



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 03:22 PM EDT

PDB ID : 3OZX / pdb\_00003ozx  
Title : Crystal structure of ABCE1 of Sulfolobus solfataricus (-FeS domain)  
Authors : Barthelme, D.; Tampe, R.  
Deposited on : 2010-09-27  
Resolution : 2.05 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

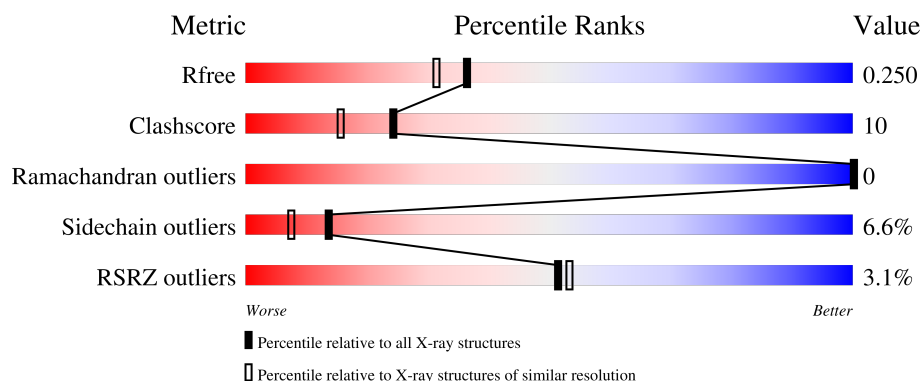
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.05 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))
$R_{free}$	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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  $\geq 3$ , 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	538	
1	B	538	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8757 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 RNase L inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4118	2640	703	767	8			
1	B	515	Total	C	N	O	S	0	0	0
			4127	2645	705	769	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	expression tag	UNP Q980K5
A	238	GLN	GLU	engineered mutation	UNP Q980K5
A	485	GLN	GLU	engineered mutation	UNP Q980K5
A	601	GLY	-	expression tag	UNP Q980K5
A	602	SER	-	expression tag	UNP Q980K5
A	603	ILE	-	expression tag	UNP Q980K5
A	604	GLU	-	expression tag	UNP Q980K5
A	605	GLY	-	expression tag	UNP Q980K5
A	606	ARG	-	expression tag	UNP Q980K5
A	607	HIS	-	expression tag	UNP Q980K5
A	608	HIS	-	expression tag	UNP Q980K5
A	609	HIS	-	expression tag	UNP Q980K5
A	610	HIS	-	expression tag	UNP Q980K5
A	611	HIS	-	expression tag	UNP Q980K5
A	612	HIS	-	expression tag	UNP Q980K5
B	75	MET	-	expression tag	UNP Q980K5
B	238	GLN	GLU	engineered mutation	UNP Q980K5
B	485	GLN	GLU	engineered mutation	UNP Q980K5
B	601	GLY	-	expression tag	UNP Q980K5
B	602	SER	-	expression tag	UNP Q980K5
B	603	ILE	-	expression tag	UNP Q980K5
B	604	GLU	-	expression tag	UNP Q980K5
B	605	GLY	-	expression tag	UNP Q980K5
B	606	ARG	-	expression tag	UNP Q980K5
B	607	HIS	-	expression tag	UNP Q980K5

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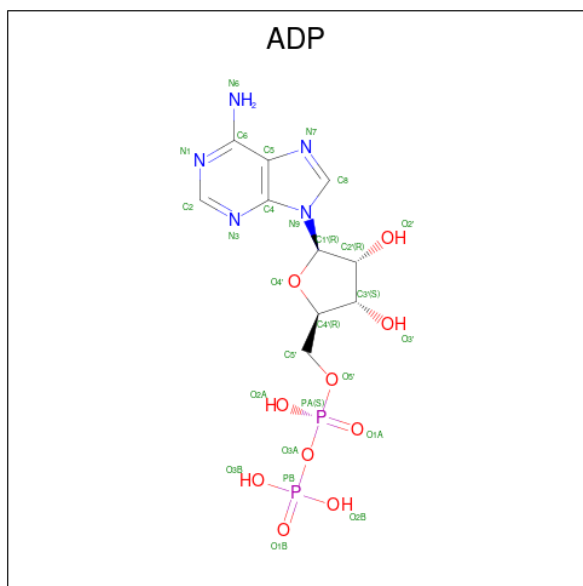
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Chain	Residue	Modelled	Actual	Comment	Reference
B	608	HIS	-	expression tag	UNP Q980K5
B	609	HIS	-	expression tag	UNP Q980K5
B	610	HIS	-	expression tag	UNP Q980K5
B	611	HIS	-	expression tag	UNP Q980K5
B	612	HIS	-	expression tag	UNP Q980K5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	191	Total	O	0	0
			191	191		
5	B	204	Total	O	0	0
			204	204		



GLY  
SER  
ILE  
GLU  
GLY  
ARG  
HIS  
HIS  
HIS  
HIS  
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.37Å 63.66Å 81.78Å 89.15° 84.47° 69.82°	Depositor
Resolution (Å)	20.00 – 2.05 20.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.3 (20.00-2.05) 91.2 (20.00-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, $R_{free}$	0.186 , 0.245 0.200 , 0.250	Depositor DCC
$R_{free}$ test set	3182 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, PO4

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	0.90	1/4187 (0.0%)	1.01	4/5640 (0.1%)
1	B	1.00	3/4196 (0.1%)	1.05	3/5652 (0.1%)
All	All	0.95	4/8383 (0.0%)	1.03	7/11292 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	373	ILE	CA-CB	6.58	1.62	1.54
1	A	124	ILE	CA-CB	5.94	1.60	1.53
1	B	515	ILE	CA-CB	5.78	1.61	1.54
1	B	514	PHE	CA-C	-5.08	1.46	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ASP	N-CA-C	7.62	120.99	109.41
1	B	526	ILE	N-CA-C	6.42	119.81	113.71
1	A	526	ILE	N-CA-C	6.14	119.54	113.71
1	A	514	PHE	CA-C-N	-6.02	114.62	122.99
1	A	514	PHE	C-N-CA	-6.02	114.62	122.99
1	B	429	SER	N-CA-C	5.96	117.19	108.14
1	A	219	GLN	N-CA-C	-5.05	105.69	111.14

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	4118	0	4237	81	0
1	B	4127	0	4245	85	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	54	0	24	0	0
3	B	54	0	24	1	0
4	A	5	0	0	0	0
5	A	191	0	0	7	0
5	B	204	0	0	7	0
All	All	8757	0	8530	165	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 10.

