



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 05:07 pm GMT

PDB ID : 4WW0
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

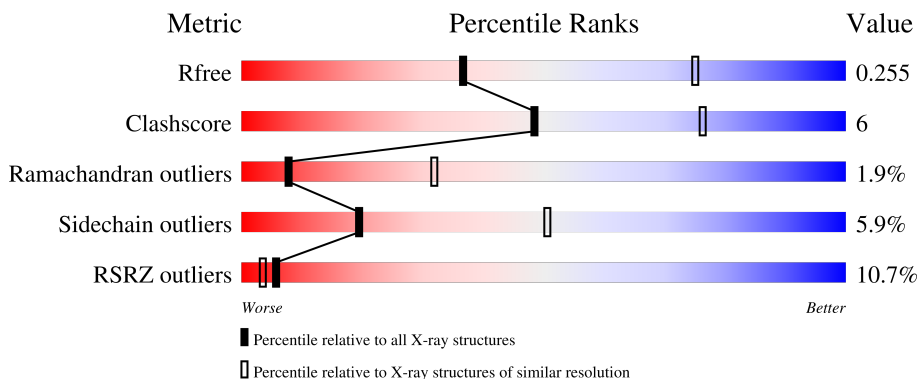
1 Overall quality at a glance

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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	 7% 67% 16% • 15%
1	B	497	 9% 67% 16% • 14%
1	C	497	 11% 64% 17% • 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
			Total	C	N	O	S			
1	A	420	3310	2112	560	625	13	0	0	0
1	B	425	3345	2132	566	633	14	0	0	0
1	C	412	3236	2060	548	617	11	0	0	0

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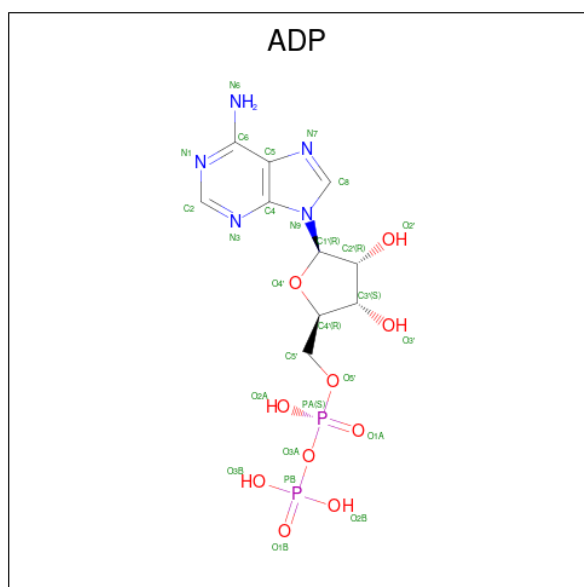
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Chain	Residue	Modelled	Actual	Comment	Reference
C	627	GLY	GLU	engineered mutation	UNP O67077

- Molecule 2 is ZINC ION (three-letter code: 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

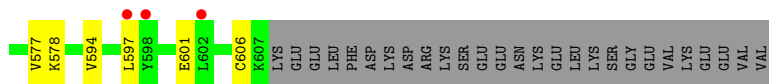
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



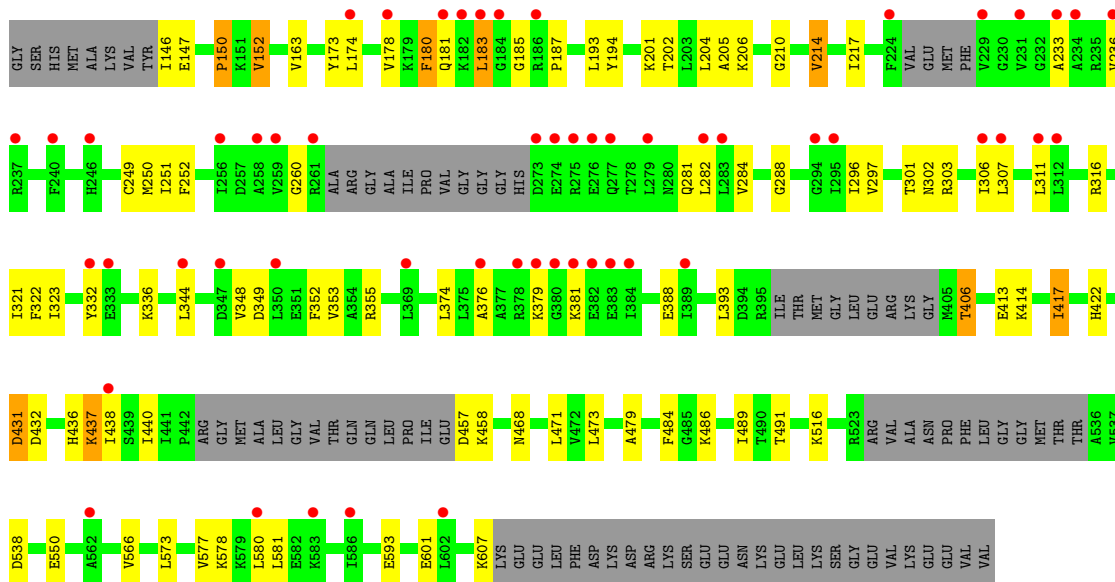
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0
3	C	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 4 is water.

