



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:32 am BST

PDB ID : 3OZX
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

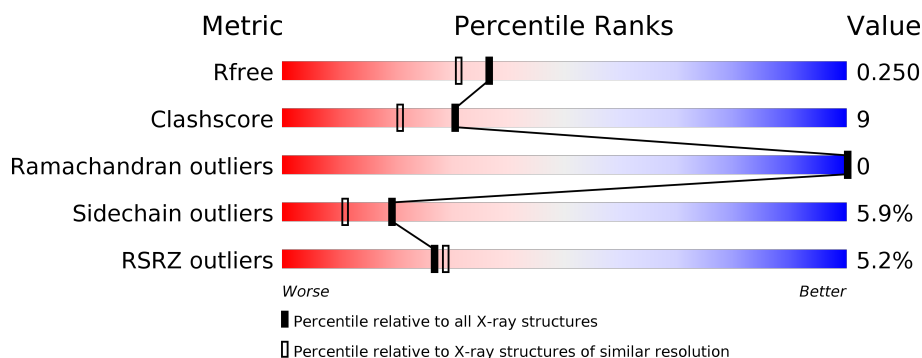
1 Overall quality at a glance

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 on 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	538	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	538	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>

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

Continued on next page...

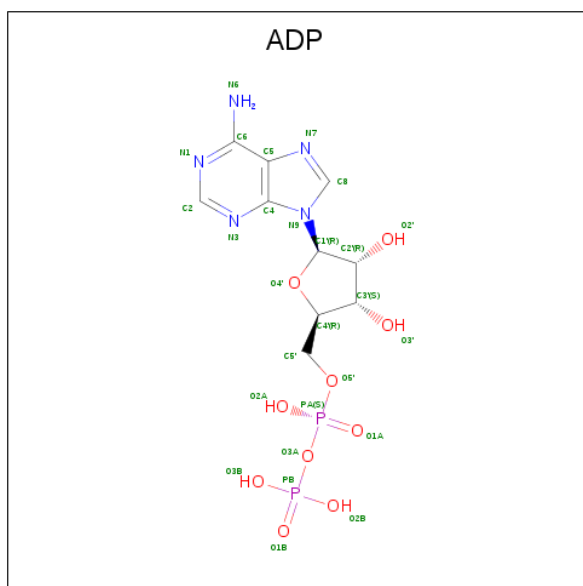
Continued from previous page...

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 (three-letter code: MG) (formula: Mg).

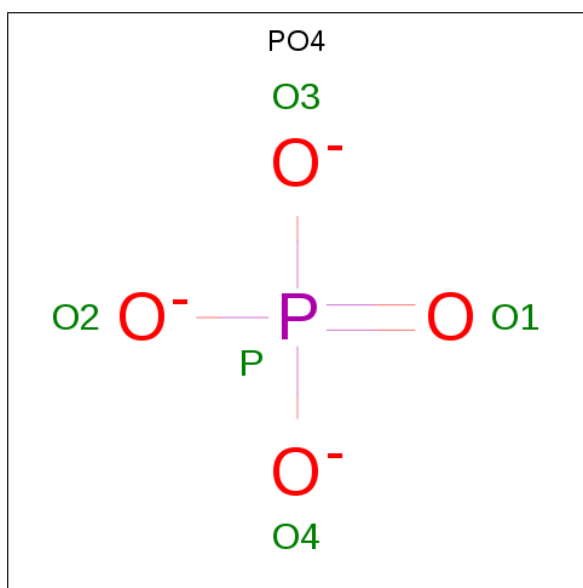
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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 (three-letter code: PO4) (formula: O₄P).



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

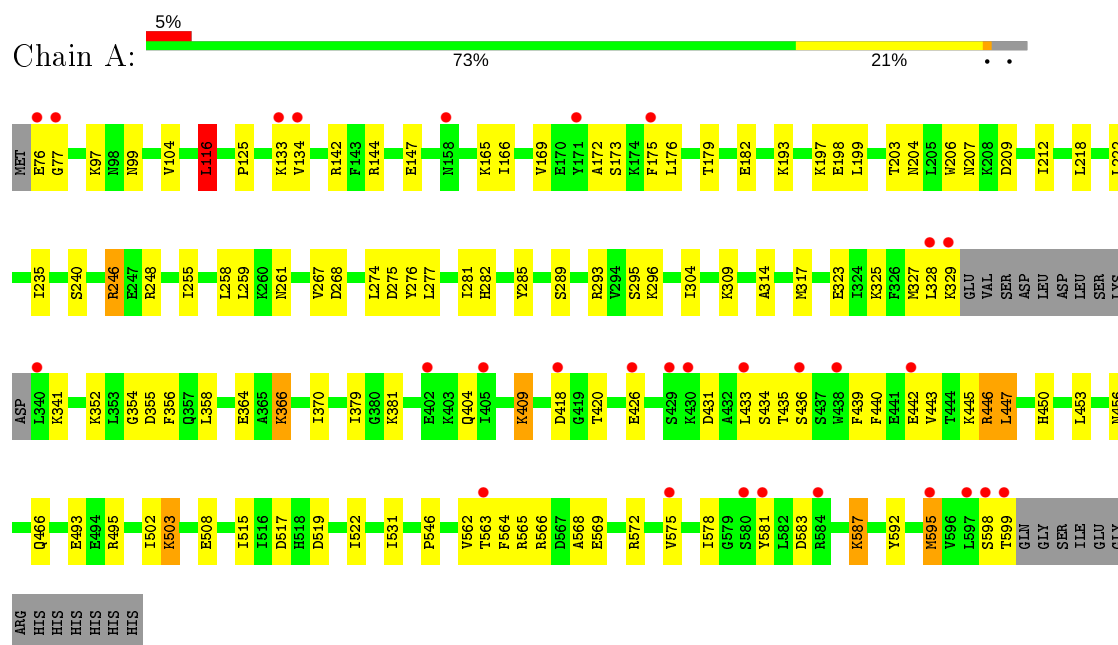
- Molecule 5 is water.

