



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:48 AM UTC

PDB ID : 1IOV / pdb_00001io
Title : COMPLEX OF D-ALA:D-ALA LIGASE WITH ADP AND A PHOSPHORYL PHOSPHONATE
Authors : Knox, J.R.; Moews, P.C.; Fan, C.
Deposited on : 1996-09-20
Resolution : 2.20 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

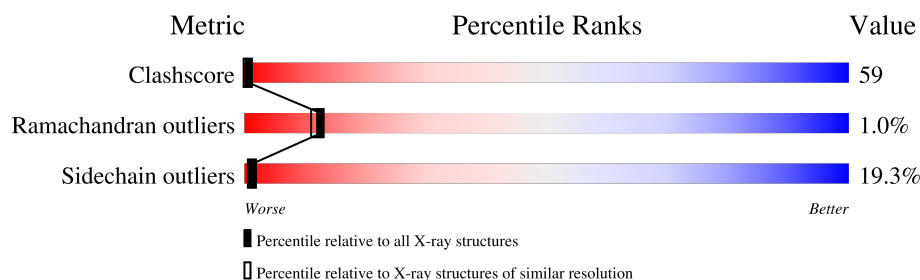
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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	28% 52% 18% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2615 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.

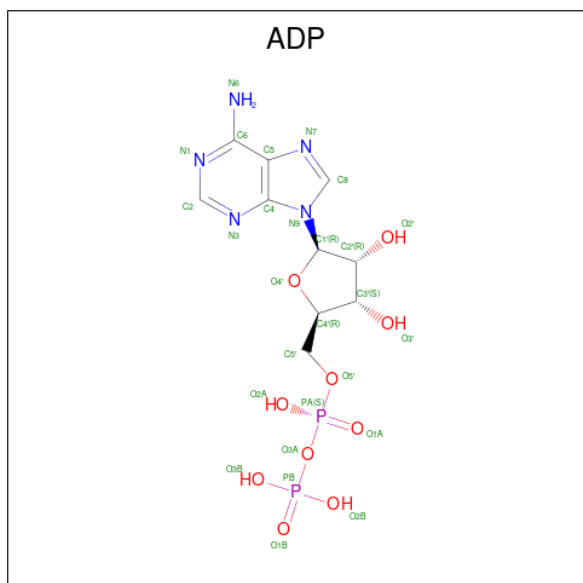
- Molecule 1 is a protein called D-ALA\;D-ALA LIGASE.

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	3	Total	Mg	0	0
			3	3		

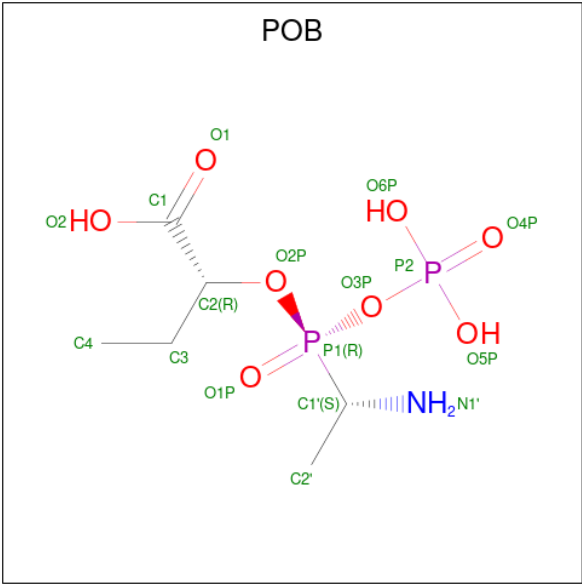
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is 2-[(1-AMINO-ETHYL)-PHOSPHATE-PHOSPHINOXYLOXY]-BUTYRIC

ACID (CCD ID: POB) (formula: C₆H₁₅NO₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			17	6	1	8	2		

- Molecule 5 is water.

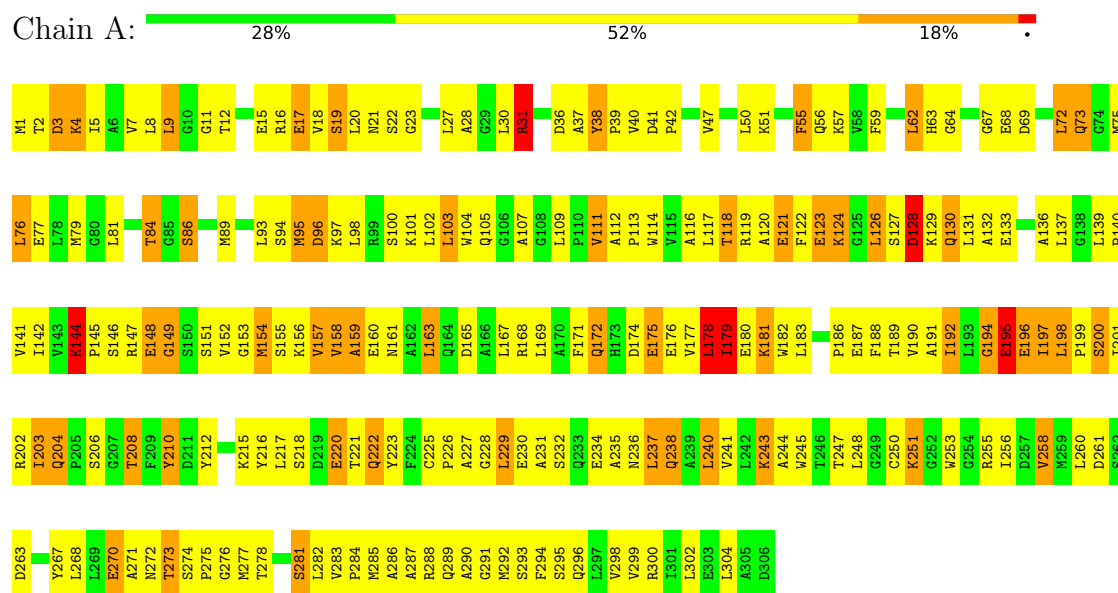
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	263	Total	O	0	0
			263	263		