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



• 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 44.75 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.01-2.96) 98.1 (44.75-2.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.96Å)	Xtrriage
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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtrriage
Anisotropy	0.211	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 87.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtrriage
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

Xtrriage'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 [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	0.48	0/3357	0.66	1/4511 (0.0%)
1	B	0.49	0/3392	0.68	0/4556
1	C	0.47	0/3280	0.66	1/4408 (0.0%)
All	All	0.48	0/10029	0.67	2/13475 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ASP	C-N-CA	6.92	139.00	121.70
1	C	431	ASP	C-N-CA	5.69	135.93	121.70

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	3310	0	3410	41	0
1	B	3345	0	3433	41	0
1	C	3236	0	3322	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:205:ALA:HB1	1:A:250:MET:HE1	2.00	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: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:C:205:ALA:HB1	1:C:250:MET:HE1	2.01	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: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
1:B:205:ALA:HB1	1:B:250:MET:HE1	2.03	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	10	38
1	B	413/497 (83%)	382 (92%)	21 (5%)	10 (2%)	6	26
1	C	400/497 (80%)	380 (95%)	13 (3%)	7 (2%)	8	33
All	All	1223/1491 (82%)	1148 (94%)	52 (4%)	23 (2%)	8	32

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	LYS
1	B	229	VAL
1	B	429	SER
1	C	150	PRO
1	C	152	VAL

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Mol	Chain	Res	Type
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 [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	355/415 (86%)	337 (95%)	18 (5%)	24 56
1	B	358/415 (86%)	334 (93%)	24 (7%)	16 45
1	C	347/415 (84%)	326 (94%)	21 (6%)	18 49
All	All	1060/1245 (85%)	997 (94%)	63 (6%)	19 50

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	MET
1	A	147	GLU
1	A	214	VAL
1	A	219	VAL

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Mol	Chain	Res	Type
1	A	303	ARG
1	A	328	VAL
1	A	374	LEU
1	A	397	THR
1	A	417	ILE
1	A	431	ASP
1	A	436	HIS
1	A	459	HIS
1	A	468	ASN
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	199	VAL
1	B	214	VAL
1	B	219	VAL
1	B	226	GLU
1	B	302	ASN
1	B	374	LEU
1	B	396	ILE
1	B	405	MET
1	B	417	ILE
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	471	LEU
1	B	491	THR
1	B	573	LEU
1	B	578	LYS
1	B	601	GLU
1	C	146	ILE
1	C	180	PHE
1	C	183	LEU
1	C	214	VAL

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Mol	Chain	Res	Type
1	C	302	ASN
1	C	316	ARG
1	C	374	LEU
1	C	393	LEU
1	C	406	THR
1	C	417	ILE
1	C	431	ASP
1	C	436	HIS
1	C	437	LYS
1	C	457	ASP
1	C	468	ASN
1	C	471	LEU
1	C	491	THR
1	C	578	LYS
1	C	593	GLU
1	C	601	GLU
1	C	607	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	B	140	HIS
1	B	558	GLN
1	C	370	ASN

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 monosaccharides 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	B	702	-	24,29,29	0.78	0	29,45,45	0.77	1 (3%)
3	ADP	A	702	-	24,29,29	0.72	0	29,45,45	0.99	2 (6%)
3	ADP	C	702	-	24,29,29	0.72	0	29,45,45	1.02	2 (6%)

