



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:10 am GMT

PDB ID : 2DLN  
Title : VANCOMYCIN RESISTANCE: STRUCTURE OF D-ALANINE:D-ALANINE LIGASE AT 2.3 ANGSTROMS RESOLUTION  
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Deposited on : 1994-07-18  
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

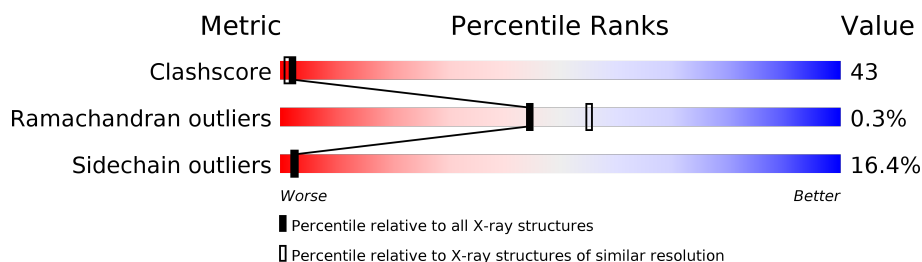
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2642 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.

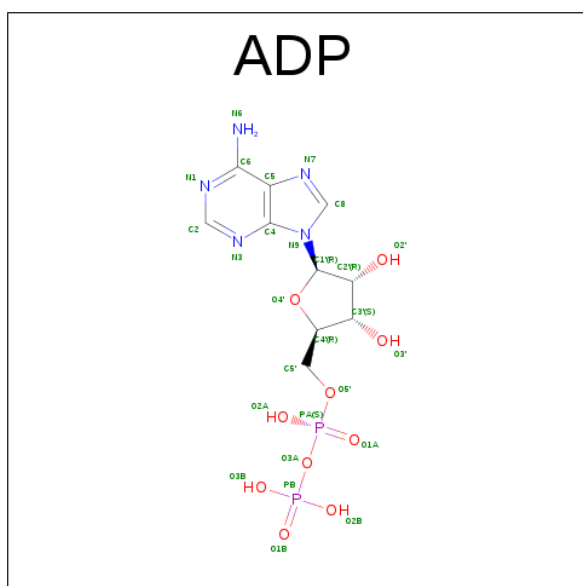
- Molecule 1 is a protein called D-ALANINE–D-ALANINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2305	1464	382	446	13			

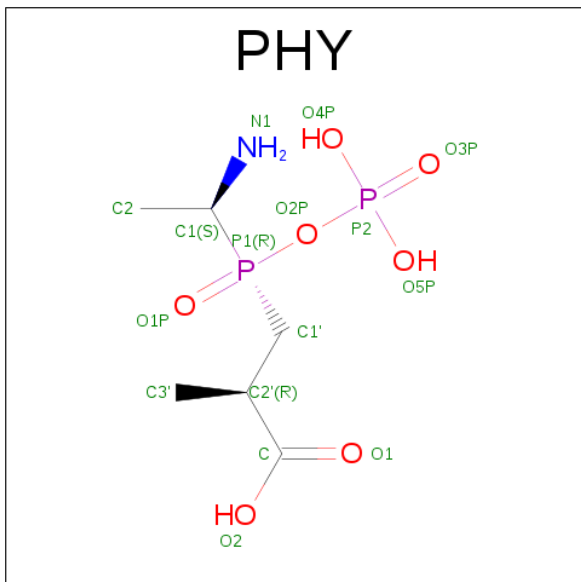
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



- Molecule 4 is 1(S)-AMINOETHYL-(2-CARBOXYPROPYL)PHOSPHORYL-PHOSPHINIC ACID (three-letter code: PHY) (formula:  $C_6H_{15}NO_7P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	6	1	7	2		

- Molecule 5 is water.

