



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:54 AM UTC

PDB ID : 5BPF / pdb_00005bpf
Title : Crystal structure of ADP complexed D-alanine-D-alanine ligase(DDL) from *Yersinia pestis*
Authors : Tran, H.T.; Kang, L.W.; Hong, M.K.
Deposited on : 2015-05-28
Resolution : 2.28 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

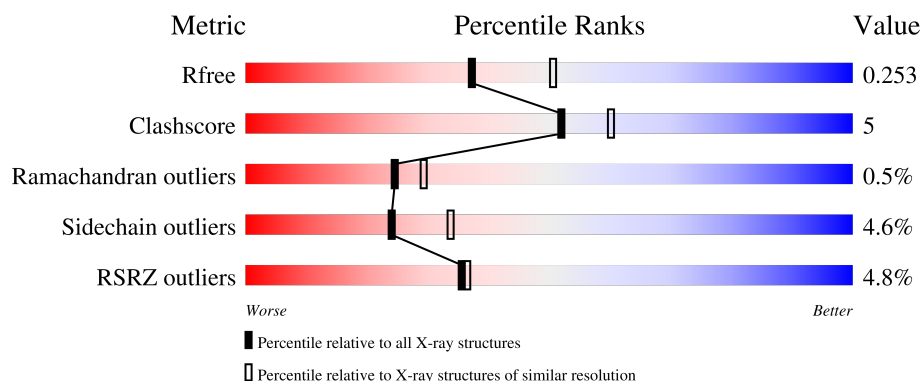
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 $\leq 5\%$. 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	306	2% 80% 14% 5%
1	B	306	10% 83% 13% ..
1	C	306	% 90% 9% .
1	D	306	6% 83% 13% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9628 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	291	Total	C	N	O	S	0	0	0
			2212	1409	368	424	11			
1	B	301	Total	C	N	O	S	0	0	0
			2291	1462	377	441	11			
1	C	306	Total	C	N	O	S	0	0	0
			2332	1487	384	450	11			
1	D	296	Total	C	N	O	S	0	0	0
			2251	1436	373	431	11			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

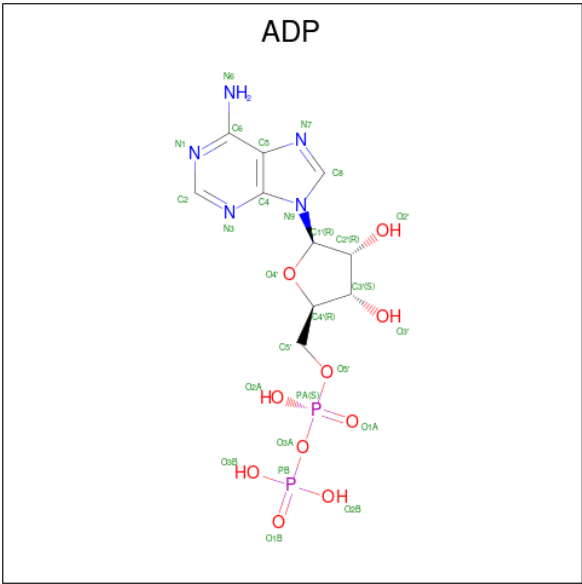
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



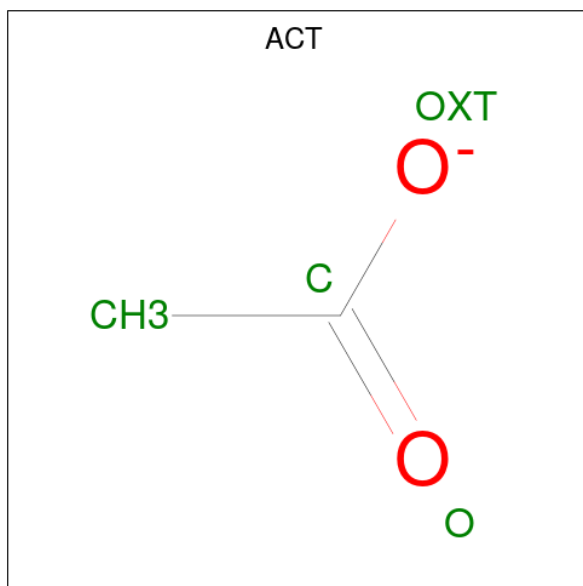
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	81	Total	O	0	0
			81	81		
6	C	149	Total	O	0	0
			149	149		

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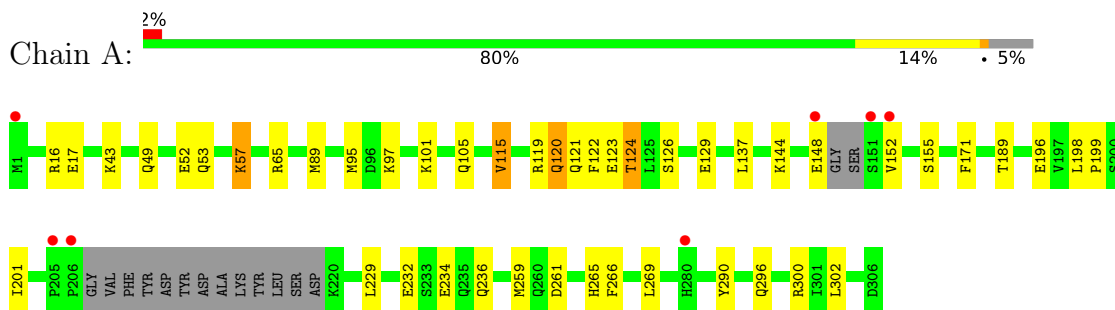
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	70	Total	O	0	0
			70	70		

