



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:14 PM UTC

PDB ID : 2DLN / pdb_00002dlh
Title : VANCOMYCIN RESISTANCE: STRUCTURE OF D-ALANINE:D-ALANINE LIGASE AT 2.3 ANGSTROMS RESOLUTION
Authors : Knox, J.R.; Moews, P.C.; Fan, C.
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

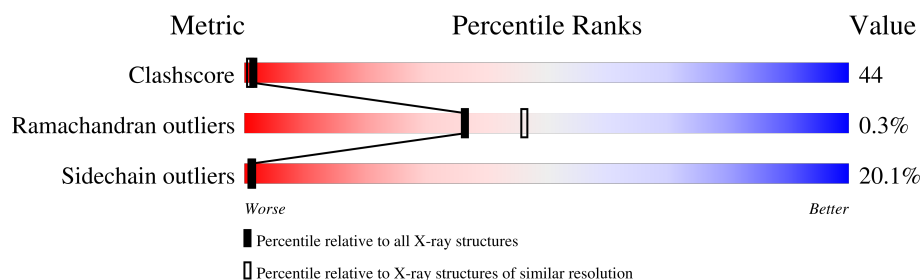
1 Overall quality at a glance

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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.

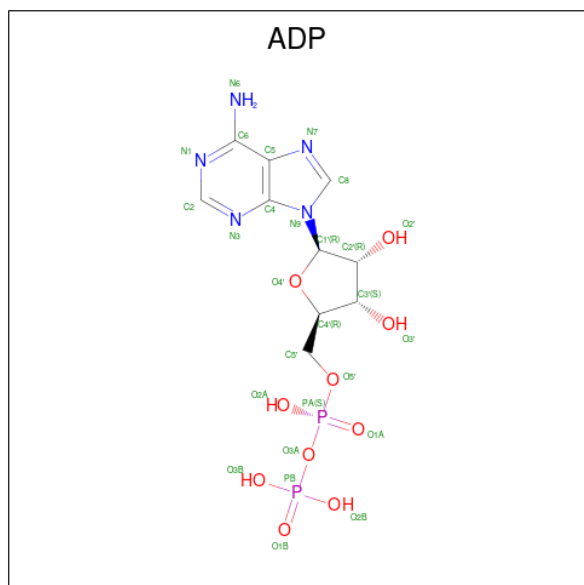
- Molecule 1 is a protein called D-ALANINE–D-ALANINE LIGASE.

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 (CCD ID: MG) (formula: Mg).

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

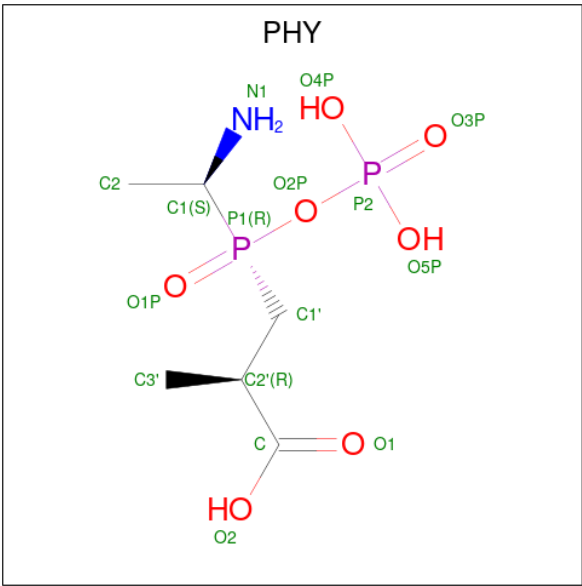
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 1(S)-AMINOETHYL-(2-CARBOXYPROPYL)PHOSPHORYL-PHOSPHINI

C ACID (CCD ID: PHY) (formula: C₆H₁₅NO₇P₂).



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.