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

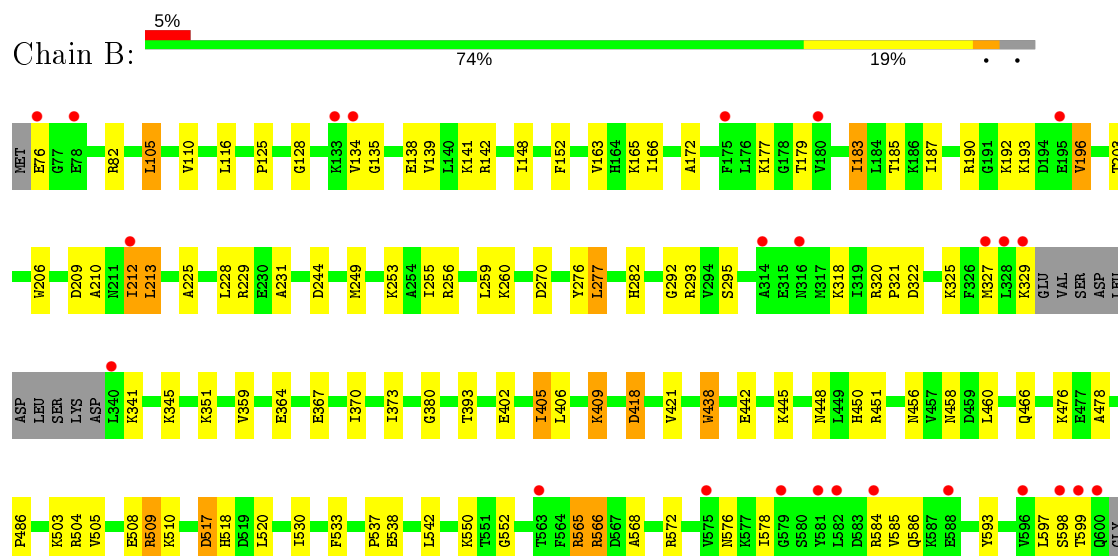
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNase L inhibitor



• Molecule 1: RNase L inhibitor



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, α , β , γ	58.37Å 63.66Å 81.78Å 89.15° 84.47° 69.82°	Depositor
Resolution (Å)	20.00 – 2.05 19.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.3 (20.00-2.05) 91.3 (19.89-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	27.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	0/4187	0.76	1/5640 (0.0%)
1	B	0.80	0/4196	0.82	3/5652 (0.1%)
All	All	0.76	0/8383	0.79	4/11292 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	LEU	CA-CB-CG	6.28	129.75	115.30
1	B	566	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	116	LEU	CB-CG-CD1	5.57	120.48	111.00
1	B	270	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	75	0
1	B	4127	0	4245	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	54	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
All	All	8757	0	8530	155	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 9.

All (155) 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:HG3	1:A:446:ARG:HH11	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:405:ILE:HG13	1:B:478:ALA:HA	1.89	0.53
1:A:446:ARG:CG	1:A:446:ARG:HH11	2.11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	1:B:418:ASP:OD2	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:138:GLU:CD	1:B:142:ARG:HH11	2.17	0.47
1:B:276:TYR:OH	1:B:578:ILE:HD12	2.13	0.47
1:A:179:THR:HG22	1:A:182:GLU:CD	2.34	0.47
1:A:77:GLY:O	5:A:3162:HOH:O	2.21	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:A:309:LYS:HZ2	1:A:569:GLU:HG2	1.81	0.45
1:B:110:VAL:O	1:B:292:GLY:HA3	2.15	0.45
1:A:565:ARG:CD	1:A:599:THR:HB	2.46	0.45
1:B:405:ILE:HD12	1:B:405:ILE:C	2.37	0.45
1:B:438:TRP:O	1:B:442:GLU:HG2	2.16	0.45
1:B:409:LYS:HZ3	1:B:466:GLN:HE22	1.63	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:B:187:ILE:CD1	1:B:225:ALA:HB1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:LYS:NZ	1:A:147:GLU:OE2	2.36	0.43
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: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:HE3	1:A:329:LYS:HB2	1.94	0.43
1:A:565:ARG:HD2	1:A:599:THR:HB	2.01	0.43
1:A:495:ARG:HB2	1:A:522:ILE:HD11	2.01	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:A:531:ILE:HD11	1:A:546:PRO:HG3	2.01	0.42
1:B:520:LEU:HD23	1:B:520:LEU:HA	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:OG1	1:A:207:ASN:HA	2.20	0.41
1:A:179:THR:HG22	1:A:182:GLU:CG	2.51	0.41
1:A:364:GLU:OE2	1:A:366:LYS:HE2	2.19	0.41
1:A:434:SER:C	1:A:436:SER:H	2.23	0.41
1:B:530:ILE:HD11	1:B:552:GLY:HA3	2.03	0.41
1:B:421:VAL:HG22	1:B:460:LEU:HD11	2.01	0.41
1:B:380:GLY:HA2	3:B:615:ADP:O1A	2.21	0.41
1:A:274:LEU:HA	1:A:274:LEU:HD23	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:309:LYS:HZ1	1:A:569:GLU:CD	2.24	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:HD13	1:A:502:ILE:HG21	1.83	0.41
1:B:190:ARG:HD2	1:B:229:ARG:O	2.19	0.41
1:B:148:ILE:CD1	1:B:152:PHE:CE2	3.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	100	100
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 [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	449/471 (95%)	425 (95%)	24 (5%)	22	14
1	B	450/471 (96%)	421 (94%)	29 (6%)	17	9
All	All	899/942 (95%)	846 (94%)	53 (6%)	19	11

