



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:09 PM UTC

PDB ID : 4WW0 / pdb_00004ww0
Title : Truncated FtsH from *A. aeolicus*
Authors : Vostrukhina, M.; Baumann, U.; Schacherl, M.; Bieniossek, C.; Lanz, M.; Baumgartner, R.
Deposited on : 2014-11-09
Resolution : 2.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

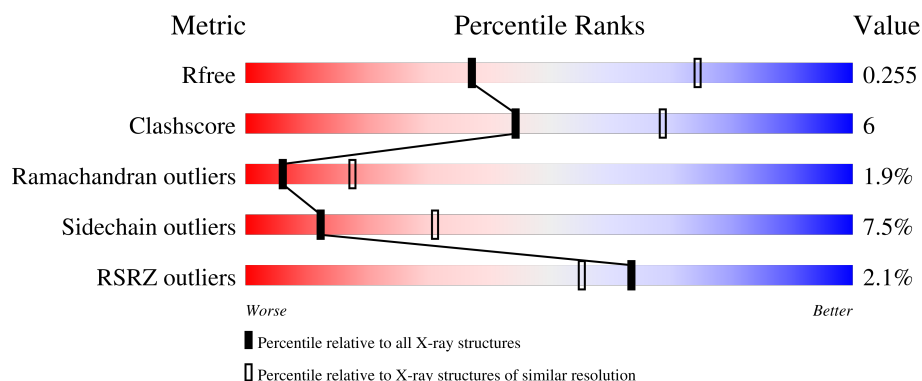
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	0% 66% 16% • 15%
1	B	497	2% 64% 18% • 14%
1	C	497	2% 62% 19% • 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9978 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 ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3310	2112	560	625	13			
1	B	425	Total	C	N	O	S	0	0	0
			3345	2132	566	633	14			
1	C	412	Total	C	N	O	S	0	0	0
			3236	2060	548	617	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLY	-	expression tag	UNP O67077
A	139	SER	-	expression tag	UNP O67077
A	140	HIS	-	expression tag	UNP O67077
A	141	MET	-	engineered mutation	UNP O67077
A	250	MET	ILE	engineered mutation	UNP O67077
A	360	LEU	PHE	engineered mutation	UNP O67077
A	552	ARG	LYS	engineered mutation	UNP O67077
A	627	GLY	GLU	engineered mutation	UNP O67077
B	138	GLY	-	expression tag	UNP O67077
B	139	SER	-	expression tag	UNP O67077
B	140	HIS	-	expression tag	UNP O67077
B	141	MET	-	engineered mutation	UNP O67077
B	250	MET	ILE	engineered mutation	UNP O67077
B	360	LEU	PHE	engineered mutation	UNP O67077
B	552	ARG	LYS	engineered mutation	UNP O67077
B	627	GLY	GLU	engineered mutation	UNP O67077
C	138	GLY	-	expression tag	UNP O67077
C	139	SER	-	expression tag	UNP O67077
C	140	HIS	-	expression tag	UNP O67077
C	141	MET	-	engineered mutation	UNP O67077
C	250	MET	ILE	engineered mutation	UNP O67077
C	360	LEU	PHE	engineered mutation	UNP O67077
C	552	ARG	LYS	engineered mutation	UNP O67077

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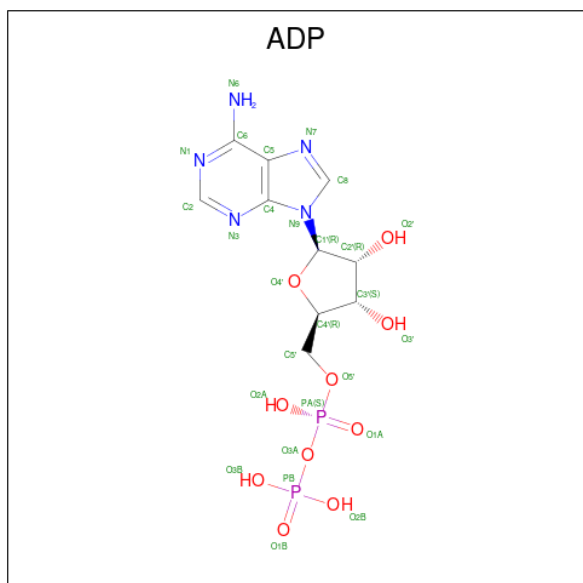
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Chain	Residue	Modelled	Actual	Comment	Reference
C	627	GLY	GLU	engineered mutation	UNP O67077

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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	B	1	Total C N O P 27 10 5 10 2	0	0
3	C	1	Total C N O P 27 10 5 10 2	0	0

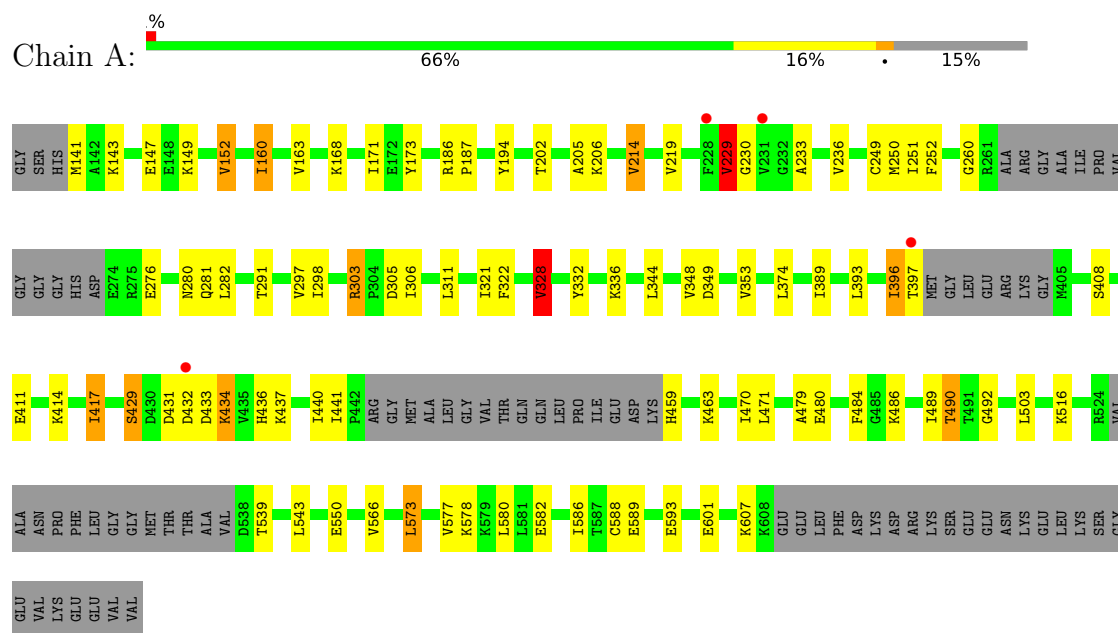
- Molecule 4 is water.

