (3%)	6 (1%)	30	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	HIS
1	B	257	LYS
1	B	139	LEU
1	D	125	ILE
1	D	124	GLU
1	D	139	LEU

### 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	210/220 (96%)	196 (93%)	14 (7%)	20	21
1	B	213/220 (97%)	197 (92%)	16 (8%)	17	17
1	C	205/220 (93%)	182 (89%)	23 (11%)	7	6
1	D	210/220 (96%)	191 (91%)	19 (9%)	12	11
All	All	838/880 (95%)	766 (91%)	72 (9%)	13	12

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	60	ARG
1	A	93	ARG

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Mol	Chain	Res	Type
1	A	103	LEU
1	A	104	PHE
1	A	128	LEU
1	A	135	ARG
1	A	140	GLU
1	A	172	ARG
1	A	221	GLU
1	A	240	LEU
1	A	243	ARG
1	A	251	GLU
1	A	259	GLN
1	B	4	ILE
1	B	10	ARG
1	B	17	ARG
1	B	29	THR
1	B	31	LYS
1	B	118	LEU
1	B	120	LYS
1	B	142	GLU
1	B	166	ARG
1	B	187	ARG
1	B	228	GLU
1	B	243	ARG
1	B	247	THR
1	B	248	LYS
1	B	251	GLU
1	B	257	LYS
1	C	10	ARG
1	C	14	LEU
1	C	20	ILE
1	C	29	THR
1	C	47	ILE
1	C	103	LEU
1	C	104	PHE
1	C	106	ARG
1	C	109	ASP
1	C	110	ARG
1	C	124	GLU
1	C	128	LEU
1	C	131	ASN
1	C	135	ARG
1	C	166	ARG

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Mol	Chain	Res	Type
1	C	187	ARG
1	C	204	TYR
1	C	221	GLU
1	C	240	LEU
1	C	248	LYS
1	C	251	GLU
1	C	257	LYS
1	C	258	LYS
1	D	17	ARG
1	D	25	GLU
1	D	29	THR
1	D	31	LYS
1	D	47	ILE
1	D	105	TYR
1	D	109	ASP
1	D	118	LEU
1	D	124	GLU
1	D	139	LEU
1	D	140	GLU
1	D	166	ARG
1	D	204	TYR
1	D	215	LYS
1	D	228	GLU
1	D	243	ARG
1	D	245	ARG
1	D	247	THR
1	D	248	LYS

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	71	ASN
1	A	141	HIS
1	C	131	ASN
1	D	102	ASN
1	D	259	GLN

### 5.3.3 RNA ⓘ

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 [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	301	3	24,33,33	0.98	1 (4%)	31,52,52	2.02	6 (19%)
2	ATP	B	301	-	24,33,33	1.13	3 (12%)	31,52,52	1.80	4 (12%)
2	ATP	C	301	-	24,33,33	0.93	2 (8%)	31,52,52	2.05	5 (16%)
2	ATP	D	301	-	24,33,33	0.89	1 (4%)	31,52,52	2.37	7 (22%)

