



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:45 pm GMT

PDB ID : 3R5X  
Title : Crystal Structure of D-alanine–D-Alanine Ligase from *Bacillus anthracis* complexed with ATP  
Authors : Kim, Y.; Mulligan, R.; Hasseman, J.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-03-20  
Resolution : 2.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

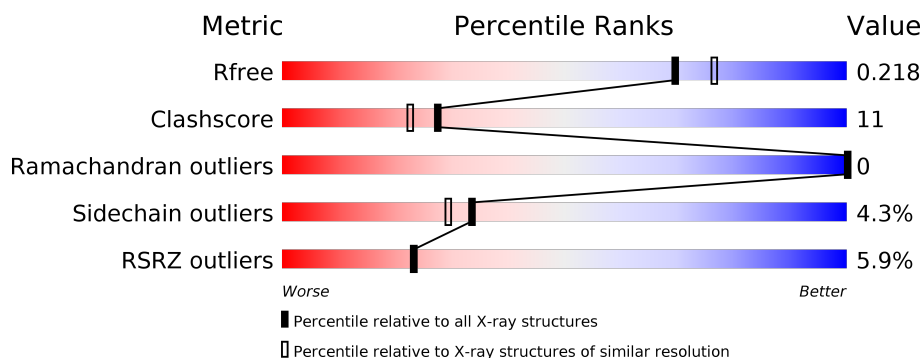
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	307	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>••</div> </div>
1	B	307	<div> <div>8%</div> <div>71%</div> <div>21%</div> <div>• 5%</div> </div>
1	C	307	<div> <div>8%</div> <div>67%</div> <div>22%</div> <div>• 7%</div> </div>
1	D	307	<div> <div>3%</div> <div>83%</div> <div>17%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	D	404	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10379 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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	Se	0	8	0
			2422	1535	386	482	4	15			
1	B	291	Total	C	N	O	S	Se	0	7	0
			2324	1477	371	457	4	15			
1	C	284	Total	C	N	O	S	Se	0	7	0
			2270	1445	360	445	4	16			
1	D	306	Total	C	N	O	S	Se	0	11	0
			2473	1569	392	490	4	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81Q29
A	-1	ASN	-	EXPRESSION TAG	UNP Q81Q29
A	0	ALA	-	EXPRESSION TAG	UNP Q81Q29
B	-2	SER	-	EXPRESSION TAG	UNP Q81Q29
B	-1	ASN	-	EXPRESSION TAG	UNP Q81Q29
B	0	ALA	-	EXPRESSION TAG	UNP Q81Q29
C	-2	SER	-	EXPRESSION TAG	UNP Q81Q29
C	-1	ASN	-	EXPRESSION TAG	UNP Q81Q29
C	0	ALA	-	EXPRESSION TAG	UNP Q81Q29
D	-2	SER	-	EXPRESSION TAG	UNP Q81Q29
D	-1	ASN	-	EXPRESSION TAG	UNP Q81Q29
D	0	ALA	-	EXPRESSION TAG	UNP Q81Q29

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

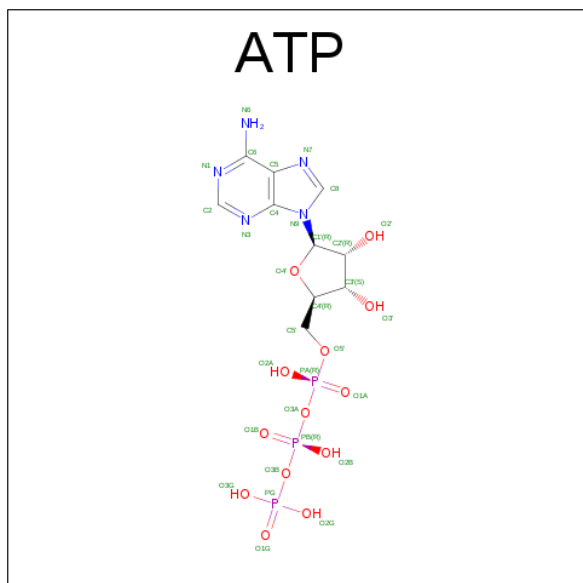
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