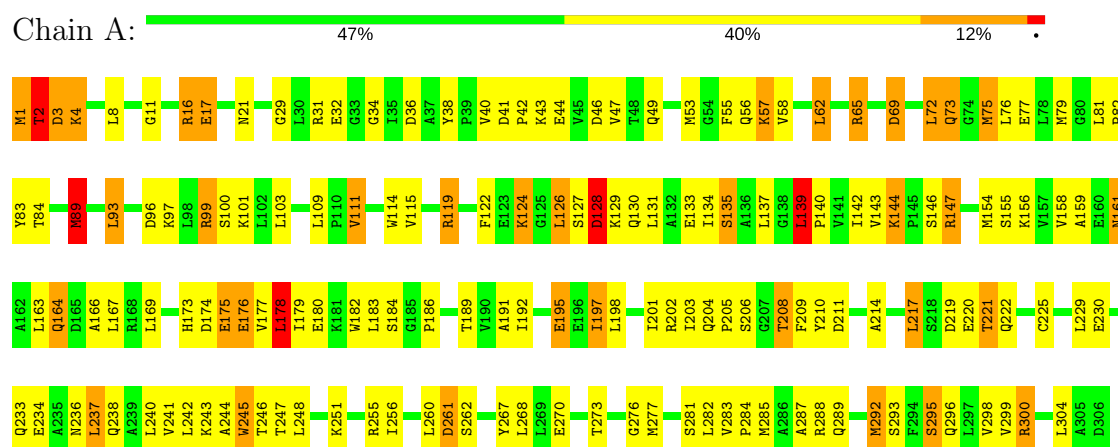
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	292	Total	O	0	0
			292	292		

### 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 ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: D-ALANINE-D-ALANINE LIGASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.30 Å 51.40 Å 51.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2642	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PHY, ADP

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	0.87	0/2346	1.64	34/3175 (1.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ARG	NE-CZ-NH1	-15.42	112.59	120.30
1	A	139	LEU	CA-CB-CG	13.20	145.66	115.30
1	A	65	ARG	NE-CZ-NH1	12.65	126.62	120.30
1	A	16	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	99	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	A	178	LEU	CA-CB-CG	8.64	135.18	115.30
1	A	288	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	99	ARG	CD-NE-CZ	7.22	133.71	123.60
1	A	176	GLU	OE1-CD-OE2	-7.13	114.74	123.30
1	A	41	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	84	THR	N-CA-C	6.92	129.67	111.00
1	A	65	ARG	CD-NE-CZ	6.90	133.26	123.60
1	A	139	LEU	CB-CA-C	6.89	123.28	110.20
1	A	210	TYR	CB-CG-CD2	-6.41	117.15	121.00
1	A	16	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	292	MET	CA-CB-CG	6.20	123.85	113.30
1	A	210	TYR	CB-CG-CD1	6.20	124.72	121.00
1	A	62	LEU	CA-CB-CG	5.87	128.81	115.30
1	A	2	THR	N-CA-CB	5.80	121.33	110.30
1	A	96	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	230	GLU	CA-CB-CG	5.71	125.96	113.40
1	A	69	ASP	CB-CA-C	5.65	121.70	110.40
1	A	65	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
1	A	84	THR	CA-C-N	5.28	126.76	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	147	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	261	ASP	N-CA-CB	5.24	120.03	110.60
1	A	119	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	A	178	LEU	N-CA-CB	5.21	120.81	110.40
1	A	180	GLU	CA-CB-CG	5.20	124.85	113.40
1	A	195	GLU	CG-CD-OE1	-5.20	107.91	118.30
1	A	128	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	119	ARG	CD-NE-CZ	-5.09	116.47	123.60
1	A	89	MET	CA-CB-CG	-5.07	104.69	113.30

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	2305	0	2321	200	2
2	A	2	0	0	0	0
3	A	27	0	12	2	0
4	A	16	0	11	3	0
5	A	292	0	0	57	7
All	All	2642	0	2344	202	8

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 43.