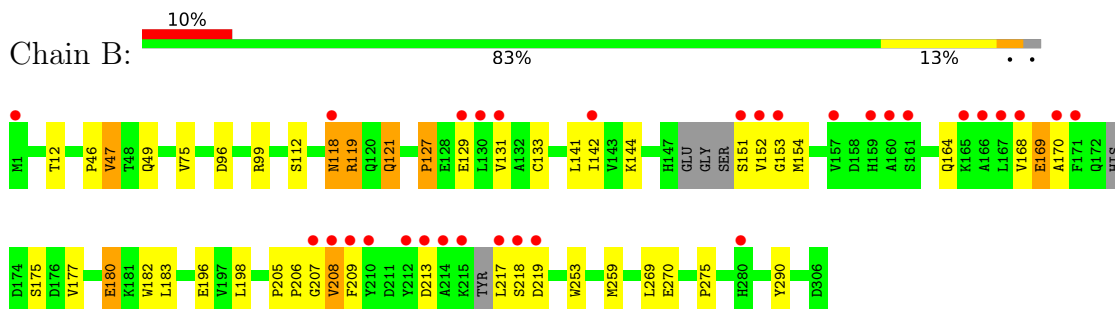
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

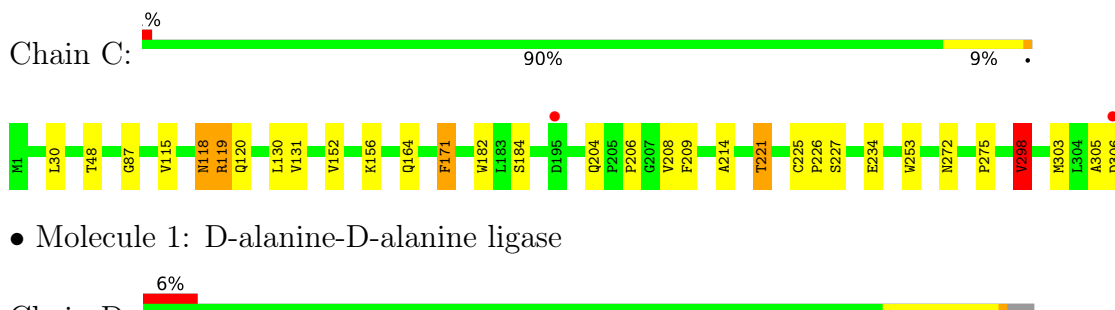
- Molecule 1: D-alanine-D-alanine ligase



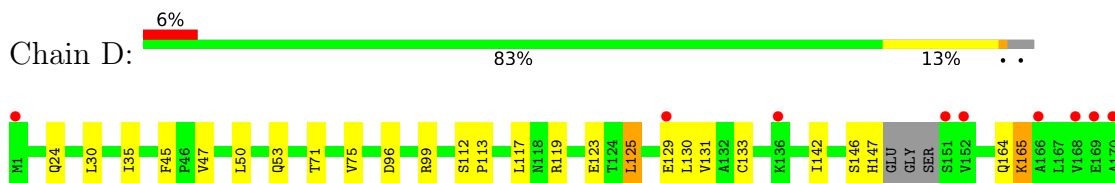
- Molecule 1: D-alanine-D-alanine ligase

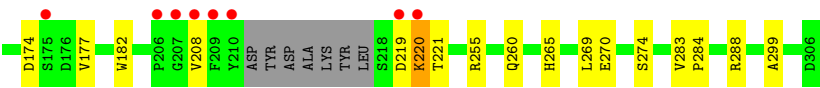


- Molecule 1: D-alanine-D-alanine ligase



- Molecule 1: D-alanine-D-alanine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.87Å 106.47Å 211.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.51 – 2.28 37.51 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.51-2.28) 100.0 (37.51-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.26 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.253 0.191 , 0.253	Depositor DCC
R_{free} test set	3336 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9628	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, NA, ADP, ACT

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	1.10	2/2253 (0.1%)	1.02	2/3052 (0.1%)
1	B	1.07	0/2333	1.02	1/3159 (0.0%)
1	C	1.13	2/2379 (0.1%)	1.12	3/3226 (0.1%)
1	D	1.01	1/2294 (0.0%)	1.06	3/3108 (0.1%)
All	All	1.08	5/9259 (0.1%)	1.05	9/12545 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	GLY	C-O	5.75	1.28	1.23
1	D	274	SER	N-CA	5.73	1.52	1.46
1	A	266	PHE	C-O	-5.45	1.17	1.23
1	C	171	PHE	C-O	-5.15	1.17	1.24
1	A	97	LYS	C-O	-5.04	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	GLU	N-CA-C	-7.95	100.08	110.33
1	A	89	MET	N-CA-C	-6.30	104.03	111.03
1	C	298	VAL	CB-CA-C	6.08	120.61	112.22
1	C	152	VAL	N-CA-C	5.78	117.48	109.45
1	A	144	LYS	N-CA-C	5.71	115.47	108.11
1	D	174	ASP	N-CA-C	5.11	116.29	108.52
1	D	146	SER	N-CA-C	5.09	117.56	111.71
1	C	119	ARG	N-CA-C	5.05	116.86	111.36
1	D	299	ALA	N-CA-C	-5.04	105.88	112.23

