



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 12:07 am BST

PDB ID : 6GCN  
Title : Truncated FtsH from *A. aeolicus* in R32  
Authors : Uthoff, M.; Baumann, U.  
Deposited on : 2018-04-18  
Resolution : 2.95 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.

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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

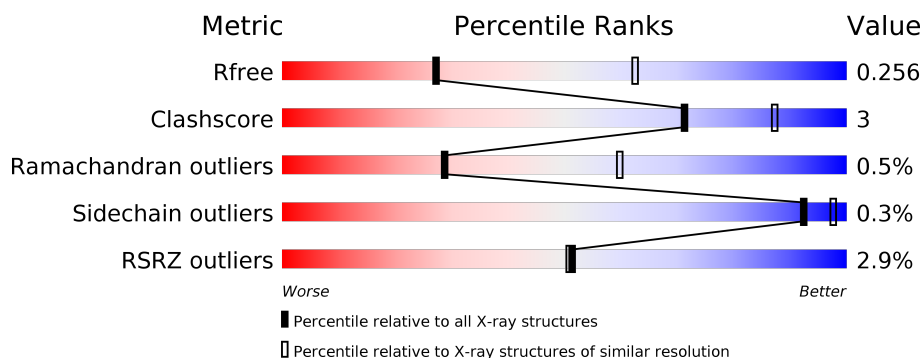
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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  $\geq 3$ , 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	479	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>13%</div> </div> </div>
1	B	479	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>9%</div> </div> </div>
1	C	479	<div> <div></div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>
1	D	479	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ALA	B	703	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25382 atoms, of which 12469 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 ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	H	N	O	S	0	4	0
			6132	1994	3022	509	596	11			
1	B	438	Total	C	H	N	O	S	0	3	0
			6340	2072	3105	527	624	12			
1	C	424	Total	C	H	N	O	S	0	1	0
			6329	2043	3140	520	615	11			
1	D	437	Total	C	H	N	O	S	0	2	0
			6401	2079	3149	534	626	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	MET	-	initiating methionine	UNP O67077
A	131	GLY	-	expression tag	UNP O67077
A	132	SER	-	expression tag	UNP O67077
A	133	SER	-	expression tag	UNP O67077
A	134	HIS	-	expression tag	UNP O67077
A	135	HIS	-	expression tag	UNP O67077
A	136	HIS	-	expression tag	UNP O67077
A	137	HIS	-	expression tag	UNP O67077
A	138	HIS	-	expression tag	UNP O67077
A	139	HIS	-	expression tag	UNP O67077
A	140	SER	-	expression tag	UNP O67077
A	141	SER	-	expression tag	UNP O67077
A	142	GLY	-	expression tag	UNP O67077
A	143	LEU	-	expression tag	UNP O67077
A	144	VAL	-	expression tag	UNP O67077
A	145	PRO	-	expression tag	UNP O67077
A	146	ARG	-	expression tag	UNP O67077
A	147	GLY	-	expression tag	UNP O67077
A	148	SER	-	expression tag	UNP O67077
A	149	HIS	-	expression tag	UNP O67077
A	150	MET	-	expression tag	UNP O67077

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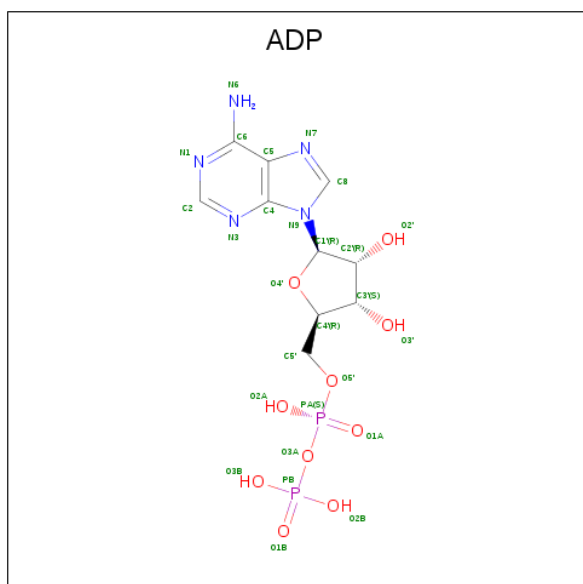
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	MET	-	initiating methionine	UNP O67077
B	131	GLY	-	expression tag	UNP O67077
B	132	SER	-	expression tag	UNP O67077
B	133	SER	-	expression tag	UNP O67077
B	134	HIS	-	expression tag	UNP O67077
B	135	HIS	-	expression tag	UNP O67077
B	136	HIS	-	expression tag	UNP O67077
B	137	HIS	-	expression tag	UNP O67077
B	138	HIS	-	expression tag	UNP O67077
B	139	HIS	-	expression tag	UNP O67077
B	140	SER	-	expression tag	UNP O67077
B	141	SER	-	expression tag	UNP O67077
B	142	GLY	-	expression tag	UNP O67077
B	143	LEU	-	expression tag	UNP O67077
B	144	VAL	-	expression tag	UNP O67077
B	145	PRO	-	expression tag	UNP O67077
B	146	ARG	-	expression tag	UNP O67077
B	147	GLY	-	expression tag	UNP O67077
B	148	SER	-	expression tag	UNP O67077
B	149	HIS	-	expression tag	UNP O67077
B	150	MET	-	expression tag	UNP O67077
C	130	MET	-	initiating methionine	UNP O67077
C	131	GLY	-	expression tag	UNP O67077
C	132	SER	-	expression tag	UNP O67077
C	133	SER	-	expression tag	UNP O67077
C	134	HIS	-	expression tag	UNP O67077
C	135	HIS	-	expression tag	UNP O67077
C	136	HIS	-	expression tag	UNP O67077
C	137	HIS	-	expression tag	UNP O67077
C	138	HIS	-	expression tag	UNP O67077
C	139	HIS	-	expression tag	UNP O67077
C	140	SER	-	expression tag	UNP O67077
C	141	SER	-	expression tag	UNP O67077
C	142	GLY	-	expression tag	UNP O67077
C	143	LEU	-	expression tag	UNP O67077
C	144	VAL	-	expression tag	UNP O67077
C	145	PRO	-	expression tag	UNP O67077
C	146	ARG	-	expression tag	UNP O67077
C	147	GLY	-	expression tag	UNP O67077
C	148	SER	-	expression tag	UNP O67077
C	149	HIS	-	expression tag	UNP O67077
C	150	MET	-	expression tag	UNP O67077