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-ALA\;D-ALA 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	98.60 Å 51.00 Å 51.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	75.0 (15.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.156 , 0.204	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2615	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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, POB, 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	1.04	0/2346	1.99	57/3175 (1.8%)

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

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	THR	N-CA-C	11.20	123.57	111.36
1	A	128	ASP	N-CA-C	-9.54	101.80	113.15
1	A	273	THR	CA-C-N	8.55	130.32	122.37
1	A	273	THR	C-N-CA	8.55	130.32	122.37
1	A	84	THR	CA-C-O	-8.40	111.51	120.42
1	A	36	ASP	CA-CB-CG	8.02	120.61	112.60
1	A	281	SER	CA-C-N	7.27	130.32	120.44
1	A	281	SER	C-N-CA	7.27	130.32	120.44
1	A	236	ASN	CA-CB-CG	7.16	119.76	112.60
1	A	41	ASP	O-C-N	7.06	126.95	121.23
1	A	18	VAL	N-CA-C	-6.64	104.02	110.72
1	A	278	THR	CA-CB-OG1	-6.48	99.89	109.60
1	A	130	GLN	N-CA-C	-6.36	104.78	113.30
1	A	22	SER	CA-C-N	6.20	127.00	119.99
1	A	22	SER	C-N-CA	6.20	127.00	119.99
1	A	76	LEU	CA-C-N	6.17	128.54	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	LEU	C-N-CA	6.17	128.54	120.28
1	A	132	ALA	N-CA-C	-6.04	104.82	111.82
1	A	136	ALA	N-CA-C	-5.96	105.59	112.92
1	A	15	GLU	CA-C-N	5.92	129.03	120.38
1	A	15	GLU	C-N-CA	5.92	129.03	120.38
1	A	163	LEU	N-CA-C	5.87	118.56	111.40
1	A	96	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	158	VAL	CB-CA-C	5.68	119.08	111.19
1	A	194	GLY	N-CA-C	-5.58	99.95	113.18
1	A	19	SER	CA-C-N	5.54	128.46	120.38
1	A	19	SER	C-N-CA	5.54	128.46	120.38
1	A	103	LEU	CB-CA-C	5.53	120.25	110.85
1	A	121	GLU	CA-CB-CG	5.48	125.06	114.10
1	A	157	VAL	CB-CA-C	5.47	118.10	110.99
1	A	178	LEU	CA-CB-CG	5.45	135.37	116.30
1	A	144	LYS	N-CA-C	5.42	117.98	108.82
1	A	204	GLN	O-C-N	5.40	125.59	121.27
1	A	165	ASP	CA-CB-CG	5.39	118.00	112.60
1	A	290	ALA	N-CA-C	-5.38	107.02	113.21
1	A	64	GLY	N-CA-C	5.34	119.65	112.17
1	A	149	GLY	CA-C-O	-5.32	115.51	121.31
1	A	183	LEU	CB-CA-C	5.26	119.01	110.22
1	A	179	ILE	O-C-N	5.25	129.24	123.10
1	A	210	TYR	O-C-N	5.25	129.63	122.29
1	A	157	VAL	CA-C-O	5.24	126.24	120.48
1	A	168	ARG	CA-C-N	5.23	131.53	121.54
1	A	168	ARG	C-N-CA	5.23	131.53	121.54
1	A	229	LEU	N-CA-CB	-5.23	101.88	110.41
1	A	84	THR	CA-CB-OG1	-5.22	101.76	109.60
1	A	38	TYR	CA-C-O	5.19	124.44	119.72
1	A	28	ALA	O-C-N	5.18	127.41	122.07
1	A	118	THR	N-CA-CB	5.15	118.37	110.70
1	A	158	VAL	N-CA-C	-5.14	99.77	107.37
1	A	55	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	118	THR	N-CA-C	-5.09	102.65	110.14
1	A	176	GLU	N-CA-CB	5.07	118.72	110.77
1	A	195	GLU	CG-CD-OE1	-5.05	106.78	118.40
1	A	260	LEU	O-C-N	5.02	128.69	123.06
1	A	238	GLN	CA-C-N	5.02	127.77	120.79
1	A	238	GLN	C-N-CA	5.02	127.77	120.79
1	A	121	GLU	N-CA-C	-5.02	106.67	112.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	ARG	Sidechain

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	278	9
2	A	3	0	0	0	0
3	A	27	0	12	6	0
4	A	17	0	11	2	0
5	A	263	0	0	57	29
All	All	2615	0	2344	279	31

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 59.