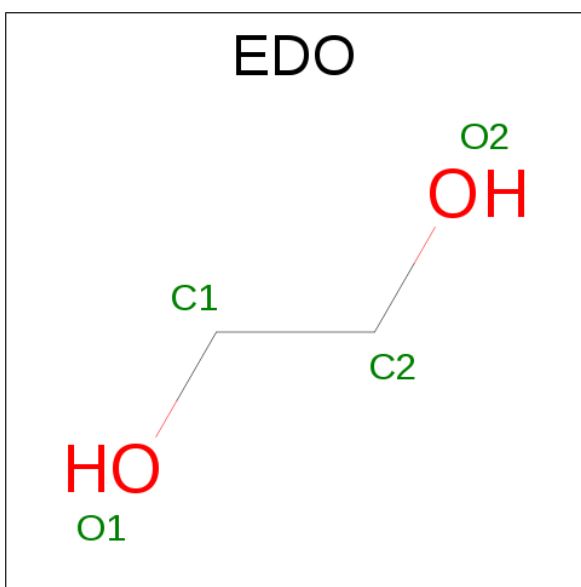


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

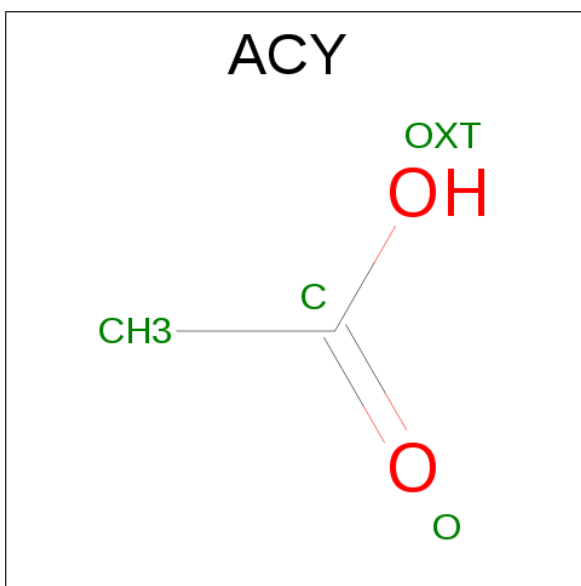
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		

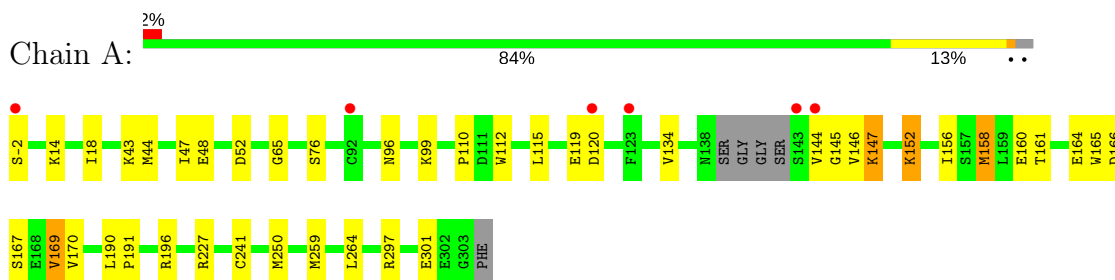
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	207	Total 207	O 207	0	0
7	B	152	Total 152	O 152	0	0
7	C	165	Total 165	O 165	0	0
7	D	226	Total 226	O 226	0	0

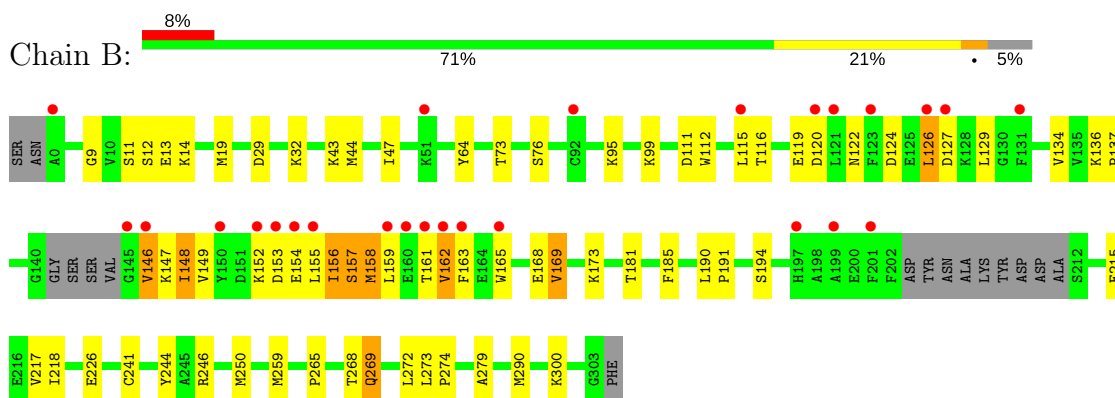
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 ( $\text{RSRZ} > 2$ ). 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.

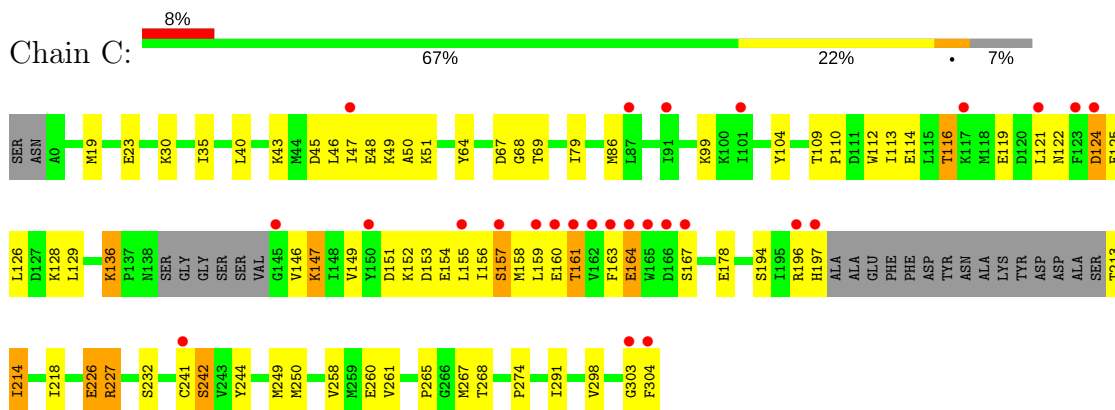
#### • Molecule 1: D-alanine–D-alanine ligase