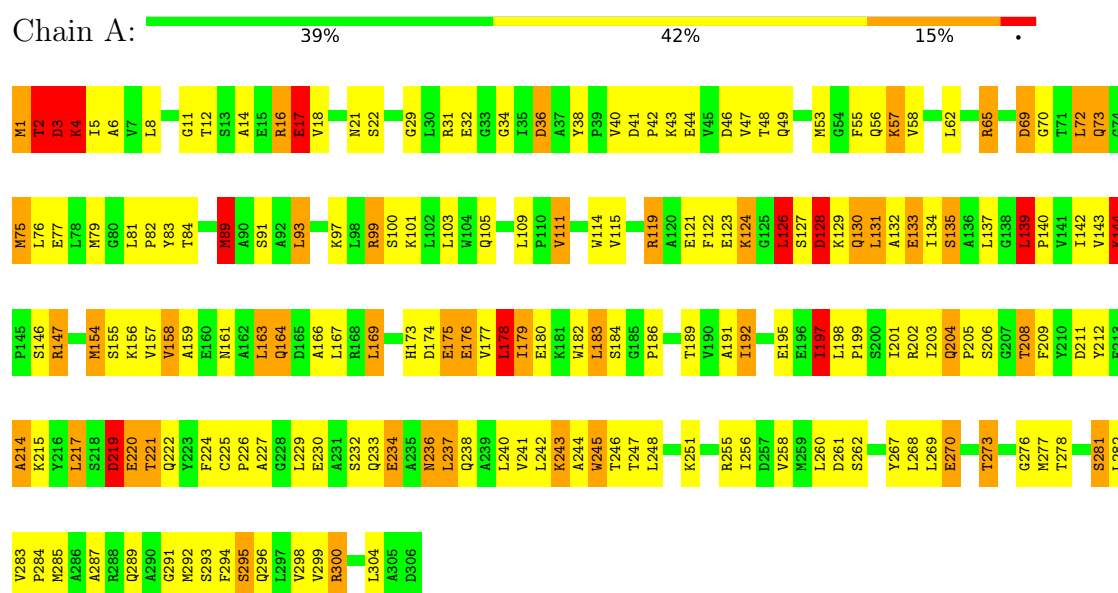
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	292	Total	O	0	0
			292	292		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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, α , β , γ	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 ²)	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: ADP, MG, PHY

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	1.08	3/2346 (0.1%)	2.08	79/3175 (2.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	THR	C-O	6.83	1.31	1.24
1	A	84	THR	CA-CB	5.87	1.62	1.53
1	A	139	LEU	CA-CB	-5.33	1.45	1.53