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	A	133	LYS
1	A	165	LYS
1	A	175	PHE
1	A	198	GLU
1	A	246	ARG
1	A	268	ASP
1	A	289	SER
1	A	341	LYS
1	A	366	LYS
1	A	409	LYS
1	A	418	ASP
1	A	426	GLU
1	A	431	ASP
1	A	446	ARG
1	A	447	LEU
1	A	493	GLU
1	A	503	LYS
1	A	508	GLU
1	A	515	ILE
1	A	517	ASP
1	A	581	TYR
1	A	587	LYS
1	A	595	MET
1	B	105	LEU
1	B	116	LEU
1	B	165	LYS
1	B	177	LYS
1	B	183	ILE
1	B	196	VAL
1	B	203	THR
1	B	212	ILE
1	B	213	LEU
1	B	260	LYS
1	B	277	LEU
1	B	318	LYS
1	B	322	ASP
1	B	329	LYS
1	B	341	LYS
1	B	402	GLU
1	B	405	ILE
1	B	409	LYS
1	B	418	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	438	TRP
1	B	509	ARG
1	B	517	ASP
1	B	537	PRO
1	B	538	GLU
1	B	565	ARG
1	B	584	ARG
1	B	585	VAL
1	B	598	SER
1	B	599	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	282	HIS
1	A	306	ASN
1	A	416	ASN
1	A	422	GLN
1	A	448	ASN
1	A	466	GLN
1	A	485	GLN
1	A	554	ASN
1	B	201	ASN
1	B	204	ASN
1	B	238	GLN
1	B	282	HIS
1	B	306	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	0.93	0	6,6,6	0.77	0
3	ADP	A	615	2	24,29,29	1.08	3 (12%)	29,45,45	1.55	6 (20%)
3	ADP	B	616	2	24,29,29	0.92	1 (4%)	29,45,45	1.60	5 (17%)
3	ADP	A	616	2	24,29,29	1.10	3 (12%)	29,45,45	1.54	4 (13%)
3	ADP	B	615	2	24,29,29	0.93	1 (4%)	29,45,45	1.63	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	616	2	-	1/12/32/32	0/3/3/3
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	B	615	2	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	616	ADP	C2-N3	2.70	1.36	1.32
3	A	616	ADP	PB-O2B	-2.56	1.45	1.54
3	A	616	ADP	O4'-C1'	2.51	1.44	1.41
3	A	615	ADP	O4'-C1'	2.41	1.44	1.41
3	A	615	ADP	C2-N3	2.40	1.36	1.32
3	B	615	ADP	O4'-C1'	2.32	1.44	1.41
3	A	616	ADP	C2-N3	2.26	1.35	1.32
3	A	615	ADP	PB-O2B	-2.13	1.46	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	615	ADP	N3-C2-N1	-5.04	120.80	128.68
3	B	615	ADP	N3-C2-N1	-4.99	120.89	128.68
3	A	616	ADP	N3-C2-N1	-4.89	121.04	128.68
3	B	616	ADP	N3-C2-N1	-4.81	121.16	128.68
3	A	616	ADP	O3'-C3'-C4'	-3.50	100.94	111.05
3	A	616	ADP	O4'-C1'-C2'	-3.02	102.52	106.93
3	A	616	ADP	O3'-C3'-C2'	-3.00	102.11	111.82
3	A	615	ADP	O2A-PA-O1A	2.99	127.02	112.24
3	B	616	ADP	O4'-C1'-C2'	-2.99	102.56	106.93
3	B	616	ADP	C3'-C2'-C1'	2.94	105.40	100.98
3	B	615	ADP	O3'-C3'-C2'	-2.86	102.56	111.82
3	B	616	ADP	O3'-C3'-C2'	-2.79	102.80	111.82
3	B	615	ADP	O3'-C3'-C4'	-2.51	103.79	111.05
3	A	615	ADP	O2A-PA-O5'	-2.45	96.37	107.75
3	B	615	ADP	O3B-PB-O2B	2.22	116.12	107.64
3	A	615	ADP	C1'-N9-C4	-2.19	122.79	126.64
3	B	615	ADP	O4'-C1'-C2'	-2.18	103.73	106.93
3	A	615	ADP	C3'-C2'-C1'	2.12	104.17	100.98
3	B	615	ADP	O2A-PA-O5'	-2.11	97.96	107.75
3	A	615	ADP	O3B-PB-O2B	2.07	115.54	107.64
3	B	616	ADP	O5'-PA-O1A	-2.05	101.07	109.07

