



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:18 pm BST

PDB ID : 4Z8X
Title : Truncated FtsH from *A. aeolicus*
Authors : Vostrukhina, M.; Baumann, U.; Schacherl, M.; Bieniossek, C.; Lanz, M.; Baumgartner, R.
Deposited on : 2015-04-09
Resolution : 3.25 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

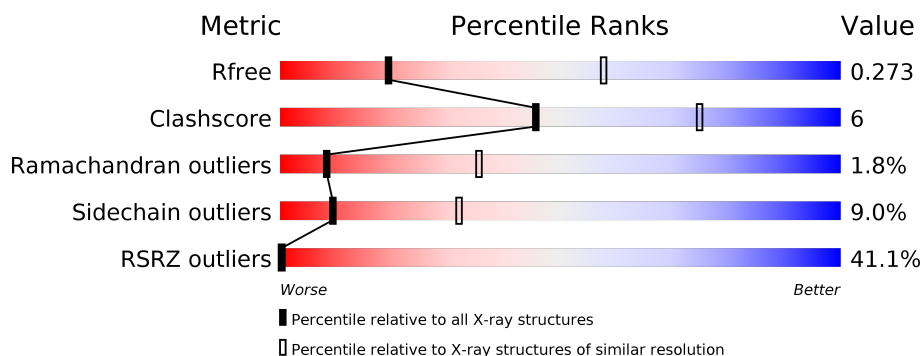
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	497	<div> <div>37%</div> <div> <div>66%</div> <div>18%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	497	<div> <div>33%</div> <div> <div>65%</div> <div>18%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	497	<div> <div>35%</div> <div> <div>65%</div> <div>19%</div> <div>•</div> <div>15%</div> </div> </div>

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10110 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	425	Total	C	N	O	S	0	0	0
			3351	2137	566	636	12			
1	B	425	Total	C	N	O	S	0	0	0
			3351	2137	566	636	12			
1	C	423	Total	C	N	O	S	0	0	0
			3333	2125	562	634	12			

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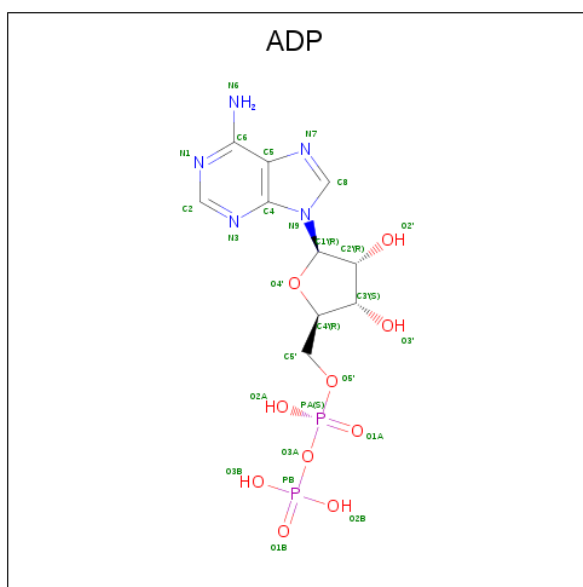
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Chain	Residue	Modelled	Actual	Comment	Reference
C	627	GLY	GLU	engineered mutation	UNP O67077

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- 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	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