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	B	702	-	-	3/12/32/32	0/3/3/3
3	ADP	A	702	-	-	1/12/32/32	0/3/3/3
3	ADP	C	702	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	ADP	C3'-C2'-C1'	2.51	104.75	100.98
3	B	702	ADP	C5-C6-N6	2.34	123.91	120.35
3	C	702	ADP	C5-C6-N6	2.28	123.82	120.35
3	A	702	ADP	O3B-PB-O3A	2.28	112.27	104.64
3	A	702	ADP	C5-C6-N6	2.27	123.80	120.35

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

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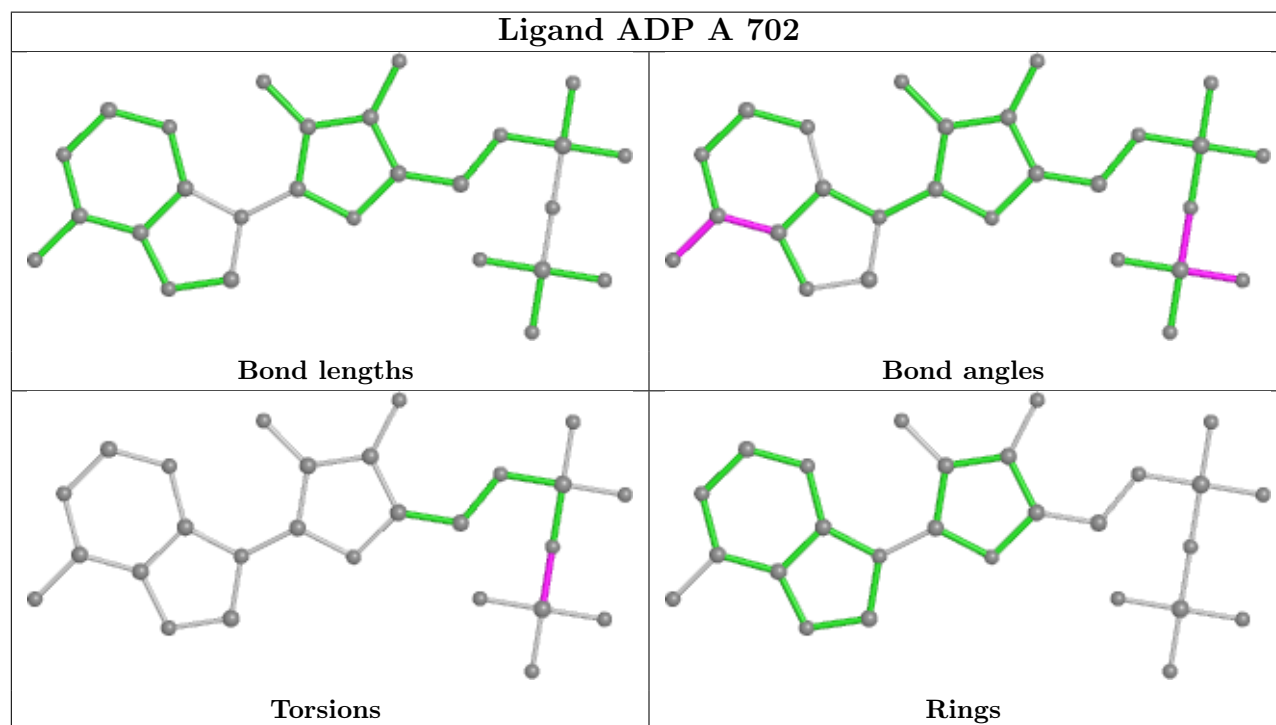
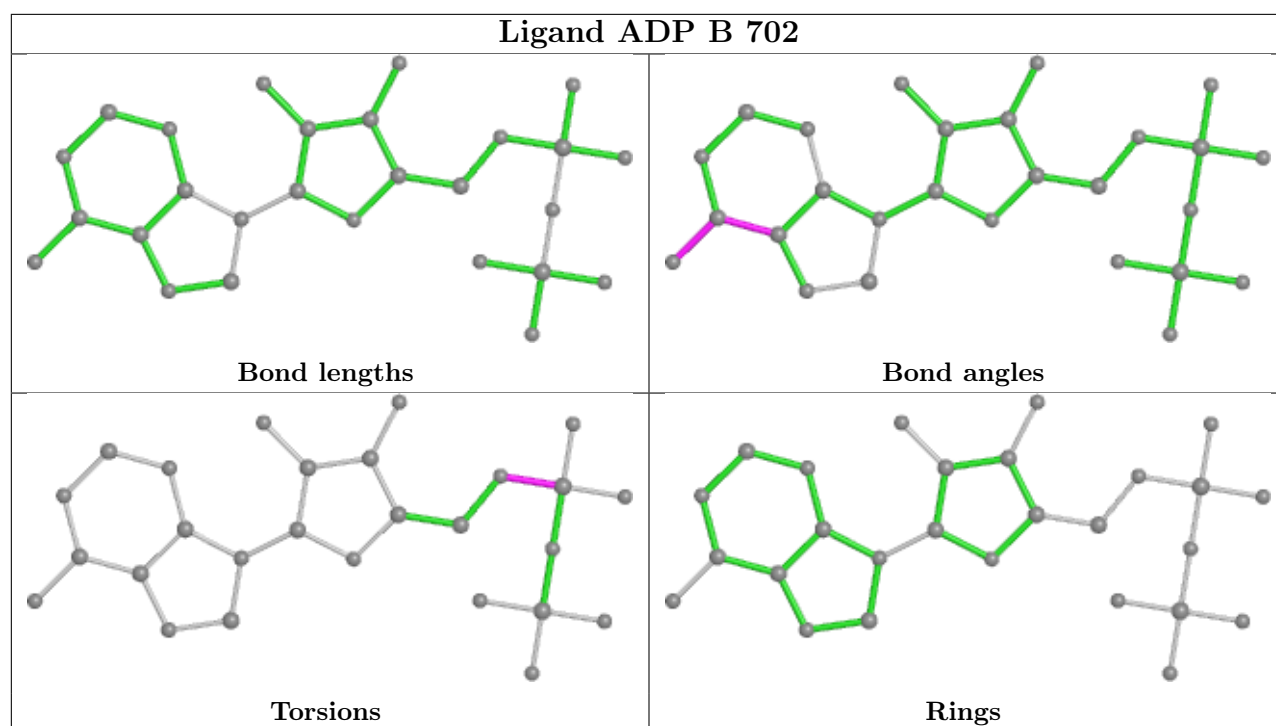
Mol	Chain	Res	Type	Atoms
3	B	702	ADP	C5'-O5'-PA-O1A
3	B	702	ADP	C5'-O5'-PA-O3A
3	B	702	ADP	C5'-O5'-PA-O2A
3	C	702	ADP	PB-O3A-PA-O2A