All (279) 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:163:LEU:HD13	5:A:646:HOH:O	1.35	1.26
1:A:89:MET:O	1:A:93:LEU:HD13	1.46	1.15
1:A:271:ALA:HB1	5:A:549:HOH:O	1.56	1.06
1:A:126:LEU:HB3	5:A:572:HOH:O	1.56	1.05
1:A:103:LEU:HD21	1:A:247:THR:HG22	1.38	0.99
1:A:159:ALA:HB1	1:A:161:ASN:ND2	1.77	0.99
1:A:4:LYS:HG3	1:A:38:TYR:CE2	1.97	0.99
1:A:159:ALA:HB1	1:A:161:ASN:HD21	1.27	0.98
1:A:197:ILE:CD1	1:A:238:GLN:HB3	1.95	0.96
1:A:1:MET:HG3	5:A:459:HOH:O	1.66	0.94
1:A:127:SER:C	1:A:129:LYS:H	1.74	0.94
1:A:285:MET:SD	5:A:407:HOH:O	2.25	0.94
1:A:142:ILE:HD11	1:A:154:MET:CE	1.97	0.93
1:A:244:ALA:HB1	5:A:415:HOH:O	1.66	0.93
1:A:206:SER:HB3	1:A:220:GLU:HB2	1.51	0.92
1:A:120:ALA:O	1:A:124:LYS:HE3	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:CD2	1:A:247:THR:HG22	2.03	0.88
1:A:75:MET:SD	1:A:79:MET:HE3	2.14	0.87
1:A:4:LYS:HG3	1:A:38:TYR:HE2	1.35	0.87
1:A:142:ILE:HD11	1:A:154:MET:HE3	1.53	0.87
1:A:140:PRO:HB3	1:A:158:VAL:HG22	1.57	0.86
1:A:197:ILE:HD11	1:A:238:GLN:HB3	1.57	0.86
1:A:188:PHE:HB2	1:A:258:VAL:HG12	1.58	0.85
1:A:75:MET:SD	1:A:79:MET:CE	2.65	0.85
1:A:130:GLN:HA	5:A:657:HOH:O	1.75	0.85
1:A:159:ALA:HB2	5:A:640:HOH:O	1.75	0.85
1:A:77:GLU:HA	5:A:541:HOH:O	1.75	0.85
1:A:195:GLU:HA	5:A:417:HOH:O	1.76	0.84
1:A:31:ARG:NH1	1:A:37:ALA:O	2.10	0.84
1:A:304:LEU:HD11	5:A:457:HOH:O	1.77	0.83
1:A:200:SER:O	1:A:226:PRO:HA	1.79	0.83
1:A:1:MET:O	1:A:3:ASP:N	2.12	0.82
1:A:189:THR:HG21	1:A:282:LEU:HD13	1.62	0.81
1:A:117:LEU:HD22	5:A:572:HOH:O	1.80	0.81
1:A:240:LEU:HD11	1:A:268:LEU:HD21	1.60	0.80
1:A:191:ALA:HB3	1:A:198:LEU:HD12	1.64	0.79
1:A:133:GLU:HG2	5:A:657:HOH:O	1.83	0.79
1:A:72:LEU:HD23	1:A:75:MET:HE2	1.65	0.79
1:A:1:MET:C	1:A:3:ASP:H	1.91	0.77
1:A:240:LEU:HD12	1:A:240:LEU:O	1.85	0.77
1:A:295:SER:O	1:A:299:VAL:HB	1.85	0.77
1:A:126:LEU:HD22	5:A:572:HOH:O	1.83	0.77
1:A:284:PRO:HB2	5:A:421:HOH:O	1.86	0.75
1:A:191:ALA:CB	1:A:198:LEU:HD12	2.18	0.74
1:A:142:ILE:CD1	1:A:154:MET:CE	2.66	0.73
1:A:203:ILE:HD12	1:A:282:LEU:HD21	1.70	0.73
1:A:248:LEU:HD23	1:A:250:CYS:SG	2.28	0.73
1:A:104:TRP:CZ2	5:A:415:HOH:O	2.43	0.71
1:A:285:MET:HB3	5:A:407:HOH:O	1.89	0.71
1:A:72:LEU:CD2	1:A:75:MET:HE2	2.20	0.71
1:A:97:LYS:HG2	1:A:146:SER:O	1.91	0.71
1:A:128:ASP:HA	1:A:131:LEU:HD12	1.73	0.71
1:A:127:SER:C	1:A:129:LYS:N	2.50	0.70
1:A:101:LYS:NZ	1:A:112:ALA:O	2.24	0.70
1:A:208:THR:HG23	5:A:606:HOH:O	1.90	0.70
1:A:72:LEU:HD22	1:A:76:LEU:HG	1.74	0.70
1:A:75:MET:HE3	1:A:76:LEU:HD23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:HIS:ND1	1:A:274:SER:O	2.26	0.69
1:A:8:LEU:HD12	1:A:72:LEU:HD11	1.74	0.69
1:A:197:ILE:HD13	1:A:238:GLN:HB3	1.75	0.69
1:A:221:THR:HG23	1:A:223:TYR:CE2	2.28	0.68
1:A:181:LYS:CD	5:A:618:HOH:O	2.42	0.67
1:A:69:ASP:O	1:A:73:GLN:NE2	2.28	0.67
1:A:187:GLU:OE2	3:A:310:ADP:O3'	2.11	0.67
1:A:218:SER:HA	5:A:427:HOH:O	1.94	0.67
1:A:201:ILE:HG22	1:A:203:ILE:HD13	1.77	0.66
1:A:203:ILE:HG21	1:A:210:TYR:CZ	2.29	0.66
1:A:145:PRO:HG2	1:A:152:VAL:O	1.95	0.66