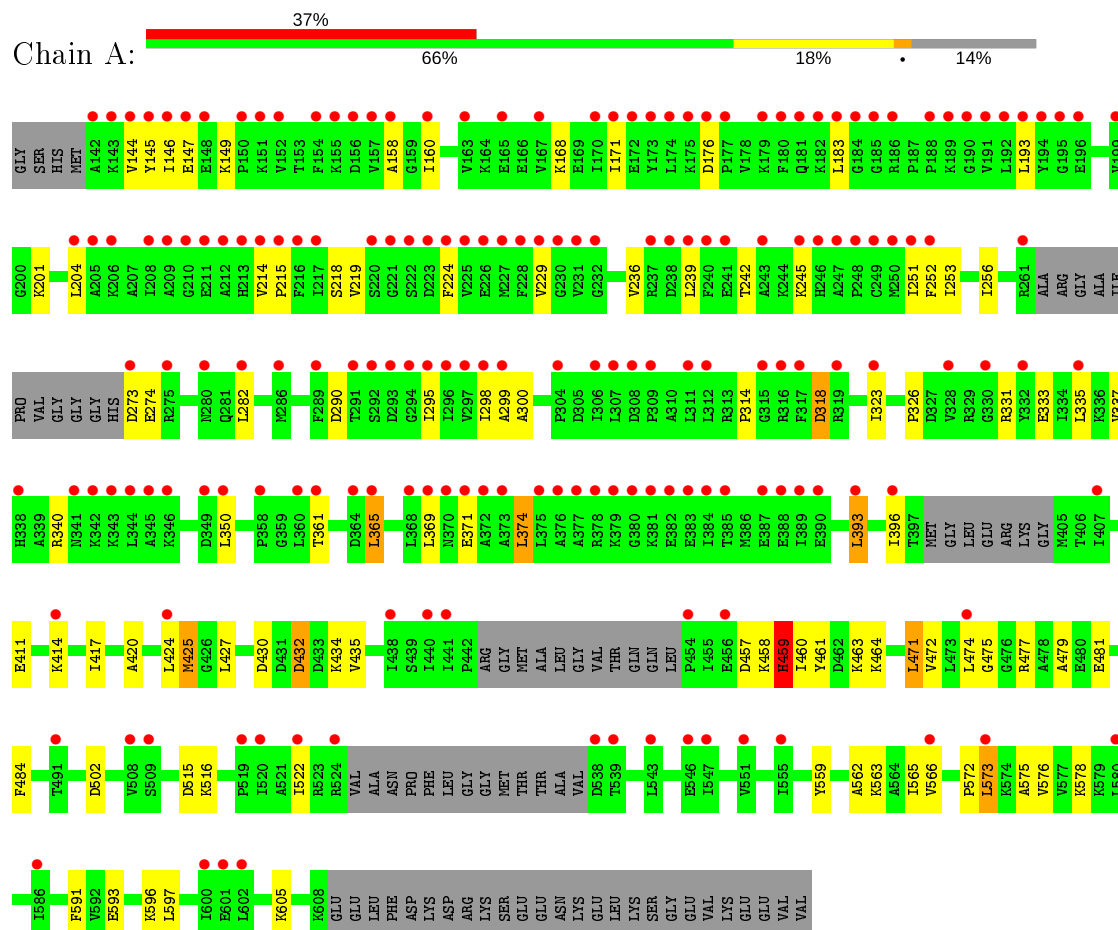
- Molecule 5 is water.