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	THR	N-CA-C	17.38	129.67	111.07
1	A	36	ASP	CA-CB-CG	10.04	122.64	112.60
1	A	147	ARG	NE-CZ-NH1	-8.91	112.59	121.50
1	A	139	LEU	CA-CB-CG	8.39	145.66	116.30
1	A	144	LYS	O-C-N	7.84	127.45	121.88
1	A	232	SER	CA-C-N	7.59	130.45	120.28
1	A	232	SER	C-N-CA	7.59	130.45	120.28
1	A	176	GLU	CB-CG-CD	7.58	125.48	112.60
1	A	131	LEU	N-CA-C	-7.41	103.97	113.16
1	A	226	PRO	CA-C-N	7.33	132.44	120.63
1	A	226	PRO	C-N-CA	7.33	132.44	120.63
1	A	219	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	130	GLN	N-CA-C	-6.86	106.80	114.62
1	A	227	ALA	N-CA-C	6.84	121.23	112.34
1	A	89	MET	N-CA-C	6.72	118.27	111.07
1	A	163	LEU	N-CA-C	6.71	118.59	111.28
1	A	139	LEU	CB-CA-C	6.66	123.28	110.17
1	A	99	ARG	CD-NE-CZ	6.65	133.71	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	LYS	CA-C-N	6.62	129.04	120.44
1	A	243	LYS	C-N-CA	6.62	129.04	120.44
1	A	4	LYS	N-CA-C	-6.59	98.49	108.96
1	A	70	GLY	N-CA-C	6.46	121.77	114.67
1	A	128	ASP	N-CA-C	-6.46	104.50	112.38
1	A	204	GLN	O-C-N	6.45	126.43	121.27
1	A	2	THR	N-CA-CB	6.41	121.33	110.49
1	A	65	ARG	CD-NE-CZ	6.33	133.26	124.40
1	A	178	LEU	N-CA-CB	6.29	120.81	110.69
1	A	214	ALA	N-CA-C	-6.26	104.53	111.36
1	A	224	PHE	CA-CB-CG	-6.19	107.61	113.80
1	A	281	SER	CA-C-N	6.09	131.00	120.58
1	A	281	SER	C-N-CA	6.09	131.00	120.58
1	A	236	ASN	CA-CB-CG	6.08	118.68	112.60
1	A	128	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	18	VAL	N-CA-C	-5.95	104.72	110.72
1	A	230	GLU	CA-CB-CG	5.93	125.96	114.10
1	A	158	VAL	N-CA-CB	5.89	119.26	111.25
1	A	158	VAL	N-CA-C	-5.88	99.93	108.17
1	A	197	ILE	CB-CA-C	5.85	119.08	110.77
1	A	12	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	84	THR	CA-C-O	-5.80	114.73	120.82
1	A	180	GLU	CA-C-N	5.76	129.02	120.95
1	A	180	GLU	C-N-CA	5.76	129.02	120.95
1	A	91	SER	N-CA-C	-5.75	104.61	111.69
1	A	230	GLU	CA-C-O	-5.71	115.49	121.55
1	A	16	ARG	CA-C-O	-5.71	114.46	120.63
1	A	209	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	147	ARG	N-CA-C	5.70	120.59	111.81
1	A	41	ASP	CB-CA-C	5.68	117.56	109.38
1	A	119	ARG	CD-NE-CZ	-5.67	116.47	124.40
1	A	183	LEU	CB-CA-C	5.64	119.05	109.80
1	A	158	VAL	O-C-N	5.64	129.10	123.18
1	A	126	LEU	CB-CA-C	5.59	118.98	109.53
1	A	154	MET	O-C-N	5.53	129.21	122.96
1	A	132	ALA	N-CA-C	-5.43	105.38	112.23
1	A	3	ASP	N-CA-CB	5.43	117.29	110.45
1	A	230	GLU	N-CA-C	-5.40	103.01	110.35
1	A	178	LEU	CA-CB-CG	5.39	135.18	116.30
1	A	123	GLU	CA-C-N	5.38	132.06	122.06
1	A	123	GLU	C-N-CA	5.38	132.06	122.06
1	A	180	GLU	CA-CB-CG	5.37	124.85	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	CB-CG-CD	5.32	123.53	111.30
1	A	270	GLU	CB-CA-C	-5.24	100.72	110.56
1	A	294	PHE	CA-C-O	-5.23	114.34	120.20
1	A	17	GLU	CB-CG-CD	5.23	121.49	112.60
1	A	105	GLN	OE1-CD-NE2	5.23	127.83	122.60
1	A	22	SER	CA-C-N	5.19	125.74	119.98
1	A	22	SER	C-N-CA	5.19	125.74	119.98
1	A	14	ALA	N-CA-C	-5.16	106.50	112.89
1	A	6	ALA	O-C-N	5.15	129.37	123.29
1	A	278	THR	CA-C-O	-5.14	115.59	121.82
1	A	121	GLU	N-CA-C	-5.14	105.76	111.36
1	A	65	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	273	THR	CA-C-N	5.10	127.12	122.37
1	A	273	THR	C-N-CA	5.10	127.12	122.37
1	A	183	LEU	N-CA-C	-5.10	100.99	109.46
1	A	215	LYS	CA-C-O	-5.08	115.48	120.82
1	A	91	SER	CA-CB-OG	5.07	121.25	111.10
1	A	69	ASP	CB-CA-C	5.05	121.70	111.60
1	A	291	GLY	N-CA-C	5.01	122.08	114.61

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	205	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	207	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 44.