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	2212	0	2219	24	0
1	B	2291	0	2290	32	0
1	C	2332	0	2323	17	0
1	D	2251	0	2252	20	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	16	0	0
3	C	6	0	8	0	0
3	D	12	0	16	1	0
4	B	27	0	12	5	0
4	C	27	0	12	0	0
4	D	27	0	12	2	0
5	B	8	0	6	1	0
5	C	8	0	6	0	0
6	A	110	0	0	0	0
6	B	81	0	0	0	0
6	C	149	0	0	0	0
6	D	70	0	0	2	0
All	All	9628	0	9172	94	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 5.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:PRO:HG2	1:B:49:GLN:HG3	1.57	0.85
1:C:214:ALA:O	1:C:221:THR:HG21	1.82	0.79
1:C:119:ARG:NH2	1:C:171:PHE:O	2.22	0.73
1:B:144:LYS:NZ	1:B:180:GLU:OE1	2.20	0.73
1:A:259:MET:HE3	1:A:269:LEU:HD11	1.74	0.70
1:A:57:LYS:HD3	1:A:302:LEU:HD11	1.73	0.70
1:A:95:MET:HE3	1:A:148:GLU:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ILE:HD11	1:D:182:TRP:CE3	2.26	0.69
1:A:126:SER:OG	1:A:129:GLU:HG2	1.92	0.69
1:D:270:GLU:OE1	4:D:401:ADP:O2A	2.15	0.65
1:B:196:GLU:OE1	1:B:290:TYR:OH	2.09	0.63
1:D:119:ARG:O	1:D:123:GLU:HG3	1.97	0.63
1:C:208:VAL:HG23	1:C:209:PHE:CD2	2.33	0.63
1:C:206:PRO:HD3	1:C:221:THR:HB	1.82	0.61
1:C:30:LEU:CD2	1:C:298:VAL:HG13	2.32	0.60
1:D:142:ILE:HD11	1:D:182:TRP:CZ3	2.37	0.59
1:B:169:GLU:O	1:B:170:ALA:HB3	2.03	0.58
1:A:122:PHE:O	1:A:123:GLU:HB2	2.05	0.56
1:B:46:PRO:HG2	1:B:49:GLN:CG	2.32	0.56
1:D:47:VAL:HG12	1:D:75:VAL:HG11	1.88	0.56
1:B:142:ILE:HD11	1:B:182:TRP:HD1	1.72	0.54
1:B:259:MET:HE1	4:B:401:ADP:C4	2.43	0.53
1:A:189:THR:HG22	1:A:201:ILE:HB	1.91	0.53
1:B:152:VAL:HG12	1:B:153:GLY:N	2.24	0.53
1:D:142:ILE:HD11	1:D:182:TRP:HE3	1.71	0.53
1:B:118:ASN:H	1:B:121:GLN:NE2	2.06	0.52
1:B:12:THR:H	5:B:403:ACT:H2	1.73	0.52
1:B:207:GLY:O	1:B:208:VAL:HG12	2.10	0.52
1:A:196:GLU:OE1	1:A:300:ARG:NH1	2.43	0.52
1:C:227:SER:OG	1:C:234:GLU:OE2	2.28	0.51
1:A:57:LYS:HD3	1:A:302:LEU:CD1	2.39	0.51
1:B:47:VAL:HG13	1:B:75:VAL:HG11	1.93	0.51
1:A:229:LEU:HB2	1:A:234:GLU:HG2	1.93	0.49
1:B:259:MET:HE1	4:B:401:ADP:H2'	1.95	0.49
1:B:168:VAL:C	1:B:169:GLU:O	2.49	0.48
1:A:121:GLN:C	1:A:122:PHE:O	2.52	0.48
1:B:259:MET:HE2	1:B:269:LEU:HD21	1.95	0.48
3:D:403:GOL:H31	3:D:404:GOL:H11	1.96	0.47
1:D:96:ASP:OD2	1:D:99:ARG:HD2	2.14	0.47
1:B:270:GLU:OE2	4:B:401:ADP:O1A	2.33	0.47
1:D:130:LEU:O	1:D:133:CYS:HB2	2.15	0.47
1:A:196:GLU:OE2	1:A:290:TYR:OH	2.32	0.47
1:A:198:LEU:HB3	1:A:199:PRO:CD	2.43	0.47
1:B:253:TRP:CH2	1:B:275:PRO:HD2	2.50	0.47
1:B:259:MET:CE	4:B:401:ADP:C4	2.97	0.47
1:D:142:ILE:HG13	4:D:401:ADP:C6	2.50	0.47
1:B:127:PRO:HB3	1:B:164:GLN:HG3	1.97	0.47
1:C:305:ALA:O	1:C:306:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HG13	1:B:209:PHE:N	2.31	0.46
1:C:253:TRP:CH2	1:C:275:PRO:HD2	2.51	0.46
1:D:30:LEU:HD22	1:D:35:ILE:HD13	1.97	0.46
1:C:118:ASN:HD22	1:C:118:ASN:C	2.23	0.46
1:A:119:ARG:NH1	1:A:171:PHE:O	2.50	0.45
1:B:259:MET:HE3	4:B:401:ADP:C2	2.51	0.45
1:C:130:LEU:O	1:C:131:VAL:C	2.60	0.45
1:A:198:LEU:HD22	1:A:290:TYR:CD2	2.52	0.44
1:D:112:SER:O	1:D:113:PRO:C	2.61	0.44
1:A:296:GLN:O	1:A:300:ARG:HG3	2.17	0.44
1:B:169:GLU:O	1:B:170:ALA:CB	2.66	0.44
1:B:112:SER:HB3	1:B:183:LEU:HD11	2.00	0.43
1:C:118:ASN:C	1:C:118:ASN:ND2	2.76	0.43
1:D:125:LEU:HG	1:D:129:GLU:CG	2.48	0.43
1:D:147:HIS:HE1	6:D:541:HOH:O	2.01	0.43
1:B:152:VAL:O	1:B:154:MET:N	2.51	0.43
1:D:125:LEU:HG	1:D:129:GLU:HG2	1.99	0.43
1:A:115:VAL:HG13	1:A:137:LEU:HD11	2.00	0.43
1:B:198:LEU:HD22	1:B:290:TYR:CD2	2.54	0.42
1:B:96:ASP:OD2	1:B:99:ARG:HD2	2.19	0.42
1:A:16:ARG:CZ	1:A:43:LYS:HE2	2.49	0.42
1:B:205:PRO:O	1:B:207:GLY:N	2.53	0.42
1:C:130:LEU:HD12	1:C:164:GLN:HE22	1.85	0.42
1:D:220:LYS:O	1:D:221:THR:C	2.62	0.42
1:D:260:GLN:HA	1:D:265:HIS:O	2.20	0.42
1:A:49:GLN:HG2	1:A:52:GLU:OE2	2.20	0.42
1:A:122:PHE:O	1:A:124:THR:N	2.49	0.42
1:B:118:ASN:OD1	1:B:118:ASN:N	2.53	0.42
1:B:47:VAL:CG1	1:B:75:VAL:HG11	2.49	0.41
1:B:144:LYS:CE	1:B:180:GLU:OE1	2.68	0.41
1:B:119:ARG:O	1:B:121:GLN:N	2.49	0.41
1:C:182:TRP:CZ3	1:C:184:SER:HA	2.54	0.41
1:D:71:THR:HG21	6:D:513:HOH:O	2.20	0.41
1:D:283:VAL:HB	1:D:284:PRO:HD3	2.01	0.41
1:D:164:GLN:O	1:D:165:LYS:C	2.64	0.41
1:A:101:LYS:O	1:A:105:GLN:HG3	2.21	0.41
1:A:198:LEU:HB3	1:A:199:PRO:HD2	2.03	0.41
1:C:30:LEU:HD21	1:C:298:VAL:HG13	2.03	0.41
1:C:182:TRP:CH2	1:C:184:SER:HA	2.56	0.41
1:A:120:GLN:O	1:A:122:PHE:O	2.38	0.41
1:D:45:PHE:CZ	1:D:53:GLN:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:CYS:HA	1:C:226:PRO:C	2.46	0.40
1:A:259:MET:HE3	1:A:269:LEU:CD1	2.47	0.40
1:A:261:ASP:OD2	1:A:265:HIS:HD2	2.05	0.40
1:B:170:ALA:HB1	1:B:177:VAL:HG21	2.03	0.40
1:C:272:ASN:OD1	1:C:272:ASN:C	2.64	0.40