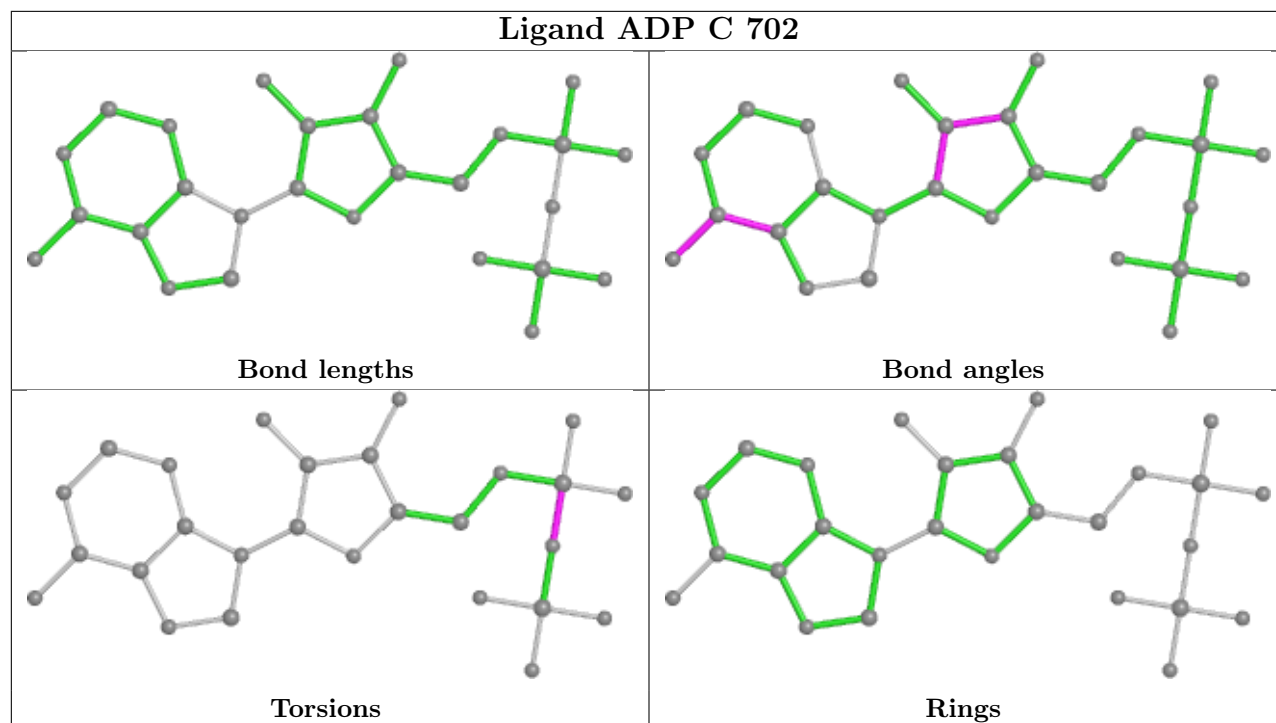
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	ADP	2	0
3	A	702	ADP	1	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%)	0.63	34 (8%) 12 6	59, 97, 167, 197	0
1	B	425/497 (85%)	0.70	46 (10%) 5 3	64, 108, 164, 214	0
1	C	412/497 (82%)	0.89	55 (13%) 3 2	65, 112, 175, 215	0
All	All	1257/1491 (84%)	0.74	135 (10%) 6 3	59, 105, 170, 215	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	PHE	8.1
1	B	228	PHE	7.4
1	A	375	LEU	7.1
1	C	183	LEU	7.0
1	C	261	ARG	6.3
1	C	306	ILE	5.8
1	C	380	GLY	5.3
1	A	391	GLU	5.2
1	A	374	LEU	5.1
1	B	231	VAL	5.1
1	C	231	VAL	5.1
1	A	379	LYS	5.0
1	C	350	LEU	5.0
1	A	227	MET	4.8
1	A	344	LEU	4.8
1	B	227	MET	4.7
1	C	182	LYS	4.5
1	B	184	GLY	4.4
1	C	275	ARG	4.3
1	C	259	VAL	4.2
1	A	384	ILE	4.2
1	B	341	ASN	4.1
1	B	182	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	276	GLU	4.0
1	C	307	LEU	4.0
1	C	229	VAL	3.9
1	A	382	GLU	3.9
1	C	282	LEU	3.8
1	B	378	ARG	3.8
1	C	240	PHE	3.7
1	A	229	VAL	3.7
1	B	602	LEU	3.7
1	A	343	LYS	3.6
1	B	180	PHE	3.6
1	A	383	GLU	3.5
1	B	183	LEU	3.5
1	C	181	GLN	3.4
1	C	344	LEU	3.4
1	B	374	LEU	3.4
1	A	345	ALA	3.4
1	A	341	ASN	3.3
1	C	583	LYS	3.3
1	A	182	LYS	3.3
1	A	378	ARG	3.3
1	C	381	LYS	3.3
1	B	375	LEU	3.3
1	C	233	ALA	3.2
1	B	189	LYS	3.2
1	B	311	LEU	3.2
1	B	431	ASP	3.1
1	A	376	ALA	3.1
1	C	224	PHE	3.1
1	C	389	ILE	3.1
1	B	381	LYS	3.0
1	A	368	LEU	3.0