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

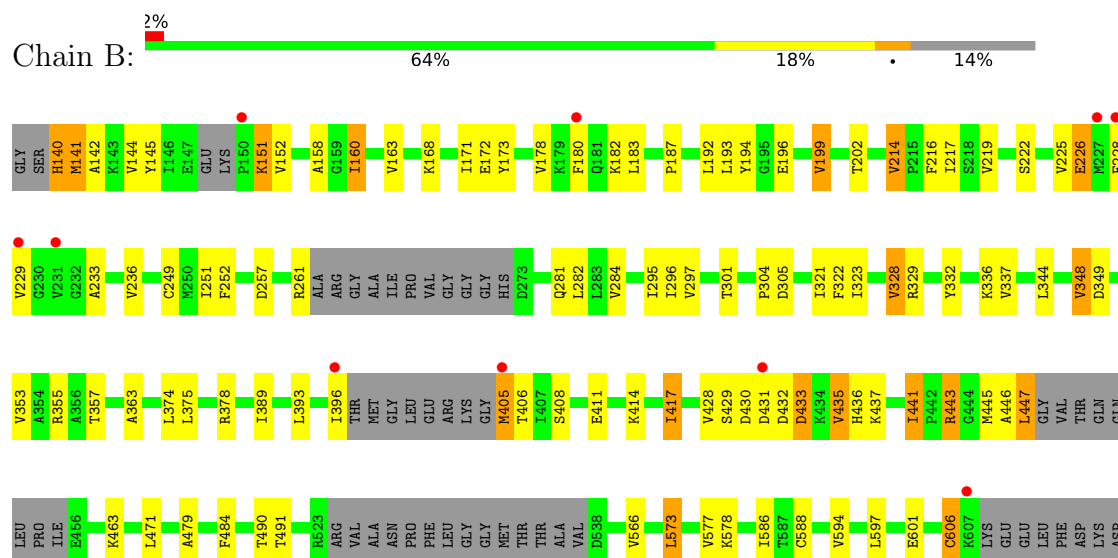
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: ATP-dependent zinc metalloprotease FtsH