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	616	ADP	PA-O3A-PB-O2B
3	A	615	ADP	PA-O3A-PB-O2B
3	B	616	ADP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

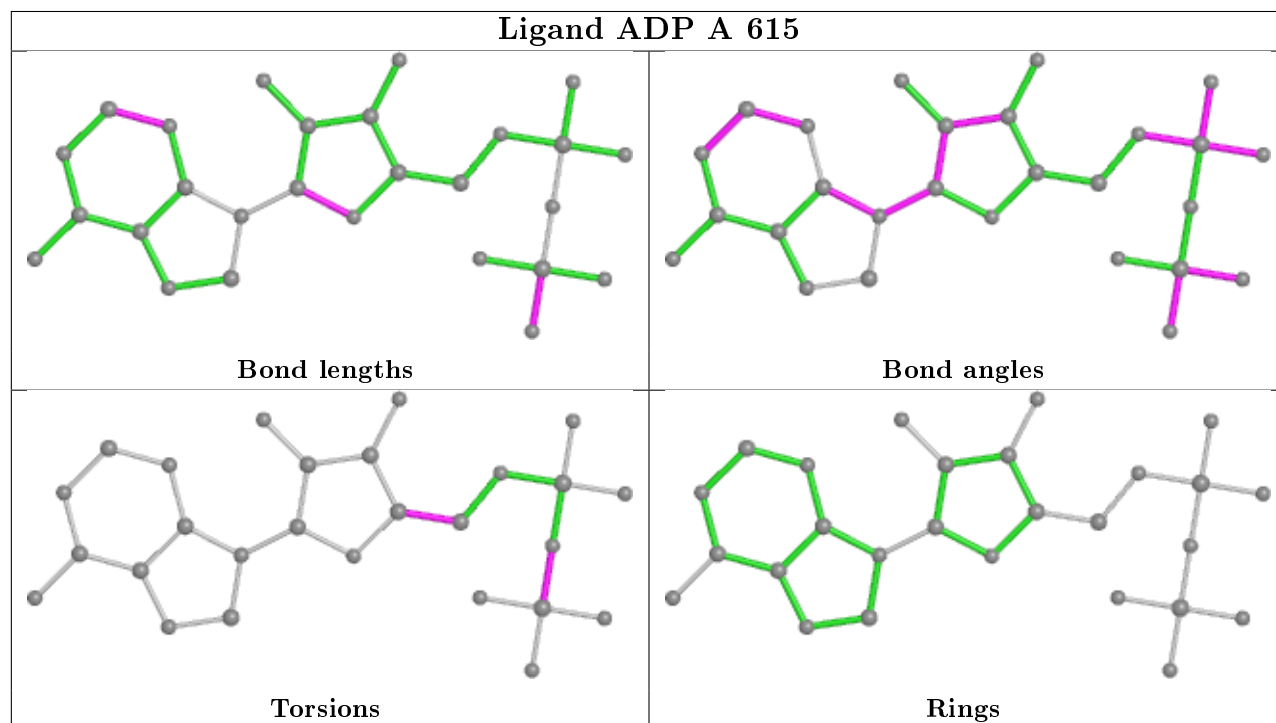
Mol	Chain	Res	Type	Atoms
3	A	615	ADP	O4'-C4'-C5'-O5'
3	A	615	ADP	C3'-C4'-C5'-O5'
3	B	616	ADP	C5'-O5'-PA-O1A