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Chain	Residue	Modelled	Actual	Comment	Reference
D	130	MET	-	initiating methionine	UNP O67077
D	131	GLY	-	expression tag	UNP O67077
D	132	SER	-	expression tag	UNP O67077
D	133	SER	-	expression tag	UNP O67077
D	134	HIS	-	expression tag	UNP O67077
D	135	HIS	-	expression tag	UNP O67077
D	136	HIS	-	expression tag	UNP O67077
D	137	HIS	-	expression tag	UNP O67077
D	138	HIS	-	expression tag	UNP O67077
D	139	HIS	-	expression tag	UNP O67077
D	140	SER	-	expression tag	UNP O67077
D	141	SER	-	expression tag	UNP O67077
D	142	GLY	-	expression tag	UNP O67077
D	143	LEU	-	expression tag	UNP O67077
D	144	VAL	-	expression tag	UNP O67077
D	145	PRO	-	expression tag	UNP O67077
D	146	ARG	-	expression tag	UNP O67077
D	147	GLY	-	expression tag	UNP O67077
D	148	SER	-	expression tag	UNP O67077
D	149	HIS	-	expression tag	UNP O67077
D	150	MET	-	expression tag	UNP O67077

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

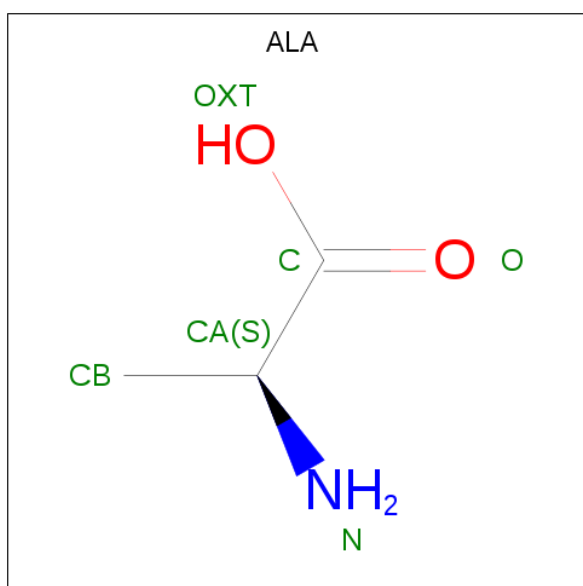


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	
			38	10	11	5	10	2	
2	B	1	Total	C	H	N	O	P	
			38	10	11	5	10	2	
2	C	1	Total	C	H	N	O	P	
			38	10	11	5	10	2	
2	D	1	Total	C	H	N	O	P	
			38	10	11	5	10	2	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn		
			1	1	0	0
3	A	1	Total	Zn		
			1	1	0	0
3	D	1	Total	Zn		
			1	1	0	0
3	C	1	Total	Zn		
			1	1	0	0

- Molecule 4 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



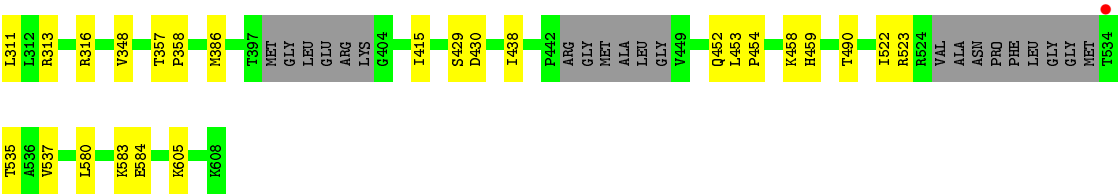
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O		
			9	3	4	1	1	0	0
4	B	1	Total	C	H	N	O		
			11	3	5	1	2	0	0

- Molecule 5 is water.

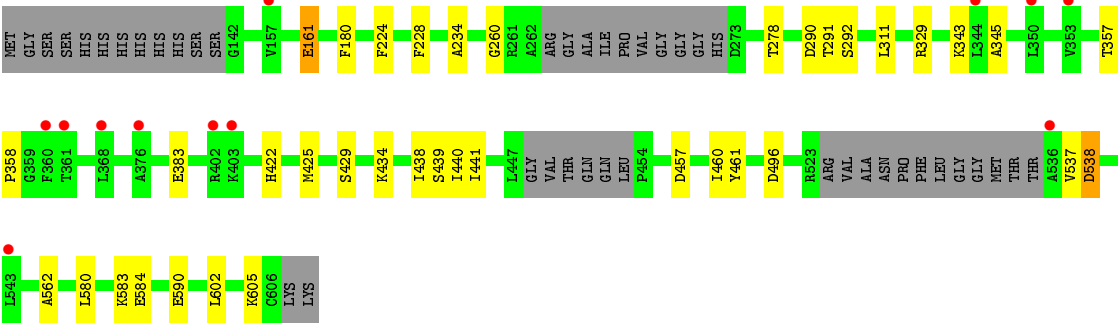
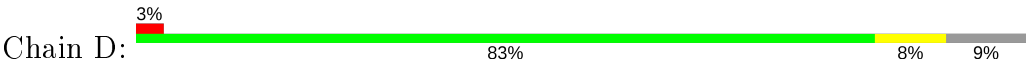
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	C	2	Total 2	O 2	0	0
5	D	1	Total 1	O 1	0	0







● Molecule 1: ATP-dependent zinc metalloprotease FtsH



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.55Å 197.55Å 323.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.59 – 2.95 72.88 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.59-2.95) 94.8 (72.88-2.95)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.213 , 0.256 0.213 , 0.256	Depositor DCC
$R_{free}$ test set	1540 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.1	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.27	0/3166	0.44	0/4292
1	B	0.28	0/3293	0.45	0/4469
1	C	0.27	0/3236	0.44	0/4378
1	D	0.28	0/3308	0.45	0/4483
All	All	0.27	0/13003	0.45	0/17622

There are no bond length outliers.