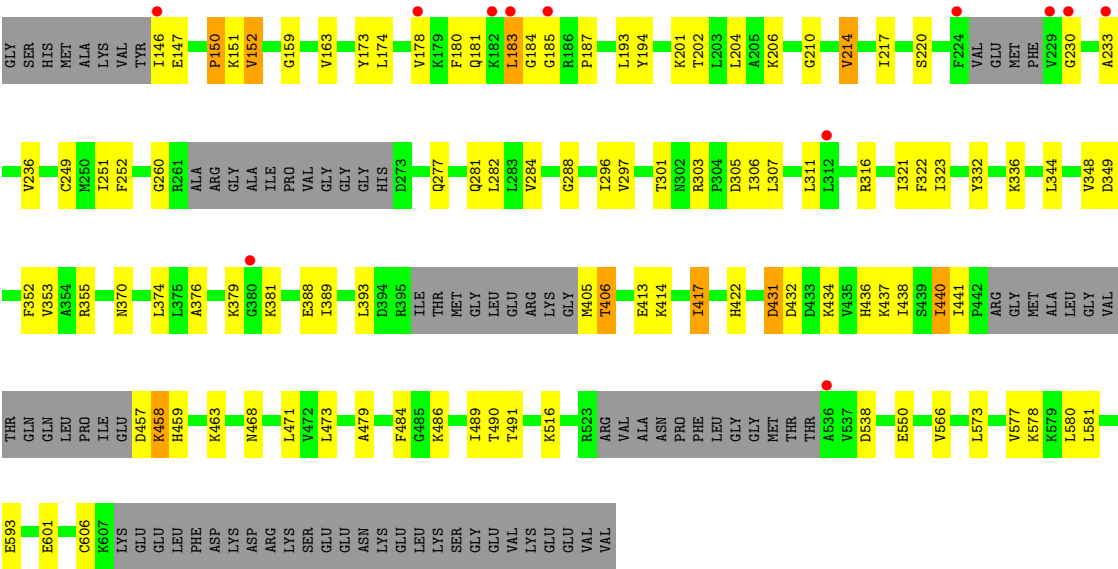


• Molecule 1: ATP-dependent zinc metalloprotease FtsH



ARG
LYS
SER
GLU
GLU
ASN
LYS
GLU
LEU
LYS
SER
GLY
GLU
VAL
LYS
GLU
VAL
VAL

● Molecule 1: ATP-dependent zinc metalloprotease FtsH



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.23Å 162.26Å 170.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.01 – 2.96 43.01 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.01-2.96) 98.2 (43.01-2.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.209 , 0.248 0.220 , 0.255	Depositor DCC
R_{free} test set	1975 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 96.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9978	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.82	0/3357	1.40	10/4511 (0.2%)
1	B	0.85	1/3392 (0.0%)	1.41	12/4556 (0.3%)
1	C	0.83	2/3280 (0.1%)	1.40	20/4408 (0.5%)
All	All	0.83	3/10029 (0.0%)	1.40	42/13475 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	606	CYS	CA-C	8.38	1.57	1.52
1	B	606	CYS	CA-C	5.80	1.58	1.53
1	C	441	ILE	CA-C	5.48	1.58	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ASP	CA-C-N	9.14	139.00	121.54
1	A	433	ASP	C-N-CA	9.14	139.00	121.54
1	C	431	ASP	CA-C-N	7.53	135.93	121.54
1	C	431	ASP	C-N-CA	7.53	135.93	121.54
1	A	152	VAL	N-CA-CB	7.12	118.48	110.72
1	B	428	VAL	CA-C-N	6.57	134.08	121.54
1	B	428	VAL	C-N-CA	6.57	134.08	121.54
1	C	490	THR	CA-C-N	6.52	131.03	120.60
1	C	490	THR	C-N-CA	6.52	131.03	120.60
1	B	180	PHE	CA-CB-CG	-6.28	107.52	113.80
1	A	429	SER	CA-C-N	6.14	133.28	121.54
1	A	429	SER	C-N-CA	6.14	133.28	121.54
1	B	433	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	228	PHE	CA-C-N	5.95	132.69	121.97
1	B	228	PHE	C-N-CA	5.95	132.69	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	GLY	CA-C-N	5.95	132.67	121.97
1	C	159	GLY	C-N-CA	5.95	132.67	121.97
1	B	490	THR	CA-C-N	5.65	129.63	120.60
1	B	490	THR	C-N-CA	5.65	129.63	120.60
1	C	230	GLY	CA-C-N	5.50	129.94	121.19
1	C	230	GLY	C-N-CA	5.50	129.94	121.19
1	C	184	GLY	CA-C-N	5.44	125.51	120.34
1	C	184	GLY	C-N-CA	5.44	125.51	120.34
1	C	220	SER	CA-C-N	5.41	126.90	120.14
1	C	220	SER	C-N-CA	5.41	126.90	120.14
1	C	305	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	588	CYS	CA-C-N	5.28	127.30	120.44
1	B	588	CYS	C-N-CA	5.28	127.30	120.44
1	C	370	ASN	CA-CB-CG	-5.22	107.38	112.60
1	C	151	LYS	CA-C-N	5.21	131.34	121.97
1	C	151	LYS	C-N-CA	5.21	131.34	121.97
1	C	277	GLN	CA-C-N	5.21	127.26	120.28
1	C	277	GLN	C-N-CA	5.21	127.26	120.28
1	A	588	CYS	CA-C-N	5.19	127.24	120.28
1	A	588	CYS	C-N-CA	5.19	127.24	120.28
1	A	433	ASP	N-CA-C	5.17	117.88	109.24
1	B	348	VAL	N-CA-CB	5.16	116.66	110.31
1	A	328	VAL	N-CA-CB	5.12	116.19	110.51
1	B	305	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	459	HIS	CA-C-N	5.11	130.21	122.91
1	C	459	HIS	C-N-CA	5.11	130.21	122.91
1	A	305	ASP	CA-CB-CG	5.08	117.68	112.60

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	3310	0	3410	41	0
1	B	3345	0	3433	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3236	0	3322	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	9978	0	10201	121	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 6.