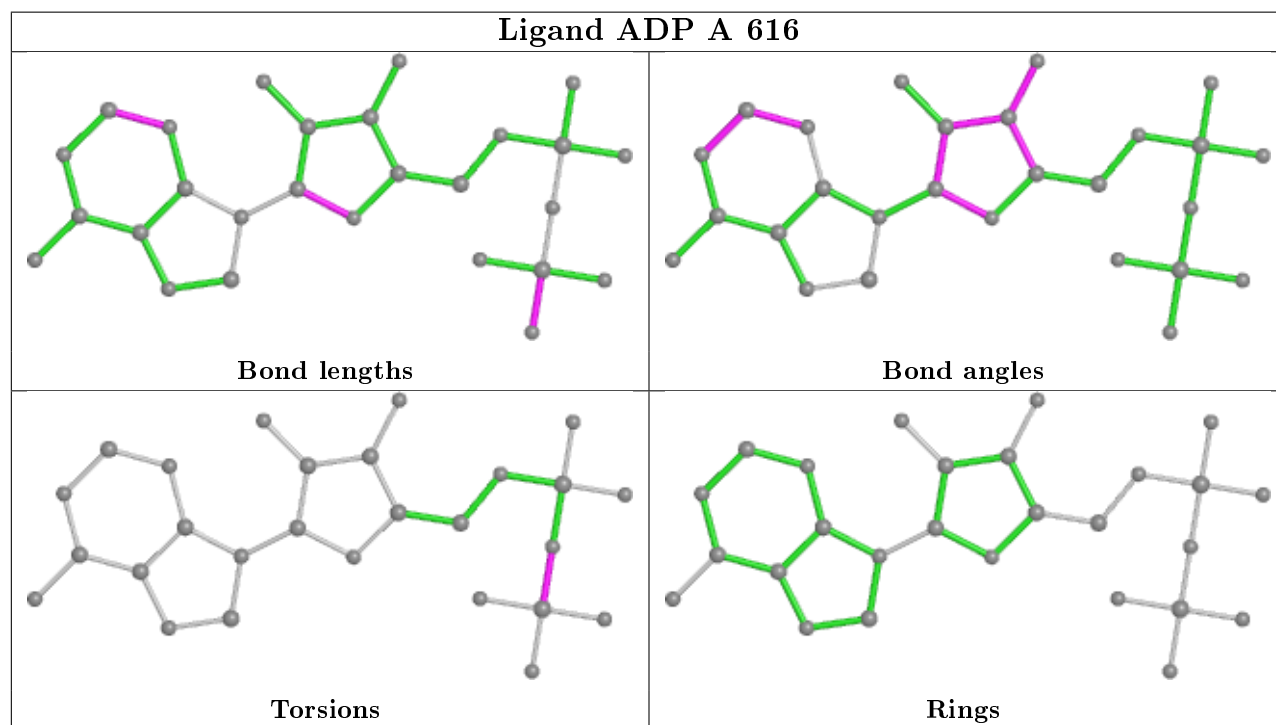
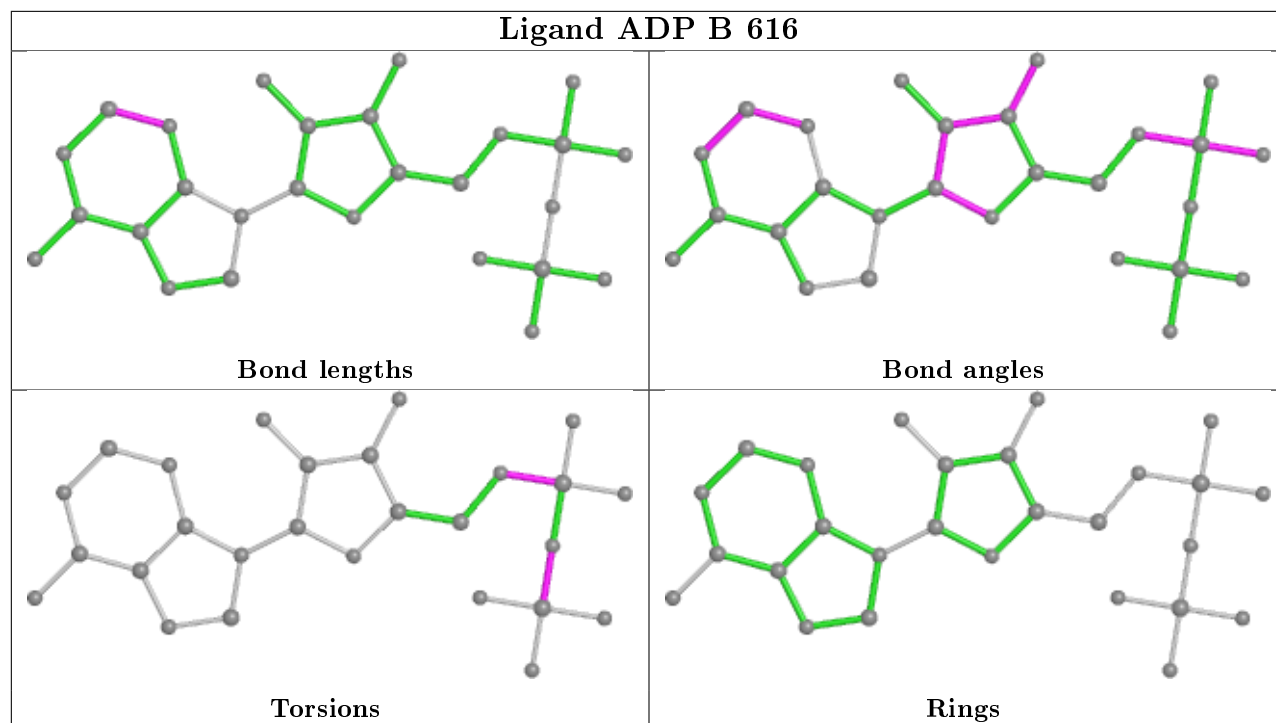
There are no ring outliers.