There are no bond angle outliers.

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	3110	3022	3022	19	0
1	B	3235	3105	3105	27	0
1	C	3189	3140	3140	24	0
1	D	3252	3149	3149	23	0
2	A	27	11	12	1	0
2	B	27	11	12	2	0
2	C	27	11	12	1	0
2	D	27	11	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	11	9	9	0	0
5	A	1	0	0	0	0
5	C	2	0	0	1	0
5	D	1	0	0	0	0
All	All	12913	12469	12473	88	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 3.

All (88) 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:C:429:SER:O	1:C:605:LYS:NZ	2.00	0.93
1:C:189:LYS:NZ	1:C:289:PHE:O	2.14	0.79
1:A:429:SER:O	1:A:605:LYS:NZ	2.14	0.77
1:B:287:ASP:OD2	1:B:316:ARG:NH2	2.20	0.74
1:D:425:MET:HE1	1:D:562:ALA:HA	1.74	0.70
1:A:583:LYS:NZ	1:A:590:GLU:OE2	2.25	0.70
1:B:224:PHE:HB3	1:B:278:THR:HG21	1.73	0.69
1:B:439:SER:OG	1:B:441:ILE:HG12	1.94	0.66
1:D:161:GLU:OE2	1:D:329:ARG:NH2	2.31	0.62
1:D:583:LYS:NZ	1:D:590:GLU:OE2	2.32	0.62
1:B:385:THR:OG1	1:B:388:GLU:OE1	2.18	0.59
1:D:224:PHE:HB3	1:D:278:THR:HG21	1.86	0.57
1:B:422:HIS:CE1	1:B:496:ASP:OD2	2.58	0.56
1:D:228:PHE:HA	1:D:234:ALA:O	2.05	0.56
1:A:328:VAL:N	1:A:584:GLU:OE1	2.38	0.56
1:D:422:HIS:CE1	1:D:496:ASP:OD2	2.59	0.55
1:B:260:GLY:O	1:B:308:ASP:N	2.36	0.53
1:D:457:ASP:N	1:D:461:TYR:OH	2.36	0.53
1:B:154:PHE:HA	1:B:157:VAL:HG22	1.91	0.53
1:B:198:GLY:N	2:B:701:ADP:O1B	2.35	0.53
1:B:537:VAL:O	1:B:537:VAL:HG23	2.09	0.52
1:B:345:ALA:HB3	1:B:384:ILE:O	2.10	0.51
1:C:490:THR:HB	1:D:460:ILE:HG23	1.93	0.50
1:C:430:ASP:OD1	1:C:430:ASP:N	2.42	0.50
1:C:580:LEU:O	1:C:584:GLU:N	2.38	0.49
1:B:143:LEU:CD1	1:C:215:PRO:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ARG:NH1	5:C:801:HOH:O	2.47	0.48
1:D:439:SER:OG	1:D:441:ILE:HG12	2.14	0.48
1:A:329:ARG:NH1	1:A:351:GLU:OE2	2.47	0.48
1:B:226:GLU:O	1:C:246:HIS:NE2	2.39	0.48
1:B:291:THR:HG23	1:B:295:ILE:HG13	1.95	0.48
1:C:522:ILE:HG13	1:C:523:ARG:H	1.79	0.48
1:A:201:LYS:NZ	2:A:701:ADP:O1B	2.44	0.47
1:A:440:ILE:HD11	1:A:584:GLU:HG3	1.97	0.47
1:D:537:VAL:HG23	1:D:537:VAL:O	2.15	0.47
1:A:348:VAL:HA	1:A:386:MET:HG2	1.96	0.46
1:B:583:LYS:NZ	1:B:590:GLU:OE2	2.48	0.46
1:C:535:THR:HG21	1:D:538:ASP:OD2	2.15	0.46
1:A:332:TYR:CE2	1:A:336:LYS:HE3	2.50	0.46
1:A:553:ARG:O	1:A:557:GLU:HG3	2.15	0.46
1:B:143:LEU:HB3	1:B:234:ALA:HB2	1.98	0.46
1:B:583:LYS:O	1:B:584:GLU:HB2	2.14	0.46
1:B:173:TYR:CE1	1:B:187:PRO:HG3	2.51	0.46
1:C:452:GLN:HA	1:C:452:GLN:OE1	2.15	0.46
1:D:260:GLY:HA3	1:D:311:LEU:HD11	1.99	0.46
1:D:345:ALA:HB2	1:D:383:GLU:HB3	1.97	0.45
1:D:434:LYS:HB3	1:D:605:LYS:O	2.17	0.45
1:A:433:ASP:OD2	1:A:469:LYS:NZ	2.43	0.45
1:D:429:SER:O	1:D:605:LYS:NZ	2.38	0.45
1:C:215:PRO:HD2	1:C:248:PRO:O	2.16	0.45
1:C:357:THR:N	1:C:358:PRO:HD3	2.31	0.44
1:A:357:THR:N	1:A:358:PRO:HD3	2.32	0.44
1:A:225:VAL:HG13	1:A:226:GLU:N	2.32	0.44
1:B:273:ASP:N	1:B:273:ASP:OD1	2.48	0.44
1:B:348:VAL:HG11	1:B:389:ILE:HD12	1.99	0.44
1:C:535:THR:HG23	1:C:535:THR:O	2.17	0.43
1:C:415:ILE:CG1	1:D:460:ILE:HD11	2.47	0.43
1:C:348:VAL:HA	1:C:386:MET:HG2	1.98	0.43
1:D:438:ILE:N	1:D:438:ILE:HD12	2.33	0.43
1:A:428:VAL:O	1:A:603:LYS:NZ	2.38	0.43
1:B:438:ILE:HD12	1:B:438:ILE:N	2.34	0.43
1:D:580:LEU:O	1:D:584:GLU:N	2.48	0.43
1:A:222:SER:OG	1:A:255:GLU:OE1	2.37	0.43
1:C:229:VAL:O	1:C:229:VAL:HG12	2.19	0.43
1:D:357:THR:N	1:D:358:PRO:HD3	2.34	0.43
1:D:440:ILE:HD11	1:D:584:GLU:HG2	2.01	0.43
1:B:291:THR:HG22	1:B:291:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:LEU:O	1:C:316:ARG:O	2.38	0.42
1:D:583:LYS:O	1:D:584:GLU:HB2	2.19	0.42
1:C:458:LYS:O	1:C:459:HIS:ND1	2.52	0.42
1:A:345:ALA:O	1:A:348:VAL:HG22	2.20	0.42
1:C:537:VAL:O	1:C:537:VAL:HG23	2.20	0.42
1:A:303:ARG:NH2	1:A:305:ASP:OD2	2.53	0.41
1:B:338:HIS:CE1	1:B:366:GLU:HB2	2.56	0.41
1:A:479:ALA:HA	1:A:566:VAL:HG11	2.03	0.41
1:C:522:ILE:HG13	1:C:523:ARG:N	2.35	0.41
1:D:291:THR:HG22	1:D:291:THR:O	2.21	0.41
1:B:457:ASP:N	1:B:461:TYR:OH	2.53	0.41
1:C:201:LYS:NZ	2:C:701:ADP:O3B	2.49	0.41
1:C:583:LYS:O	1:C:584:GLU:HB2	2.21	0.41
1:A:338:HIS:CE1	1:A:366[A]:GLU:HB2	2.56	0.41
1:B:203:LEU:HD22	2:B:701:ADP:H2'	2.03	0.41
1:B:348:VAL:HG12	1:B:386:MET:HG2	2.03	0.41
1:A:339:ALA:HB1	1:A:344:LEU:HD23	2.03	0.40
1:D:290:ASP:OD1	1:D:292:SER:OG	2.39	0.40
1:B:187:PRO:HB2	1:B:188:PRO:HD2	2.04	0.40
1:C:438:ILE:HD12	1:C:438:ILE:N	2.36	0.40
1:B:348:VAL:HG12	1:B:386:MET:CG	2.52	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	410/479 (86%)	396 (97%)	13 (3%)	1 (0%)	47	76
1	B	431/479 (90%)	407 (94%)	21 (5%)	3 (1%)	22	52
1	C	413/479 (86%)	395 (96%)	16 (4%)	2 (0%)	29	60
1	D	431/479 (90%)	412 (96%)	17 (4%)	2 (0%)	29	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1685/1916 (88%)	1610 (96%)	67 (4%)	8 (0%)	29	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	538	ASP
1	C	454	PRO
1	D	343	LYS
1	D	538	ASP
1	A	494	GLU
1	B	343	LYS
1	B	494	GLU
1	C	160	ILE