All (121) 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:214:VAL:HG13	1:C:249:CYS:HA	1.52	0.92
1:A:490:THR:HG23	1:A:492:GLY:H	1.35	0.90
1:A:214:VAL:HG13	1:A:249:CYS:HA	1.62	0.81
1:B:214:VAL:HG13	1:B:249:CYS:HA	1.64	0.79
1:B:435:VAL:O	1:B:606:CYS:HA	1.91	0.71
1:B:202:THR:HG23	3:B:702:ADP:O1B	1.92	0.69
1:A:186:ARG:HD3	1:A:291:THR:HG21	1.75	0.69
1:C:183:LEU:HG	1:C:185:GLY:H	1.60	0.66
1:C:147:GLU:HG3	1:C:217:ILE:HG12	1.79	0.64
1:A:580:LEU:HD13	1:A:586:ILE:HG12	1.78	0.64
1:B:357:THR:HG22	1:B:393:LEU:HD11	1.80	0.63
1:C:150:PRO:HB3	1:C:210:GLY:HA2	1.81	0.62
1:B:225:VAL:HG21	1:C:288:GLY:HA2	1.82	0.61
1:A:480:GLU:OE2	1:A:490:THR:HG22	2.01	0.61
1:B:199:VAL:HG13	1:B:323:ILE:HG22	1.83	0.60
1:B:145:TYR:HB2	1:B:216:PHE:HB3	1.83	0.59
1:A:152:VAL:HG21	1:A:206:LYS:HB3	1.85	0.59
1:B:168:LYS:O	1:B:172:GLU:HG2	2.03	0.58
1:C:180:PHE:HA	1:C:183:LEU:HD23	1.85	0.58
1:B:363:ALA:HB2	3:B:702:ADP:H5'1	1.87	0.57
1:B:151:LYS:HD3	1:B:152:VAL:HG23	1.87	0.56
1:C:479:ALA:HA	1:C:566:VAL:HG11	1.88	0.56
1:A:152:VAL:CG2	1:A:206:LYS:HB3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:GLY:HA3	1:C:311:LEU:HD11	1.87	0.56
1:B:144:VAL:HG22	1:B:217:ILE:HG12	1.88	0.55
1:C:202:THR:HG23	3:C:702:ADP:O1B	2.06	0.55
1:C:152:VAL:HG11	1:C:206:LYS:HB3	1.88	0.55
1:B:479:ALA:HA	1:B:566:VAL:HG11	1.89	0.54
1:A:393:LEU:O	1:A:396:ILE:HG12	2.08	0.54
1:A:479:ALA:HA	1:A:566:VAL:HG11	1.90	0.54
1:B:417:ILE:HG13	1:B:577:VAL:HG21	1.90	0.53
1:C:417:ILE:HG13	1:C:577:VAL:HG21	1.90	0.52
1:C:251:ILE:HD12	1:C:297:VAL:HG22	1.91	0.51
1:A:276:GLU:O	1:A:280:ASN:HB2	2.11	0.50
1:B:251:ILE:HD12	1:B:297:VAL:HG22	1.94	0.50
1:A:417:ILE:HG13	1:A:577:VAL:HG21	1.93	0.49
1:A:260:GLY:HA3	1:A:311:LEU:HD11	1.93	0.49
1:A:251:ILE:HD12	1:A:297:VAL:HG22	1.93	0.49
1:B:163:VAL:HG13	1:B:321:ILE:HG21	1.94	0.49
1:C:163:VAL:HG13	1:C:321:ILE:HG21	1.94	0.49
1:A:202:THR:HG23	3:A:702:ADP:O1B	2.12	0.49
1:B:236:VAL:HG11	1:B:282:LEU:HA	1.94	0.49
1:C:236:VAL:HG11	1:C:282:LEU:HA	1.95	0.49
1:A:490:THR:HG23	1:A:492:GLY:N	2.16	0.49
1:A:236:VAL:HG11	1:A:282:LEU:HA	1.95	0.48
1:B:594:VAL:HA	1:B:597:LEU:HD12	1.95	0.48
1:C:281:GLN:HA	1:C:284:VAL:HG22	1.95	0.48
1:C:301:THR:HG21	1:C:307:LEU:HD11	1.96	0.48
1:A:163:VAL:HG13	1:A:321:ILE:HG21	1.95	0.48
1:B:344:LEU:HB3	1:B:348:VAL:HG21	1.96	0.48
1:A:194:TYR:CZ	1:A:322:PHE:HB2	2.49	0.48
1:A:589:GLU:O	1:A:593:GLU:HG2	2.14	0.48
1:C:422:HIS:HE1	1:C:473:LEU:O	1.97	0.47
1:C:303:ARG:HB3	1:C:306:ILE:HG12	1.96	0.47
1:C:344:LEU:HB3	1:C:348:VAL:HG21	1.96	0.47
1:A:229:VAL:HG13	1:A:230:GLY:N	2.30	0.47
1:A:434:LYS:HD2	1:A:607:LYS:HA	1.97	0.47
1:C:194:TYR:CZ	1:C:322:PHE:HB2	2.51	0.46
1:B:192:LEU:HD11	1:B:301:THR:HG22	1.97	0.46
1:C:233:ALA:O	1:C:281:GLN:HG2	2.16	0.46
1:A:328:VAL:HG21	1:A:582:GLU:O	2.15	0.46
1:B:281:GLN:HA	1:B:284:VAL:HG22	1.97	0.46
1:C:573:LEU:HD23	1:C:573:LEU:HA	1.83	0.46
1:C:438:ILE:HG22	1:C:580:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:THR:HG23	1:A:543:LEU:HD23	1.97	0.45
1:C:178:VAL:HA	1:C:181:GLN:HB2	1.97	0.45
1:C:352:PHE:HA	1:C:355:ARG:HD3	1.97	0.45
1:B:375:LEU:HA	1:B:378:ARG:HG2	1.98	0.45
1:A:344:LEU:HB3	1:A:348:VAL:HG21	1.99	0.45
1:A:303:ARG:HB2	1:A:306:ILE:HG12	1.99	0.45
1:B:194:TYR:CZ	1:B:322:PHE:HB2	2.52	0.45
1:B:443:ARG:O	1:C:458:LYS:HA	2.17	0.45
1:B:196:GLU:HG2	1:B:445:MET:HE3	1.98	0.45
1:C:174:LEU:HD21	1:C:296:ILE:HG22	1.98	0.45
1:C:332:TYR:CE2	1:C:336:LYS:HD2	2.52	0.44
1:A:332:TYR:CE2	1:A:336:LYS:HD2	2.52	0.44
1:B:417:ILE:HD13	1:B:484:PHE:CZ	2.53	0.44
1:A:414:LYS:HD3	1:A:484:PHE:CE2	2.52	0.44
1:B:233:ALA:O	1:B:281:GLN:HG2	2.18	0.44
1:A:573:LEU:HD23	1:A:573:LEU:HA	1.85	0.44
1:A:233:ALA:O	1:A:281:GLN:HG2	2.18	0.43
1:C:376:ALA:HB2	1:C:388:GLU:HG2	2.00	0.43
1:C:417:ILE:HD13	1:C:484:PHE:CZ	2.54	0.43
1:A:173:TYR:CE1	1:A:187:PRO:HG3	2.53	0.43
1:B:408:SER:HB3	1:B:411:GLU:HB2	2.01	0.43
1:A:349:ASP:O	1:A:353:VAL:HG23	2.19	0.43
1:B:178:VAL:O	1:B:182:LYS:HG2	2.19	0.43
1:B:405:MET:HE2	1:B:406:THR:HB	1.99	0.43
1:B:158:ALA:HB2	1:B:337:VAL:HG21	1.99	0.43
1:B:222:SER:O	1:B:225:VAL:HG22	2.19	0.43
1:B:414:LYS:HD3	1:B:484:PHE:CE2	2.53	0.42
1:B:257:ASP:O	1:B:261:ARG:HG3	2.19	0.42
1:C:173:TYR:CE1	1:C:187:PRO:HG3	2.54	0.42
1:B:332:TYR:CE2	1:B:336:LYS:HD2	2.53	0.42
1:B:173:TYR:CE1	1:B:187:PRO:HG3	2.53	0.42
1:C:414:LYS:HD3	1:C:484:PHE:CE2	2.53	0.42
1:A:205:ALA:HB1	1:A:250:MET:HE1	2.02	0.42
1:A:168:LYS:HA	1:A:171:ILE:HD12	2.01	0.42
1:A:486:LYS:O	1:A:489:ILE:HG12	2.20	0.42
1:B:573:LEU:HD23	1:B:573:LEU:HA	1.89	0.42
1:C:486:LYS:O	1:C:489:ILE:HG12	2.19	0.41
1:B:304:PRO:HB2	1:B:447:LEU:HD23	2.02	0.41
1:A:429:SER:OG	1:A:432:ASP:HB3	2.19	0.41
1:A:470:ILE:HG13	1:A:503:LEU:HD23	2.02	0.41
1:C:413:GLU:HA	1:C:581:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:THR:HG22	1:B:252:PHE:CZ	2.55	0.41
1:C:201:LYS:HG2	1:C:323:ILE:HD12	2.03	0.41
1:C:349:ASP:O	1:C:353:VAL:HG23	2.20	0.41
1:C:202:THR:HG22	1:C:252:PHE:CZ	2.56	0.41
1:A:202:THR:HG22	1:A:252:PHE:CZ	2.56	0.41
1:A:250:MET:SD	1:A:298:ILE:HD12	2.61	0.41
1:B:441:ILE:HG22	1:B:445:MET:HB2	2.02	0.41
1:A:186:ARG:HA	1:A:187:PRO:HD2	1.90	0.40
1:C:379:LYS:HD3	1:C:381:LYS:HE3	2.02	0.40
1:C:516:LYS:HE2	1:C:550:GLU:HG2	2.02	0.40
1:A:516:LYS:HE2	1:A:550:GLU:HG2	2.03	0.40
1:B:140:HIS:CE1	1:B:141:MET:HB2	2.56	0.40
1:B:328:VAL:HG11	1:B:355:ARG:HG2	2.03	0.40
1:B:349:ASP:O	1:B:353:VAL:HG23	2.21	0.40
1:A:408:SER:HB3	1:A:411:GLU:HB2	2.04	0.40
1:C:193:LEU:HD21	1:C:204:LEU:HD23	2.04	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	410/497 (82%)	386 (94%)	18 (4%)	6 (2%)	8	23
1	B	413/497 (83%)	382 (92%)	21 (5%)	10 (2%)	4	13
1	C	400/497 (80%)	380 (95%)	13 (3%)	7 (2%)	6	19
All	All	1223/1491 (82%)	1148 (94%)	52 (4%)	23 (2%)	6	17