All (165) 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:ASN:HB2	5:A:3246:HOH:O	1.54	1.08
1:B:76:GLU:HA	1:B:293:ARG:HH22	1.18	1.04
1:B:196:VAL:HG21	1:B:228:LEU:HD21	1.46	0.98
1:B:359:VAL:HB	1:B:542:LEU:HD13	1.45	0.98
1:A:446:ARG:HH11	1:A:446:ARG:HG3	1.25	0.97
1:A:309:LYS:HA	1:A:323:GLU:HG3	1.49	0.95
1:B:196:VAL:CG2	1:B:228:LEU:HD21	1.99	0.92
1:B:565:ARG:HD2	1:B:586:GLN:NE2	1.93	0.83
1:B:456:ASN:HD22	1:B:458:ASN:H	1.29	0.79
1:B:210:ALA:HA	1:B:213:LEU:HD22	1.68	0.76
1:A:276:TYR:OH	1:A:578:ILE:HG12	1.86	0.76
1:B:405:ILE:CD1	1:B:476:LYS:HE2	2.17	0.75
1:B:138:GLU:HA	1:B:141:LYS:HE2	1.67	0.75
1:B:282:HIS:HD2	1:B:295:SER:O	1.71	0.74
1:B:135:GLY:O	1:B:139:VAL:HG23	1.90	0.71
1:A:442:GLU:O	1:A:446:ARG:HB2	1.91	0.71
1:B:405:ILE:HD11	1:B:476:LYS:HE2	1.73	0.71
1:A:355:ASP:O	5:A:3183:HOH:O	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ASN:HD21	1:B:451:ARG:NH1	1.89	0.70
1:B:76:GLU:CA	1:B:293:ARG:HH22	2.01	0.69
1:A:327:MET:SD	1:A:566:ARG:HD2	2.33	0.69
1:B:456:ASN:ND2	1:B:458:ASN:H	1.90	0.69
1:B:448:ASN:HD21	1:B:451:ARG:HH11	1.40	0.69
1:A:325:LYS:HD2	1:A:328:LEU:HD11	1.75	0.68
1:B:148:ILE:HG12	1:B:152:PHE:CD2	2.30	0.67
1:B:166:ILE:HD11	1:B:172:ALA:HB2	1.77	0.67
1:A:281:ILE:HD13	1:A:304:ILE:HG13	1.77	0.66
1:B:409:LYS:NZ	1:B:466:GLN:HE22	1.95	0.65
1:A:404:GLN:NE2	5:A:3249:HOH:O	2.27	0.65
1:B:209:ASP:O	1:B:212:ILE:HG22	1.96	0.65
1:B:76:GLU:HA	1:B:293:ARG:NH2	2.02	0.65
1:A:197:LYS:HE2	1:A:203:THR:HG22	1.79	0.64
1:A:409:LYS:NZ	1:A:466:GLN:HE22	1.96	0.64
1:A:246:ARG:HB3	1:A:246:ARG:HH11	1.63	0.63
1:B:320:ARG:HG2	1:B:321:PRO:HD2	1.82	0.62
1:B:505:VAL:O	1:B:509:ARG:HG3	2.00	0.62
1:B:192:LYS:O	1:B:196:VAL:HG23	1.99	0.62
1:A:76:GLU:O	1:A:293:ARG:NH2	2.33	0.62
1:B:327:MET:SD	1:B:566:ARG:HD2	2.40	0.61
1:A:420:THR:HA	1:A:456:ASN:HA	1.82	0.61
1:B:373:ILE:HG23	1:B:533:PHE:CE2	2.36	0.61
1:B:196:VAL:HG21	1:B:228:LEU:CD2	2.25	0.61
1:A:285:TYR:CE2	1:A:317:MET:HG2	2.35	0.61
1:A:104:VAL:HB	1:A:267:VAL:HG22	1.82	0.60
1:B:193:LYS:HE2	1:B:206:TRP:HZ2	1.66	0.60
1:B:370:ILE:HD11	1:B:503:LYS:HA	1.83	0.59
1:A:519:ASP:HB3	1:A:522:ILE:HD12	1.84	0.59
1:B:486:PRO:HD2	1:B:517:ASP:OD2	2.02	0.59
1:A:255:ILE:HB	1:A:277:LEU:HD21	1.85	0.59
1:A:125:PRO:O	1:A:134:VAL:HG21	2.02	0.59
1:A:166:ILE:HD11	1:A:172:ALA:HB2	1.85	0.58
1:B:405:ILE:HD12	1:B:406:LEU:N	2.18	0.58
1:B:255:ILE:HB	1:B:277:LEU:HD11	1.84	0.58
1:A:99:ASN:OD1	1:A:261:ASN:HA	2.04	0.57
1:B:568:ALA:HA	1:B:597:LEU:HD22	1.86	0.57
1:B:572:ARG:HD2	5:B:3110:HOH:O	2.03	0.57
1:A:568:ALA:HB2	1:A:598:SER:HB2	1.87	0.56
1:A:144:ARG:NH2	5:A:3197:HOH:O	2.39	0.56
1:A:255:ILE:HG23	1:A:259:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:ARG:HD2	1:B:586:GLN:HE21	1.70	0.55
1:A:562:VAL:HG12	1:A:578:ILE:HD11	1.87	0.55
1:B:367:GLU:HG2	1:B:510:LYS:HB3	1.89	0.55
1:A:370:ILE:HD11	1:A:503:LYS:HA	1.90	0.53
1:B:185:THR:CG2	1:B:193:LYS:HE3	2.37	0.53
1:B:576:ASN:HD21	1:B:586:GLN:NE2	2.06	0.53
1:A:577:LYS:O	1:A:580:SER:OG	2.21	0.53
1:B:405:ILE:HG13	1:B:478:ALA:HA	1.89	0.53
1:A:446:ARG:HH11	1:A:446:ARG:CG	2.11	0.52
1:B:138:GLU:CD	1:B:142:ARG:HH11	2.17	0.52
1:A:142:ARG:NE	5:A:3153:HOH:O	2.43	0.52
1:A:209:ASP:O	1:A:212:ILE:HG13	2.09	0.52
1:B:138:GLU:HG2	1:B:141:LYS:HE2	1.90	0.52
1:B:245:VAL:H	1:B:518:HIS:HD1	1.56	0.52
1:A:179:THR:HG22	1:A:182:GLU:CD	2.34	0.52
1:B:393:THR:HG22	5:B:3286:HOH:O	2.10	0.52
1:B:445:LYS:HG3	1:B:450:HIS:CE1	2.45	0.52
1:A:275:ASP:OD1	1:A:572:ARG:NH2	2.44	0.51
1:B:179:THR:O	1:B:183:ILE:CG1	2.58	0.51
1:B:255:ILE:HG23	1:B:259:LEU:HD12	1.93	0.51
1:A:199:LEU:HD12	1:A:258:LEU:HD11	1.92	0.51
1:A:116:LEU:HG	1:A:235:ILE:CG2	2.41	0.51
1:B:249:MET:O	1:B:253:LYS:HG3	2.11	0.51
1:A:193:LYS:HE3	1:A:206:TRP:HZ2	1.76	0.51
1:A:446:ARG:HG3	1:A:446:ARG:NH1	2.04	0.50
1:B:163:VAL:HG23	1:B:231:ALA:HB2	1.94	0.50
1:B:293:ARG:HD3	5:B:3415:HOH:O	2.12	0.50