All (202) 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:A:204:GLN:HG2	5:A:568:HOH:O	1.35	1.21
1:A:2:THR:H	1:A:4:LYS:HE3	1.19	1.03
1:A:197:ILE:HD11	1:A:238:GLN:HG2	1.41	1.01
1:A:244:ALA:CB	5:A:677:HOH:O	2.08	1.00
1:A:192:ILE:HG13	5:A:572:HOH:O	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:N	1:A:4:LYS:HE3	1.78	0.98
1:A:295:SER:O	1:A:299:VAL:HG23	1.65	0.97
1:A:240:LEU:HA	1:A:243:LYS:HE3	1.46	0.96
1:A:159:ALA:HB3	1:A:161:ASN:ND2	1.84	0.93
1:A:164:GLN:HB2	5:A:578:HOH:O	1.70	0.92
1:A:233:GLN:HA	5:A:636:HOH:O	1.70	0.90
4:A:320:PHY:O2	5:A:654:HOH:O	1.89	0.90
1:A:2:THR:H	1:A:4:LYS:CE	1.85	0.90
1:A:281:SER:OG	5:A:654:HOH:O	1.61	0.89
1:A:268:LEU:CD2	5:A:677:HOH:O	2.21	0.89
1:A:34:GLY:O	5:A:613:HOH:O	1.90	0.89
1:A:143:VAL:HG21	1:A:166:ALA:HB1	1.52	0.88
1:A:2:THR:O	1:A:56:GLN:HG2	1.73	0.88
1:A:197:ILE:HD11	1:A:238:GLN:CG	2.05	0.87
1:A:159:ALA:CB	1:A:161:ASN:ND2	2.36	0.86
1:A:103:LEU:HD21	1:A:247:THR:HG22	1.59	0.85
1:A:159:ALA:HB3	1:A:161:ASN:HD21	1.36	0.84
1:A:220:GLU:HB3	5:A:665:HOH:O	1.78	0.83
1:A:124:LYS:HE3	5:A:569:HOH:O	1.78	0.82
1:A:69:ASP:O	1:A:73:GLN:NE2	2.12	0.82
1:A:133:GLU:HG3	5:A:683:HOH:O	1.80	0.81
1:A:268:LEU:HD21	5:A:677:HOH:O	1.79	0.81
1:A:284:PRO:HB2	5:A:454:HOH:O	1.79	0.81
1:A:131:LEU:O	1:A:135:SER:HB2	1.80	0.80
1:A:43:LYS:O	1:A:43:LYS:HG2	1.82	0.80
1:A:189:THR:HG21	1:A:282:LEU:HD13	1.63	0.80
1:A:134:ILE:HA	1:A:137:LEU:HD12	1.65	0.77
1:A:219:ASP:HA	5:A:652:HOH:O	1.84	0.76
1:A:103:LEU:CD2	1:A:247:THR:HG22	2.16	0.75
1:A:214:ALA:O	1:A:221:THR:HG21	1.85	0.75
1:A:133:GLU:HA	1:A:133:GLU:OE1	1.84	0.75
1:A:143:VAL:HG21	1:A:166:ALA:CB	2.15	0.75
1:A:99:ARG:NH1	1:A:176:GLU:OE1	2.18	0.74
1:A:109:LEU:HD11	1:A:243:LYS:HD2	1.69	0.74
1:A:89:MET:HG2	1:A:93:LEU:HD13	1.70	0.74
1:A:89:MET:HG2	1:A:93:LEU:CD1	2.18	0.74
1:A:164:GLN:HB3	5:A:506:HOH:O	1.87	0.74
1:A:244:ALA:HB2	5:A:677:HOH:O	1.74	0.74
1:A:293:SER:H	1:A:296:GLN:HE21	1.36	0.73
1:A:197:ILE:HD11	1:A:238:GLN:CB	2.19	0.73
1:A:167:LEU:HD21	1:A:179:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:NH2	5:A:637:HOH:O	2.22	0.71
1:A:220:GLU:OE1	5:A:665:HOH:O	2.08	0.70
1:A:159:ALA:CB	1:A:161:ASN:HD22	2.04	0.70
1:A:285:MET:SD	5:A:472:HOH:O	2.51	0.68
1:A:159:ALA:HB1	1:A:161:ASN:HD22	1.58	0.67
1:A:57:LYS:HD3	5:A:469:HOH:O	1.92	0.67
1:A:133:GLU:CA	1:A:133:GLU:OE1	2.39	0.66