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	LYS

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Mol	Chain	Res	Type
1	B	229	VAL
1	B	429	SER
1	C	150	PRO
1	C	152	VAL
1	C	432	ASP
1	A	229	VAL
1	A	437	LYS
1	B	437	LYS
1	C	437	LYS
1	B	430	ASP
1	C	538	ASP
1	B	446	ALA
1	A	149	LYS
1	B	142	ALA
1	B	160	ILE
1	B	226	GLU
1	B	431	ASP
1	A	160	ILE
1	B	151	LYS
1	C	406	THR
1	C	440	ILE
1	A	396	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	355/415 (86%)	331 (93%)	24 (7%)	14	35
1	B	358/415 (86%)	325 (91%)	33 (9%)	8	23
1	C	347/415 (84%)	324 (93%)	23 (7%)	15	37
All	All	1060/1245 (85%)	980 (92%)	80 (8%)	12	31

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	MET
1	A	143	LYS
1	A	147	GLU
1	A	160	ILE
1	A	214	VAL
1	A	219	VAL
1	A	229	VAL
1	A	303	ARG
1	A	328	VAL
1	A	374	LEU
1	A	389	ILE
1	A	397	THR
1	A	417	ILE
1	A	431	ASP
1	A	436	HIS
1	A	440	ILE
1	A	441	ILE
1	A	459	HIS
1	A	463	LYS
1	A	471	LEU
1	A	490	THR
1	A	573	LEU
1	A	578	LYS
1	A	601	GLU
1	B	140	HIS
1	B	141	MET
1	B	160	ILE
1	B	171	ILE
1	B	183	LEU
1	B	193	LEU
1	B	199	VAL
1	B	214	VAL
1	B	219	VAL
1	B	226	GLU
1	B	295	ILE
1	B	296	ILE
1	B	328	VAL
1	B	329	ARG
1	B	374	LEU
1	B	389	ILE
1	B	396	ILE
1	B	405	MET
1	B	417	ILE

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Mol	Chain	Res	Type
1	B	432	ASP
1	B	433	ASP
1	B	435	VAL
1	B	436	HIS
1	B	441	ILE
1	B	443	ARG
1	B	447	LEU
1	B	463	LYS
1	B	471	LEU
1	B	491	THR
1	B	573	LEU
1	B	578	LYS
1	B	586	ILE
1	B	601	GLU
1	C	146	ILE
1	C	183	LEU
1	C	214	VAL
1	C	316	ARG
1	C	374	LEU
1	C	389	ILE
1	C	393	LEU
1	C	405	MET
1	C	406	THR
1	C	417	ILE
1	C	431	ASP
1	C	434	LYS
1	C	436	HIS
1	C	440	ILE
1	C	457	ASP
1	C	458	LYS
1	C	463	LYS
1	C	468	ASN
1	C	471	LEU
1	C	491	THR
1	C	578	LYS
1	C	593	GLU
1	C	601	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	213	HIS
1	A	277	GLN
1	A	367	ASN
1	A	459	HIS
1	B	140	HIS
1	B	213	HIS
1	B	246	HIS
1	B	558	GLN
1	C	246	HIS
1	C	370	ASN