### 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	306/397 (77%)	306 (100%)	0	100	100
1	B	314/397 (79%)	314 (100%)	0	100	100
1	C	321/397 (81%)	320 (100%)	1 (0%)	92	97
1	D	320/397 (81%)	317 (99%)	3 (1%)	78	92
All	All	1261/1588 (79%)	1257 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	453	LEU
1	D	161	GLU
1	D	180	PHE
1	D	602	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 5.3.3 RNA [i](#)

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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$
2	ADP	B	701	-	24,29,29	0.96	2 (8%)	29,45,45	1.52	5 (17%)
2	ADP	A	701	-	24,29,29	0.97	2 (8%)	29,45,45	1.48	4 (13%)
2	ADP	D	701	-	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	C	701	-	24,29,29	0.94	1 (4%)	29,45,45	1.52	5 (17%)

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
2	ADP	B	701	-	-	0/12/32/32	0/3/3/3
2	ADP	A	701	-	-	1/12/32/32	0/3/3/3
2	ADP	D	701	-	-	1/12/32/32	0/3/3/3
2	ADP	C	701	-	-	1/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ADP	C5-C4	2.48	1.47	1.40
2	C	701	ADP	C5-C4	2.47	1.47	1.40
2	B	701	ADP	C5-C4	2.40	1.47	1.40
2	D	701	ADP	C5-C4	2.39	1.47	1.40
2	B	701	ADP	C2-N3	2.07	1.35	1.32
2	A	701	ADP	C2-N3	2.03	1.35	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	ADP	C3'-C2'-C1'	3.73	106.59	100.98
2	B	701	ADP	C3'-C2'-C1'	3.70	106.55	100.98
2	A	701	ADP	N3-C2-N1	-3.57	123.09	128.68
2	D	701	ADP	PA-O3A-PB	-3.55	120.63	132.83
2	C	701	ADP	N3-C2-N1	-3.55	123.13	128.68
2	D	701	ADP	C3'-C2'-C1'	3.55	106.32	100.98
2	B	701	ADP	N3-C2-N1	-3.54	123.15	128.68
2	D	701	ADP	N3-C2-N1	-3.53	123.15	128.68
2	A	701	ADP	C3'-C2'-C1'	3.45	106.18	100.98
2	C	701	ADP	PA-O3A-PB	-3.43	121.06	132.83
2	A	701	ADP	PA-O3A-PB	-3.33	121.40	132.83
2	B	701	ADP	PA-O3A-PB	-3.32	121.45	132.83
2	A	701	ADP	C4-C5-N7	-2.37	106.93	109.40
2	D	701	ADP	C4-C5-N7	-2.24	107.06	109.40
2	B	701	ADP	C4-C5-N7	-2.14	107.17	109.40
2	C	701	ADP	C4-C5-N7	-2.12	107.19	109.40
2	C	701	ADP	O3B-PB-O2B	2.08	115.61	107.64
2	B	701	ADP	N6-C6-N1	2.08	122.89	118.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