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

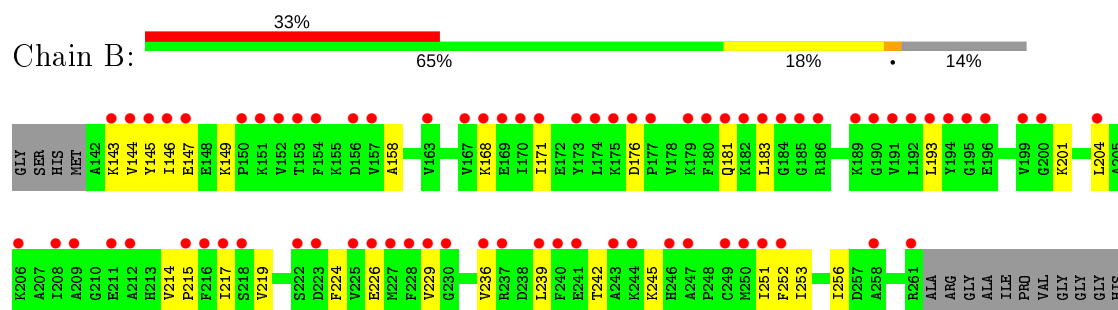
3 Residue-property plots

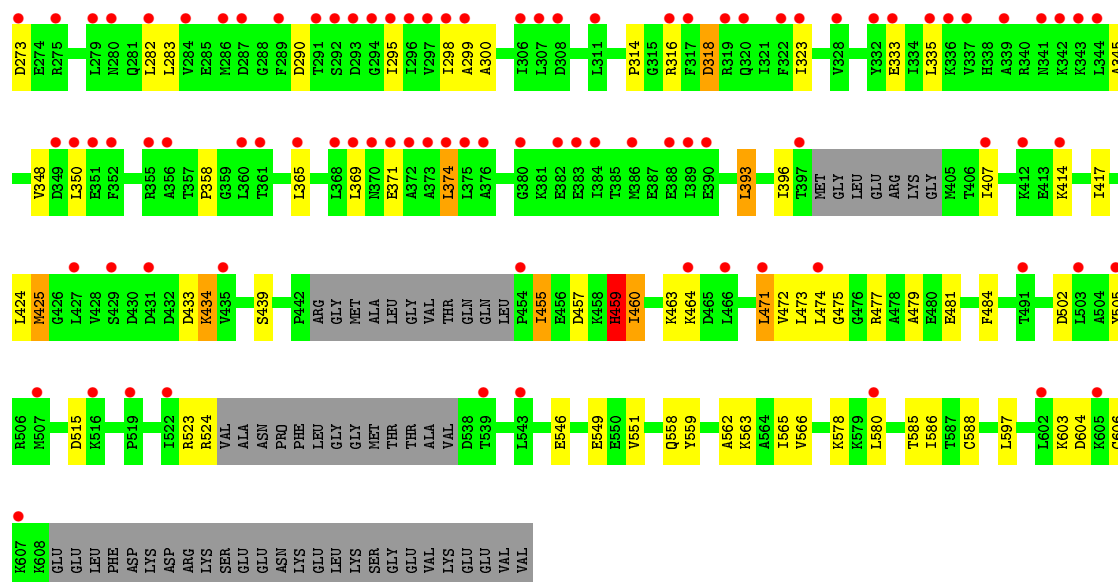
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