1:B:405:ILE:HD12	1:B:405:ILE:C	2.37	0.50
1:A:445:LYS:HG3	1:A:450:HIS:CE1	2.47	0.49
1:B:456:ASN:HD22	1:B:458:ASN:N	2.05	0.49
1:B:418:ASP:OD2	1:B:418:ASP:N	2.40	0.49
1:A:169:VAL:HG12	1:A:222:LEU:HD12	1.95	0.49
1:B:565:ARG:HD2	1:B:586:GLN:HE22	1.73	0.49
1:B:282:HIS:HE1	5:B:3317:HOH:O	1.95	0.49
1:B:504:ARG:NH1	1:B:508:GLU:OE2	2.46	0.48
1:B:256:ARG:NH1	1:B:277:LEU:O	2.43	0.48
1:A:447:LEU:HD12	1:A:447:LEU:HA	1.65	0.48
1:A:282:HIS:HD2	1:A:295:SER:O	1.97	0.47
1:A:296:LYS:HD3	1:A:314:ALA:CB	2.45	0.47
1:B:276:TYR:OH	1:B:578:ILE:HD12	2.13	0.47
1:A:77:GLY:O	5:A:3162:HOH:O	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LYS:HZ2	1:A:569:GLU:HG2	1.80	0.47
1:B:82:ARG:HB2	1:B:128:GLY:HA2	1.96	0.46
1:B:179:THR:O	1:B:183:ILE:HG12	2.16	0.46
1:B:351:LYS:NZ	5:B:3286:HOH:O	2.48	0.46
1:B:125:PRO:O	1:B:134:VAL:HG21	2.16	0.46
1:B:110:VAL:O	1:B:292:GLY:HA3	2.15	0.45
1:A:434:SER:C	1:A:436:SER:H	2.23	0.45
1:A:565:ARG:CD	1:A:599:THR:HB	2.46	0.45
1:B:409:LYS:HZ3	1:B:466:GLN:HE22	1.63	0.45
1:B:438:TRP:O	1:B:442:GLU:HG2	2.16	0.45
1:B:148:ILE:HG12	1:B:152:PHE:CE2	2.52	0.45
1:B:325:LYS:HG2	5:B:3223:HOH:O	2.17	0.45
1:A:563:THR:HG22	1:A:592:TYR:HA	1.99	0.44
1:A:309:LYS:HZ1	1:A:569:GLU:CD	2.25	0.44
1:B:187:ILE:CD1	1:B:225:ALA:HB1	2.47	0.44
1:B:467:LYS:NZ	5:B:3383:HOH:O	2.36	0.44
1:A:240:SER:HB2	1:A:248:ARG:HG2	2.00	0.44
1:B:148:ILE:HD13	1:B:152:PHE:HE2	1.83	0.44
1:A:433:LEU:HD21	1:A:453:LEU:HD21	1.99	0.43
1:A:173:SER:HA	1:A:176:LEU:HD22	2.00	0.43
1:B:179:THR:O	1:B:183:ILE:HG13	2.17	0.43
1:A:564:PHE:CE1	1:A:575:VAL:HB	2.54	0.43
1:B:345:LYS:HA	1:B:364:GLU:HA	1.99	0.43
1:B:421:VAL:CG2	1:B:460:LEU:HD11	2.48	0.43
1:A:97:LYS:NZ	1:A:147:GLU:OE2	2.36	0.43
1:A:445:LYS:HA	1:A:450:HIS:ND1	2.34	0.43
1:A:282:HIS:HE1	5:A:3045:HOH:O	2.00	0.43
1:A:595:MET:H	1:A:595:MET:HG3	1.57	0.43
1:A:179:THR:HG23	1:A:182:GLU:H	1.84	0.43
1:A:329:LYS:HB2	1:A:329:LYS:HE3	1.94	0.43
1:A:565:ARG:HD2	1:A:599:THR:HB	2.01	0.43
1:A:409:LYS:HZ2	1:A:466:GLN:HE22	1.67	0.42
1:B:431:ASP:O	1:B:432:ALA:C	2.62	0.42
1:A:495:ARG:HB2	1:A:522:ILE:HD11	2.01	0.42
1:A:536:GLU:OE1	1:B:348:LYS:NZ	2.44	0.42
1:A:434:SER:C	1:A:436:SER:N	2.78	0.42
1:A:102:LEU:C	1:A:102:LEU:HD23	2.45	0.42
1:A:435:THR:HA	1:A:440:PHE:CD2	2.55	0.42
1:B:244:ASP:HB2	1:B:518:HIS:CE1	2.55	0.42
1:B:249:MET:HE3	1:B:562:VAL:HG21	2.02	0.42
1:A:531:ILE:HD11	1:A:546:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LEU:HA	1:B:520:LEU:HD23	1.82	0.42
1:A:446:ARG:HD2	1:A:446:ARG:HA	1.88	0.42
1:A:495:ARG:HD3	1:A:522:ILE:HD11	2.02	0.41
1:B:187:ILE:HD11	1:B:225:ALA:HA	2.01	0.41
1:A:179:THR:HG22	1:A:182:GLU:CG	2.51	0.41
1:A:179:THR:OG1	1:A:207:ASN:HA	2.20	0.41
1:A:364:GLU:OE2	1:A:366:LYS:HE2	2.19	0.41
1:B:530:ILE:HD11	1:B:552:GLY:HA3	2.03	0.41
1:B:380:GLY:HA2	3:B:615:ADP:O1A	2.21	0.41
1:B:421:VAL:HG22	1:B:460:LEU:HD11	2.01	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.84	0.41
1:A:218:LEU:O	1:A:222:LEU:HG	2.21	0.41
1:B:550:LYS:HA	1:B:593:TYR:CD2	2.56	0.41
1:A:356:PHE:CE2	1:A:358:LEU:HB2	2.56	0.41
1:A:439:PHE:CE2	1:A:443:VAL:HG21	2.56	0.41
1:A:502:ILE:HG21	1:A:502:ILE:HD13	1.83	0.41
1:B:148:ILE:CD1	1:B:152:PHE:CE2	3.03	0.41
1:B:190:ARG:HD2	1:B:229:ARG:O	2.19	0.41
1:B:359:VAL:HB	1:B:542:LEU:CD1	2.33	0.41
1:A:281:ILE:CD1	1:A:304:ILE:HG13	2.48	0.40
1:A:352:LYS:HE3	1:A:354:GLY:O	2.20	0.40
1:A:379:ILE:HG22	1:A:381:LYS:HG3	2.03	0.40
1:A:583:ASP:O	1:A:587:LYS:HB2	2.21	0.40
1:A:400:THR:HA	1:A:401:PRO:C	2.46	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	510/538 (95%)	496 (97%)	14 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	511/538 (95%)	498 (98%)	13 (2%)	0	100	100
All	All	1021/1076 (95%)	994 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	449/471 (95%)	420 (94%)	29 (6%)	14	7
1	B	450/471 (96%)	420 (93%)	30 (7%)	13	7
All	All	899/942 (95%)	840 (93%)	59 (7%)	14	7