1:A:245:TRP:HD1	1:A:256:ILE:HD11	1.61	0.66
1:A:295:SER:O	1:A:299:VAL:CG2	2.44	0.66
1:A:159:ALA:HB1	1:A:161:ASN:ND2	2.10	0.65
1:A:142:ILE:HD11	1:A:154:MET:CE	2.27	0.64
1:A:1:MET:C	1:A:3:ASP:H	1.99	0.64
1:A:72:LEU:HD23	1:A:75:MET:HE2	1.79	0.64
1:A:276:GLY:C	1:A:277:MET:HG2	2.16	0.64
1:A:242:LEU:O	1:A:246:THR:HG23	1.98	0.64
1:A:154:MET:SD	3:A:310:ADP:H5'1	2.39	0.63
1:A:8:LEU:CD1	1:A:72:LEU:HD11	2.29	0.63
1:A:128:ASP:OD2	1:A:129:LYS:NZ	2.25	0.62
1:A:140:PRO:HB3	1:A:158:VAL:HG22	1.81	0.62
1:A:75:MET:SD	1:A:79:MET:HE1	2.41	0.61
1:A:124:LYS:HG2	5:A:569:HOH:O	2.00	0.61
1:A:101:LYS:HE2	5:A:614:HOH:O	1.98	0.61
1:A:36:ASP:HA	5:A:582:HOH:O	2.01	0.60
1:A:38:TYR:CD1	1:A:55:PHE:HE1	2.20	0.60
1:A:75:MET:SD	1:A:79:MET:CE	2.90	0.60
1:A:31:ARG:NE	5:A:671:HOH:O	2.34	0.60
1:A:134:ILE:O	1:A:137:LEU:HB2	2.02	0.59
1:A:268:LEU:HD22	5:A:677:HOH:O	1.96	0.59
1:A:56:GLN:O	1:A:82:PRO:HD2	2.02	0.59
1:A:58:VAL:O	1:A:83:TYR:HA	2.01	0.59
1:A:143:VAL:CG2	1:A:166:ALA:HB1	2.29	0.59
1:A:282:LEU:HD12	5:A:637:HOH:O	2.02	0.59
1:A:142:ILE:HD11	1:A:154:MET:HE3	1.85	0.58
1:A:197:ILE:HD11	1:A:238:GLN:HB3	1.83	0.58
1:A:109:LEU:HD21	5:A:646:HOH:O	2.05	0.57
1:A:163:LEU:HD11	1:A:179:ILE:HD13	1.85	0.57
1:A:29:GLY:O	1:A:295:SER:HB3	2.05	0.57
1:A:300:ARG:O	1:A:304:LEU:HG	2.05	0.56
1:A:208:THR:CB	5:A:402:HOH:O	2.54	0.56
1:A:1:MET:C	1:A:3:ASP:N	2.59	0.56
1:A:109:LEU:CD2	5:A:646:HOH:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:HA	1:A:126:LEU:HD23	1.88	0.56
1:A:129:LYS:HD2	1:A:129:LYS:N	2.20	0.56
1:A:229:LEU:HG	1:A:233:GLN:HB2	1.88	0.56
1:A:293:SER:H	1:A:296:GLN:NE2	2.03	0.56
1:A:115:VAL:HG23	1:A:137:LEU:HD11	1.87	0.56
1:A:201:ILE:HG21	5:A:472:HOH:O	2.05	0.55
1:A:57:LYS:HG3	1:A:82:PRO:HB2	1.87	0.55
1:A:128:ASP:HB3	5:A:684:HOH:O	2.07	0.55
1:A:17:GLU:CD	5:A:562:HOH:O	2.44	0.55
1:A:89:MET:CG	1:A:93:LEU:HD13	2.37	0.55
1:A:97:LYS:HG3	1:A:146:SER:O	2.07	0.55
1:A:76:LEU:HD13	1:A:83:TYR:HB3	1.89	0.55
1:A:3:ASP:O	5:A:462:HOH:O	2.18	0.54
1:A:72:LEU:HD23	1:A:75:MET:CE	2.38	0.54
1:A:126:LEU:HG	5:A:681:HOH:O	2.07	0.54
1:A:11:GLY:O	1:A:16:ARG:NH1	2.34	0.53
1:A:101:LYS:HD2	1:A:114:TRP:CD2	2.43	0.53
1:A:111:VAL:HG22	5:A:614:HOH:O	2.09	0.53
1:A:283:VAL:N	1:A:284:PRO:CD	2.71	0.53
1:A:201:ILE:HG22	1:A:203:ILE:HD13	1.90	0.53
1:A:8:LEU:HD12	1:A:72:LEU:HD11	1.91	0.53