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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	702	-	28,29,29	0.48	0	43,45,45	0.71	1 (2%)
3	ADP	B	702	-	28,29,29	0.58	1 (3%)	43,45,45	0.54	0
3	ADP	C	702	-	28,29,29	0.50	0	43,45,45	0.76	0

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	702	-	-	1/16/32/32	0/3/3/3
3	ADP	B	702	-	-	3/16/32/32	0/3/3/3
3	ADP	C	702	-	-	1/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ADP	PB-O3B	-2.03	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ADP	O3B-PB-O3A	2.28	112.27	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	ADP	PA-O3A-PB-O2B
3	B	702	ADP	C5'-O5'-PA-O1A
3	B	702	ADP	C5'-O5'-PA-O2A
3	B	702	ADP	C5'-O5'-PA-O3A
3	C	702	ADP	PB-O3A-PA-O2A

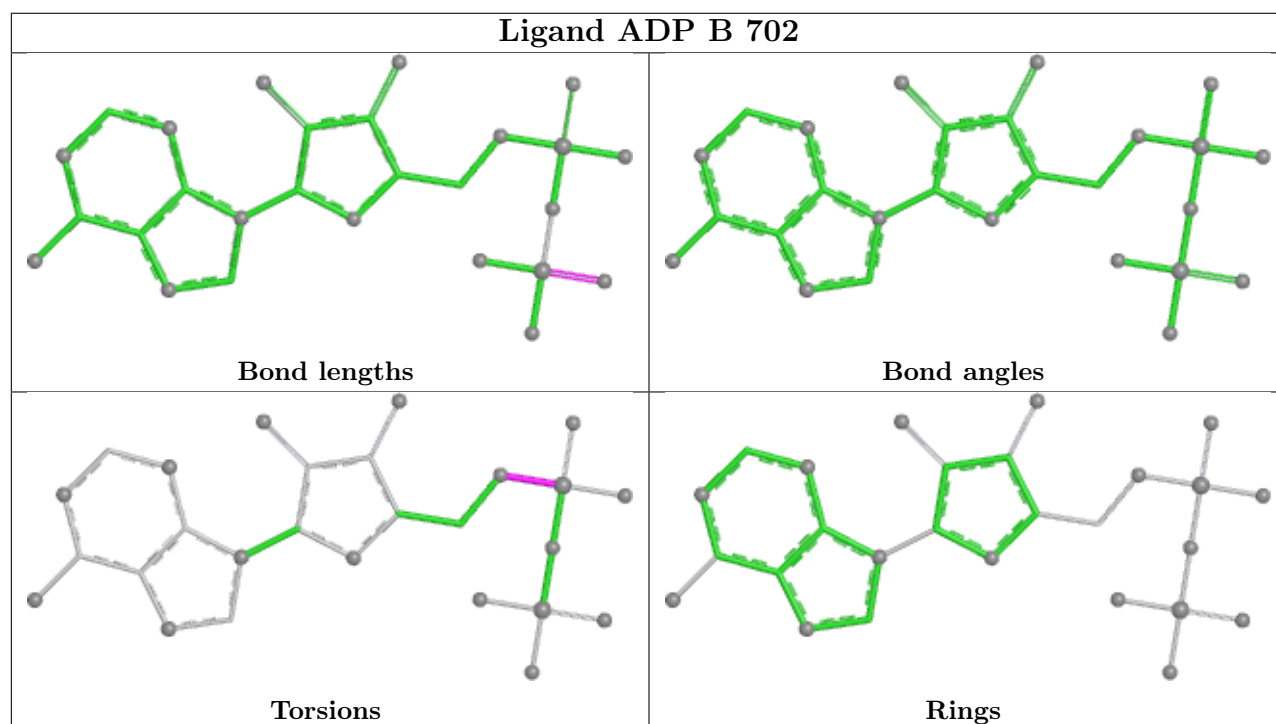
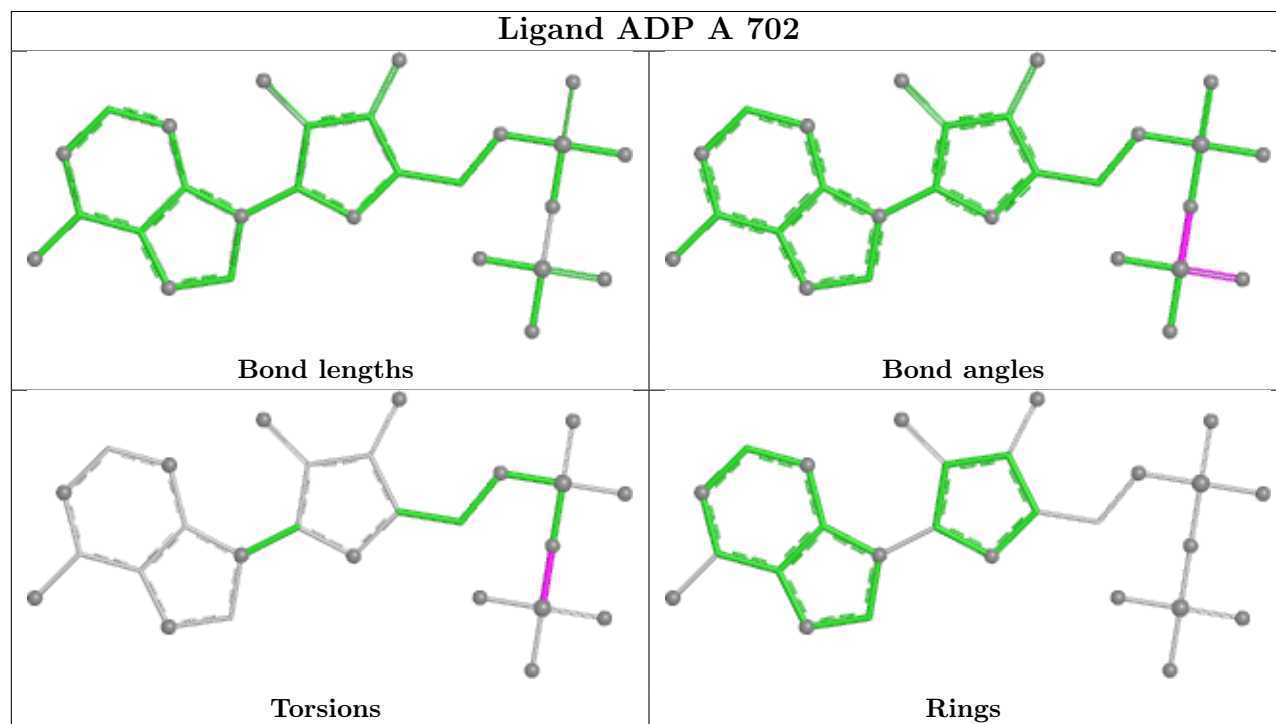
There are no ring outliers.