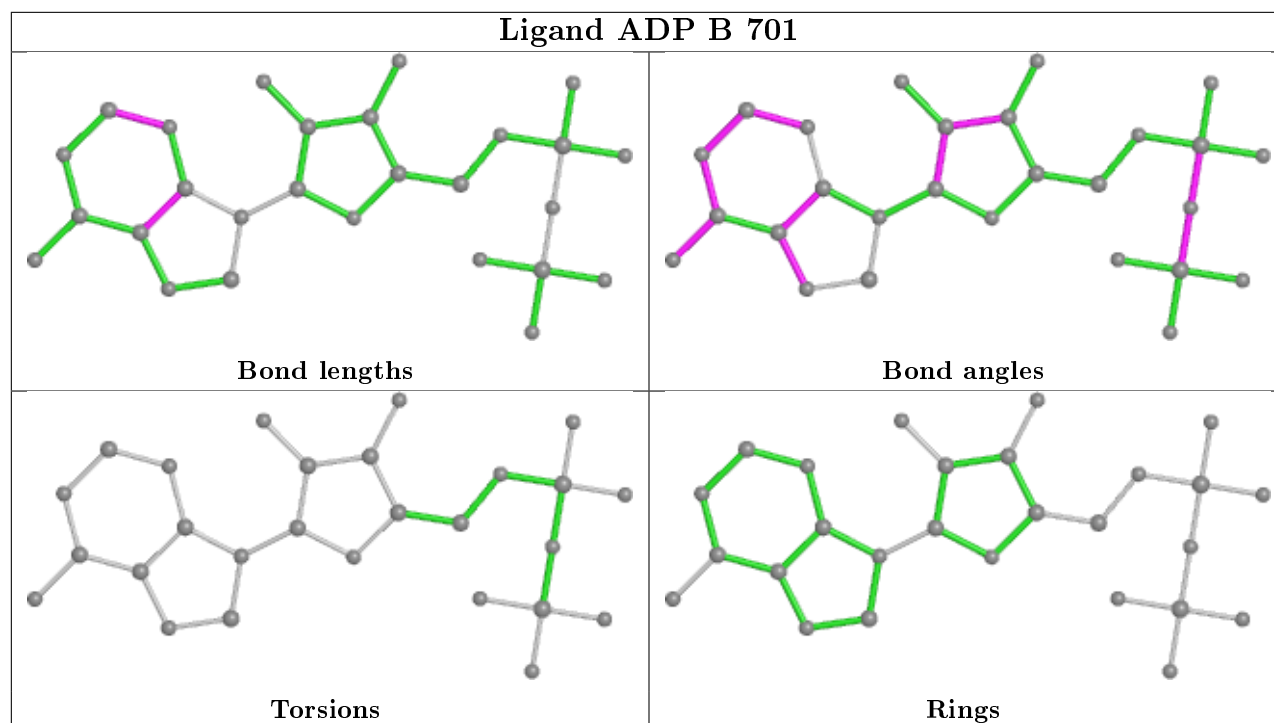
Mol	Chain	Res	Type	Atoms
2	A	701	ADP	PA-O3A-PB-O1B
2	D	701	ADP	PA-O3A-PB-O3B
2	C	701	ADP	PA-O3A-PB-O3B