1:A:31:ARG:NH1	5:A:582:HOH:O	2.41	0.53
1:A:144:LYS:CG	1:A:178:LEU:HD23	2.39	0.53
1:A:142:ILE:HD12	1:A:182:TRP:HZ3	1.73	0.53
1:A:128:ASP:CB	5:A:684:HOH:O	2.57	0.53
1:A:208:THR:HB	5:A:402:HOH:O	2.09	0.53
1:A:49:GLN:O	1:A:53:MET:HG3	2.09	0.52
1:A:142:ILE:HD12	1:A:182:TRP:CZ3	2.45	0.52
1:A:201:ILE:HD13	5:A:472:HOH:O	2.10	0.51
1:A:73:GLN:O	1:A:77:GLU:HG2	2.10	0.51
1:A:127:SER:C	1:A:129:LYS:N	2.63	0.51
1:A:122:PHE:HD1	1:A:126:LEU:HD21	1.76	0.50
1:A:214:ALA:O	1:A:221:THR:CG2	2.57	0.50
1:A:281:SER:OG	4:A:320:PHY:O2	2.29	0.50
1:A:89:MET:SD	1:A:93:LEU:HD13	2.52	0.50
1:A:261:ASP:HB3	1:A:267:TYR:HE2	1.76	0.50
1:A:43:LYS:CG	1:A:43:LYS:O	2.56	0.49
1:A:173:HIS:CE1	5:A:625:HOH:O	2.66	0.49
1:A:245:TRP:CH2	1:A:251:LYS:HA	2.48	0.49
1:A:293:SER:N	1:A:296:GLN:HE21	2.09	0.49
1:A:119:ARG:O	1:A:122:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:TRP:CD1	1:A:256:ILE:HD11	2.44	0.49
1:A:46:ASP:O	1:A:49:GLN:HG2	2.13	0.49
1:A:241:VAL:HG13	1:A:256:ILE:HD12	1.94	0.49
1:A:268:LEU:CD1	5:A:677:HOH:O	2.61	0.49
1:A:197:ILE:CD1	1:A:238:GLN:HG2	2.28	0.48
1:A:244:ALA:HB1	5:A:677:HOH:O	1.94	0.48
1:A:287:ALA:HB1	1:A:292:MET:HG3	1.95	0.48
1:A:292:MET:CE	5:A:509:HOH:O	2.62	0.48
1:A:42:PRO:HG2	1:A:62:LEU:HD11	1.94	0.48
1:A:139:LEU:HD12	1:A:158:VAL:HG13	1.96	0.47
1:A:65:ARG:HD2	1:A:147:ARG:HE	1.79	0.47
1:A:75:MET:SD	1:A:79:MET:HE3	2.54	0.47
1:A:270:GLU:HG3	1:A:270:GLU:O	2.14	0.47
1:A:1:MET:HA	1:A:4:LYS:HE2	1.97	0.47
1:A:130:GLN:O	1:A:133:GLU:HB2	2.15	0.46
1:A:174:ASP:OD1	1:A:175:GLU:N	2.49	0.46
1:A:57:LYS:HB2	1:A:57:LYS:HE2	1.43	0.46
1:A:247:THR:HG21	5:A:646:HOH:O	2.15	0.46
1:A:127:SER:HB2	1:A:130:GLN:HB2	1.98	0.46
1:A:225:CYS:SG	1:A:289:GLN:HG2	2.56	0.46
1:A:236:ASN:ND2	5:A:636:HOH:O	2.27	0.46
1:A:273:THR:O	5:A:446:HOH:O	2.20	0.46
1:A:72:LEU:CD2	1:A:75:MET:CE	2.93	0.46
1:A:101:LYS:HD3	1:A:114:TRP:CE3	2.50	0.46
1:A:292:MET:HE2	5:A:509:HOH:O	2.16	0.46
1:A:191:ALA:HB3	1:A:198:LEU:HD12	1.99	0.45
1:A:127:SER:C	1:A:129:LYS:H	2.19	0.45
1:A:183:LEU:HD22	1:A:261:ASP:HB2	1.97	0.45
1:A:186:PRO:HD2	1:A:260:LEU:HB2	1.99	0.45
1:A:229:LEU:HD23	1:A:234:GLU:CA	2.47	0.44
1:A:93:LEU:HD21	1:A:103:LEU:HD13	1.99	0.44
1:A:154:MET:HE2	1:A:209:PHE:CE2	2.52	0.44
1:A:229:LEU:HD23	1:A:234:GLU:HA	1.99	0.44
1:A:73:GLN:HB2	1:A:73:GLN:HE21	1.56	0.44
1:A:167:LEU:HD21	1:A:179:ILE:CD1	2.43	0.44