All (207) 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
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:HG2	1:A:43:LYS:O	1.82	0.80
1:A:75:MET:SD	1:A:79:MET:HE3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:255:ARG:NH2	5:A:637:HOH:O	2.22	0.71
1:A:276:GLY:C	1:A:277:MET:HG2	2.16	0.70
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:1:MET:C	1:A:3:ASP:H	1.99	0.69
1:A:292:MET:HE1	5:A:509:HOH:O	1.92	0.68
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:OE1	1:A:133:GLU:CA	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:HE3	1.78	0.65
1:A:142:ILE:HD11	1:A:154:MET:CE	2.27	0.64
1:A:242:LEU:O	1:A:246:THR:HG23	1.98	0.64
1:A:8:LEU:CD1	1:A:72:LEU:HD11	2.29	0.63
1:A:154:MET:SD	3:A:310:ADP:H5'1	2.39	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:124:LYS:HG2	5:A:569:HOH:O	2.00	0.61
1:A:1:MET:C	1:A:3:ASP:N	2.59	0.61
1:A:72:LEU:HD23	1:A:75:MET:HE2	1.82	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:31:ARG:NE	5:A:671:HOH:O	2.34	0.60
1:A:17:GLU:CD	5:A:562:HOH:O	2.44	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:75:MET:SD	1:A:79:MET:CE	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:GLY:O	1:A:295:SER:HB3	2.05	0.57
1:A:163:LEU:HD11	1:A:179:ILE:HD13	1.85	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:109:LEU:CD2	5:A:646:HOH:O	2.53	0.56
1:A:122:PHE:HA	1:A:126:LEU:HD23	1.88	0.56
1:A:129:LYS:N	1:A:129:LYS:HD2	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:49:GLN:HE21	1:A:53:MET:HE3	1.71	0.55
1:A:127:SER:C	1:A:129:LYS:N	2.63	0.55
1:A:57:LYS:HG3	1:A:82:PRO:HB2	1.87	0.55
1:A:89:MET:CG	1:A:93:LEU:HD13	2.37	0.55
1:A:128:ASP:HB3	5:A:684:HOH:O	2.07	0.55
1:A:76:LEU:HD13	1:A:83:TYR:HB3	1.89	0.55
1:A:97:LYS:HG3	1:A:146:SER:O	2.07	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:8:LEU:HD12	1:A:72:LEU:HD11	1.91	0.53
1:A:201:ILE:HG22	1:A:203:ILE:HD13	1.90	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:73:GLN:O	1:A:77:GLU:HG2	2.10	0.51
1:A:201:ILE:HD13	5:A:472:HOH:O	2.10	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:89:MET:SD	1:A:93:LEU:HD13	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:C	1:A:129:LYS:H	2.19	0.50
1:A:261:ASP:HB3	1:A:267:TYR:HE2	1.76	0.50
1:A:43:LYS:O	1:A:43:LYS:CG	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:46:ASP:O	1:A:49:GLN:HG2	2.13	0.49
1:A:119:ARG:O	1:A:122:PHE:HB3	2.12	0.49
1:A:245:TRP:CD1	1:A:256:ILE:HD11	2.44	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:135:SER:C	1:A:137:LEU:H	2.21	0.48
1:A:154:MET:HE1	3:A:310:ADP:O4'	2.13	0.48
1:A:197:ILE:CD1	1:A:238:GLN:HG2	2.28	0.48
1:A:281:SER:OG	4:A:320:PHY:O2	2.29	0.48
1:A:244:ALA:HB1	5:A:677:HOH:O	1.94	0.48
1:A:42:PRO:HG2	1:A:62:LEU:HD11	1.94	0.48
1:A:287:ALA:HB1	1:A:292:MET:HG3	1.95	0.48
1:A:65:ARG:HD2	1:A:147:ARG:HE	1.79	0.47
1:A:139:LEU:HD12	1:A:158:VAL:HG13	1.96	0.47
1:A:1:MET:HA	1:A:4:LYS:HE2	1.97	0.47
1:A:270:GLU:O	1:A:270:GLU:HG3	2.14	0.47
1:A:57:LYS:HB2	1:A:57:LYS:HE2	1.43	0.46
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: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:191:ALA:HB3	1:A:198:LEU:HD12	1.99	0.45
1:A:75:MET:CG	1:A:79:MET:HE3	2.46	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:48:THR:HA	1:A:79:MET:HE1	1.99	0.44
1:A:285:MET:HE3	1:A:285:MET:HB2	1.68	0.44
1:A:93:LEU:HD21	1:A:103:LEU:HD13	1.99	0.44
1:A:142:ILE:CD1	1:A:154:MET:HE3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HD23	1:A:234:GLU:HA	1.99	0.44
1:A:73:GLN:HE21	1:A:73:GLN:HB2	1.56	0.44
1:A:167:LEU:HD21	1:A:179:ILE:CD1	2.43	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
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:21:ASN:HD22	1:A:21:ASN:HA	1.66	0.43
1:A:101:LYS:HG3	1:A:111:VAL:CG2	2.49	0.43
1:A:147:ARG:HD3	1:A:147:ARG:HH11	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:198:LEU:O	1:A:199:PRO:C	2.62	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:2:THR:H	1:A:4:LYS:NZ	2.17	0.42
1:A:281:SER:O	1:A:285:MET:HE3	2.20	0.42
1:A:205:PRO:HA	1:A:221:THR:HB	2.01	0.41
1:A:144:LYS:HG2	1:A:178:LEU:CD2	2.50	0.41
1:A:156:LYS:HD2	5:A:663:HOH:O	2.20	0.41
1:A:197:ILE:CD1	1:A:238:GLN:HB3	2.49	0.41
1:A:211:ASP:O	1:A:214:ALA:N	2.51	0.41
1:A:89:MET:CG	1:A:93:LEU:CD1	2.92	0.41
1:A:292:MET:CE	5:A:509:HOH:O	2.62	0.41
1:A:201:ILE:HG22	1:A:202:ARG:N	2.36	0.41
1:A:211:ASP:O	1:A:212:TYR:C	2.64	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:81:LEU:HA	1:A:82:PRO:HD3	1.85	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:161:ASN:HD22	1:A:161:ASN:H	1.69	0.40
1:A:169:LEU:C	1:A:169:LEU:CD2	2.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:CG	5:A:636:HOH:O	2.69	0.40
1:A:206:SER:OG	1:A:220:GLU:CD	2.65	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
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%)	36 46