1	B	343	LYS	3.0
1	C	369	LEU	3.0
1	C	295	ILE	3.0
1	C	258	ALA	3.0
1	A	348	VAL	3.0
1	B	229	VAL	3.0
1	B	597	LEU	3.0
1	C	379	LYS	3.0
1	A	275	ARG	2.9
1	A	339	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	376	ALA	2.8
1	C	312	LEU	2.8
1	A	395	ARG	2.8
1	C	178	VAL	2.8
1	C	383	GLU	2.8
1	C	236	VAL	2.8
1	A	377	ALA	2.8
1	B	389	ILE	2.7
1	B	261	ARG	2.7
1	B	293	ASP	2.7
1	B	383	GLU	2.7
1	C	438	ILE	2.6
1	B	282	LEU	2.6
1	B	427	LEU	2.6
1	B	368	LEU	2.6
1	C	274	GLU	2.6
1	B	294	GLY	2.5
1	C	277	GLN	2.5
1	B	384	ILE	2.5
1	A	338	HIS	2.5
1	C	186	ARG	2.5
1	A	155	LYS	2.5
1	A	346	LYS	2.5
1	C	256	ILE	2.5
1	B	430	ASP	2.5
1	A	389	ILE	2.5
1	A	352	PHE	2.4
1	A	350	LEU	2.4
1	B	393	LEU	2.4
1	B	382	GLU	2.4
1	A	175	LYS	2.4
1	B	405	MET	2.4
1	A	372	ALA	2.4
1	C	279	LEU	2.4
1	C	294	GLY	2.3
1	B	372	ALA	2.3
1	C	283	LEU	2.3
1	C	246	HIS	2.3
1	B	332	TYR	2.3
1	C	174	LEU	2.3
1	C	562	ALA	2.3
1	C	234	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	382	GLU	2.3
1	B	379	LYS	2.2
1	B	392	ALA	2.2
1	C	311	LEU	2.2
1	B	391	GLU	2.2
1	B	167	VAL	2.2
1	B	344	LEU	2.2
1	B	295	ILE	2.2
1	C	273	ASP	2.2
1	C	384	ILE	2.2
1	C	586	ILE	2.2
1	C	237	ARG	2.2
1	B	598	TYR	2.2
1	C	378	ARG	2.2
1	B	350	LEU	2.1
1	B	259	VAL	2.1
1	A	183	LEU	2.1
1	C	580	LEU	2.1
1	C	602	LEU	2.1
1	C	332	TYR	2.1
1	A	373	ALA	2.1
1	C	184	GLY	2.1
1	A	180	PHE	2.1
1	C	347	ASP	2.1
1	B	376	ALA	2.1
1	C	333	GLU	2.0
1	B	178	VAL	2.0
1	B	317	PHE	2.0