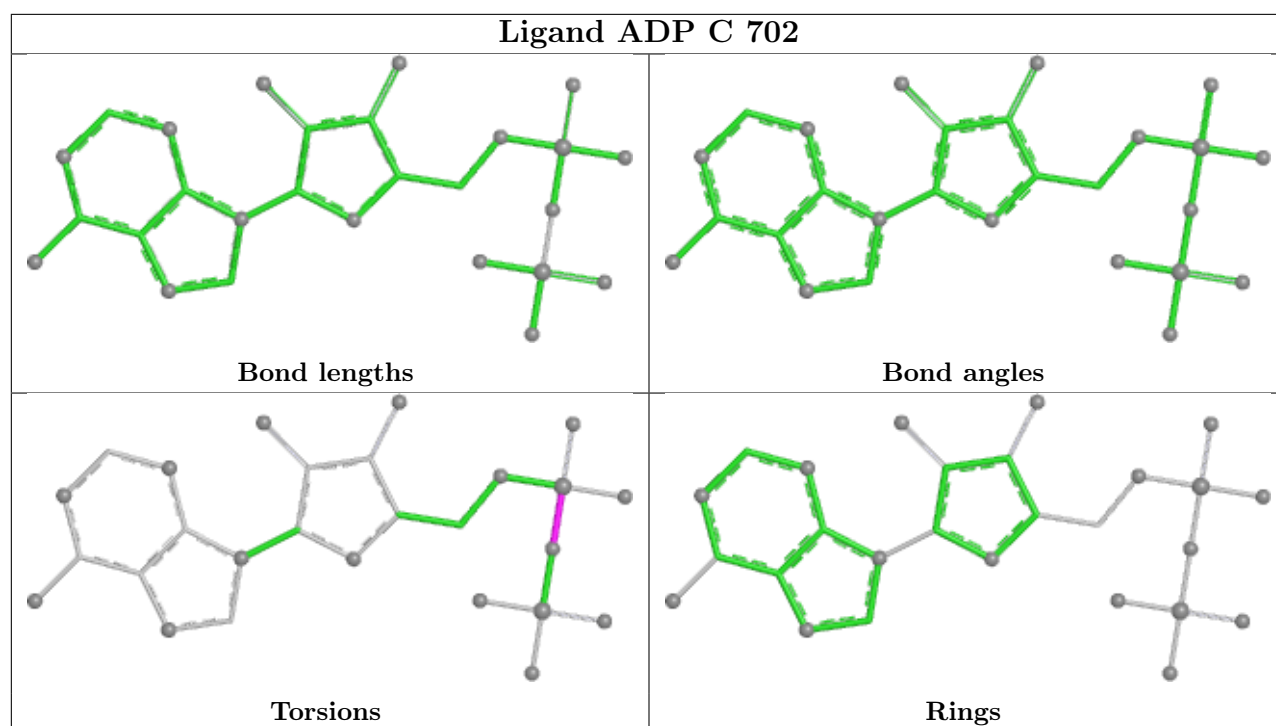
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	ADP	1	0
3	B	702	ADP	2	0
3	C	702	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	420/497 (84%)	-0.07	4 (0%) 79 74	59, 97, 167, 197	0
1	B	425/497 (85%)	0.09	10 (2%) 59 51	64, 108, 164, 214	0
1	C	412/497 (82%)	0.16	12 (2%) 53 46	65, 112, 175, 215	0
All	All	1257/1491 (84%)	0.06	26 (2%) 63 55	59, 105, 170, 215	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	VAL	4.4
1	C	183	LEU	4.2
1	C	230	GLY	3.9
1	B	227	MET	3.8
1	B	150	PRO	3.8
1	C	229	VAL	3.4
1	C	536	ALA	3.3
1	C	380	GLY	3.3
1	A	231	VAL	3.1
1	B	229	VAL	2.8
1	C	224	PHE	2.7
1	B	607	LYS	2.7
1	C	185	GLY	2.6
1	C	233	ALA	2.6
1	B	431	ASP	2.4
1	B	180	PHE	2.4
1	A	228	PHE	2.4
1	A	432	ASP	2.3
1	B	396	ILE	2.2
1	C	178	VAL	2.2
1	C	182	LYS	2.1
1	B	405	MET	2.1
1	C	146	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	312	LEU	2.1
1	B	228	PHE	2.1
1	A	397	THR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