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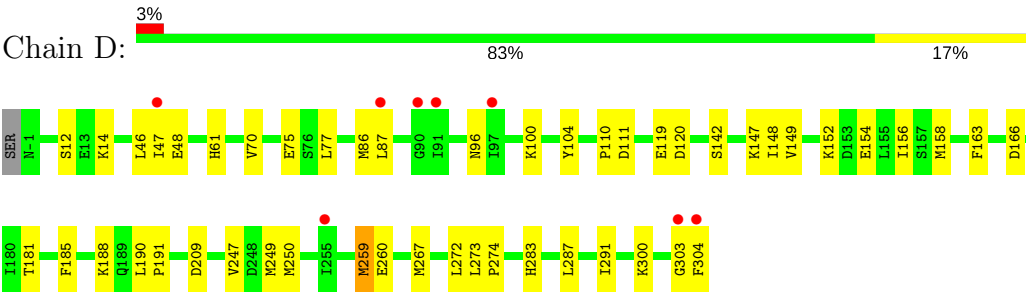


#### • Molecule 1: D-alanine–D-alanine ligase



#### • Molecule 1: D-alanine–D-alanine ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.34Å 68.99Å 92.39Å 73.36° 84.96° 75.46°	Depositor
Resolution (Å)	32.77 – 2.00 37.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (32.77-2.00) 88.7 (37.42-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.177 , 0.221 0.174 , 0.218	Depositor DCC
$R_{free}$ test set	4238 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ACY, MG, CA, ATP, EDO

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	0.51	1/2442 (0.0%)	0.59	0/3266
1	B	0.51	1/2341 (0.0%)	0.56	0/3125
1	C	0.50	1/2286 (0.0%)	0.60	0/3052
1	D	0.51	0/2495	0.63	0/3336
All	All	0.51	3/9564 (0.0%)	0.60	0/12779

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	241	CYS	CB-SG	-7.03	1.70	1.82
1	B	241	CYS	CB-SG	-5.48	1.72	1.81
1	A	241	CYS	CB-SG	-5.11	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2422	0	2438	43	0
1	B	2324	0	2362	64	0
1	C	2270	0	2319	71	0
1	D	2473	0	2488	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	31	0	12	2	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	2	0
4	C	1	0	0	0	0
5	D	4	0	6	4	0
6	D	4	0	3	0	0
7	A	207	0	0	3	0
7	B	152	0	0	1	0
7	C	165	0	0	2	0
7	D	226	0	0	6	0
All	All	10379	0	9664	218	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 11.