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	116	LEU
1	A	133	LYS
1	A	138	GLU
1	A	148	ILE
1	A	175	PHE
1	A	176	LEU
1	A	198	GLU
1	A	246	ARG
1	A	268	ASP
1	A	272	ILE
1	A	281	ILE
1	A	289	SER
1	A	341	LYS
1	A	371	ILE
1	A	379	ILE
1	A	418	ASP
1	A	426	GLU

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Mol	Chain	Res	Type
1	A	431	ASP
1	A	443	VAL
1	A	446	ARG
1	A	447	LEU
1	A	454	GLU
1	A	493	GLU
1	A	503	LYS
1	A	508	GLU
1	A	515	ILE
1	A	575	VAL
1	A	595	MET
1	B	105	LEU
1	B	116	LEU
1	B	142	ARG
1	B	177	LYS
1	B	183	ILE
1	B	193	LYS
1	B	196	VAL
1	B	203	THR
1	B	212	ILE
1	B	213	LEU
1	B	277	LEU
1	B	322	ASP
1	B	341	LYS
1	B	374	LEU
1	B	402	GLU
1	B	405	ILE
1	B	409	LYS
1	B	418	ASP
1	B	438	TRP
1	B	509	ARG
1	B	517	ASP
1	B	537	PRO
1	B	538	GLU
1	B	554	ASN
1	B	565	ARG
1	B	582	LEU
1	B	584	ARG
1	B	585	VAL
1	B	598	SER
1	B	599	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)



such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	238	GLN
1	A	261	ASN
1	A	282	HIS
1	A	306	ASN
1	A	416	ASN
1	A	422	GLN
1	A	427	ASN
1	A	448	ASN
1	A	466	GLN
1	A	485	GLN
1	B	98	ASN
1	B	201	ASN
1	B	204	ASN
1	B	207	ASN
1	B	238	GLN
1	B	282	HIS
1	B	306	ASN
1	B	404	GLN
1	B	448	ASN
1	B	456	ASN
1	B	458	ASN
1	B	466	GLN
1	B	485	GLN
1	B	586	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	PO4	A	1	-	4,4,4	0.99	0	6,6,6	0.81	0
3	ADP	A	616	2	24,29,29	1.40	4 (16%)	29,45,45	1.74	4 (13%)
3	ADP	A	615	2	24,29,29	1.51	4 (16%)	29,45,45	1.66	6 (20%)
3	ADP	B	616	2	24,29,29	1.45	2 (8%)	29,45,45	1.58	2 (6%)
3	ADP	B	615	2	24,29,29	1.02	1 (4%)	29,45,45	1.71	6 (20%)