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	301	3	-	0/18/38/38	0/3/3/3
2	ATP	B	301	-	-	0/18/38/38	0/3/3/3
2	ATP	C	301	-	-	0/18/38/38	0/3/3/3
2	ATP	D	301	-	-	0/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ATP	C2-N3	2.03	1.35	1.32
2	B	301	ATP	C2-N3	2.41	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ATP	O4'-C1'	2.63	1.44	1.41
2	C	301	ATP	C5-C4	2.84	1.46	1.40
2	A	301	ATP	C5-C4	2.86	1.47	1.40
2	D	301	ATP	C5-C4	2.93	1.47	1.40
2	B	301	ATP	C5-C4	3.34	1.48	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	ATP	N3-C2-N1	-8.59	122.32	128.89
2	A	301	ATP	N3-C2-N1	-8.09	122.70	128.89
2	B	301	ATP	N3-C2-N1	-7.07	123.48	128.89
2	C	301	ATP	N3-C2-N1	-7.06	123.49	128.89
2	C	301	ATP	PA-O3A-PB	-5.12	118.34	132.73
2	D	301	ATP	PB-O3B-PG	-4.94	116.10	132.67
2	D	301	ATP	PA-O3A-PB	-4.86	119.08	132.73
2	A	301	ATP	PB-O3B-PG	-3.72	120.20	132.67
2	C	301	ATP	PB-O3B-PG	-3.44	121.14	132.67
2	C	301	ATP	C4-C5-N7	-3.38	106.37	109.48
2	B	301	ATP	PA-O3A-PB	-3.29	123.49	132.73
2	D	301	ATP	C4-C5-N7	-2.98	106.74	109.48
2	B	301	ATP	C2'-C1'-N9	-2.64	110.26	114.29
2	A	301	ATP	PA-O3A-PB	-2.57	125.52	132.73
2	D	301	ATP	C1'-N9-C4	-2.49	123.19	126.94
2	A	301	ATP	C4-C5-N7	-2.46	107.22	109.48
2	B	301	ATP	C4-C5-N7	-2.45	107.22	109.48
2	A	301	ATP	C2'-C1'-N9	-2.44	110.57	114.29
2	D	301	ATP	O3A-PA-O5'	-2.18	97.16	102.94
2	C	301	ATP	C1'-N9-C4	-2.09	123.80	126.94
2	A	301	ATP	C2-N1-C6	2.09	122.51	118.77
2	D	301	ATP	O3G-PG-O2G	2.31	116.17	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ATP	4	0
2	B	301	ATP	1	0
2	C	301	ATP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	ATP	5	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	252/261 (96%)	0.06	5 (1%) 68 67	24, 40, 74, 116	1 (0%)
1	B	257/261 (98%)	0.21	16 (6%) 24 23	21, 39, 80, 118	0
1	C	246/261 (94%)	0.37	19 (7%) 16 16	26, 46, 81, 120	1 (0%)
1	D	254/261 (97%)	0.32	21 (8%) 14 13	23, 46, 90, 130	0
All	All	1009/1044 (96%)	0.24	61 (6%) 25 25	21, 43, 82, 130	2 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	HIS	6.7
1	B	141	HIS	6.0
1	D	7	SER	5.4
1	D	9	PRO	5.3
1	C	105	TYR	5.2
1	D	12	TRP	5.2
1	B	140	GLU	5.2
1	C	11	TYR	4.8
1	D	10	ARG	4.6
1	D	140	GLU	4.6
1	D	14	LEU	4.5
1	C	258	LYS	4.3
1	C	259	GLN	4.2
1	A	105	TYR	4.2
1	B	105	TYR	4.2
1	A	141	HIS	4.0
1	D	139	LEU	3.7
1	B	139	LEU	3.7
1	D	11	TYR	3.7
1	B	142	GLU	3.4
1	B	252	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	104	PHE	3.2
1	D	105	TYR	3.1
1	C	161	LEU	3.1
1	A	142	GLU	3.0
1	C	136	ILE	3.0
1	B	104	PHE	2.9
1	B	143	ARG	2.9
1	D	15	TYR	2.8
1	C	135	ARG	2.8
1	B	74	VAL	2.7
1	B	158	VAL	2.7
1	C	9	PRO	2.7
1	C	12	TRP	2.6
1	D	142	GLU	2.6
1	B	180	ILE	2.6
1	C	130	ILE	2.6
1	D	138	GLY	2.5
1	C	149	ASN	2.5
1	C	145	LYS	2.5
1	D	108	GLU	2.4
1	C	124	GLU	2.4
1	A	104	PHE	2.4
1	C	115	ALA	2.4
1	D	136	ILE	2.4
1	D	172	ARG	2.3
1	B	2	VAL	2.3
1	C	180	ILE	2.3
1	C	126	GLU	2.3
1	B	12	TRP	2.3
1	B	135	ARG	2.3
1	D	261	ASP	2.2
1	B	4	ILE	2.2
1	D	141	HIS	2.2
1	D	200	ILE	2.1
1	C	121	TYR	2.1
1	C	146	VAL	2.1
1	D	96	ASN	2.1
1	B	3	LYS	2.0
1	A	139	LEU	2.0
1	D	80	VAL	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	C	301	31/31	0.90	0.17	-0.23	34,53,134,138	0
2	ATP	D	301	31/31	0.92	0.13	-0.50	35,49,104,109	0
2	ATP	A	301	31/31	0.93	0.15	-0.54	24,36,108,129	0
2	ATP	B	301	31/31	0.91	0.12	-0.63	25,50,92,105	0
3	MG	A	302	1/1	0.97	0.23	-	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.