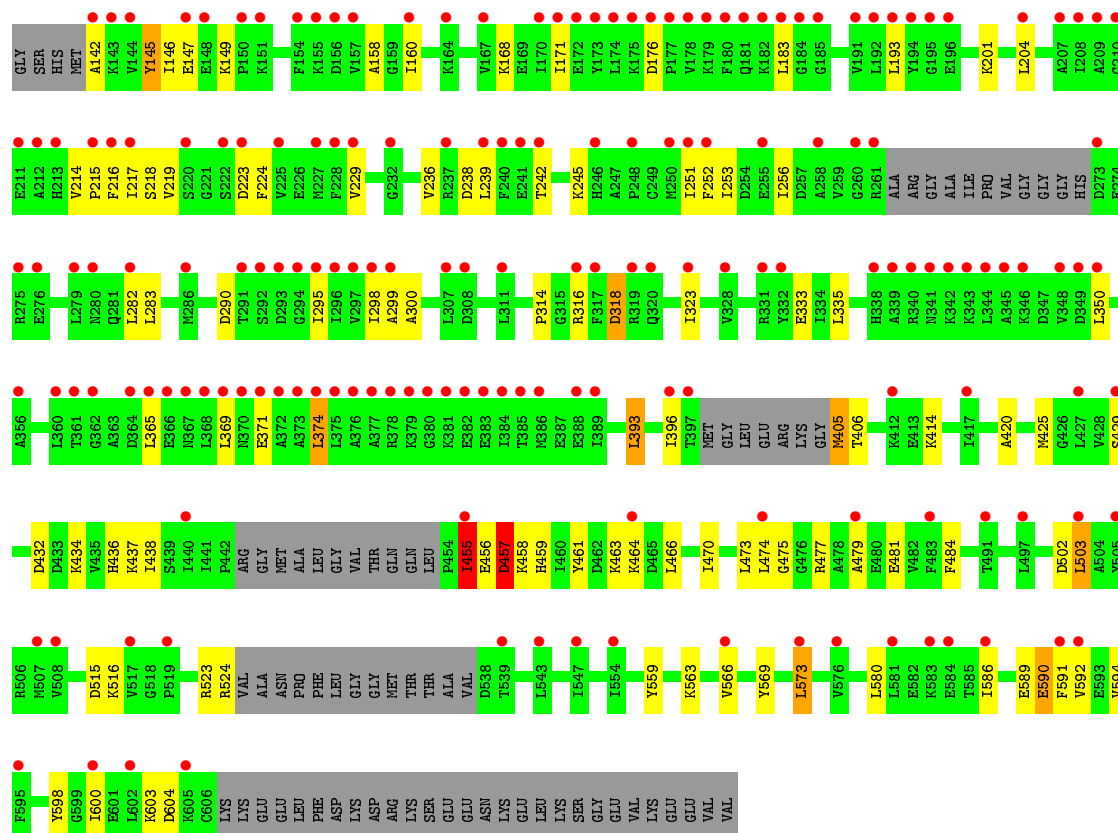


- Molecule 1: ATP-dependent zinc metalloprotease FtsH





• 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	127.86 Å 188.48 Å 206.22 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.51 – 3.25 94.24 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (64.51-3.25) 99.3 (94.24-3.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.26 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.226 , 0.253 0.245 , 0.273	Depositor DCC
R_{free} test set	2006 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	124.1	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 203.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10110	wwPDB-VP
Average B, all atoms (Å ²)	221.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% 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, SO4, 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	0.52	0/3399	0.67	1/4568 (0.0%)
1	B	0.51	0/3399	0.66	1/4568 (0.0%)
1	C	0.50	0/3381	0.66	0/4546
All	All	0.51	0/10179	0.66	2/13682 (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	459	HIS	C-N-CA	5.16	134.61	121.70
1	B	459	HIS	C-N-CA	5.16	134.60	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	3351	0	3449	41	0
1	B	3351	0	3449	43	0
1	C	3333	0	3423	47	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	0	0
3	C	27	0	12	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	10110	0	10345	130	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 (130) 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:B:146:ILE:O	1:B:217:ILE:HA	1.70	0.91
1:B:147:GLU:HG2	1:B:217:ILE:HG12	1.59	0.84
1:C:142:ALA:N	1:C:223:ASP:HB3	2.02	0.76
1:A:424:LEU:HD21	1:A:565:ILE:HG22	1.74	0.69
1:A:479:ALA:HA	1:A:566:VAL:HG11	1.77	0.67
1:A:144:VAL:HB	1:A:219:VAL:HG23	1.82	0.62
1:C:436:HIS:CG	1:C:437:LYS:H	2.17	0.61
1:C:158:ALA:HB1	1:C:333:GLU:HB3	1.81	0.61
1:C:466:LEU:HD22	1:C:503:LEU:HD21	1.83	0.61
1:C:459:HIS:HD2	1:C:461:TYR:CZ	2.18	0.60
1:A:572:PRO:O	1:A:575:ALA:HB3	2.01	0.59
1:B:425:MET:HG3	1:B:471:LEU:HD13	1.84	0.59
1:B:144:VAL:HB	1:B:219:VAL:HG23	1.87	0.57
1:C:335:LEU:HB3	1:C:350:LEU:HD22	1.87	0.57
1:A:427:LEU:HG	1:A:435:VAL:HG21	1.85	0.56
1:A:411:GLU:OE2	1:B:459:HIS:HD2	1.88	0.56
1:A:158:ALA:HB1	1:A:333:GLU:HB3	1.87	0.56
1:A:477:ARG:HG3	1:A:559:TYR:CE1	2.42	0.55
1:C:470:ILE:HG13	1:C:503:LEU:HD13	1.89	0.55
1:A:335:LEU:HB3	1:A:350:LEU:HD22	1.89	0.54
1:B:588:CYS:HG	1:B:606:CYS:HG	1.52	0.54
1:A:146:ILE:HD13	1:A:218:SER:HB3	1.90	0.53