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	615	2	-	3/12/32/32	0/3/3/3
3	ADP	B	616	2	-	3/12/32/32	0/3/3/3
3	ADP	A	616	2	-	1/12/32/32	0/3/3/3
3	ADP	B	615	2	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	616	ADP	PA-O3A	5.27	1.65	1.59
3	A	615	ADP	PA-O3A	4.97	1.64	1.59
3	A	616	ADP	PA-O3A	4.37	1.64	1.59
3	A	616	ADP	O4'-C1'	2.81	1.44	1.40
3	B	616	ADP	C2-N3	2.81	1.36	1.32
3	A	615	ADP	O4'-C1'	2.70	1.44	1.40
3	A	616	ADP	PB-O2B	-2.65	1.45	1.54
3	B	615	ADP	O4'-C1'	2.61	1.44	1.40
3	A	615	ADP	C2-N3	2.50	1.36	1.32
3	A	616	ADP	C2-N3	2.36	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	615	ADP	PB-O2B	-2.20	1.46	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	615	ADP	N3-C2-N1	-5.80	120.80	128.67
3	B	615	ADP	N3-C2-N1	-5.74	120.89	128.67
3	A	616	ADP	N3-C2-N1	-5.62	121.04	128.67
3	B	616	ADP	N3-C2-N1	-5.53	121.16	128.67
3	A	616	ADP	O4'-C1'-N9	4.34	114.50	108.75
3	A	616	ADP	O3'-C3'-C4'	-3.53	100.94	111.08
3	A	615	ADP	O2A-PA-O1A	3.13	127.02	112.44
3	A	616	ADP	O3'-C3'-C2'	-3.03	102.11	111.82
3	B	615	ADP	O3'-C3'-C2'	-2.89	102.56	111.82
3	B	616	ADP	O3'-C3'-C2'	-2.81	102.80	111.82
3	B	615	ADP	O2A-PA-O3A	2.68	114.52	107.27
3	B	615	ADP	O3'-C3'-C4'	-2.54	103.79	111.08
3	A	615	ADP	O2A-PA-O5'	-2.47	96.37	107.57
3	A	615	ADP	O4'-C1'-N9	-2.45	105.49	108.75
3	B	615	ADP	O3B-PB-O2B	2.22	116.12	107.80
3	A	615	ADP	C1'-N9-C4	-2.19	122.79	126.64
3	B	615	ADP	O2A-PA-O5'	-2.12	97.96	107.57
3	A	615	ADP	O3B-PB-O2B	2.06	115.54	107.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

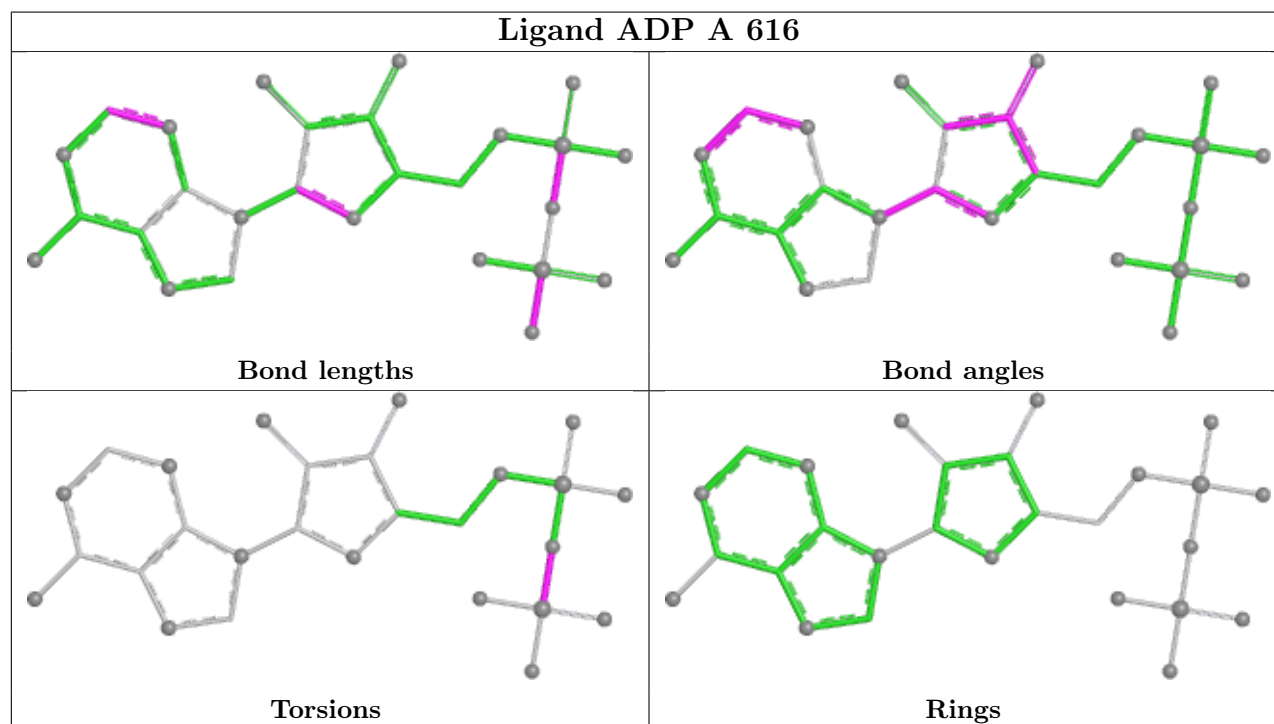
Mol	Chain	Res	Type	Atoms
3	B	616	ADP	PA-O3A-PB-O2B
3	A	615	ADP	PA-O3A-PB-O2B
3	A	616	ADP	PA-O3A-PB-O2B
3	B	616	ADP	C5'-O5'-PA-O1A
3	A	615	ADP	C3'-C4'-C5'-O5'
3	B	616	ADP	PA-O3A-PB-O1B
3	A	615	ADP	O4'-C4'-C5'-O5'