There are no symmetry-related clashes.

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	285/306 (93%)	277 (97%)	7 (2%)	1 (0%)	30	36
1	B	293/306 (96%)	276 (94%)	13 (4%)	4 (1%)	9	8
1	C	304/306 (99%)	297 (98%)	7 (2%)	0	100	100
1	D	290/306 (95%)	277 (96%)	12 (4%)	1 (0%)	36	44
All	All	1172/1224 (96%)	1127 (96%)	39 (3%)	6 (0%)	24	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	VAL
1	B	121	GLN
1	D	219	ASP
1	A	152	VAL
1	B	206	PRO
1	B	127	PRO

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	239/251 (95%)	229 (96%)	10 (4%)	26	37
1	B	247/251 (98%)	233 (94%)	14 (6%)	18	25
1	C	251/251 (100%)	242 (96%)	9 (4%)	31	44
1	D	243/251 (97%)	231 (95%)	12 (5%)	22	31
All	All	980/1004 (98%)	935 (95%)	45 (5%)	24	34

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	53	GLN
1	A	57	LYS
1	A	65	ARG
1	A	115	VAL
1	A	120	GLN
1	A	124	THR
1	A	155	SER
1	A	232	GLU
1	A	236	GLN
1	B	47	VAL
1	B	118	ASN
1	B	119	ARG
1	B	129	GLU
1	B	131	VAL
1	B	133	CYS
1	B	141	LEU
1	B	151	SER
1	B	175	SER
1	B	180	GLU
1	B	213	ASP
1	B	217	LEU
1	B	218	SER
1	B	219	ASP

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Mol	Chain	Res	Type
1	C	48	THR
1	C	115	VAL
1	C	118	ASN
1	C	120	GLN
1	C	156	LYS
1	C	204	GLN
1	C	221	THR
1	C	298	VAL
1	C	303	MET
1	D	24	GLN
1	D	50	LEU
1	D	117	LEU
1	D	125	LEU
1	D	131	VAL
1	D	165	LYS
1	D	177	VAL
1	D	208	VAL
1	D	220	LYS
1	D	255	ARG
1	D	269	LEU
1	D	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	53	GLN
1	A	265	HIS
1	B	121	GLN
1	C	49	GLN
1	C	118	ASN
1	C	164	GLN
1	C	172	GLN
1	C	235	GLN
1	C	243	GLN
1	D	24	GLN
1	D	121	GLN
1	D	147	HIS
1	D	236	GLN
1	D	243	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 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	ADP	D	401	-	28,29,29	1.98	5 (17%)	43,45,45	1.92	10 (23%)
5	ACT	B	404	-	3,3,3	0.82	0	3,3,3	0.71	0
3	GOL	D	403	-	5,5,5	0.61	0	5,5,5	1.00	0
3	GOL	A	402	-	5,5,5	0.44	0	5,5,5	0.50	0
3	GOL	C	405	-	5,5,5	0.96	0	5,5,5	1.00	0
5	ACT	C	403	-	3,3,3	0.98	0	3,3,3	0.54	0
5	ACT	C	404	-	3,3,3	0.81	0	3,3,3	1.21	0
3	GOL	A	403	-	5,5,5	0.84	0	5,5,5	0.67	0
3	GOL	D	404	-	5,5,5	0.55	0	5,5,5	0.84	0
5	ACT	B	403	-	3,3,3	0.88	0	3,3,3	0.86	0
4	ADP	B	401	-	28,29,29	1.94	5 (17%)	43,45,45	1.79	11 (25%)
4	ADP	C	401	-	28,29,29	1.60	6 (21%)	43,45,45	1.66	10 (23%)