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%)	195 (80%)	49 (20%)	1 1

All (49) 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	5	ILE
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	133	GLU
1	A	135	SER
1	A	139	LEU
1	A	144	LYS
1	A	155	SER
1	A	157	VAL
1	A	164	GLN
1	A	169	LEU
1	A	175	GLU
1	A	177	VAL
1	A	178	LEU
1	A	179	ILE
1	A	184	SER
1	A	192	ILE
1	A	195	GLU
1	A	197	ILE

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Mol	Chain	Res	Type
1	A	208	THR
1	A	217	LEU
1	A	219	ASP
1	A	220	GLU
1	A	221	THR
1	A	234	GLU
1	A	237	LEU
1	A	245	TRP
1	A	248	LEU
1	A	258	VAL
1	A	262	SER
1	A	269	LEU
1	A	295	SER
1	A	298	VAL
1	A	300	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	49	GLN
1	A	56	GLN
1	A	73	GLN
1	A	105	GLN
1	A	130	GLN
1	A	161	ASN
1	A	173	HIS
1	A	204	GLN
1	A	289	GLN
1	A	296	GLN

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 [i](#)

There are no oligosaccharides 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$
4	PHY	A	320	2	10,15,15	8.95	1 (10%)	12,23,23	1.87	4 (33%)
3	ADP	A	310	2	28,29,29	0.88	2 (7%)	43,45,45	1.08	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PHY	A	320	2	-	1/12/21/21	-
3	ADP	A	310	2	-	6/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	320	PHY	P1-C1'	-28.08	1.52	1.79
3	A	310	ADP	C5'-C4'	2.29	1.58	1.51
3	A	310	ADP	PB-O2B	-2.09	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	320	PHY	O4P-P2-O2P	4.34	119.20	104.64
3	A	310	ADP	O5'-C5'-C4'	-3.31	97.73	108.99
4	A	320	PHY	O1-C-C2'	-2.54	114.54	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	320	PHY	O5P-P2-O4P	2.48	117.09	107.80
3	A	310	ADP	O2B-PB-O3A	2.29	112.30	104.64
3	A	310	ADP	O4'-C1'-N9	-2.08	104.09	108.09
4	A	320	PHY	O2P-P2-O3P	-2.05	100.27	111.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