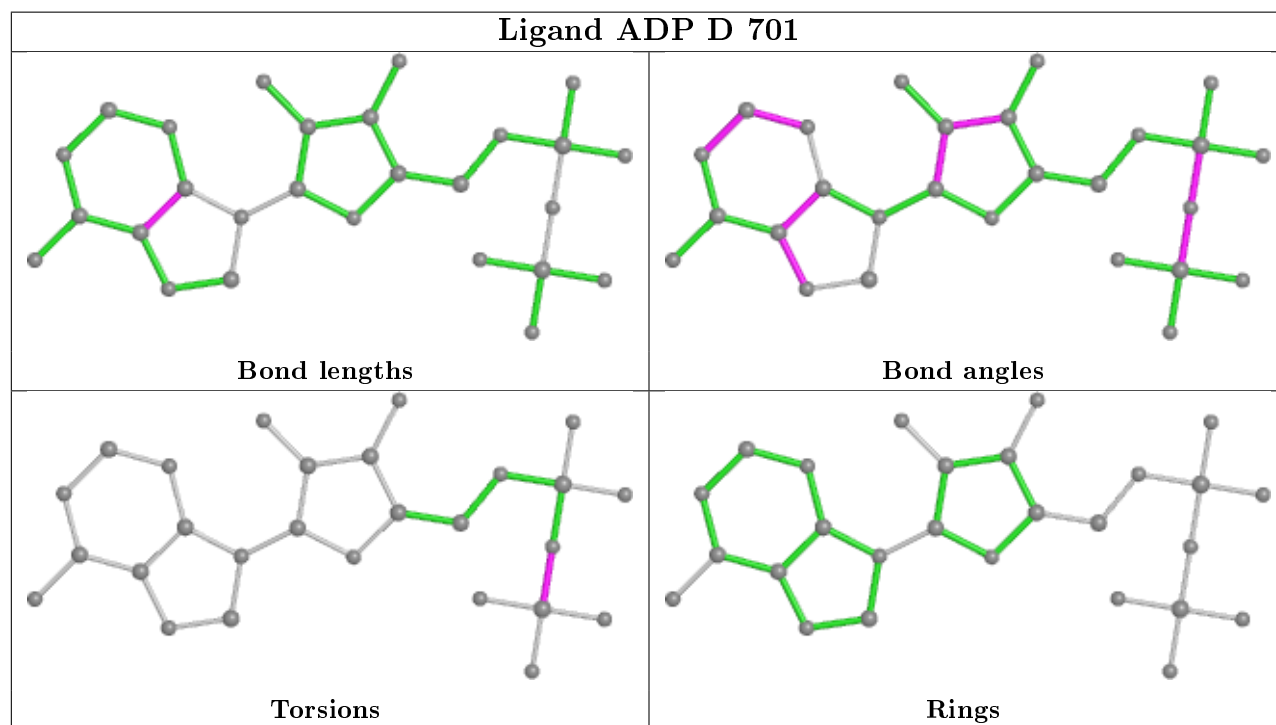
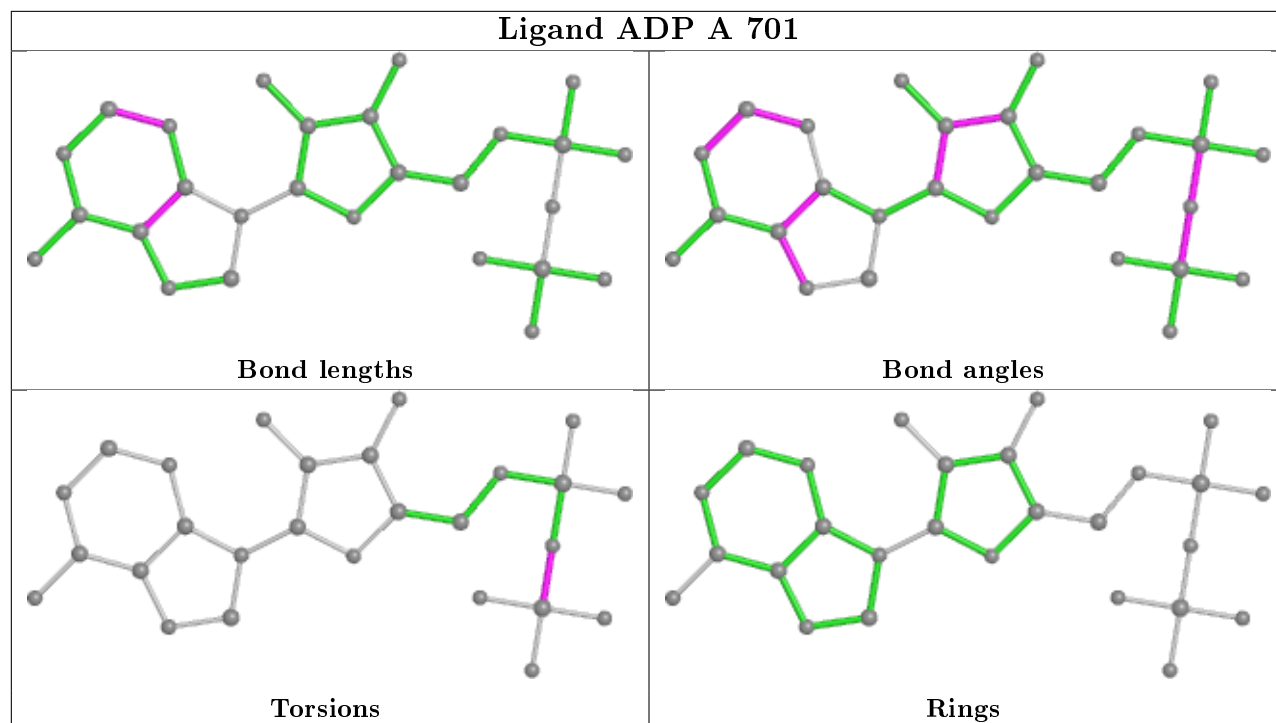
There are no ring outliers.

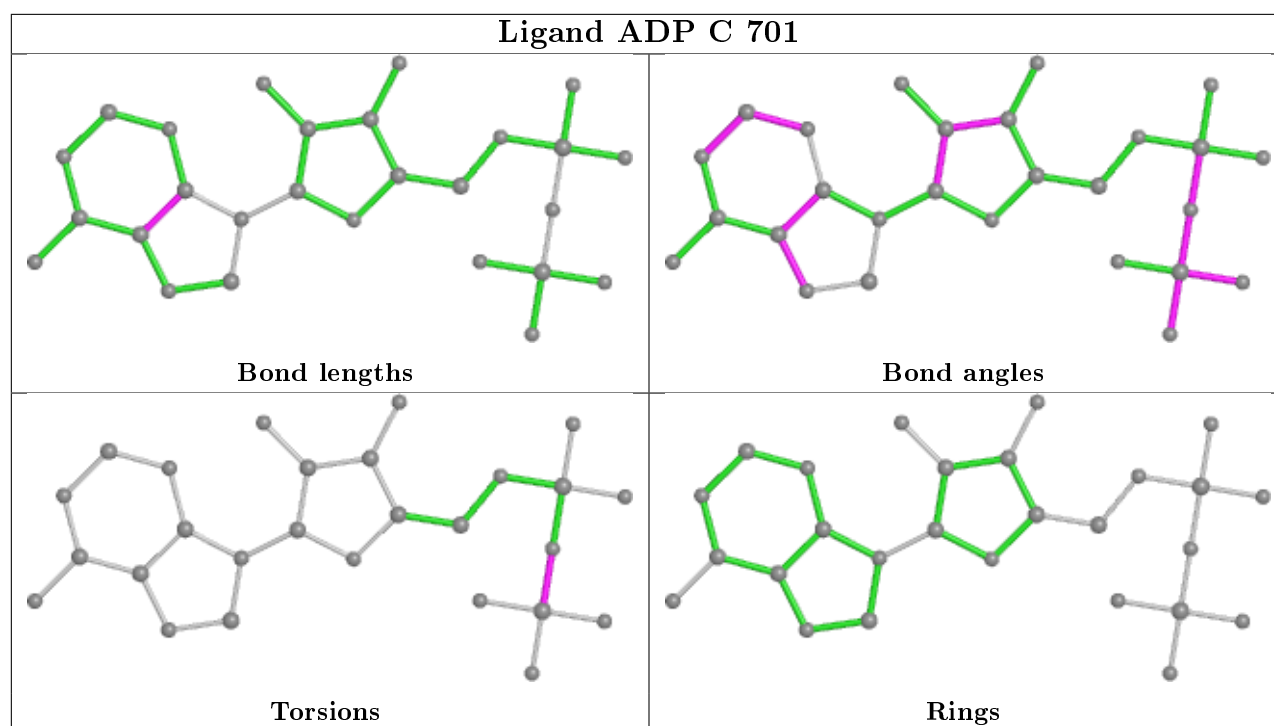
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ADP	2	0
2	A	701	ADP	1	0
2	C	701	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	418/479 (87%)	0.48	25 (5%) 21 20	58, 97, 136, 157	0
1	B	438/479 (91%)	0.31	11 (2%) 57 58	55, 95, 148, 162	0
1	C	424/479 (88%)	0.31	2 (0%) 91 91	56, 89, 133, 154	0
1	D	437/479 (91%)	0.31	12 (2%) 54 54	54, 91, 139, 166	0
All	All	1717/1916 (89%)	0.35	50 (2%) 51 51	54, 92, 139, 166	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	376	ALA	4.6
1	A	295	ILE	4.0
1	A	226	GLU	3.8
1	A	160	ILE	3.8
1	B	447	LEU	3.6
1	A	191	VAL	3.3
1	D	353	VAL	3.3
1	A	176	ASP	3.3
1	A	259	VAL	3.1
1	A	383	GLU	3.1
1	A	597[A]	LEU	3.1
1	A	178	VAL	3.0
1	D	360	PHE	3.0
1	D	403	LYS	3.0
1	A	384	ILE	3.0
1	A	323	ILE	2.9
1	A	177	PRO	2.9
1	B	368	LEU	2.9
1	B	535	THR	2.8
1	A	523	ARG	2.7
1	B	365	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	433	ASP	2.7
1	B	143	LEU	2.7
1	D	344	LEU	2.7
1	A	294	GLY	2.6
1	A	307	LEU	2.6
1	C	534	THR	2.6
1	A	440	ILE	2.5
1	A	175	LYS	2.5
1	B	376	ALA	2.5
1	A	204	LEU	2.5
1	B	606	CYS	2.4
1	D	536	ALA	2.4
1	D	350	LEU	2.3
1	C	225	VAL	2.3
1	A	203	LEU	2.3
1	A	534	THR	2.2
1	A	167	VAL	2.2
1	A	350	LEU	2.2
1	A	262	ALA	2.2
1	A	296	ILE	2.1
1	D	543	LEU	2.1
1	B	573	LEU	2.1
1	A	369	LEU	2.1
1	D	368	LEU	2.1
1	D	157	VAL	2.1
1	D	361	THR	2.1
1	D	402	ARG	2.0
1	B	289	PHE	2.0
1	B	183	LEU	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, 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.