All (218) 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:C:147:LYS:HD3	1:C:158:MSE:SE	2.02	1.08
1:D:147:LYS:HE2	1:D:158[A]:MSE:SE	2.15	0.97
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.31	0.94
1:C:152:LYS:HE2	1:C:156:ILE:HD11	1.48	0.93
1:C:109[A]:THR:HG22	1:C:110:PRO:HD2	1.54	0.88
1:B:147:LYS:HB3	1:B:158:MSE:HE3	1.60	0.84
1:A:110:PRO:CG	1:A:259[B]:MSE:HE1	2.08	0.83
1:D:267:MSE:CE	1:D:287:LEU:HD21	2.08	0.83
1:C:157:SER:O	1:C:160:GLU:HG3	1.80	0.81
1:B:194:SER:HB2	1:B:218:ILE:HD13	1.62	0.81
1:B:119:GLU:HG2	1:B:120:ASP:H	1.46	0.81
1:A:147:LYS:HG3	1:A:158:MSE:SE	2.31	0.80
1:A:110:PRO:HG3	1:A:259[B]:MSE:HE1	1.64	0.79
1:C:125:GLU:H	1:C:125:GLU:CD	1.85	0.79
1:C:109[A]:THR:HG23	1:C:258:VAL:O	1.82	0.79
1:C:99:LYS:HG2	1:C:109[A]:THR:HG21	1.67	0.77
1:A:96[B]:ASN:OD1	1:A:170:VAL:HG22	1.85	0.77
1:B:146:VAL:HG23	1:B:148:ILE:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:SER:HB2	1:B:218:ILE:CD1	2.17	0.74
1:C:126:LEU:HD21	1:C:155:LEU:HD21	1.67	0.74
1:B:162:VAL:CG1	1:B:163:PHE:N	2.53	0.71
1:A:110:PRO:CG	1:A:259[B]:MSE:CE	2.68	0.71
1:A:147:LYS:HZ3	1:A:158:MSE:SE	2.23	0.71
1:A:76:SER:OG	1:B:44:MSE:HE3	1.90	0.71
1:D:267:MSE:HE3	1:D:287:LEU:HD21	1.73	0.71
1:A:44:MSE:HB3	1:B:47:ILE:HD13	1.74	0.70
1:B:43:LYS:HA	1:B:64:TYR:OH	1.92	0.69
1:B:147:LYS:HB3	1:B:158:MSE:CE	2.22	0.69
1:D:104:TYR:HB2	7:D:512:HOH:O	1.93	0.69
1:C:227:ARG:HG2	1:C:227:ARG:NH1	2.06	0.68
1:B:162:VAL:O	1:B:165:TRP:HB2	1.94	0.68
1:B:159:LEU:O	1:B:162:VAL:HG12	1.94	0.68
1:B:13[B]:GLU:HA	1:B:13[B]:GLU:OE1	1.94	0.68
1:C:125:GLU:HA	1:C:128:LYS:HD2	1.75	0.67
1:D:267:MSE:HE1	1:D:287:LEU:HD21	1.76	0.67
1:A:158:MSE:HA	1:A:158:MSE:HE2	1.77	0.67
1:B:19:MSE:HE3	1:B:268:THR:HG21	1.75	0.67
1:C:124:ASP:O	1:C:128:LYS:HG3	1.94	0.67
1:B:119:GLU:HG2	1:B:120:ASP:N	2.10	0.65
1:C:48:GLU:HG2	1:C:49:LYS:HG2	1.78	0.65
1:A:165:TRP:C	1:A:166[B]:ASP:OD1	2.35	0.64
1:B:115:LEU:HB3	1:B:169:VAL:HG12	1.79	0.64
1:D:110:PRO:HB2	1:D:172:GLU:HG2	1.78	0.64
1:C:157:SER:O	1:C:160:GLU:CG	2.44	0.64
1:A:166[B]:ASP:N	1:A:166[B]:ASP:OD1	2.30	0.64
1:C:153:ASP:O	1:C:157:SER:HB2	1.97	0.64
1:C:121:LEU:HD21	1:C:159:LEU:CD1	2.29	0.62
1:C:242:SER:HB2	7:C:561:HOH:O	2.00	0.62
1:B:217:VAL:HG21	1:B:279:ALA:HB2	1.81	0.62
5:D:404:EDO:H21	7:D:726:HOH:O	2.00	0.62
1:D:267:MSE:HE3	1:D:287:LEU:CD2	2.30	0.61
1:A:44:MSE:HE3	1:B:47:ILE:HD11	1.81	0.60
1:C:68:GLY:O	1:C:86[B]:MSE:HG3	2.01	0.60
1:B:155:LEU:O	1:B:159:LEU:HG	2.01	0.60
1:C:104:TYR:HB2	7:D:512:HOH:O	2.02	0.60
1:C:151:ASP:HB3	1:C:154[A]:GLU:HG3	1.81	0.60
1:C:126:LEU:HD21	1:C:155:LEU:CD2	2.32	0.60
1:B:181[B]:THR:HG21	7:B:610:HOH:O	2.03	0.59
1:B:153:ASP:O	1:B:157:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:HD3	7:A:676:HOH:O	2.04	0.58
1:A:110:PRO:HG2	1:A:259[B]:MSE:HE1	1.85	0.58
1:D:267:MSE:CE	1:D:287:LEU:CD2	2.79	0.58
1:A:110:PRO:HG2	1:A:259[B]:MSE:CE	2.33	0.58
1:C:109[A]:THR:HG22	1:C:110:PRO:CD	2.31	0.57
1:D:96:ASN:HB2	7:D:559:HOH:O	2.04	0.57
1:C:232:SER:HB3	1:C:249:MSE:CE	2.34	0.57
1:A:44:MSE:CE	1:B:47:ILE:HD11	2.34	0.57
1:B:244:TYR:HE1	1:B:265:PRO:HD2	1.70	0.56
1:C:147:LYS:CD	1:C:158:MSE:SE	2.92	0.56
1:A:145:GLY:O	1:A:147:LYS:HE3	2.06	0.56
3:A:402:ATP:O1G	7:A:688:HOH:O	2.17	0.55
1:B:13[B]:GLU:CA	1:B:13[B]:GLU:OE1	2.54	0.55
1:B:153:ASP:HA	1:B:156:ILE:HD11	1.88	0.55
1:D:283:HIS:CD2	1:D:283:HIS:H	2.24	0.55
5:D:404:EDO:C1	7:D:726:HOH:O	2.55	0.55