1:A:62:LEU:HD22	1:A:67:GLY:HA3	1.77	0.66
1:A:38:TYR:CD2	1:A:55:PHE:HE1	2.14	0.66
1:A:142:ILE:CD1	1:A:154:MET:HE1	2.27	0.65
1:A:177:VAL:HB	5:A:573:HOH:O	1.96	0.65
1:A:181:LYS:HE3	5:A:618:HOH:O	1.96	0.65
1:A:153:GLY:HA2	1:A:169:LEU:CD2	2.26	0.65
1:A:283:VAL:HB	1:A:284:PRO:HD3	1.79	0.65
1:A:240:LEU:CD1	1:A:268:LEU:HD21	2.27	0.64
1:A:1:MET:C	1:A:3:ASP:N	2.50	0.64
1:A:240:LEU:HD11	1:A:268:LEU:CD2	2.28	0.64
1:A:75:MET:CE	1:A:79:MET:HE3	2.27	0.64
1:A:237:LEU:HD21	1:A:258:VAL:HG11	1.80	0.64
1:A:75:MET:HE3	1:A:79:MET:HE3	1.79	0.63
1:A:304:LEU:CD1	5:A:457:HOH:O	2.43	0.62
1:A:197:ILE:HD11	1:A:238:GLN:CB	2.28	0.62
1:A:190:VAL:HG21	1:A:241:VAL:HG21	1.81	0.62
1:A:289:GLN:C	1:A:291:GLY:H	2.08	0.61
1:A:159:ALA:CB	1:A:161:ASN:HD21	2.06	0.61
1:A:240:LEU:HD12	1:A:240:LEU:C	2.25	0.61
1:A:119:ARG:NH2	1:A:171:PHE:O	2.32	0.61
1:A:216:TYR:HB2	1:A:217:LEU:HD12	1.82	0.61
1:A:182:TRP:NE1	5:A:627:HOH:O	2.32	0.60
1:A:89:MET:HB3	5:A:589:HOH:O	1.99	0.60
1:A:217:LEU:HA	5:A:556:HOH:O	2.00	0.60
1:A:197:ILE:CD1	1:A:238:GLN:CB	2.78	0.60
1:A:126:LEU:CD2	5:A:572:HOH:O	2.45	0.59
1:A:217:LEU:C	5:A:556:HOH:O	2.44	0.59
1:A:146:SER:HA	1:A:178:LEU:CD1	2.33	0.59
1:A:244:ALA:CB	5:A:415:HOH:O	2.37	0.59
1:A:144:LYS:HE3	5:A:635:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:OE1	1:A:300:ARG:NH1	2.35	0.59
1:A:167:LEU:HD21	1:A:179:ILE:HD11	1.84	0.58
1:A:241:VAL:O	1:A:245:TRP:HB2	2.03	0.58
1:A:263:ASP:OD2	1:A:267:TYR:OH	2.20	0.58
1:A:142:ILE:CD1	1:A:154:MET:HE3	2.28	0.58
3:A:310:ADP:O3B	4:A:321:POB:O4P	2.21	0.58
1:A:89:MET:HE3	1:A:93:LEU:HD22	1.85	0.57
1:A:140:PRO:CB	1:A:158:VAL:HG22	2.33	0.57
1:A:253:TRP:CZ3	1:A:277:MET:HE2	2.39	0.57
1:A:156:LYS:HE3	1:A:158:VAL:CG2	2.34	0.57
1:A:218:SER:N	5:A:556:HOH:O	2.36	0.57
1:A:188:PHE:HB2	1:A:258:VAL:CG1	2.34	0.57
1:A:177:VAL:CB	5:A:573:HOH:O	2.53	0.56
1:A:144:LYS:CE	5:A:635:HOH:O	2.52	0.56
1:A:158:VAL:O	1:A:159:ALA:HB3	2.03	0.56
1:A:101:LYS:HE2	1:A:111:VAL:HG13	1.86	0.56
1:A:51:LYS:HD3	1:A:81:LEU:HD11	1.86	0.56
1:A:146:SER:HA	1:A:178:LEU:HD11	1.88	0.56
1:A:225:CYS:SG	1:A:289:GLN:HG2	2.46	0.56
1:A:27:LEU:CD2	1:A:39:PRO:HG3	2.36	0.55
1:A:27:LEU:HD21	1:A:39:PRO:HG3	1.88	0.55
1:A:128:ASP:C	1:A:129:LYS:HD2	2.32	0.55
1:A:133:GLU:OE1	1:A:133:GLU:HA	2.07	0.55
1:A:142:ILE:HD13	1:A:154:MET:HE1	1.89	0.55
1:A:253:TRP:CH2	1:A:277:MET:HE2	2.42	0.55
1:A:101:LYS:HD3	1:A:114:TRP:CD2	2.41	0.55
1:A:23:GLY:O	1:A:27:LEU:HB2	2.07	0.55
1:A:93:LEU:HG	5:A:521:HOH:O	2.05	0.54
1:A:140:PRO:HG2	1:A:182:TRP:CB	2.37	0.54
1:A:144:LYS:HD2	1:A:178:LEU:HD22	1.89	0.54
1:A:206:SER:CB	1:A:220:GLU:HB2	2.32	0.54
1:A:27:LEU:O	1:A:31:ARG:HG3	2.06	0.54
1:A:140:PRO:HG2	1:A:182:TRP:CG	2.43	0.54
1:A:73:GLN:NE2	1:A:73:GLN:H	2.05	0.54
1:A:160:GLU:HG3	5:A:650:HOH:O	2.07	0.53
1:A:235:ALA:HA	5:A:479:HOH:O	2.07	0.53
1:A:274:SER:N	1:A:275:PRO:HD3	2.22	0.53
1:A:300:ARG:HG2	5:A:447:HOH:O	2.09	0.53
1:A:181:LYS:CE	5:A:618:HOH:O	2.55	0.53
1:A:119:ARG:O	1:A:122:PHE:HB3	2.09	0.52