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 monosaccharides in this entry.

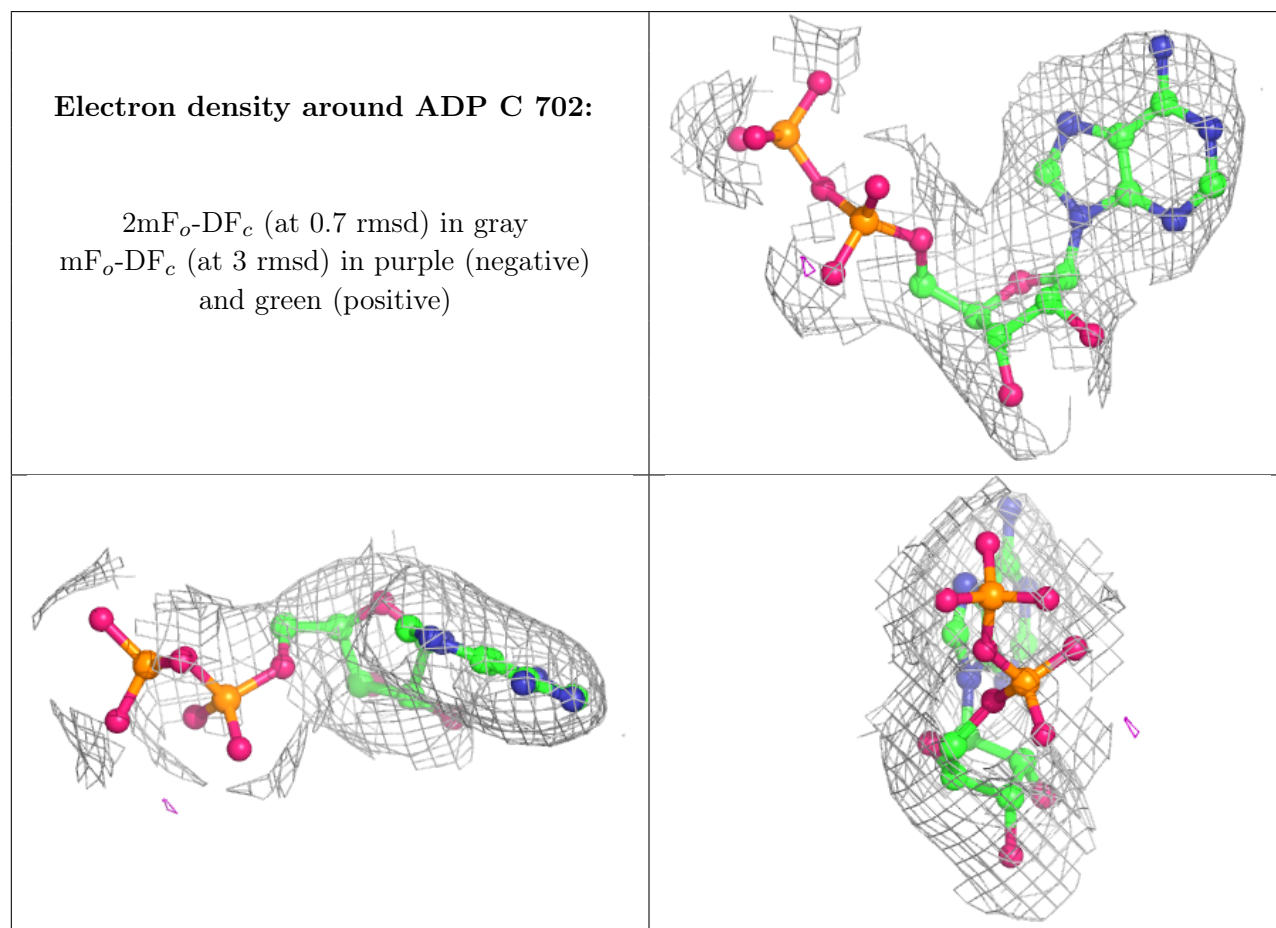
6.4 Ligands [i](#)