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	ADP	D	401	-	-	3/16/32/32	0/3/3/3
3	GOL	D	403	-	-	2/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	C	405	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	D	404	-	-	4/4/4/4	-
4	ADP	B	401	-	-	5/16/32/32	0/3/3/3
4	ADP	C	401	-	-	0/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	ADP	PA-O3A	6.35	1.66	1.59
4	D	401	ADP	C5-C4	6.23	1.50	1.39
4	D	401	ADP	PA-O3A	5.71	1.65	1.59
4	B	401	ADP	C5-C4	5.65	1.49	1.39
4	C	401	ADP	C5-C4	5.14	1.48	1.39
4	D	401	ADP	C5-C6	3.28	1.50	1.41
4	C	401	ADP	C8-N7	3.14	1.37	1.31
4	B	401	ADP	C5-C6	2.85	1.48	1.41
4	D	401	ADP	C8-N7	2.69	1.36	1.31
4	C	401	ADP	C5-N7	-2.65	1.34	1.39
4	C	401	ADP	C2-N1	2.31	1.38	1.33
4	D	401	ADP	C4-N3	2.19	1.38	1.34
4	B	401	ADP	C8-N7	2.10	1.35	1.31
4	C	401	ADP	C4-N9	-2.07	1.33	1.37
4	B	401	ADP	C5-N7	-2.06	1.35	1.39
4	C	401	ADP	C5-C6	2.04	1.46	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	ADP	C5-C4-N3	-5.92	118.57	126.72
4	D	401	ADP	N3-C4-N9	4.92	135.53	127.17
4	C	401	ADP	C5-C4-N3	-4.45	120.59	126.72
4	B	401	ADP	C5-C4-N3	-4.39	120.67	126.72
4	D	401	ADP	C2-N3-C4	4.18	122.04	111.83
4	D	401	ADP	N3-C2-N1	-4.00	122.53	128.58
4	B	401	ADP	N3-C4-N9	3.96	133.90	127.17
4	D	401	ADP	C4-C5-N7	-3.54	106.53	110.58
4	B	401	ADP	N3-C2-N1	-3.45	123.36	128.58
4	C	401	ADP	N3-C4-N9	3.33	132.82	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ADP	C4-C5-N7	-3.28	106.83	110.58
4	C	401	ADP	C4-C5-N7	-3.28	106.84	110.58
4	B	401	ADP	C4-N9-C8	3.25	109.15	105.74
4	B	401	ADP	C2-N1-C6	3.10	123.83	118.73
4	B	401	ADP	C2-N3-C4	3.02	119.22	111.83
4	D	401	ADP	C4-N9-C8	2.87	108.75	105.74
4	C	401	ADP	C5-N7-C8	2.71	107.71	103.45
4	C	401	ADP	C4-N9-C8	2.70	108.58	105.74
4	C	401	ADP	O3B-PB-O3A	2.70	113.69	104.64
4	D	401	ADP	C6-C5-N7	2.67	137.23	132.09
4	C	401	ADP	N9-C8-N7	-2.59	110.26	113.94
4	B	401	ADP	C5-N7-C8	2.55	107.45	103.45
4	D	401	ADP	O2A-PA-O3A	2.38	113.71	107.27
4	C	401	ADP	C2-N3-C4	2.37	117.63	111.83
4	D	401	ADP	C5-N7-C8	2.37	107.17	103.45
4	C	401	ADP	N3-C2-N1	-2.37	125.00	128.58
4	B	401	ADP	N6-C6-N1	2.36	123.64	118.38
4	D	401	ADP	C2-N1-C6	2.17	122.30	118.73
4	B	401	ADP	O2B-PB-O3A	2.15	111.86	104.64
4	B	401	ADP	C6-C5-N7	2.08	136.10	132.09
4	C	401	ADP	O2B-PB-O1B	2.03	118.74	110.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	404	GOL	C1-C2-C3-O3
4	B	401	ADP	PA-O3A-PB-O2B
4	D	401	ADP	C5'-O5'-PA-O2A
4	D	401	ADP	C5'-O5'-PA-O3A
3	A	403	GOL	C1-C2-C3-O3
3	C	405	GOL	C1-C2-C3-O3
3	D	403	GOL	O1-C1-C2-C3
3	D	404	GOL	O1-C1-C2-C3
3	A	403	GOL	O2-C2-C3-O3
3	C	405	GOL	O2-C2-C3-O3
3	D	404	GOL	O1-C1-C2-O2
4	D	401	ADP	PA-O3A-PB-O1B
4	B	401	ADP	PA-O3A-PB-O3B
3	D	404	GOL	O2-C2-C3-O3
3	D	403	GOL	C1-C2-C3-O3
4	B	401	ADP	PB-O3A-PA-O5'