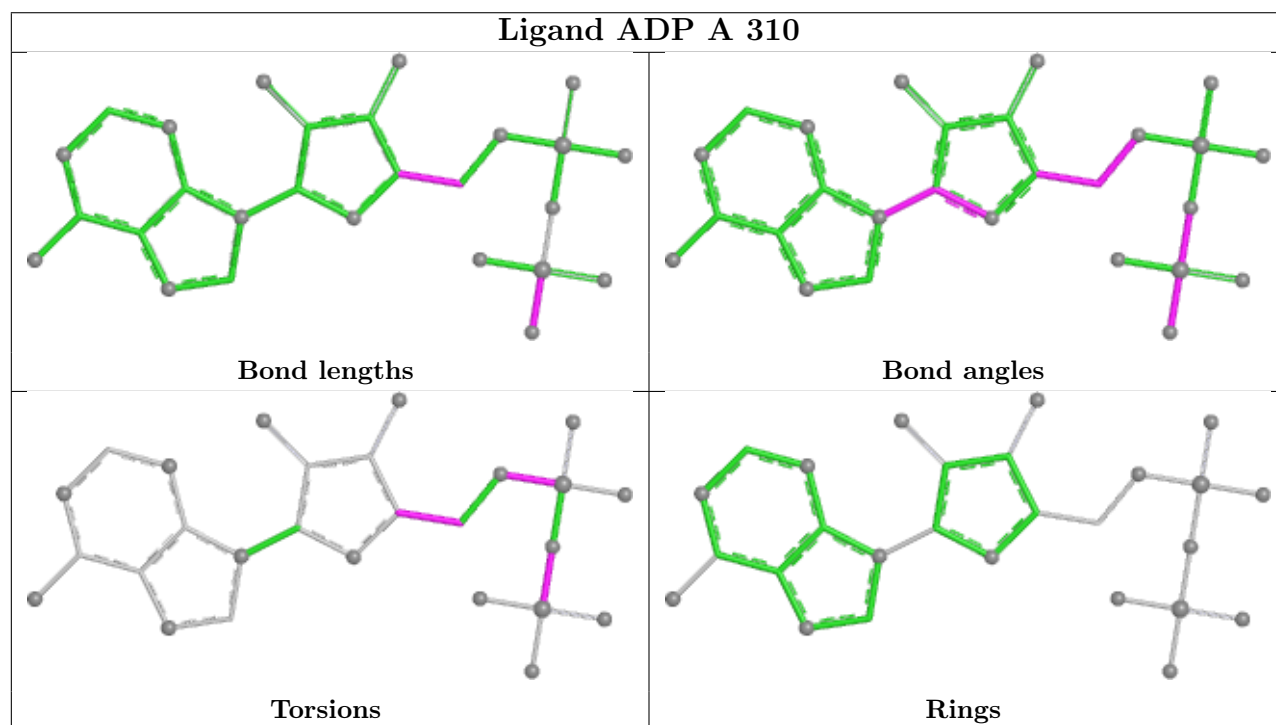
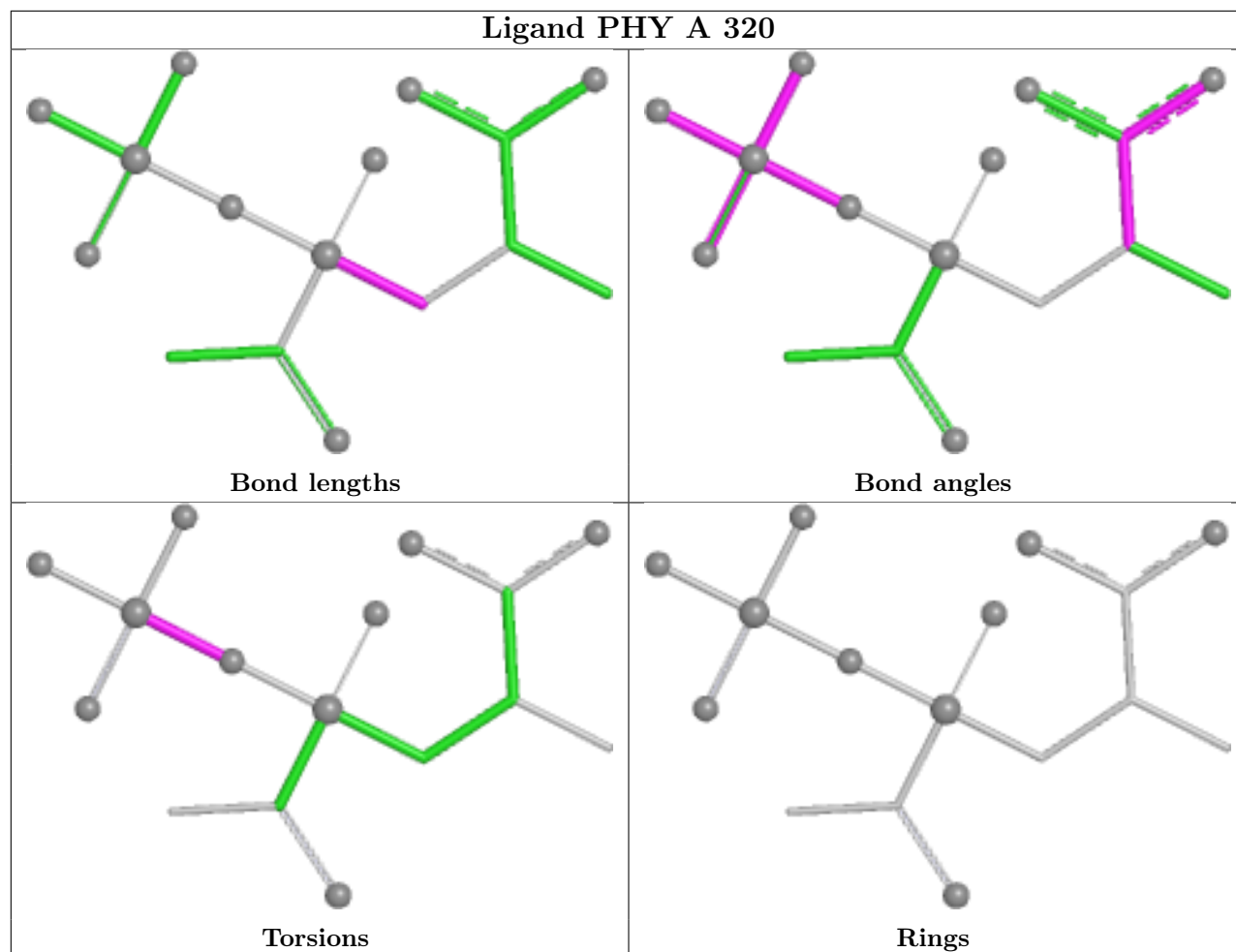
Mol	Chain	Res	Type	Atoms
3	A	310	ADP	PA-O3A-PB-O3B
3	A	310	ADP	C5'-O5'-PA-O1A
3	A	310	ADP	C5'-O5'-PA-O2A
4	A	320	PHY	P1-O2P-P2-O4P
3	A	310	ADP	C5'-O5'-PA-O3A
3	A	310	ADP	C3'-C4'-C5'-O5'
3	A	310	ADP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.