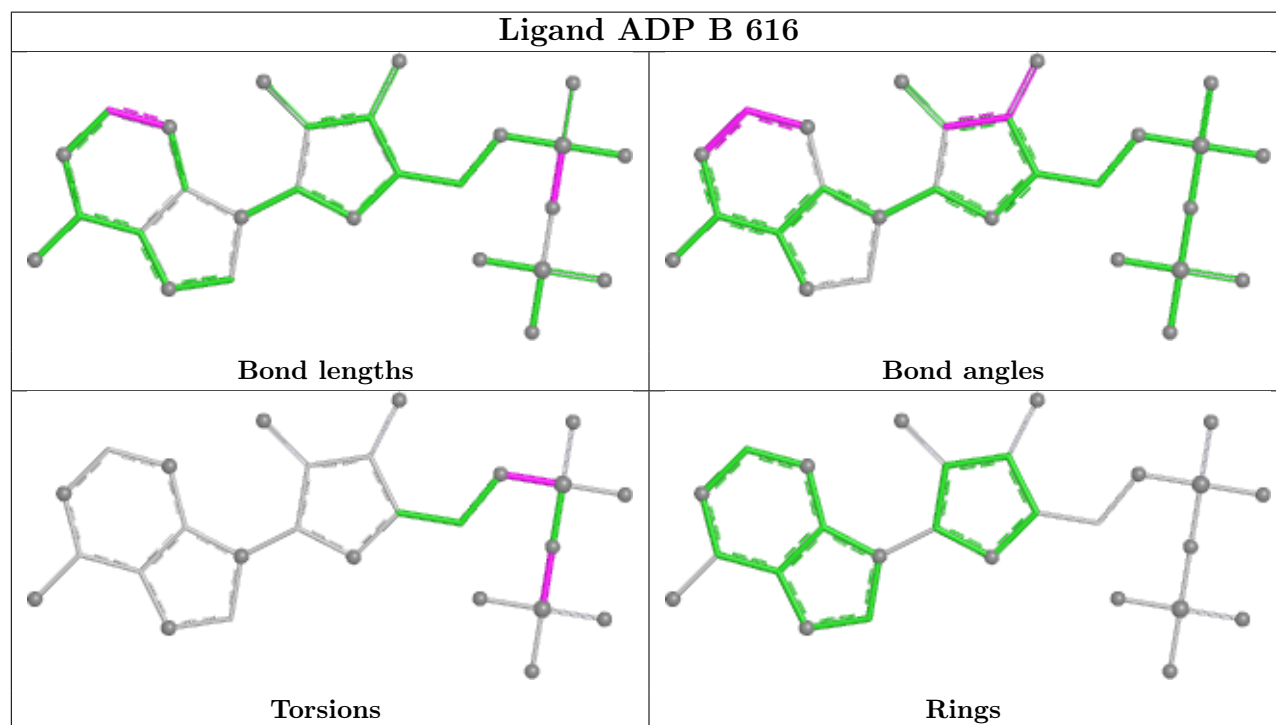
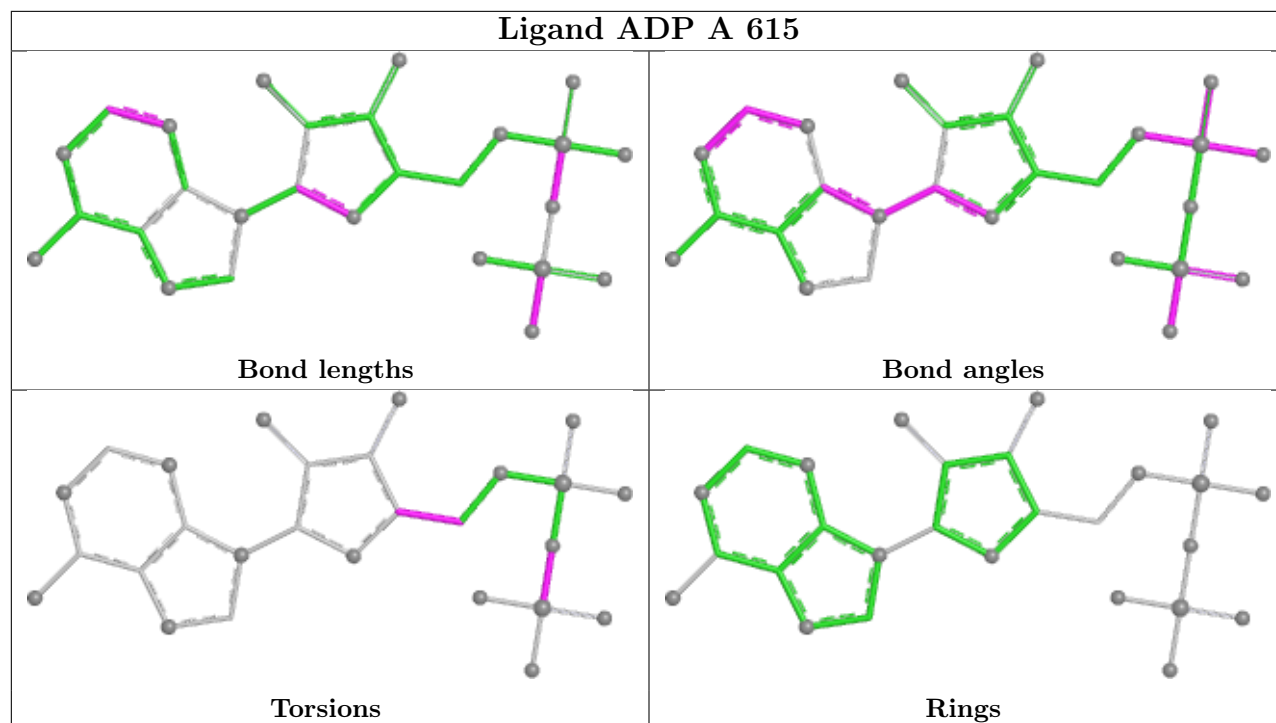
There are no ring outliers.