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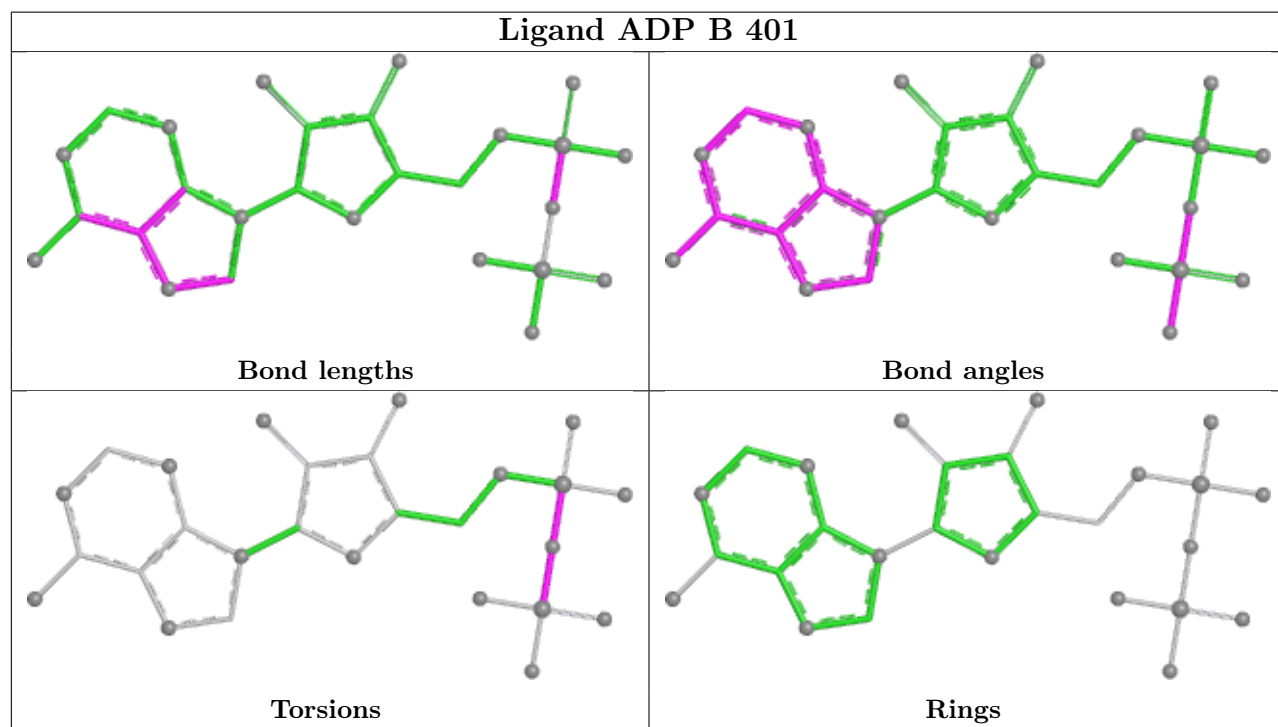
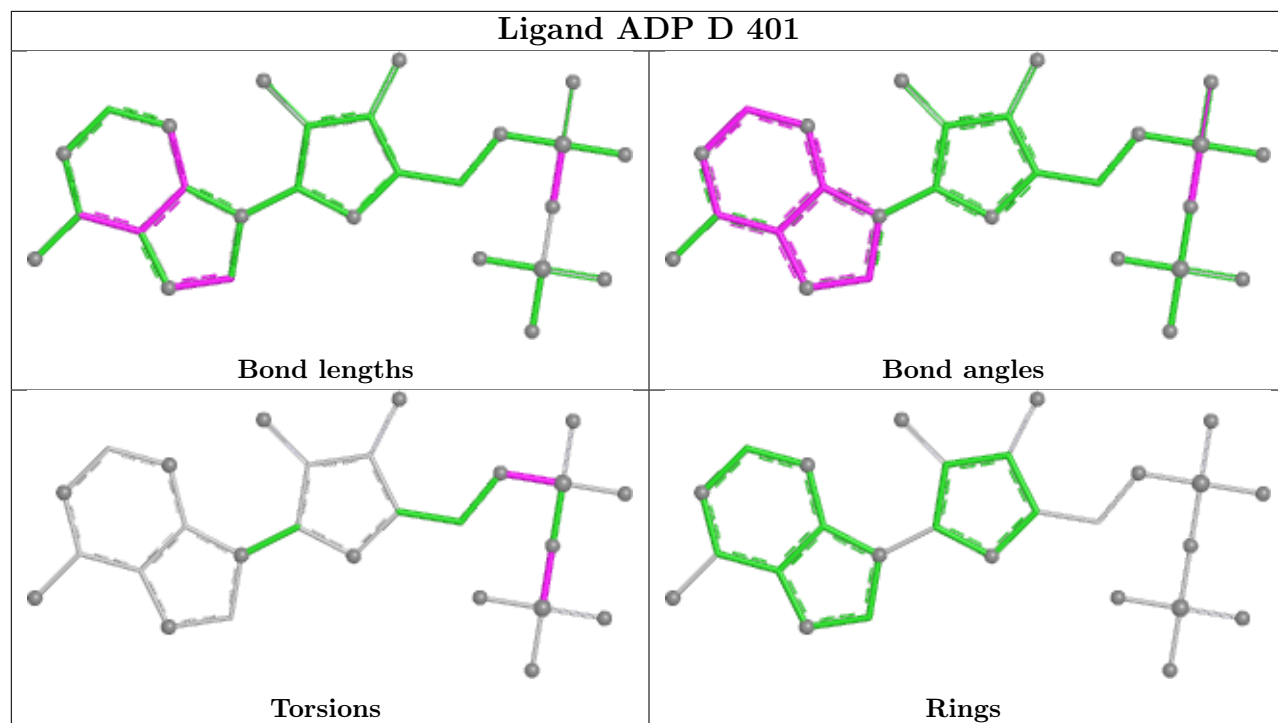
Mol	Chain	Res	Type	Atoms
4	B	401	ADP	PA-O3A-PB-O1B
4	B	401	ADP	PB-O3A-PA-O2A

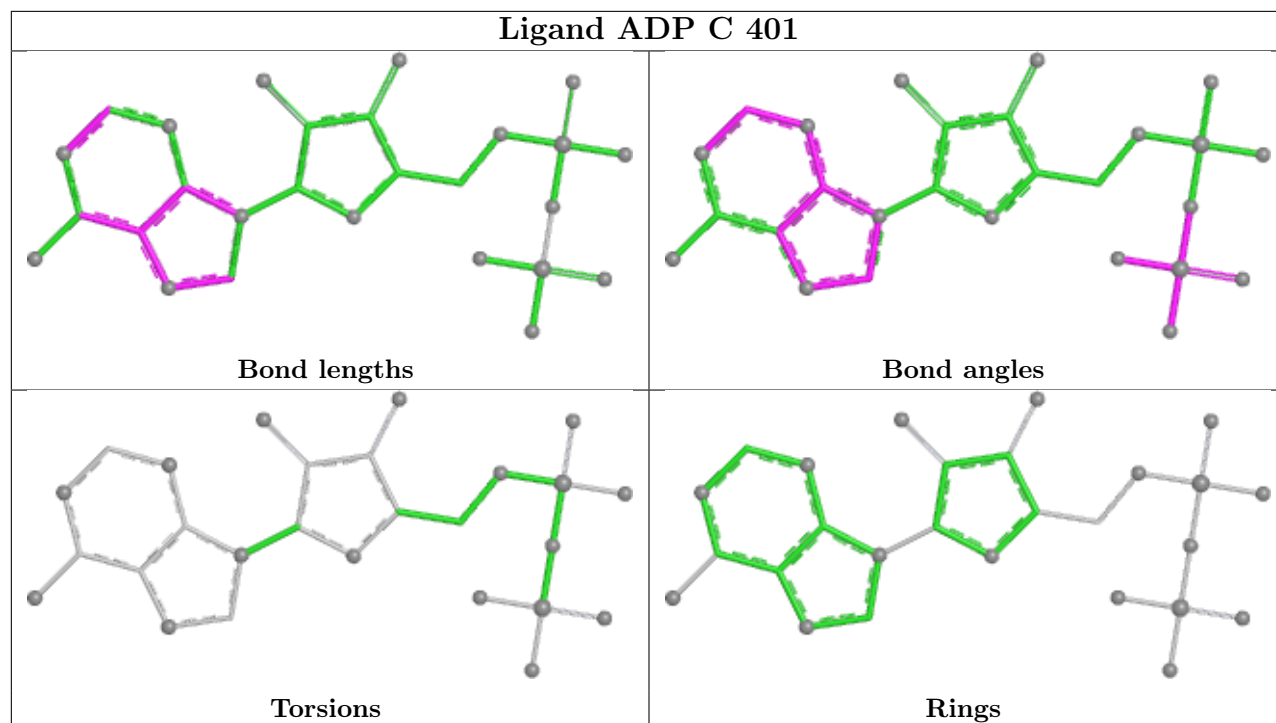
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	ADP	2	0
3	D	403	GOL	1	0
3	D	404	GOL	1	0
5	B	403	ACT	1	0
4	B	401	ADP	5	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