1:A:420:ALA:HB1	1:A:573:LEU:HD22	1.91	0.53
1:B:393:LEU:HA	1:B:396:ILE:HD12	1.91	0.52
1:B:477:ARG:HG3	1:B:559:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HA	1:A:396:ILE:HD12	1.92	0.51
1:B:149:LYS:HE3	1:B:215:PRO:HG3	1.93	0.51
1:C:477:ARG:HG3	1:C:559:TYR:CE1	2.45	0.51
1:B:580:LEU:HD13	1:B:586:ILE:HG12	1.93	0.51
1:C:393:LEU:HA	1:C:396:ILE:HD12	1.92	0.51
1:B:335:LEU:HB3	1:B:350:LEU:HD22	1.93	0.51
1:C:149:LYS:HE3	1:C:215:PRO:HG3	1.93	0.51
1:A:149:LYS:HE3	1:A:215:PRO:HG3	1.93	0.50
1:C:252:PHE:HA	1:C:298:ILE:O	2.12	0.49
1:B:252:PHE:HA	1:B:298:ILE:O	2.12	0.49
1:C:566:VAL:HG13	1:C:573:LEU:HD12	1.95	0.49
1:A:424:LEU:CD2	1:A:565:ILE:HG22	2.42	0.49
1:A:252:PHE:HA	1:A:298:ILE:O	2.12	0.49
1:C:420:ALA:HB1	1:C:573:LEU:CD2	2.43	0.49
1:C:590:GLU:O	1:C:594:VAL:HG23	2.12	0.48
1:A:559:TYR:CE2	1:A:563:LYS:HD2	2.48	0.48
1:B:158:ALA:HB1	1:B:333:GLU:HB3	1.94	0.48
1:B:559:TYR:CE2	1:B:563:LYS:HD2	2.47	0.48
1:B:459:HIS:O	1:B:460:ILE:HG12	2.14	0.48
1:A:168:LYS:HA	1:A:171:ILE:HD12	1.95	0.47
1:B:588:CYS:SG	1:B:606:CYS:SG	3.07	0.47
1:C:559:TYR:CE2	1:C:563:LYS:HD2	2.49	0.47
1:B:168:LYS:HA	1:B:171:ILE:HD12	1.96	0.47
1:B:242:THR:HA	1:B:245:LYS:HE3	1.95	0.47
1:B:479:ALA:HA	1:B:566:VAL:HG11	1.95	0.47
1:C:168:LYS:HA	1:C:171:ILE:HD12	1.95	0.47
1:C:242:THR:HA	1:C:245:LYS:HE3	1.96	0.47
1:B:471:LEU:HB2	1:B:558:GLN:HE21	1.81	0.47
1:A:242:THR:HA	1:A:245:LYS:HE3	1.96	0.46
1:C:580:LEU:HD13	1:C:586:ILE:HG12	1.97	0.46
1:A:471:LEU:HD22	1:A:562:ALA:HB2	1.99	0.45
1:C:459:HIS:CD2	1:C:461:TYR:CZ	3.03	0.45
1:A:326:PRO:HB2	1:A:331:ARG:HG3	1.98	0.45
1:A:420:ALA:HB1	1:A:573:LEU:CD2	2.46	0.45
1:C:239:LEU:HD21	1:C:251:ILE:HG21	1.98	0.45
1:B:256:ILE:HG21	1:B:299:ALA:HB1	1.99	0.45
1:C:256:ILE:HG21	1:C:299:ALA:HB1	1.99	0.45
1:A:432:ASP:HB2	1:A:605:LYS:HZ3	1.81	0.45
1:A:576:VAL:HG11	1:A:591:PHE:CD2	2.52	0.44
1:A:361:THR:O	1:A:365:LEU:HB2	2.18	0.44
1:A:425:MET:HB3	1:A:472:VAL:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LEU:HD21	1:B:251:ILE:HG21	1.98	0.44
1:C:146:ILE:HG22	1:C:147:GLU:H	1.81	0.44
1:C:145:TYR:HD1	1:C:219:VAL:HB	1.83	0.44
1:C:455:ILE:HD11	1:C:473:LEU:HD11	1.99	0.44
1:C:217:ILE:HB	1:C:251:ILE:HA	1.98	0.44
1:C:457:ASP:HB2	1:C:458:LYS:H	1.69	0.44
1:C:436:HIS:CG	1:C:437:LYS:N	2.86	0.44
1:C:479:ALA:HA	1:C:566:VAL:HG11	2.00	0.44
1:A:239:LEU:HD21	1:A:251:ILE:HG21	1.99	0.44
1:A:256:ILE:HG21	1:A:299:ALA:HB1	2.00	0.44
1:B:193:LEU:HD21	1:B:204:LEU:HD23	2.00	0.43
1:B:505:TYR:CE2	1:B:551:VAL:HG11	2.53	0.43
1:A:593:GLU:HA	1:A:596:LYS:HE3	2.01	0.43
1:B:439:SER:HB2	1:B:585:THR:HG23	2.00	0.43