1:A:161:THR:O	1:A:164:GLU:HG2	2.07	0.55
1:B:162:VAL:HG12	1:B:163:PHE:N	2.22	0.55
1:A:144:VAL:HG22	1:A:147:LYS:NZ	2.22	0.54
1:B:95:LYS:HE2	1:B:137:PRO:O	2.08	0.54
1:D:250[B]:MSE:HG3	1:D:259:MSE:CE	2.38	0.54
1:D:75:GLU:OE2	5:D:404:EDO:H21	2.08	0.54
1:A:152:LYS:O	1:A:156:ILE:HG12	2.08	0.54
1:D:179:GLU:HG2	1:D:250[B]:MSE:HE3	1.90	0.54
1:C:99:LYS:NZ	1:C:109[A]:THR:HG22	2.23	0.54
1:D:46:LEU:HD11	1:D:70:VAL:HG13	1.90	0.54
1:D:260:GLU:OE1	3:D:402:ATP:O3G	2.26	0.54
1:C:242:SER:OG	1:C:298:VAL:HG11	2.08	0.54
1:D:303:GLY:C	1:D:304:PHE:HD2	2.11	0.53
1:C:125:GLU:N	1:C:125:GLU:CD	2.59	0.53
1:C:125:GLU:O	1:C:128:LYS:HB2	2.09	0.53
1:B:116:THR:HG22	1:B:168:GLU:HG2	1.91	0.53
1:B:126:LEU:O	1:B:129:LEU:HB2	2.09	0.52
1:D:185:PHE:O	1:D:188:LYS:HG2	2.09	0.52
1:D:111:ASP:HB2	1:D:173:LYS:HD2	1.91	0.52
1:B:146:VAL:HG23	1:B:148:ILE:CG2	2.38	0.52
1:C:232:SER:HB3	1:C:249:MSE:HE1	1.92	0.52
1:A:115:LEU:HB3	1:A:169:VAL:HG12	1.92	0.51
1:A:144:VAL:CG2	1:A:147:LYS:HZ1	2.22	0.51
1:B:29:ASP:OD2	1:B:32:LYS:HG3	2.10	0.51
1:C:113:ILE:CD1	1:C:126:LEU:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LEU:HB3	1:C:163:PHE:CE2	2.46	0.51
1:B:273:LEU:HB3	1:B:274:PRO:HD3	1.93	0.50
1:A:166[A]:ASP:OD1	1:A:167:SER:N	2.44	0.50
1:A:158:MSE:CE	1:A:158:MSE:HA	2.41	0.50
1:C:40:LEU:HD22	1:C:45:ASP:HB2	1.93	0.50
1:D:47:ILE:HD13	1:D:77:LEU:HD11	1.92	0.50
1:D:267:MSE:HE2	1:D:291:ILE:HD11	1.92	0.50
1:D:250[B]:MSE:HG3	1:D:259:MSE:SE	2.62	0.50
1:D:110:PRO:HB2	1:D:172:GLU:CG	2.41	0.49
1:B:217:VAL:HG21	1:B:279:ALA:CB	2.42	0.49
1:C:244:TYR:HE1	1:C:265:PRO:HD2	1.78	0.49
1:C:69:THR:HA	1:D:86[B]:MSE:HE1	1.94	0.49
1:C:109[A]:THR:CG2	1:C:110:PRO:HD2	2.35	0.49
1:D:273:LEU:HB3	1:D:274:PRO:HD3	1.94	0.49
1:C:267:MSE:HE2	1:C:291:ILE:CD1	2.41	0.49
1:C:30:LYS:HD3	1:C:35:ILE:HD12	1.94	0.49
1:B:134:VAL:HG21	3:B:402:ATP:C6	2.48	0.49
1:B:162:VAL:HG13	1:B:163:PHE:N	2.24	0.48
1:C:149:VAL:HG13	1:C:154[A]:GLU:HB2	1.94	0.48
1:B:111:ASP:HB2	1:B:173:LYS:HE3	1.96	0.48
1:B:153:ASP:HA	1:B:156:ILE:CD1	2.42	0.48
1:B:181[A]:THR:HG21	1:B:246:ARG:NE	2.29	0.48
1:C:113:ILE:HG22	1:C:114:GLU:N	2.27	0.48
1:D:86[B]:MSE:HG2	1:D:87:LEU:N	2.27	0.48
1:D:120:ASP:OD1	1:D:120:ASP:N	2.41	0.48
1:C:122:ASN:OD1	1:C:122:ASN:C	2.52	0.48
1:D:304:PHE:N	1:D:304:PHE:CD2	2.82	0.48
1:B:250:MSE:HE2	1:B:259[B]:MSE:SE	2.64	0.47
1:B:155:LEU:CD1	1:B:159:LEU:HD21	2.44	0.47
1:C:147:LYS:HB2	1:C:158:MSE:HE3	1.97	0.47
3:C:402:ATP:O1A	7:C:616:HOH:O	2.20	0.47
1:B:162:VAL:O	1:B:165:TRP:N	2.47	0.47
1:C:226:GLU:HG2	1:C:227:ARG:N	2.28	0.47
1:C:303:GLY:O	1:C:304:PHE:CD2	2.68	0.47
1:A:250:MSE:HE2	1:A:250:MSE:HB2	1.80	0.46
1:A:44:MSE:HB3	1:B:47:ILE:CD1	2.43	0.46
1:C:194:SER:HB2	1:C:218:ILE:HG21	1.97	0.46
1:B:99:LYS:HE3	1:B:112:TRP:CE3	2.51	0.46
1:D:250[B]:MSE:HB3	1:D:250[B]:MSE:HE2	1.92	0.46
1:C:227:ARG:NH1	1:C:227:ARG:CG	2.70	0.46
1:C:47:ILE:O	1:C:51:LYS:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:PHE:HA	1:D:166:ASP:O	2.16	0.45
1:C:124:ASP:HB2	1:C:125:GLU:OE2	2.16	0.45
1:A:43:LYS:HE3	1:B:76:SER:HB2	1.98	0.45
1:C:116:THR:OG1	1:C:119:GLU:HB2	2.16	0.45
1:C:136:LYS:HB3	1:C:146:VAL:HG12	1.99	0.45
1:B:9:GLY:O	1:B:14:LYS:HD2	2.17	0.45
1:B:190:LEU:HB3	1:B:191:PRO:CD	2.47	0.45
1:B:190:LEU:HB3	1:B:191:PRO:HD2	1.99	0.45
1:B:126:LEU:HD12	1:B:126:LEU:HA	1.84	0.45
1:B:149:VAL:HG12	1:B:154:GLU:HB3	1.99	0.45
1:C:48:GLU:HG2	1:C:49:LYS:N	2.32	0.45