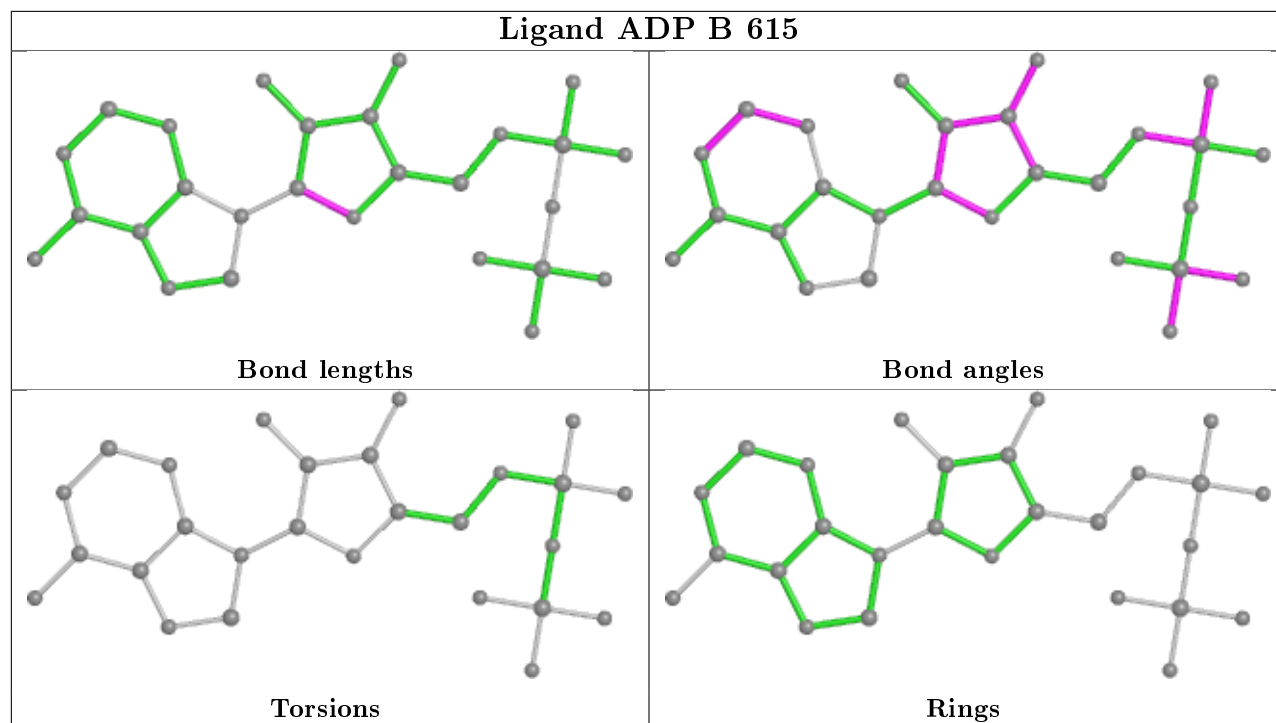
1 monomer is involved in 1 short contact:

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, 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	514/538 (95%)	0.25	29 (5%)	24 26	13, 33, 77, 101	0
1	B	515/538 (95%)	0.14	25 (4%)	29 31	11, 31, 65, 105	0
All	All	1029/1076 (95%)	0.19	54 (5%)	27 29	11, 32, 71, 105	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	TYR	8.3
1	B	328	LEU	7.4
1	A	340	LEU	6.8
1	B	599	THR	6.5
1	B	329	LYS	5.8
1	A	442	GLU	5.3
1	A	599	THR	4.9
1	A	175	PHE	4.7
1	A	329	LYS	4.6
1	A	438	TRP	4.5
1	B	340	LEU	4.4
1	B	134	VAL	4.3
1	A	429	SER	4.1
1	A	598	SER	3.9
1	B	584	ARG	3.9
1	B	600	GLN	3.9
1	B	212	ILE	3.9
1	B	327	MET	3.7
1	A	133	LYS	3.3
1	A	595	MET	3.3
1	B	588	GLU	3.2
1	A	418	ASP	3.0
1	B	598	SER	3.0
1	A	597	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	579	GLY	2.9
1	A	328	LEU	2.9
1	B	575	VAL	2.8
1	A	405	ILE	2.8
1	A	430	LYS	2.8
1	A	76	GLU	2.7
1	B	581	TYR	2.7
1	B	596	VAL	2.7
1	A	580	SER	2.6
1	A	158	ASN	2.6
1	B	314	ALA	2.6
1	A	171	TYR	2.5
1	B	316	ASN	2.4
1	A	575	VAL	2.4
1	A	134	VAL	2.3
1	A	584	ARG	2.3
1	B	582	LEU	2.3
1	B	76	GLU	2.3
1	B	175	PHE	2.2
1	A	436	SER	2.2
1	B	195	GLU	2.2
1	B	133	LYS	2.2
1	A	563	THR	2.2
1	A	402	GLU	2.1
1	A	426	GLU	2.1
1	B	180	VAL	2.1
1	B	563	THR	2.1
1	B	78	GLU	2.1
1	A	433	LEU	2.0
1	A	77	GLY	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 ⓘ