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, 95th 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 ²)	Q<0.9
1	A	291/306 (95%)	-0.18	7 (2%) 59 61	16, 29, 61, 83	0
1	B	301/306 (98%)	0.24	31 (10%) 12 13	16, 31, 90, 118	0
1	C	306/306 (100%)	-0.35	2 (0%) 84 85	18, 27, 49, 70	0
1	D	296/306 (96%)	0.30	17 (5%) 29 30	20, 38, 71, 92	0
All	All	1194/1224 (97%)	0.00	57 (4%) 35 36	16, 31, 72, 118	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	LEU	6.5
1	B	152	VAL	4.3
1	B	212	TYR	3.7
1	D	151	SER	3.5
1	D	1	MET	3.5
1	B	153	GLY	3.5
1	B	207	GLY	3.5
1	B	219	ASP	3.4
1	B	215	LYS	3.4
1	D	152	VAL	3.4
1	B	208	VAL	3.3
1	B	170	ALA	3.3
1	A	1	MET	3.3
1	B	168	VAL	3.3
1	B	209	PHE	3.2
1	D	220	LYS	3.1
1	D	170	ALA	3.1
1	A	280	HIS	3.0
1	D	210	TYR	3.0
1	A	151	SER	3.0
1	B	214	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	152	VAL	2.9
1	B	213	ASP	2.9
1	B	166	ALA	2.8
1	A	148	GLU	2.7
1	B	171	PHE	2.7
1	D	168	VAL	2.6
1	A	206	PRO	2.6
1	D	206	PRO	2.6
1	B	1	MET	2.6
1	B	157	VAL	2.6
1	B	165	LYS	2.6
1	D	208	VAL	2.5
1	B	151	SER	2.5
1	D	166	ALA	2.5
1	B	129	GLU	2.5
1	B	131	VAL	2.5
1	D	207	GLY	2.5
1	D	175	SER	2.4
1	B	159	HIS	2.4
1	A	205	PRO	2.3
1	B	218	SER	2.3
1	D	129	GLU	2.3
1	B	130	LEU	2.3
1	B	160	ALA	2.2
1	D	219	ASP	2.2
1	B	167	LEU	2.1
1	C	195	ASP	2.1
1	B	280	HIS	2.1
1	D	209	PHE	2.1
1	B	161	SER	2.1
1	D	169	GLU	2.1
1	C	306	ASP	2.0
1	B	210	TYR	2.0
1	D	136	LYS	2.0
1	B	118	ASN	2.0
1	B	142	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

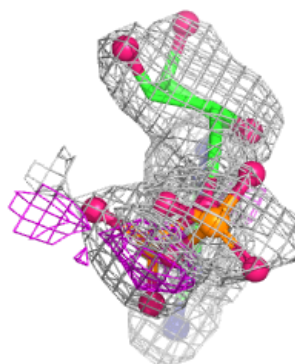
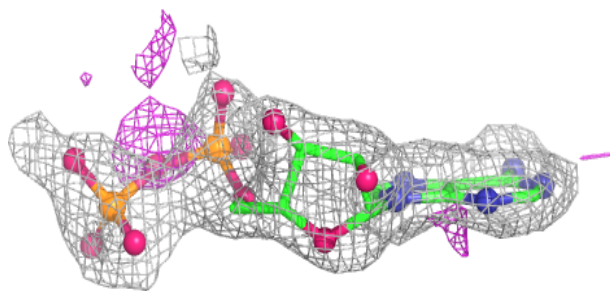
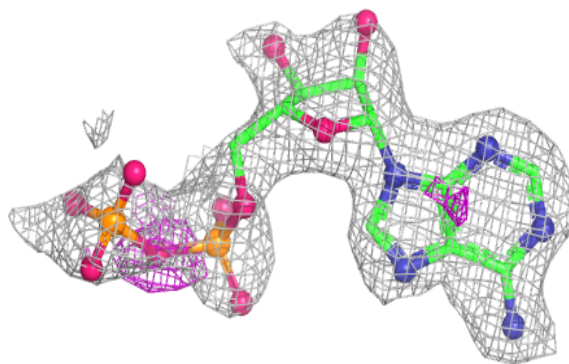
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	C	404	4/4	0.71	0.19	53,55,57,63	0
3	GOL	A	402	6/6	0.72	0.19	48,61,63,63	0
5	ACT	B	403	4/4	0.78	0.16	36,44,46,55	0
3	GOL	C	405	6/6	0.78	0.15	35,45,51,51	0
3	GOL	A	403	6/6	0.80	0.14	30,45,46,47	0
4	ADP	B	401	27/27	0.80	0.12	49,59,107,109	0
4	ADP	D	401	27/27	0.83	0.11	43,52,89,96	0
5	ACT	B	404	4/4	0.85	0.16	51,57,58,64	0
3	GOL	D	403	6/6	0.85	0.12	37,44,45,50	0
3	GOL	D	404	6/6	0.90	0.11	32,41,44,44	0
2	NA	A	404	1/1	0.91	0.18	28,28,28,28	0
2	NA	D	402	1/1	0.93	0.09	23,23,23,23	0
5	ACT	C	403	4/4	0.96	0.11	34,34,35,36	0
4	ADP	C	401	27/27	0.96	0.07	26,30,69,71	0
2	NA	A	401	1/1	0.97	0.03	19,19,19,19	0
2	NA	B	402	1/1	0.98	0.04	17,17,17,17	0
2	NA	C	402	1/1	0.99	0.05	21,21,21,21	0