1:D:96:ASN:O	1:D:100:LYS:HG3	2.17	0.45
1:D:75:GLU:OE2	5:D:404:EDO:C2	2.64	0.45
1:B:185:PHE:CE2	1:B:290:MSE:HE2	2.51	0.45
1:C:43:LYS:HG3	1:C:64:TYR:CE2	2.52	0.45
1:D:47:ILE:HB	1:D:48:GLU:OE1	2.17	0.45
1:A:96[B]:ASN:CG	1:A:170:VAL:HG22	2.36	0.45
1:B:181[A]:THR:HG21	1:B:246:ARG:CD	2.46	0.45
1:C:116:THR:H	1:C:119:GLU:HB3	1.82	0.45
1:C:113:ILE:HD11	1:C:126:LEU:HA	1.97	0.44
1:B:122:ASN:HB3	1:B:124:ASP:OD1	2.17	0.44
1:B:269:GLN:HB2	1:B:269:GLN:HE21	1.65	0.44
1:D:260:GLU:OE2	3:D:402:ATP:O3B	2.36	0.44
1:A:119:GLU:HG2	1:A:120:ASP:O	2.18	0.43
1:B:181[A]:THR:CG2	1:B:246:ARG:HG2	2.48	0.43
1:C:113:ILE:CG2	1:C:114:GLU:N	2.81	0.43
1:C:196:ARG:HH21	1:C:214:ILE:HD13	1.82	0.43
1:C:152:LYS:CE	1:C:156:ILE:HD11	2.33	0.43
1:B:155:LEU:HD12	1:B:159:LEU:HD21	2.00	0.43
1:C:161:THR:HA	1:C:164:GLU:OE1	2.19	0.43
1:A:44:MSE:HE2	1:B:73:THR:HG23	2.01	0.43
1:D:149:VAL:HB	1:D:154:GLU:HB3	2.00	0.43
1:A:44:MSE:HE3	1:A:47:ILE:CD1	2.49	0.43
1:D:190:LEU:HB3	1:D:191:PRO:HD2	2.01	0.43
1:A:146:VAL:C	1:A:147:LYS:HG2	2.38	0.42
1:A:144:VAL:CG2	1:A:147:LYS:NZ	2.82	0.42
1:A:160:GLU:HG3	7:A:506:HOH:O	2.19	0.42
1:B:13[B]:GLU:N	1:B:13[B]:GLU:CD	2.72	0.42
1:B:156:ILE:HG12	1:B:157:SER:H	1.83	0.42
1:B:163:PHE:HD1	1:B:163:PHE:HA	1.76	0.42
1:C:99:LYS:HE3	1:C:112:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LYS:O	1:B:156:ILE:HD13	2.19	0.42
1:A:227[A]:ARG:HE	1:A:227[A]:ARG:HB2	1.46	0.42
1:A:65:GLY:HA3	1:A:264:LEU:HD22	2.01	0.42
1:C:19:MSE:O	1:C:23:GLU:HG3	2.19	0.42
1:D:61:HIS:HD2	7:D:614:HOH:O	2.00	0.42
1:A:14:LYS:O	1:A:18:ILE:HG12	2.19	0.42
1:B:43:LYS:CA	1:B:64:TYR:OH	2.63	0.42
1:A:99:LYS:HE3	1:A:112:TRP:CD2	2.55	0.42
1:C:122:ASN:ND2	1:C:125:GLU:OE2	2.52	0.42
1:C:267:MSE:CE	1:C:291:ILE:CD1	2.98	0.42
1:C:250:MSE:HB2	1:C:250:MSE:HE2	1.99	0.41
1:A:144:VAL:HG22	1:A:147:LYS:HZ2	1.85	0.41
1:C:50:ALA:HB1	1:C:79:ILE:CD1	2.50	0.41
1:D:303:GLY:C	1:D:304:PHE:CD2	2.92	0.41
1:B:146:VAL:CG2	1:B:146:VAL:O	2.67	0.41
1:C:99:LYS:NZ	1:C:109[A]:THR:CG2	2.82	0.41
1:C:99:LYS:HZ2	1:C:109[A]:THR:HG22	1.85	0.41
1:C:197:HIS:HA	1:C:213:THR:HG22	2.02	0.41
1:D:179:GLU:HG2	1:D:250[A]:MSE:SE	2.70	0.41
1:D:181:THR:HG21	1:D:272:LEU:HD13	2.02	0.41
1:A:190:LEU:HB3	1:A:191:PRO:CD	2.51	0.41
1:D:152:LYS:O	1:D:156:ILE:HD13	2.21	0.41
1:D:250[B]:MSE:SE	1:D:259:MSE:HE2	2.71	0.41
1:C:244:TYR:CE1	1:C:265:PRO:HD2	2.56	0.41
1:C:268:THR:O	1:C:274:PRO:HG2	2.21	0.41
1:D:247:VAL:HG11	1:D:249:MSE:HE2	2.03	0.41
1:A:297:ARG:O	1:A:301:GLU:HG3	2.21	0.40
1:B:153:ASP:O	1:B:156:ILE:HG12	2.21	0.40
1:C:113:ILE:HG13	1:C:129:LEU:HD11	2.03	0.40
1:D:158[B]:MSE:HE3	1:D:158[B]:MSE:HA	2.03	0.40
1:C:260:GLU:CG	1:C:261:VAL:N	2.84	0.40
1:A:110:PRO:CG	1:A:259[B]:MSE:HE2	2.50	0.40
1:A:134:VAL:HG21	3:A:402:ATP:C6	2.57	0.40
1:C:46:LEU:O	1:C:50:ALA:HB3	2.21	0.40
1:B:215:GLU:CD	1:B:272:LEU:HD21	2.42	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	306/307 (100%)	302 (99%)	4 (1%)	0	100	100
1	B	292/307 (95%)	288 (99%)	4 (1%)	0	100	100
1	C	285/307 (93%)	282 (99%)	3 (1%)	0	100	100
1	D	315/307 (103%)	313 (99%)	2 (1%)	0	100	100
All	All	1198/1228 (98%)	1185 (99%)	13 (1%)	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	272/253 (108%)	264 (97%)	8 (3%)	48	47
1	B	261/253 (103%)	245 (94%)	16 (6%)	22	16
1	C	257/253 (102%)	242 (94%)	15 (6%)	23	18
1	D	277/253 (110%)	270 (98%)	7 (2%)	53	54
All	All	1067/1012 (105%)	1021 (96%)	46 (4%)	33	29