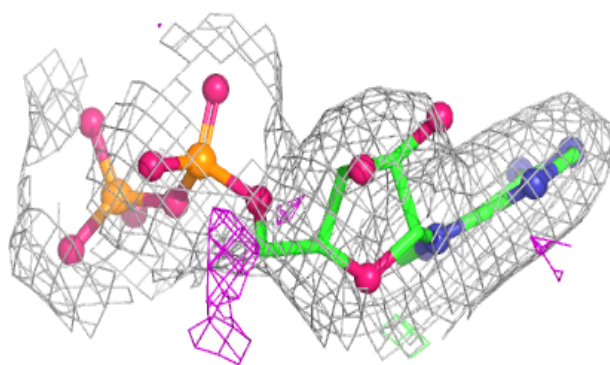
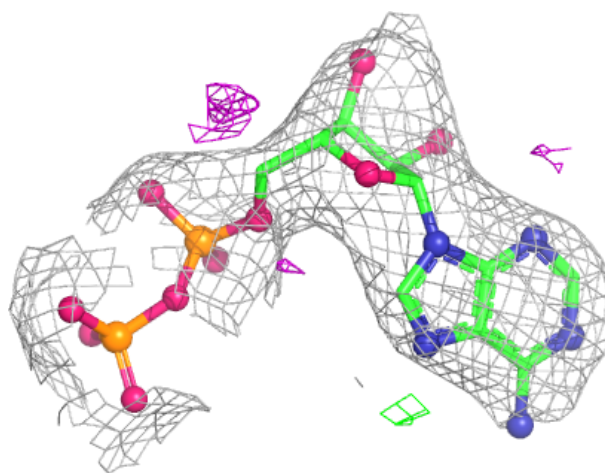
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ZN	C	701	1/1	0.88	0.14	247,247,247,247	0
3	ADP	B	702	27/27	0.96	0.07	72,82,88,93	0
3	ADP	A	702	27/27	0.97	0.06	76,81,91,98	0
3	ADP	C	702	27/27	0.98	0.06	81,85,94,97	0
2	ZN	A	701	1/1	0.99	0.05	84,84,84,84	0
2	ZN	B	701	1/1	0.99	0.03	81,81,81,81	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.

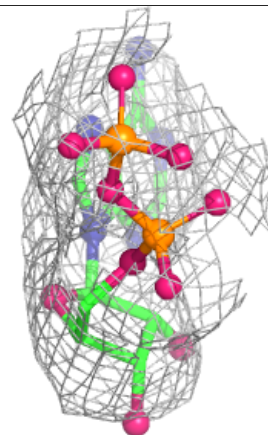
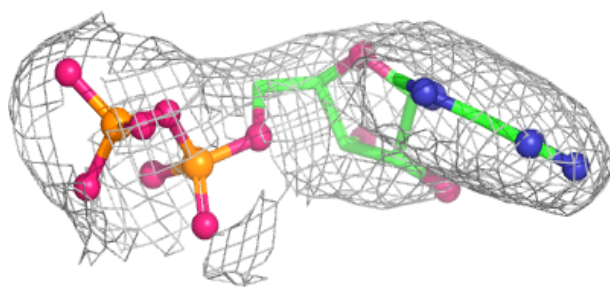
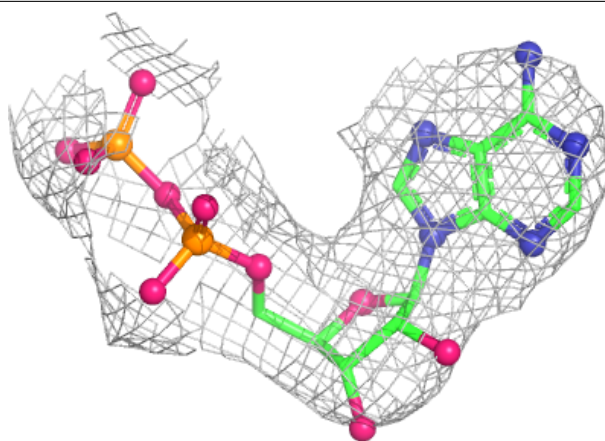
Electron density around ADP B 702:

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



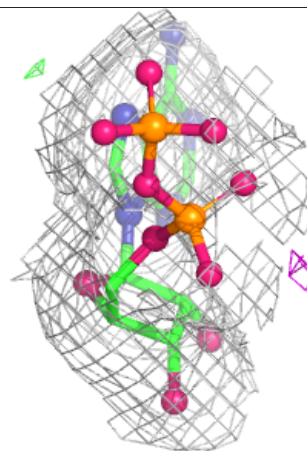
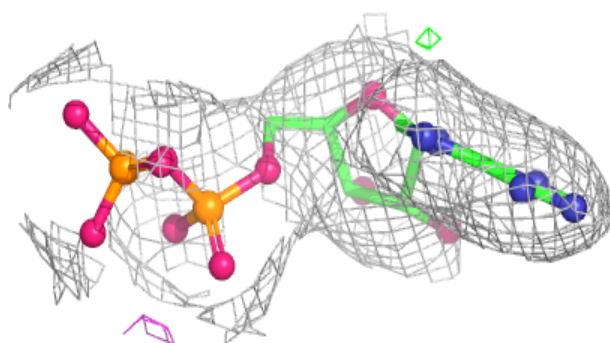
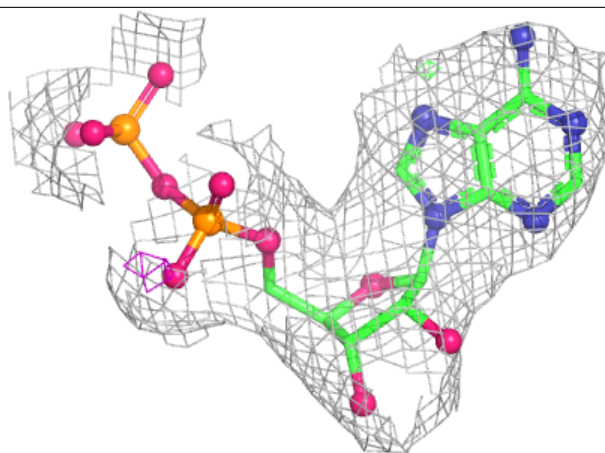
Electron density around ADP A 702:

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



Electron density around ADP C 702:

$2mF_o-DF_c$ (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.