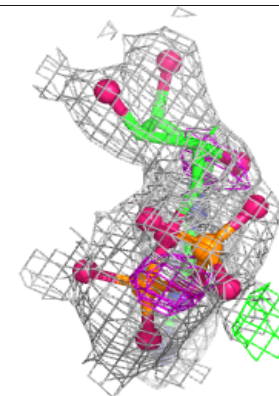
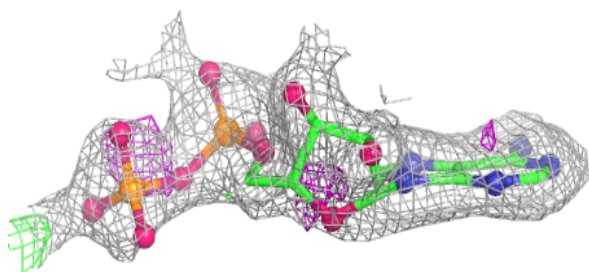
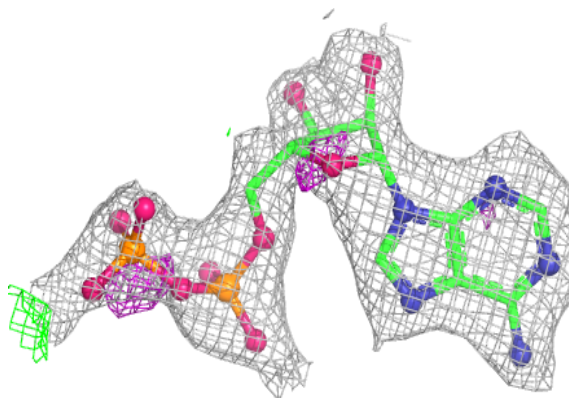
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

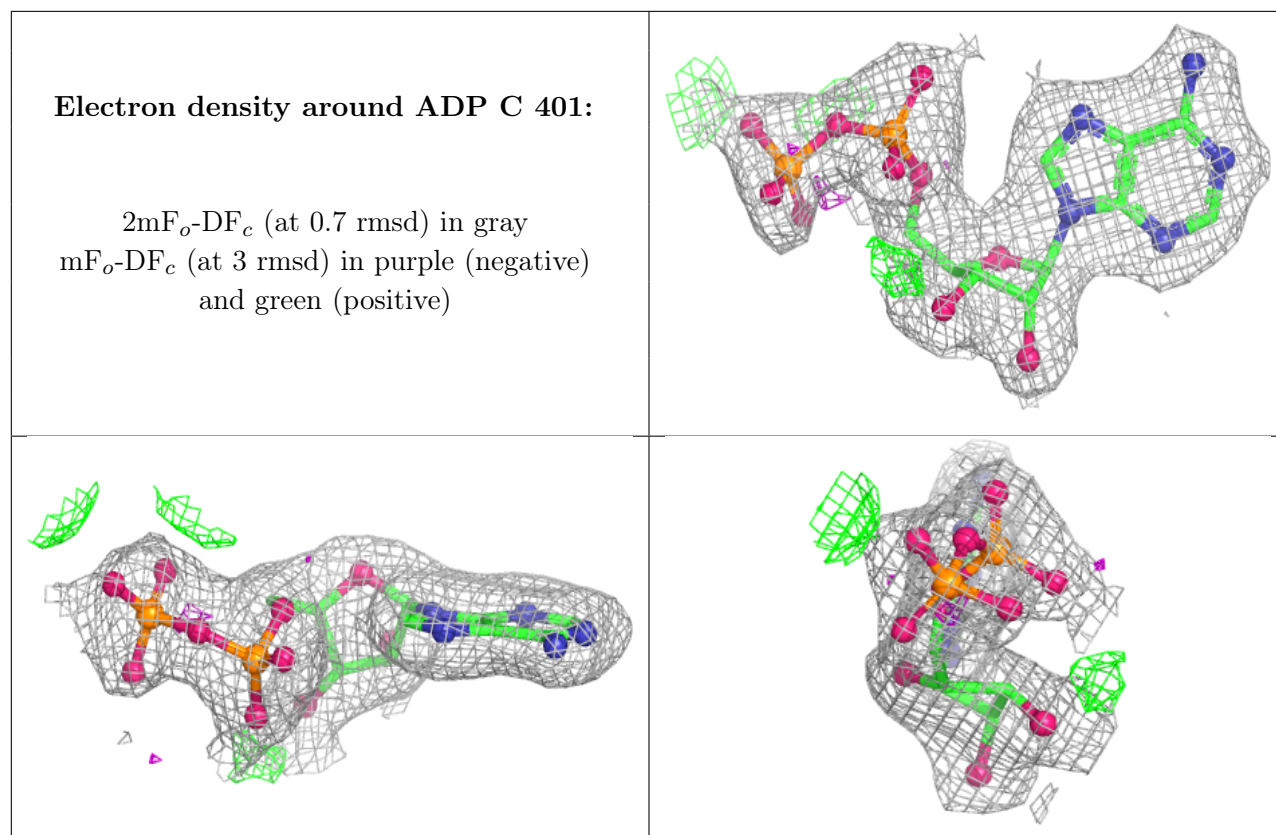
Electron density around ADP B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP D 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.