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	48	GLU

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Mol	Chain	Res	Type
1	A	52[A]	ASP
1	A	52[B]	ASP
1	A	147	LYS
1	A	152	LYS
1	A	158	MSE
1	A	169	VAL
1	B	11	SER
1	B	12	SER
1	B	126	LEU
1	B	127	ASP
1	B	136	LYS
1	B	146	VAL
1	B	148	ILE
1	B	156	ILE
1	B	157	SER
1	B	158	MSE
1	B	161	THR
1	B	162	VAL
1	B	169	VAL
1	B	226	GLU
1	B	269	GLN
1	B	300	LYS
1	C	67	ASP
1	C	116	THR
1	C	124	ASP
1	C	136	LYS
1	C	147	LYS
1	C	157	SER
1	C	161	THR
1	C	164	GLU
1	C	167	SER
1	C	178[A]	GLU
1	C	178[B]	GLU
1	C	214	ILE
1	C	226	GLU
1	C	227	ARG
1	C	242	SER
1	D	12	SER
1	D	14	LYS
1	D	119	GLU
1	D	142	SER
1	D	148	ILE

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Mol	Chain	Res	Type
1	D	259	MSE
1	D	300	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
1	B	269	GLN
1	C	41	ASN
1	C	269	GLN
1	D	41	ASN
1	D	283	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 [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z  > 2$
3	ATP	A	402	2	27,33,33	1.09	2 (7%)	25,52,52	1.46	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	B	402	-	27,33,33	1.05	1 (3%)	25,52,52	1.70	3 (12%)
3	ATP	C	402	2	27,33,33	1.05	2 (7%)	25,52,52	1.67	1 (4%)
3	ATP	D	402	2	27,33,33	1.10	2 (7%)	25,52,52	1.75	5 (20%)
5	EDO	D	404	-	3,3,3	0.32	0	2,2,2	0.46	0
6	ACY	D	405	-	1,3,3	1.43	0	0,3,3	0.00	-