1:A:192:ILE:HD13	1:A:197:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLY:C	1:A:277:MET:HG2	2.34	0.52
1:A:163:LEU:HD11	1:A:179:ILE:CD1	2.40	0.52
1:A:270:GLU:CD	1:A:272:ASN:HD21	2.18	0.51
1:A:245:TRP:CD1	1:A:256:ILE:HD11	2.46	0.51
1:A:300:ARG:O	1:A:304:LEU:HG	2.10	0.51
1:A:68:GLU:CG	1:A:274:SER:HB3	2.41	0.51
1:A:119:ARG:O	1:A:123:GLU:HG3	2.11	0.51
1:A:51:LYS:NZ	1:A:79:MET:O	2.44	0.51
1:A:258:VAL:HG23	1:A:268:LEU:HD23	1.92	0.51
1:A:47:VAL:O	1:A:50:LEU:HD12	2.10	0.50
1:A:86:SER:HA	1:A:251:LYS:HG3	1.93	0.50
1:A:237:LEU:HD22	1:A:241:VAL:CG2	2.42	0.50
1:A:94:SER:OG	1:A:248:LEU:HD21	2.12	0.50
1:A:158:VAL:O	1:A:159:ALA:CB	2.59	0.50
1:A:97:LYS:HB2	1:A:178:LEU:HD11	1.94	0.49
1:A:245:TRP:HD1	1:A:256:ILE:HD11	1.76	0.49
1:A:42:PRO:HG2	1:A:62:LEU:HD11	1.93	0.49
1:A:127:SER:HB3	1:A:129:LYS:HB2	1.94	0.49
1:A:282:LEU:CD1	5:A:510:HOH:O	2.61	0.49
1:A:7:VAL:O	1:A:9:LEU:HD23	2.13	0.49
1:A:93:LEU:O	1:A:100:SER:OG	2.26	0.49
1:A:149:GLY:HA3	5:A:536:HOH:O	2.13	0.48
1:A:97:LYS:CG	1:A:146:SER:O	2.60	0.48
1:A:47:VAL:O	1:A:79:MET:HE1	2.13	0.48
1:A:151:SER:OG	1:A:215:LYS:HE3	2.13	0.48
1:A:177:VAL:C	5:A:573:HOH:O	2.55	0.48
1:A:215:LYS:HD3	4:A:321:POB:H32	1.94	0.48
1:A:101:LYS:HG3	1:A:111:VAL:HG11	1.95	0.48
1:A:217:LEU:HD21	5:A:527:HOH:O	2.13	0.48
1:A:89:MET:HG2	1:A:93:LEU:CD1	2.43	0.48
1:A:101:LYS:NZ	1:A:180:GLU:OE1	2.47	0.48
1:A:194:GLY:HA3	5:A:457:HOH:O	2.13	0.48
1:A:62:LEU:CD2	1:A:67:GLY:HA3	2.42	0.47
1:A:9:LEU:HD12	1:A:20:LEU:HD23	1.96	0.47
1:A:189:THR:HG22	1:A:203:ILE:HD11	1.95	0.47
1:A:47:VAL:HA	1:A:50:LEU:HG	1.95	0.47
1:A:186:PRO:HB2	1:A:188:PHE:CZ	2.50	0.47
1:A:287:ALA:HB1	1:A:292:MET:HG3	1.95	0.47
1:A:244:ALA:HB2	1:A:268:LEU:HD11	1.97	0.47
1:A:130:GLN:O	1:A:133:GLU:HB2	2.15	0.47
1:A:189:THR:OG1	1:A:255:ARG:NE	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ARG:CZ	5:A:457:HOH:O	2.62	0.47
1:A:107:ALA:HB3	1:A:109:LEU:CD2	2.45	0.47
1:A:197:ILE:HD11	1:A:238:GLN:CD	2.40	0.47
1:A:228:GLY:HA3	5:A:641:HOH:O	2.15	0.47
1:A:217:LEU:HD12	1:A:217:LEU:N	2.30	0.46
1:A:293:SER:OG	1:A:296:GLN:HG3	2.15	0.46
1:A:203:ILE:CD1	1:A:282:LEU:HD21	2.42	0.46
1:A:169:LEU:O	1:A:172:GLN:HG3	2.15	0.46
1:A:89:MET:O	1:A:89:MET:HG2	2.16	0.46
1:A:181:LYS:O	3:A:310:ADP:N6	2.48	0.46
1:A:287:ALA:HB1	1:A:292:MET:CG	2.46	0.46
1:A:19:SER:OG	1:A:62:LEU:HA	2.16	0.46
1:A:96:ASP:OD1	1:A:98:LEU:HB3	2.16	0.46
1:A:118:THR:HA	1:A:175:GLU:O	2.16	0.46
1:A:167:LEU:O	1:A:171:PHE:HB2	2.16	0.46
1:A:198:LEU:HB2	1:A:286:ALA:HB1	1.97	0.46
1:A:199:PRO:HD3	5:A:600:HOH:O	2.16	0.46
1:A:98:LEU:O	1:A:102:LEU:HG	2.16	0.45
1:A:149:GLY:HA2	3:A:310:ADP:O2B	2.16	0.45
1:A:4:LYS:CG	1:A:38:TYR:CE2	2.84	0.45
1:A:94:SER:OG	1:A:248:LEU:CD2	2.65	0.45
1:A:103:LEU:CD2	1:A:247:THR:CG2	2.87	0.45
1:A:159:ALA:CB	1:A:161:ASN:ND2	2.63	0.45
1:A:221:THR:HG21	1:A:223:TYR:OH	2.17	0.45
1:A:222:GLN:HA	1:A:222:GLN:HE21	1.81	0.45
1:A:5:ILE:HG21	1:A:30:LEU:HD13	1.99	0.45
1:A:73:GLN:H	1:A:73:GLN:HE21	1.64	0.45
1:A:270:GLU:HG2	3:A:310:ADP:O2A	2.15	0.45
1:A:282:LEU:O	1:A:283:VAL:C	2.60	0.45