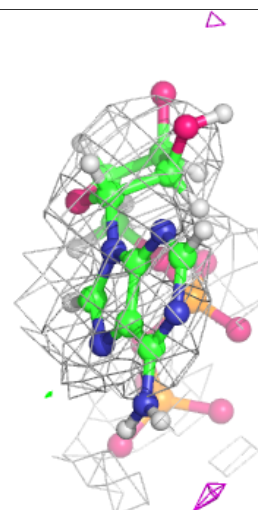
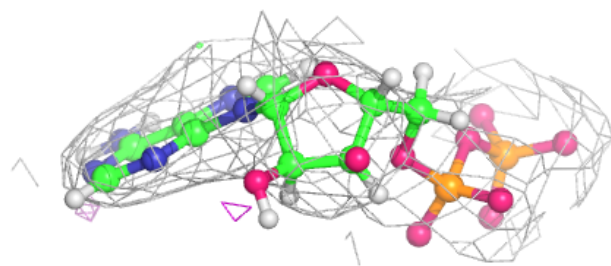
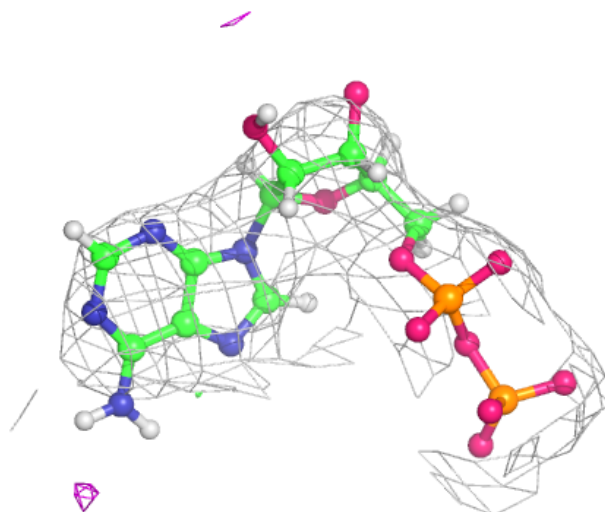
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	ALA	B	703	5/6	0.65	0.43	103,124,135,153	0
3	ZN	C	702	1/1	0.88	0.12	150,150,150,150	0
3	ZN	A	702	1/1	0.89	0.14	160,160,160,160	0
2	ADP	A	701	27/27	0.93	0.24	83,95,119,128	0
3	ZN	D	702	1/1	0.93	0.16	108,108,108,108	0
4	ALA	B	704	6/6	0.94	0.23	89,118,140,142	0
2	ADP	B	701	27/27	0.95	0.18	83,96,128,144	0
2	ADP	C	701	27/27	0.96	0.24	62,84,108,129	0
2	ADP	D	701	27/27	0.96	0.18	71,92,124,133	0
3	ZN	B	702	1/1	0.97	0.15	101,101,101,101	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.