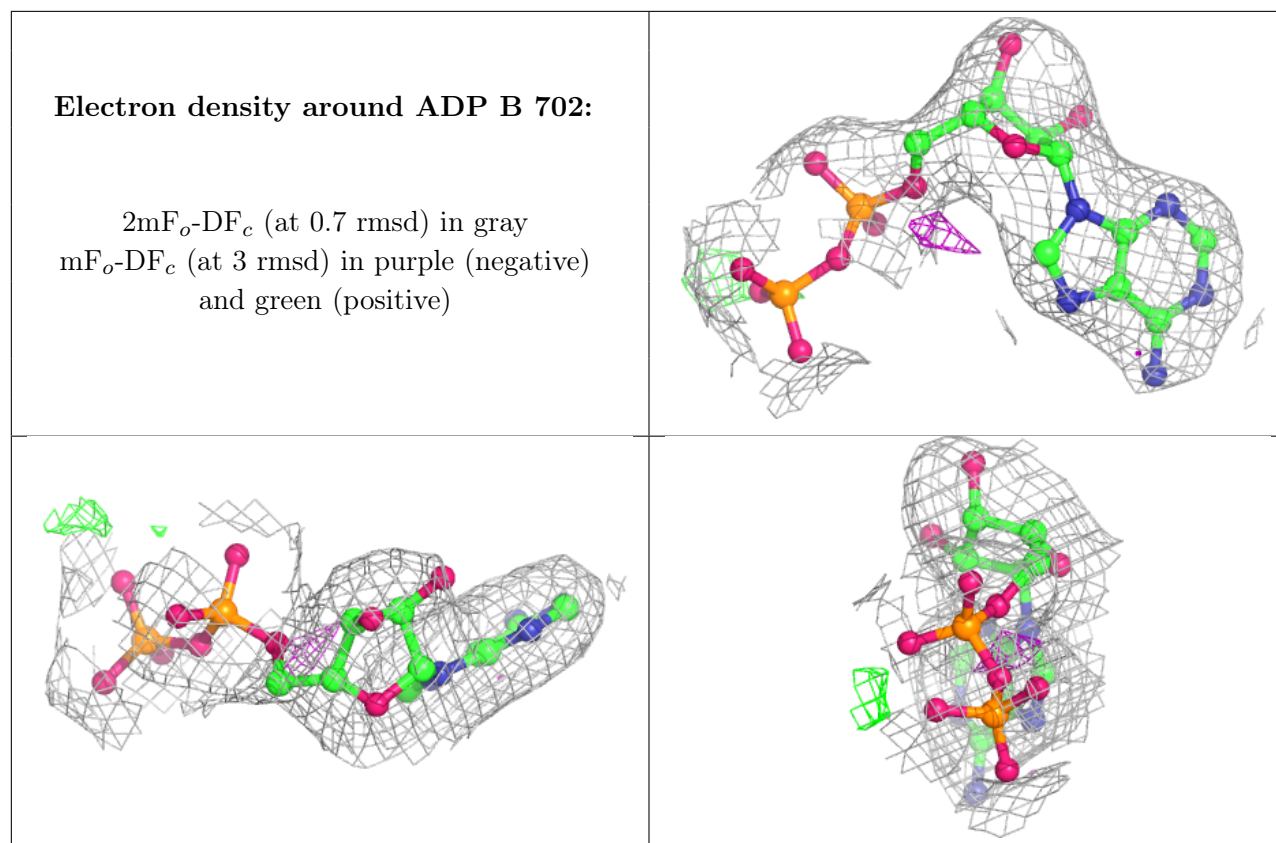
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