1:A:4:LYS:HE3	1:A:4:LYS:HB2	1.74	0.45
1:A:148:GLU:HB3	5:A:539:HOH:O	2.16	0.45
1:A:206:SER:OG	1:A:220:GLU:HG3	2.17	0.45
1:A:98:LEU:HD11	1:A:116:ALA:HB1	1.99	0.44
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.64	0.44
1:A:11:GLY:O	1:A:16:ARG:HD2	2.18	0.44
1:A:3:ASP:HA	1:A:56:GLN:HG3	1.99	0.44
1:A:73:GLN:O	1:A:77:GLU:HG2	2.16	0.44
1:A:244:ALA:HB1	1:A:268:LEU:HD13	2.00	0.44
1:A:40:VAL:HG11	1:A:50:LEU:HD21	2.00	0.44
1:A:75:MET:HE2	1:A:75:MET:HB3	1.81	0.44
1:A:281:SER:O	1:A:285:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:N	1:A:175:GLU:O	2.51	0.43
1:A:38:TYR:HA	1:A:39:PRO:HD3	1.66	0.43
1:A:89:MET:HG2	1:A:93:LEU:HD13	2.00	0.43
1:A:93:LEU:CD1	1:A:93:LEU:N	2.80	0.43
1:A:156:LYS:HE3	1:A:158:VAL:HG23	1.99	0.43
1:A:253:TRP:CH2	1:A:275:PRO:HD2	2.54	0.43
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.84	0.43
1:A:197:ILE:HD11	1:A:238:GLN:CG	2.49	0.43
1:A:221:THR:HG23	1:A:223:TYR:CZ	2.53	0.43
1:A:75:MET:CG	1:A:79:MET:HE3	2.47	0.43
1:A:117:LEU:HA	1:A:121:GLU:OE1	2.18	0.43
1:A:225:CYS:HA	1:A:226:PRO:C	2.43	0.43
1:A:38:TYR:CD2	1:A:55:PHE:CE1	3.01	0.43
1:A:89:MET:HE3	1:A:93:LEU:CD2	2.48	0.43
1:A:2:THR:O	1:A:56:GLN:HG3	2.19	0.43
1:A:240:LEU:HD11	1:A:268:LEU:CG	2.49	0.42
1:A:212:TYR:CD1	1:A:212:TYR:C	2.97	0.42
1:A:230:GLU:C	1:A:232:SER:H	2.27	0.42
1:A:9:LEU:HD21	1:A:39:PRO:HA	2.01	0.42
1:A:16:ARG:O	1:A:16:ARG:HG3	2.19	0.42
1:A:72:LEU:HD22	1:A:72:LEU:O	2.18	0.42
1:A:140:PRO:HG2	1:A:182:TRP:HB2	2.01	0.42
1:A:228:GLY:HA2	5:A:577:HOH:O	2.19	0.42
1:A:189:THR:HA	1:A:256:ILE:O	2.19	0.42
1:A:59:PHE:CD2	1:A:84:THR:HG21	2.55	0.42
1:A:59:PHE:HD2	1:A:302:LEU:HD13	1.85	0.42
1:A:63:HIS:CE1	1:A:274:SER:O	2.72	0.42
1:A:95:MET:O	1:A:147:ARG:HA	2.19	0.42
1:A:203:ILE:CD1	1:A:282:LEU:CD2	2.98	0.42
1:A:295:SER:O	1:A:299:VAL:CB	2.62	0.42
1:A:4:LYS:HG2	1:A:55:PHE:CE1	2.55	0.42
1:A:255:ARG:NH2	5:A:510:HOH:O	2.51	0.41
1:A:153:GLY:HA2	1:A:169:LEU:HD21	1.99	0.41
1:A:181:LYS:HD2	5:A:618:HOH:O	2.11	0.41
1:A:237:LEU:O	1:A:241:VAL:HG23	2.20	0.41
1:A:240:LEU:HA	1:A:243:LYS:HE3	2.01	0.41
1:A:283:VAL:HG13	5:A:546:HOH:O	2.21	0.41
1:A:123:GLU:HG3	1:A:123:GLU:H	1.72	0.41
1:A:189:THR:CG2	1:A:203:ILE:HD11	2.51	0.41
1:A:244:ALA:C	5:A:415:HOH:O	2.64	0.41
1:A:288:ARG:HG2	5:A:423:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TRP:CE2	5:A:415:HOH:O	2.71	0.41
1:A:119:ARG:NH2	1:A:174:ASP:C	2.78	0.41
1:A:261:ASP:C	1:A:263:ASP:N	2.79	0.41
1:A:57:LYS:CE	5:A:466:HOH:O	2.69	0.41
1:A:198:LEU:HA	1:A:199:PRO:HD3	1.92	0.41
1:A:277:MET:HB3	1:A:294:PHE:HZ	1.86	0.41
1:A:101:LYS:HG3	1:A:111:VAL:CG1	2.50	0.41
1:A:103:LEU:HD23	1:A:247:THR:HG22	1.97	0.41
1:A:177:VAL:HG12	5:A:573:HOH:O	2.20	0.41
1:A:289:GLN:C	1:A:291:GLY:N	2.78	0.41
1:A:96:ASP:O	1:A:100:SER:HB2	2.21	0.41
1:A:144:LYS:CD	1:A:178:LEU:HD22	2.50	0.40
1:A:169:LEU:HA	1:A:172:GLN:HG3	2.02	0.40
1:A:229:LEU:HD23	1:A:234:GLU:HA	2.03	0.40
1:A:57:LYS:HD3	5:A:466:HOH:O	2.22	0.40
1:A:154:MET:HE1	3:A:310:ADP:O4'	2.22	0.40
1:A:292:MET:HE2	1:A:292:MET:HB3	2.00	0.40