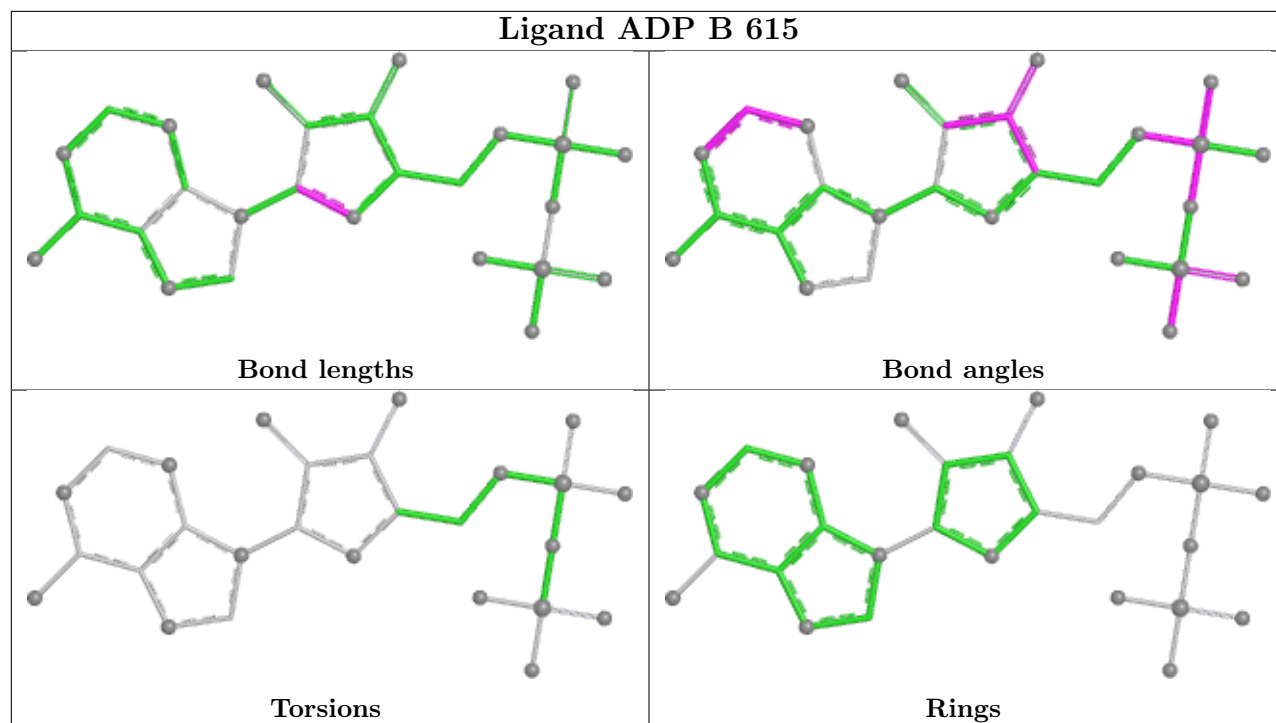
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	615	ADP	1	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	514/538 (95%)	0.14	19 (3%) 45 47	13, 33, 77, 101	0
1	B	515/538 (95%)	-0.03	13 (2%) 58 60	11, 31, 65, 105	0
All	All	1029/1076 (95%)	0.06	32 (3%) 51 53	11, 32, 71, 105	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	TRP	4.1
1	B	581	TYR	4.0
1	A	340	LEU	3.9
1	A	597	LEU	3.5
1	A	581	TYR	3.4
1	B	598	SER	3.3
1	B	597	LEU	3.1
1	A	585	VAL	3.1
1	B	150	ASN	3.0
1	B	599	THR	3.0
1	A	598	SER	3.0
1	A	432	ALA	2.9
1	A	439	PHE	2.8
1	A	329	LYS	2.8
1	A	442	GLU	2.7
1	B	314	ALA	2.6
1	A	599	THR	2.6
1	B	328	LEU	2.6
1	B	212	ILE	2.4
1	A	418	ASP	2.4
1	A	596	VAL	2.4
1	A	429	SER	2.4
1	B	135	GLY	2.3
1	A	134	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	340	LEU	2.3
1	B	596	VAL	2.2
1	A	578	ILE	2.2
1	A	582	LEU	2.1
1	A	437	SER	2.1
1	B	580	SER	2.1
1	A	328	LEU	2.1
1	B	438	TRP	2.1

## 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 monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

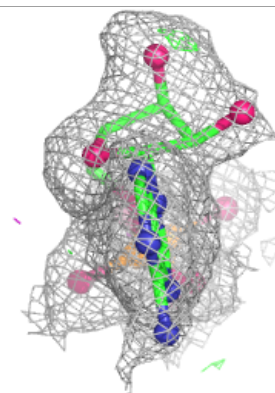
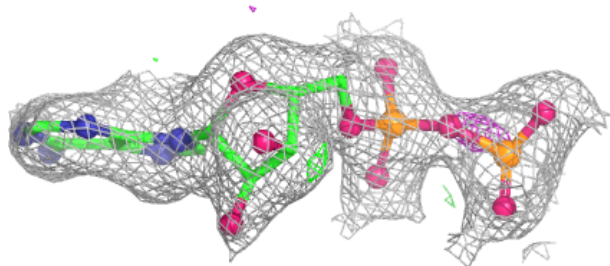
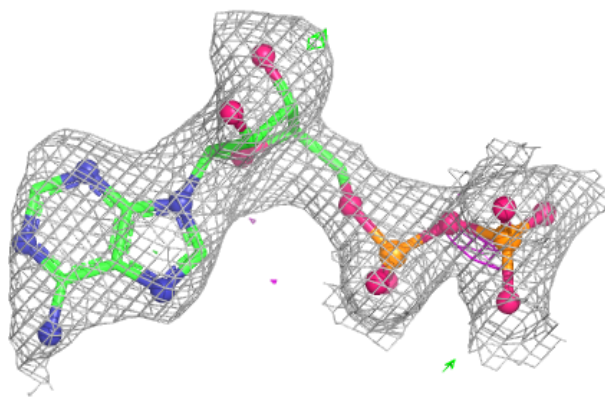
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	613	1/1	0.96	0.03	12,12,12,12	0
2	MG	B	613	1/1	0.96	0.04	15,15,15,15	0
2	MG	B	614	1/1	0.96	0.04	18,18,18,18	0
3	ADP	B	615	27/27	0.97	0.07	14,29,47,53	0
4	PO4	A	1	5/5	0.97	0.11	33,33,42,46	0
3	ADP	A	616	27/27	0.98	0.05	11,25,35,36	0
2	MG	A	614	1/1	0.98	0.02	16,16,16,16	0
3	ADP	B	616	27/27	0.98	0.05	11,22,29,32	0
3	ADP	A	615	27/27	0.98	0.05	11,20,25,27	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.