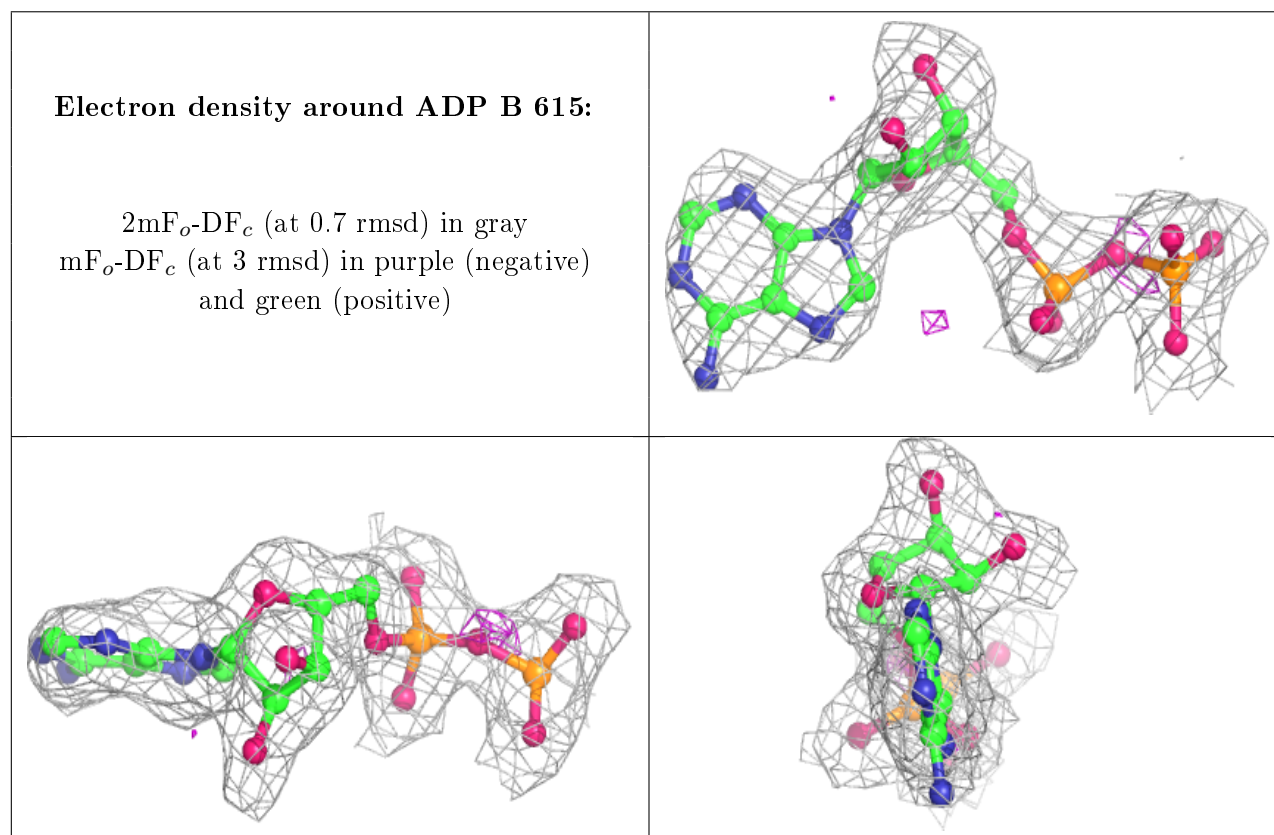
There are no carbohydrates in this entry.

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.

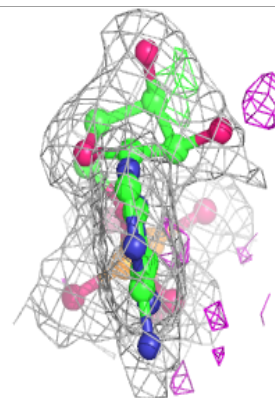
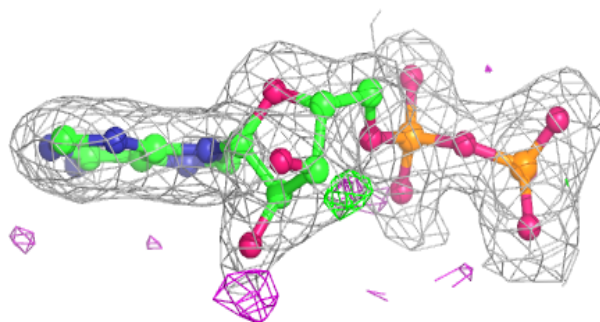
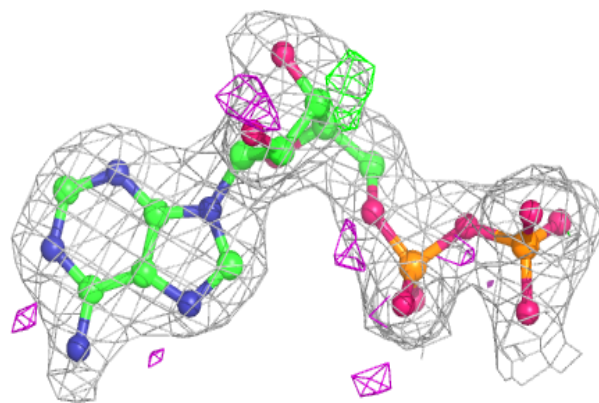
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	614	1/1	0.94	0.04	18,18,18,18	0
3	ADP	B	615	27/27	0.95	0.12	14,29,47,53	0
2	MG	B	613	1/1	0.96	0.04	15,15,15,15	0
2	MG	A	613	1/1	0.97	0.04	12,12,12,12	0
3	ADP	A	616	27/27	0.97	0.09	11,25,35,36	0
3	ADP	B	616	27/27	0.98	0.09	11,22,29,32	0
4	PO4	A	1	5/5	0.99	0.10	33,33,42,46	0
2	MG	A	614	1/1	0.99	0.03	16,16,16,16	0
3	ADP	A	615	27/27	0.99	0.07	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.