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
3	ATP	A	402	2	-	0/18/38/38	0/3/3/3
3	ATP	B	402	-	-	0/18/38/38	0/3/3/3
3	ATP	C	402	2	-	0/18/38/38	0/3/3/3
3	ATP	D	402	2	-	0/18/38/38	0/3/3/3
5	EDO	D	404	-	-	0/1/1/1	0/0/0/0
6	ACY	D	405	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	ATP	C5-N7	-2.03	1.32	1.39
3	A	402	ATP	O4'-C1'	2.03	1.44	1.41
3	D	402	ATP	C5-C4	2.25	1.45	1.40
3	C	402	ATP	O4'-C1'	2.26	1.44	1.41
3	C	402	ATP	C5-C4	3.00	1.47	1.40
3	A	402	ATP	C5-C4	3.31	1.48	1.40
3	B	402	ATP	C5-C4	3.37	1.48	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	ATP	N3-C2-N1	-6.69	123.03	128.86
3	B	402	ATP	N3-C2-N1	-6.08	123.56	128.86
3	D	402	ATP	N3-C2-N1	-5.94	123.69	128.86
3	A	402	ATP	N3-C2-N1	-4.71	124.75	128.86
3	D	402	ATP	C4-C5-N7	-3.15	106.36	109.41
3	B	402	ATP	C4-C5-N7	-2.94	106.57	109.41
3	A	402	ATP	C4-C5-N7	-2.24	107.25	109.41
3	A	402	ATP	C2-N1-C6	2.10	122.44	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	ATP	O2A-PA-O1A	2.20	123.68	112.28
3	A	402	ATP	N6-C6-N1	2.26	123.25	118.77
3	D	402	ATP	O3G-PG-O2G	2.34	117.03	107.61
3	B	402	ATP	C4'-O4'-C1'	2.37	112.29	109.77
3	D	402	ATP	O3G-PG-O1G	2.99	122.20	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	ATP	2	0
3	B	402	ATP	1	0
3	C	402	ATP	1	0
3	D	402	ATP	2	0
5	D	404	EDO	4	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	288/307 (93%)	-0.17	6 (2%) 64 63	30, 47, 87, 137	0
1	B	277/307 (90%)	0.29	26 (9%) 9 9	32, 57, 133, 187	0
1	C	270/307 (87%)	0.28	26 (9%) 9 9	29, 52, 124, 192	0
1	D	292/307 (95%)	-0.06	8 (2%) 55 54	30, 46, 78, 107	0
All	All	1127/1228 (91%)	0.08	66 (5%) 23 23	29, 50, 113, 192	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	TRP	10.6
1	C	121	LEU	8.9
1	B	123	PHE	8.7
1	A	143	SER	8.4
1	B	165	TRP	6.8
1	C	145	GLY	6.7
1	B	121	LEU	6.6
1	D	303	GLY	6.4
1	C	123	PHE	6.1
1	B	162	VAL	5.9
1	A	120	ASP	4.8
1	C	162	VAL	4.5
1	B	155	LEU	4.4
1	D	304	PHE	4.4
1	B	120	ASP	4.0
1	C	161	THR	3.9
1	C	155	LEU	3.6
1	B	126	LEU	3.6
1	C	117	LYS	3.6
1	B	0	ALA	3.5
1	B	127	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	304	PHE	3.3
1	B	161	THR	3.3
1	C	87	LEU	3.3
1	B	152	LYS	3.2
1	B	201	PHE	3.2
1	B	154	GLU	3.1
1	D	97	ILE	3.1
1	C	166	ASP	3.0
1	C	303	GLY	3.0
1	D	47	ILE	3.0
1	D	91	ILE	3.0
1	B	150	TYR	3.0
1	C	124	ASP	2.9
1	B	146	VAL	2.9
1	C	163	PHE	2.9
1	B	51	LYS	2.7
1	C	91	ILE	2.7
1	B	163	PHE	2.7
1	C	160	GLU	2.7
1	D	87	LEU	2.6
1	B	145	GLY	2.6
1	C	159	LEU	2.6
1	A	123	PHE	2.5
1	A	-2	SER	2.5
1	A	144	VAL	2.5
1	D	255	ILE	2.4
1	B	115	LEU	2.4
1	C	164	GLU	2.4
1	D	90	GLY	2.3
1	B	160	GLU	2.3
1	C	47	ILE	2.3
1	C	101	ILE	2.3
1	C	150	TYR	2.3
1	B	153	ASP	2.3
1	B	92	CYS	2.3
1	C	196	ARG	2.2
1	C	197	HIS	2.2
1	B	159	LEU	2.2
1	B	197	HIS	2.1
1	B	199	ALA	2.1
1	A	92	CYS	2.1
1	C	157	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	131	PHE	2.1
1	C	167	SER	2.0
1	C	241	CYS	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(Å <sup>2</sup> )	Q<0.9
3	ATP	B	402	31/31	0.73	0.22	1.12	71,126,226,235	0
3	ATP	A	402	31/31	0.93	0.12	0.38	32,41,64,160	21
2	CA	D	401	1/1	0.99	0.17	0.13	36,36,36,36	0
3	ATP	D	402	31/31	0.96	0.14	0.01	30,36,164,221	0
2	CA	D	403	1/1	0.97	0.13	-0.06	50,50,50,50	0
3	ATP	C	402	31/31	0.92	0.10	-0.55	48,80,168,207	0
5	EDO	D	404	4/4	0.91	0.09	-0.64	63,66,75,80	0
4	MG	C	404	1/1	0.95	0.08	-0.90	60,60,60,60	0
2	CA	B	403	1/1	0.99	0.03	-1.94	69,69,69,69	0
2	CA	C	403	1/1	0.95	0.08	-	53,53,53,53	0
2	CA	A	401	1/1	0.94	0.06	-	58,58,58,58	0
6	ACY	D	405	4/4	0.95	0.10	-	81,87,88,91	0
2	CA	B	401	1/1	0.74	0.10	-	101,101,101,101	0
2	CA	C	401	1/1	0.71	0.09	-	82,82,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.