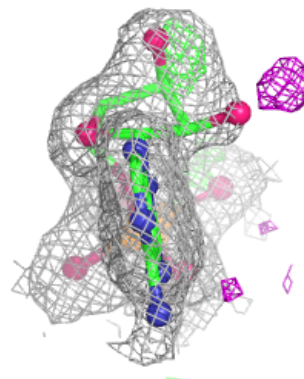
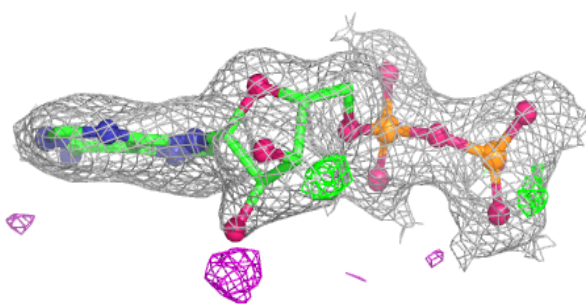
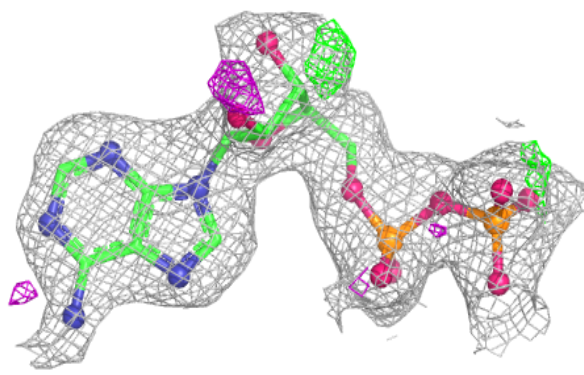


**Electron density around ADP B 615:**

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

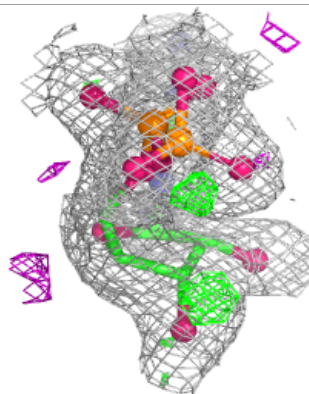
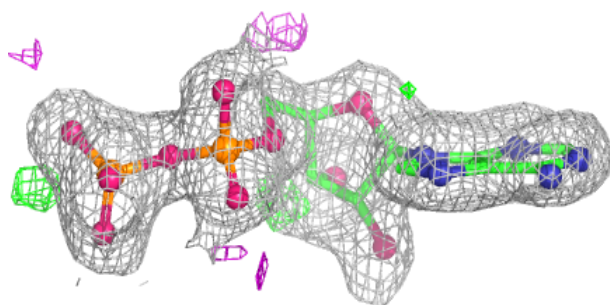
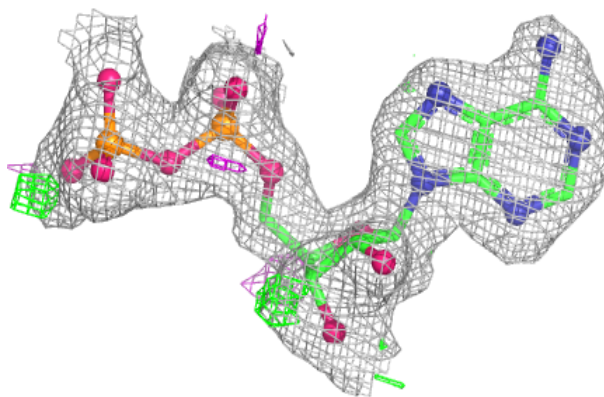
**Electron density around ADP A 616:**

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

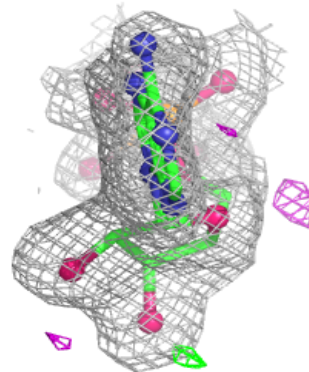
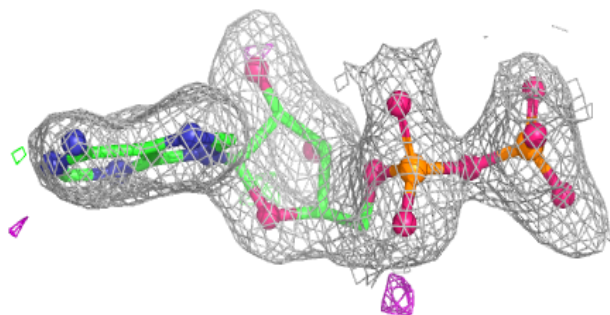
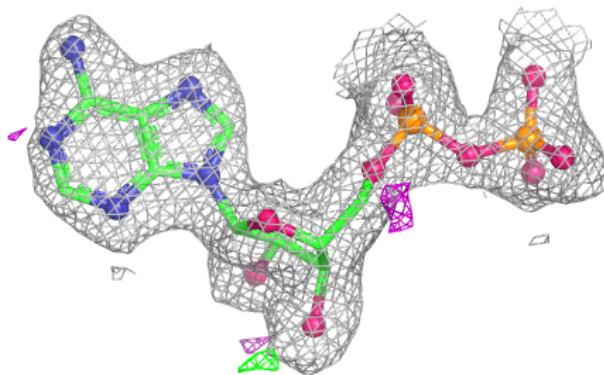


**Electron density around ADP B 616:**

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

**Electron density around ADP A 615:**

$2mF_o-DF_c$  (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.