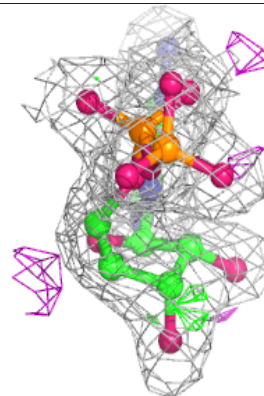
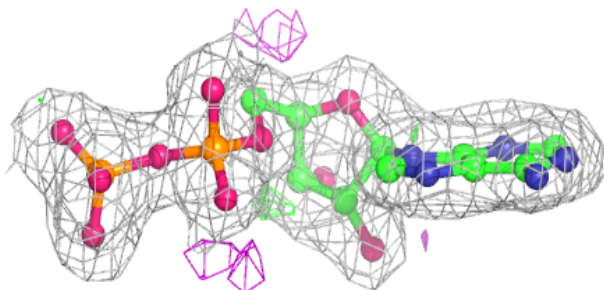
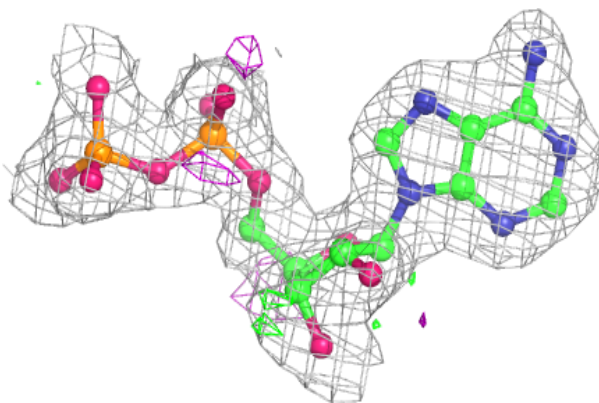


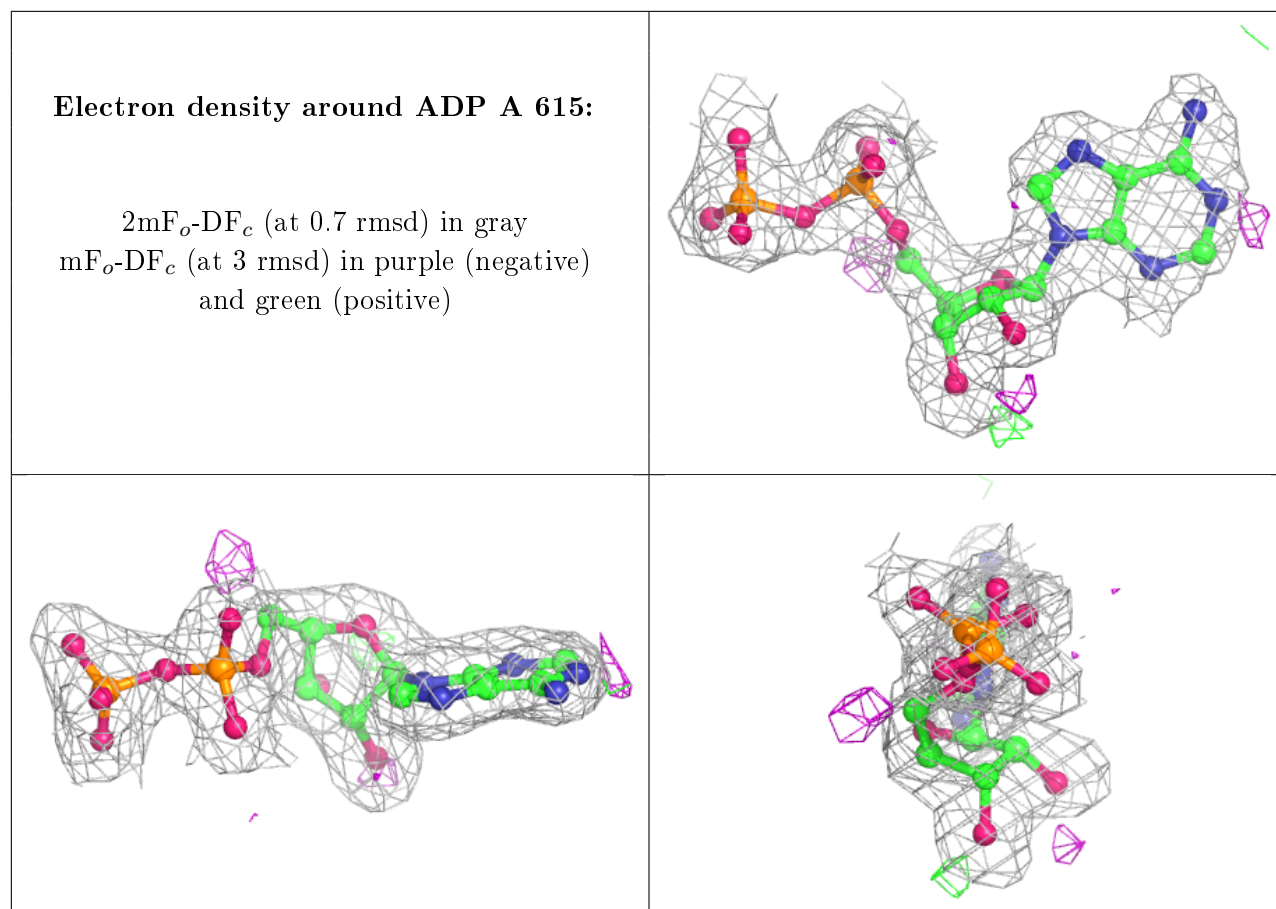
Electron density around ADP A 616:

$2mF_o-DF_c$ (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)





6.5 Other polymers ⓘ

There are no such residues in this entry.