1:B:414:LYS:HD3	1:B:484:PHE:CD2	2.54	0.43
1:A:193:LEU:HD21	1:A:204:LEU:HD23	2.00	0.43
1:C:594:VAL:O	1:C:598:TYR:HD1	2.01	0.43
1:B:236:VAL:HG11	1:B:282:LEU:HA	2.01	0.43
1:C:569:TYR:HD1	1:C:600:ILE:HD13	1.84	0.43
1:A:474:LEU:HD13	1:A:559:TYR:HB2	2.00	0.42
1:C:193:LEU:HD21	1:C:204:LEU:HD23	2.01	0.42
1:C:414:LYS:HD3	1:C:484:PHE:CE2	2.54	0.42
1:C:201:LYS:HD2	1:C:300:ALA:HB1	2.01	0.42
1:C:283:LEU:HB3	1:C:316:ARG:HD3	2.02	0.42
1:B:424:LEU:HD21	1:B:565:ILE:HG22	1.99	0.42
1:C:236:VAL:HG11	1:C:282:LEU:HA	2.00	0.42
1:B:455:ILE:N	1:B:455:ILE:HD13	2.34	0.42
1:A:371:GLU:HA	1:A:374:LEU:HB2	2.02	0.42
1:C:371:GLU:HA	1:C:374:LEU:HB2	2.02	0.42
1:B:546:GLU:O	1:B:549:GLU:HG2	2.20	0.42
1:B:473:LEU:HA	1:B:473:LEU:HD23	1.90	0.42
1:B:603:LYS:HZ2	1:B:604:ASP:H	1.67	0.42
1:C:405:MET:HB3	1:C:406:THR:H	1.74	0.42
1:C:474:LEU:HD13	1:C:559:TYR:HB2	2.01	0.42
1:A:414:LYS:HD3	1:A:484:PHE:CE2	2.55	0.42
1:B:219:VAL:HG13	1:B:253:ILE:HG23	2.01	0.42
1:B:201:LYS:HD2	1:B:300:ALA:HB1	2.02	0.41
1:A:314:PRO:HA	1:A:318:ASP:HB3	2.01	0.41
1:A:236:VAL:HG11	1:A:282:LEU:HA	2.01	0.41
1:A:201:LYS:HD2	1:A:300:ALA:HB1	2.02	0.41
1:A:414:LYS:HD3	1:A:484:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:MET:HB3	1:B:472:VAL:HA	2.02	0.41
1:C:414:LYS:HD3	1:C:484:PHE:CD2	2.55	0.41
1:A:219:VAL:HG13	1:A:253:ILE:HG23	2.02	0.41
1:A:459:HIS:HB3	1:A:461:TYR:CE1	2.55	0.41
1:B:371:GLU:HA	1:B:374:LEU:HB2	2.02	0.41
1:B:283:LEU:HD22	1:B:316:ARG:HD3	2.01	0.41
1:B:314:PRO:HA	1:B:318:ASP:HB3	2.02	0.41
1:C:314:PRO:HA	1:C:318:ASP:HB3	2.02	0.41
1:A:427:LEU:HD23	1:A:605:LYS:HB2	2.02	0.41
1:B:358:PRO:HB2	1:B:407:ILE:HB	2.02	0.41
1:B:471:LEU:HD22	1:B:562:ALA:HB2	2.02	0.41
1:C:216:PHE:CE2	1:C:218:SER:HB2	2.55	0.41
1:C:420:ALA:HB1	1:C:573:LEU:HD22	2.01	0.41
1:A:337:VAL:HG13	1:A:340:ARG:HH21	1.86	0.41
1:C:146:ILE:HD12	1:C:218:SER:HB3	2.03	0.41
1:C:219:VAL:HG13	1:C:253:ILE:HG23	2.01	0.41
1:C:438:ILE:HB	1:C:586:ILE:HG13	2.03	0.41
1:B:345:ALA:HB3	1:B:348:VAL:HG13	2.04	0.40
1:B:417:ILE:HD12	1:B:484:PHE:CZ	2.56	0.40
1:A:417:ILE:HD12	1:A:484:PHE:CZ	2.57	0.40
1:B:474:LEU:HD13	1:B:559:TYR:HB2	2.03	0.40
1:C:146:ILE:HG22	1:C:147:GLU:N	2.36	0.40
1:C:459:HIS:HD2	1:C:461:TYR:CE2	2.39	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	415/497 (84%)	379 (91%)	28 (7%)	8 (2%)	8	34
1	B	415/497 (84%)	378 (91%)	31 (8%)	6 (1%)	11	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	413/497 (83%)	373 (90%)	32 (8%)	8 (2%)	8	34
All	All	1243/1491 (83%)	1130 (91%)	91 (7%)	22 (2%)	8	35