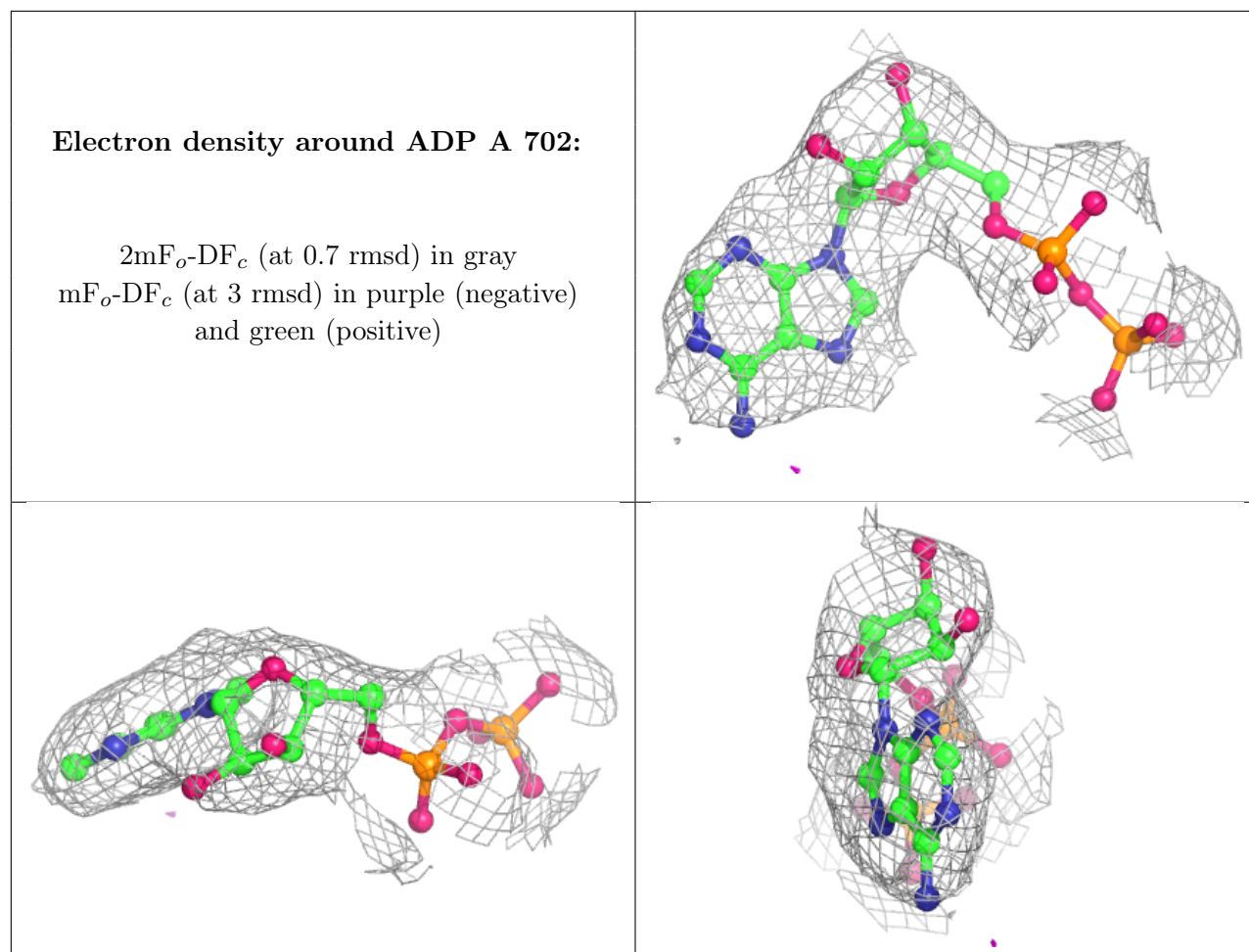
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	C	701	1/1	0.58	0.08	247,247,247,247	0
3	ADP	C	702	27/27	0.93	0.19	81,85,94,97	0
3	ADP	B	702	27/27	0.94	0.21	72,82,88,93	0
3	ADP	A	702	27/27	0.94	0.22	76,81,91,98	0
2	ZN	B	701	1/1	0.98	0.21	81,81,81,81	0
2	ZN	A	701	1/1	0.99	0.23	84,84,84,84	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.







6.5 Other polymers [i](#)

There are no such residues in this entry.