All (31) 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:489:HOH:O	5:A:506:HOH:O[1_554]	1.13	1.07
5:A:456:HOH:O	5:A:456:HOH:O[2_565]	1.16	1.04
5:A:494:HOH:O	5:A:494:HOH:O[2_565]	1.24	0.96
5:A:468:HOH:O	5:A:579:HOH:O[3_546]	1.27	0.93
5:A:413:HOH:O	5:A:653:HOH:O[2_555]	1.28	0.92
5:A:426:HOH:O	5:A:654:HOH:O[1_565]	1.29	0.91
1:A:155:SER:CB	5:A:437:HOH:O[3_547]	1.47	0.73
5:A:474:HOH:O	5:A:594:HOH:O[2_555]	1.47	0.73
5:A:504:HOH:O	5:A:663:HOH:O[3_556]	1.51	0.69
5:A:473:HOH:O	5:A:475:HOH:O[2_555]	1.68	0.52
5:A:486:HOH:O	5:A:650:HOH:O[3_556]	1.74	0.46
5:A:574:HOH:O	5:A:593:HOH:O[2_555]	1.83	0.37
5:A:533:HOH:O	5:A:565:HOH:O[3_557]	1.84	0.36
1:A:212:TYR:OH	1:A:288:ARG:NH1[3_547]	1.85	0.35
5:A:532:HOH:O	5:A:614:HOH:O[3_557]	1.85	0.35
5:A:499:HOH:O	5:A:499:HOH:O[2_565]	1.86	0.34
1:A:227:ALA:O	5:A:492:HOH:O[3_556]	1.89	0.31
5:A:446:HOH:O	5:A:662:HOH:O[1_565]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:594:HOH:O	5:A:651:HOH:O[2_555]	2.00	0.20
1:A:204:GLN:CG	5:A:609:HOH:O[3_556]	2.01	0.19
1:A:156:LYS:NZ	1:A:230:GLU:OE2[3_546]	2.03	0.17
5:A:578:HOH:O	5:A:586:HOH:O[1_565]	2.08	0.12
5:A:495:HOH:O	5:A:496:HOH:O[2_565]	2.10	0.10
5:A:587:HOH:O	5:A:588:HOH:O[2_565]	2.11	0.09
5:A:559:HOH:O	5:A:569:HOH:O[3_547]	2.13	0.07
1:A:17:GLU:OE1	5:A:652:HOH:O[3_557]	2.14	0.06
5:A:631:HOH:O	5:A:638:HOH:O[3_547]	2.15	0.05
1:A:4:LYS:CD	5:A:570:HOH:O[1_556]	2.17	0.03
1:A:17:GLU:OE2	5:A:652:HOH:O[3_557]	2.17	0.03
1:A:148:GLU:OE2	5:A:420:HOH:O[3_547]	2.18	0.02
5:A:458:HOH:O	5:A:637:HOH:O[3_556]	2.18	0.02