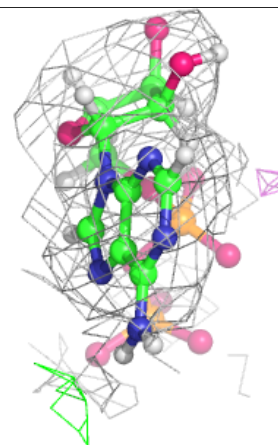
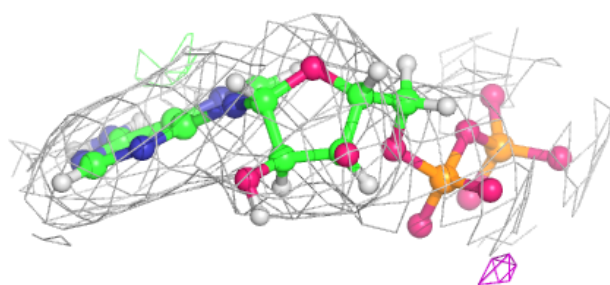
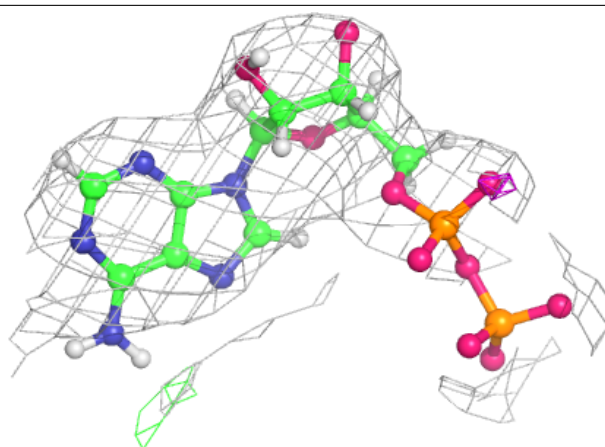
**Electron density around ADP A 701:**

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



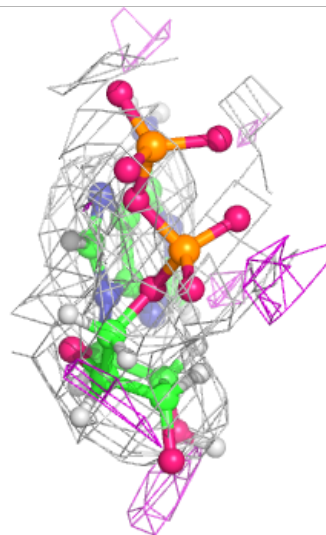
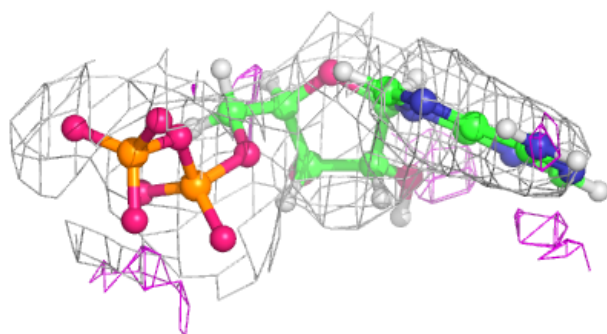
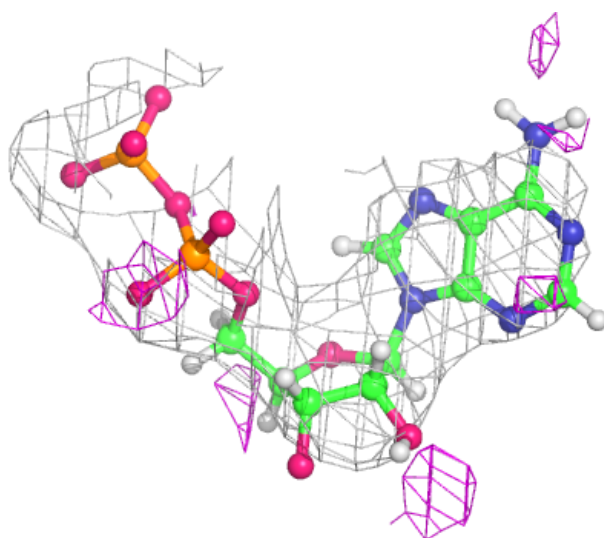
**Electron density around ADP B 701:**

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



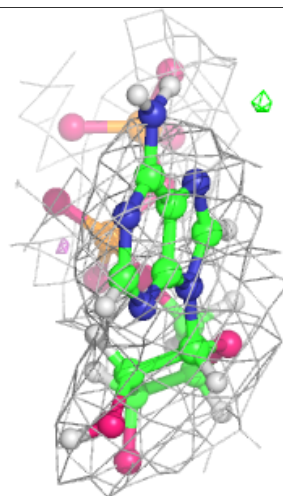
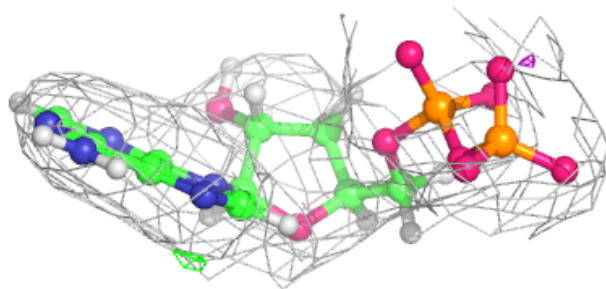
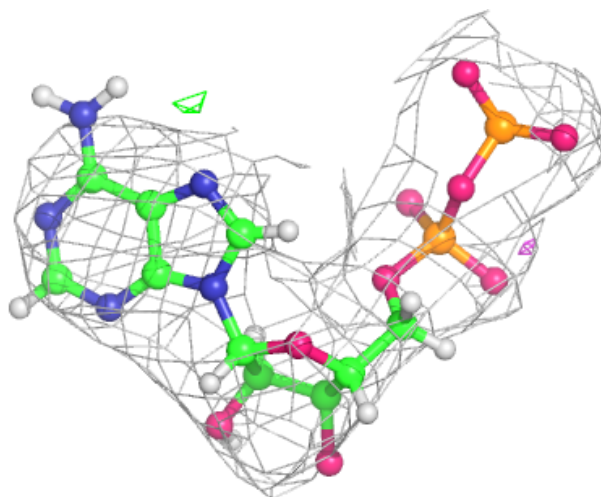
**Electron density around ADP C 701:**

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



**Electron density around ADP D 701:**

$2mF_o-DF_c$  (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.