1:A:135:SER:C	1:A:137:LEU:H	2.21	0.44
1:A:147:ARG:HD3	5:A:631:HOH:O	2.17	0.43
1:A:147:ARG:NH1	5:A:631:HOH:O	2.51	0.43
1:A:143:VAL:O	1:A:154:MET:HA	2.18	0.43
1:A:276:GLY:O	1:A:277:MET:HG2	2.18	0.43
1:A:283:VAL:N	1:A:284:PRO:HD3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:H	1:A:130:GLN:NE2	2.16	0.43
4:A:320:PHY:H2'	5:A:637:HOH:O	2.18	0.43
1:A:129:LYS:HD2	1:A:129:LYS:H	1.84	0.43
1:A:154:MET:HE1	3:A:310:ADP:O4'	2.19	0.43
1:A:101:LYS:HG3	1:A:111:VAL:CG2	2.49	0.43
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.66	0.43
1:A:147:ARG:HH11	1:A:147:ARG:HD3	1.52	0.43
1:A:191:ALA:CB	1:A:198:LEU:HD12	2.49	0.43
1:A:206:SER:HB3	1:A:220:GLU:HB2	2.01	0.43
1:A:119:ARG:HH11	1:A:119:ARG:HD2	1.59	0.42
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.77	0.42
1:A:8:LEU:HD23	1:A:40:VAL:HB	2.02	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.76	0.42
1:A:75:MET:HE3	1:A:75:MET:HB3	1.94	0.42
1:A:2:THR:H	1:A:4:LYS:NZ	2.17	0.42
1:A:205:PRO:HA	1:A:221:THR:HB	2.01	0.41
1:A:156:LYS:HD2	5:A:663:HOH:O	2.20	0.41
1:A:144:LYS:HG2	1:A:178:LEU:CD2	2.50	0.41
1:A:211:ASP:O	1:A:214:ALA:N	2.51	0.41
1:A:197:ILE:CD1	1:A:238:GLN:HB3	2.49	0.41
1:A:89:MET:HE2	1:A:89:MET:HB3	1.99	0.41
1:A:89:MET:CG	1:A:93:LEU:CD1	2.92	0.41
1:A:201:ILE:HG22	1:A:202:ARG:N	2.36	0.41
1:A:222:GLN:NE2	5:A:427:HOH:O	2.46	0.41
1:A:234:GLU:HG3	5:A:483:HOH:O	2.19	0.41
1:A:159:ALA:CB	1:A:161:ASN:HD21	2.11	0.41
1:A:173:HIS:HD2	5:A:406:HOH:O	2.02	0.41
1:A:173:HIS:HE1	5:A:625:HOH:O	2.02	0.41
1:A:217:LEU:HD12	1:A:217:LEU:N	2.35	0.41
1:A:81:LEU:HA	1:A:82:PRO:HD3	1.85	0.41
1:A:161:ASN:HD22	1:A:161:ASN:H	1.69	0.40
1:A:233:GLN:CG	5:A:636:HOH:O	2.69	0.40
1:A:154:MET:HE3	1:A:154:MET:HB3	1.72	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:456:HOH:O	5:A:644:HOH:O[3_557]	1.41	0.79
5:A:450:HOH:O	5:A:689:HOH:O[3_557]	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:523:HOH:O	5:A:530:HOH:O[3_546]	1.96	0.24
5:A:404:HOH:O	5:A:497:HOH:O[2_555]	2.07	0.13
5:A:640:HOH:O	5:A:641:HOH:O[1_556]	2.07	0.13
5:A:593:HOH:O	5:A:593:HOH:O[2_565]	2.09	0.11
1:A:32:GLU:OE1	5:A:541:HOH:O[3_557]	2.13	0.07
1:A:139:LEU:CD2	1:A:202:ARG:NH1[3_546]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	304/306 (99%)	281 (92%)	22 (7%)	1 (0%)	44 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLU

### 5.3.2 Protein sidechains [i](#)

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	244/244 (100%)	204 (84%)	40 (16%)	2 2

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	3	ASP
1	A	4	LYS
1	A	17	GLU
1	A	47	VAL
1	A	57	LYS
1	A	72	LEU
1	A	73	GLN
1	A	75	MET
1	A	89	MET
1	A	93	LEU
1	A	100	SER
1	A	111	VAL
1	A	124	LYS
1	A	126	LEU
1	A	128	ASP
1	A	135	SER
1	A	139	LEU
1	A	144	LYS
1	A	155	SER
1	A	161	ASN
1	A	164	GLN
1	A	169	LEU
1	A	175	GLU
1	A	177	VAL
1	A	178	LEU
1	A	184	SER
1	A	195	GLU
1	A	197	ILE
1	A	208	THR
1	A	217	LEU
1	A	221	THR
1	A	237	LEU
1	A	245	TRP
1	A	248	LEU
1	A	262	SER
1	A	295	SER
1	A	298	VAL
1	A	300	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	49	GLN
1	A	73	GLN
1	A	130	GLN
1	A	161	ASN
1	A	173	HIS
1	A	289	GLN
1	A	296	GLN

### 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ADP	A	310	2	25,29,29	1.22	3 (12%)	24,45,45	1.25	1 (4%)
4	PHY	A	320	2	8,15,15	10.47	1 (12%)	7,23,23	1.69	2 (28%)

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	ADP	A	310	2	-	0/12/32/32	0/3/3/3
4	PHY	A	320	2	-	0/8/21/21	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	320	PHY	P1-C1'	-29.48	1.52	1.79
3	A	310	ADP	PB-O3A	-2.26	1.56	1.60
3	A	310	ADP	C5'-C4'	2.17	1.58	1.51
3	A	310	ADP	O4'-C1'	3.46	1.46	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	310	ADP	O5'-C5'-C4'	-3.18	97.73	109.00
4	A	320	PHY	O5P-P2-O4P	2.35	117.09	107.61
4	A	320	PHY	P1-C1'-C2'	2.82	129.17	116.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	310	ADP	2	0
4	A	320	PHY	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.