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%)	271 (89%)	30 (10%)	3 (1%)	12 11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ALA
1	A	231	ALA
1	A	86	SER

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%)	197 (81%)	47 (19%)	1 1

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	4	LYS
1	A	9	LEU
1	A	12	THR
1	A	17	GLU
1	A	31	ARG
1	A	62	LEU
1	A	72	LEU
1	A	73	GLN
1	A	95	MET
1	A	105	GLN
1	A	111	VAL
1	A	123	GLU
1	A	124	LYS
1	A	126	LEU
1	A	128	ASP
1	A	137	LEU
1	A	139	LEU
1	A	141	VAL
1	A	144	LYS
1	A	148	GLU
1	A	154	MET
1	A	157	VAL
1	A	172	GLN
1	A	175	GLU
1	A	178	LEU
1	A	179	ILE
1	A	181	LYS
1	A	192	ILE
1	A	195	GLU
1	A	196	GLU
1	A	197	ILE
1	A	198	LEU
1	A	200	SER
1	A	202	ARG

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Mol	Chain	Res	Type
1	A	203	ILE
1	A	208	THR
1	A	220	GLU
1	A	222	GLN
1	A	237	LEU
1	A	240	LEU
1	A	243	LYS
1	A	251	LYS
1	A	258	VAL
1	A	270	GLU
1	A	273	THR
1	A	298	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	56	GLN
1	A	73	GLN
1	A	130	GLN
1	A	161	ASN
1	A	173	HIS
1	A	222	GLN
1	A	272	ASN
1	A	280	HIS
1	A	289	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 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	28,29,29	0.94	2 (7%)	43,45,45	1.15	3 (6%)
4	POB	A	321	2	14,16,16	5.88	2 (14%)	18,24,24	2.23	4 (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
3	ADP	A	310	2	-	5/16/32/32	0/3/3/3
4	POB	A	321	2	-	2/20/23/23	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	321	POB	P1-C1'	-21.53	1.55	1.84
4	A	321	POB	P1-O2P	-2.80	1.52	1.57
3	A	310	ADP	PB-O3B	-2.09	1.47	1.54
3	A	310	ADP	O2'-C2'	2.04	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	321	POB	O3P-P1-O1P	-6.33	102.73	114.94
3	A	310	ADP	O2'-C2'-C3'	-3.81	99.60	111.82
4	A	321	POB	O2-C1-C2	3.68	122.29	112.71
4	A	321	POB	O1-C1-C2	-3.50	115.29	122.85
3	A	310	ADP	O2B-PB-O3A	2.85	114.21	104.64
3	A	310	ADP	O3B-PB-O3A	2.11	111.70	104.64
4	A	321	POB	O1P-P1-C1'	-2.09	111.25	115.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

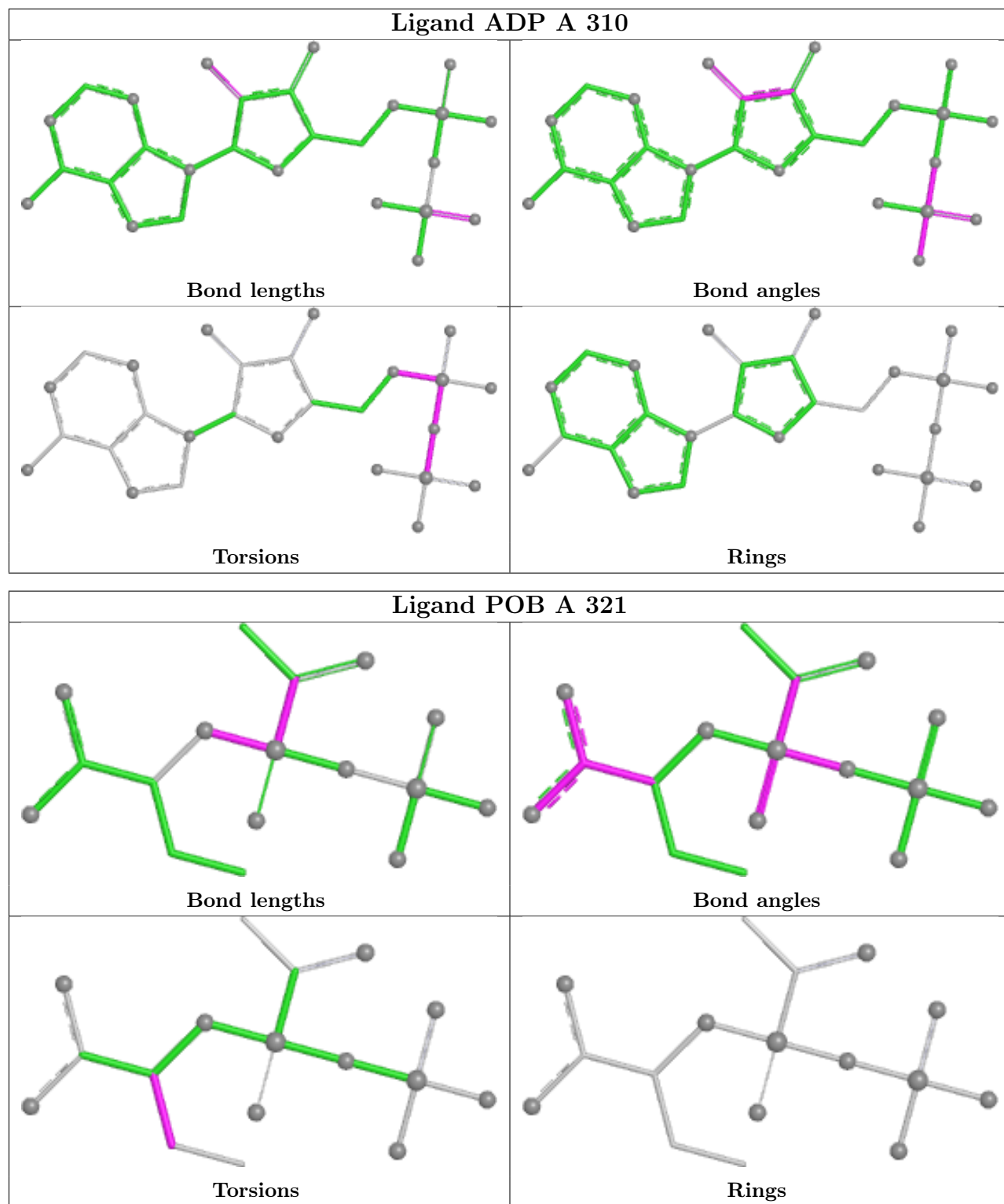
Mol	Chain	Res	Type	Atoms
3	A	310	ADP	PA-O3A-PB-O3B
4	A	321	POB	O2P-C2-C3-C4
3	A	310	ADP	PB-O3A-PA-O1A
4	A	321	POB	C1-C2-C3-C4
3	A	310	ADP	C5'-O5'-PA-O3A
3	A	310	ADP	PA-O3A-PB-O1B
3	A	310	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	310	ADP	6	0
4	A	321	POB	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.