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	ILE
1	C	434	LYS
1	C	455	ILE
1	C	604	ASP
1	A	147	GLU
1	A	229	VAL
1	B	229	VAL
1	B	460	ILE
1	C	229	VAL
1	C	589	GLU
1	A	145	TYR
1	A	434	LYS
1	A	459	HIS
1	B	434	LYS
1	C	457	ASP
1	C	523	ARG
1	A	458	LYS
1	B	145	TYR
1	B	459	HIS
1	B	475	GLY
1	A	475	GLY
1	C	475	GLY

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	360/415 (87%)	330 (92%)	30 (8%)	11	36
1	B	360/415 (87%)	328 (91%)	32 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	358/415 (86%)	323 (90%)	35 (10%)	8	29
All	All	1078/1245 (87%)	981 (91%)	97 (9%)	9	32

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ILE
1	A	176	ASP
1	A	183	LEU
1	A	214	VAL
1	A	224	PHE
1	A	273	ASP
1	A	274	GLU
1	A	290	ASP
1	A	295	ILE
1	A	318	ASP
1	A	323	ILE
1	A	365	LEU
1	A	369	LEU
1	A	374	LEU
1	A	393	LEU
1	A	425	MET
1	A	430	ASP
1	A	432	ASP
1	A	457	ASP
1	A	463	LYS
1	A	464	LYS
1	A	471	LEU
1	A	481	GLU
1	A	502	ASP
1	A	515	ASP
1	A	516	LYS
1	A	522	ILE
1	A	573	LEU
1	A	578	LYS
1	A	597	LEU
1	B	143	LYS
1	B	176	ASP
1	B	181	GLN
1	B	183	LEU
1	B	214	VAL
1	B	224	PHE

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Mol	Chain	Res	Type
1	B	226	GLU
1	B	273	ASP
1	B	290	ASP
1	B	295	ILE
1	B	318	ASP
1	B	323	ILE
1	B	365	LEU
1	B	369	LEU
1	B	374	LEU
1	B	393	LEU
1	B	425	MET
1	B	433	ASP
1	B	434	LYS
1	B	455	ILE
1	B	457	ASP
1	B	459	HIS
1	B	463	LYS
1	B	464	LYS
1	B	471	LEU
1	B	481	GLU
1	B	502	ASP
1	B	515	ASP
1	B	523	ARG
1	B	524	ARG
1	B	578	LYS
1	B	597	LEU
1	C	145	TYR
1	C	160	ILE
1	C	176	ASP
1	C	183	LEU
1	C	214	VAL
1	C	224	PHE
1	C	238	ASP
1	C	290	ASP
1	C	295	ILE
1	C	318	ASP
1	C	323	ILE
1	C	365	LEU
1	C	369	LEU
1	C	374	LEU
1	C	393	LEU
1	C	405	MET

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Mol	Chain	Res	Type
1	C	425	MET
1	C	429	SER
1	C	432	ASP
1	C	455	ILE
1	C	456	GLU
1	C	457	ASP
1	C	463	LYS
1	C	464	LYS
1	C	481	GLU
1	C	502	ASP
1	C	503	LEU
1	C	515	ASP
1	C	516	LYS
1	C	524	ARG
1	C	573	LEU
1	C	590	GLU
1	C	591	PHE
1	C	592	VAL
1	C	603	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	ASN
1	B	370	ASN
1	B	468	ASN
1	B	558	GLN
1	C	459	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 3 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	SO4	B	702	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	C	703	-	4,4,4	0.15	0	6,6,6	0.13	0
3	ADP	C	702	-	24,29,29	0.69	0	29,45,45	0.85	1 (3%)
3	ADP	A	702	-	24,29,29	0.70	0	29,45,45	0.85	1 (3%)
4	SO4	A	703	-	4,4,4	0.19	0	6,6,6	0.11	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	C	702	-	-	6/12/32/32	0/3/3/3
3	ADP	A	702	-	-	6/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	ADP	C5-C6-N6	2.27	123.80	120.35
3	A	702	ADP	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	ADP	PA-O3A-PB-O3B
3	A	702	ADP	C5'-O5'-PA-O1A
3	A	702	ADP	C5'-O5'-PA-O2A

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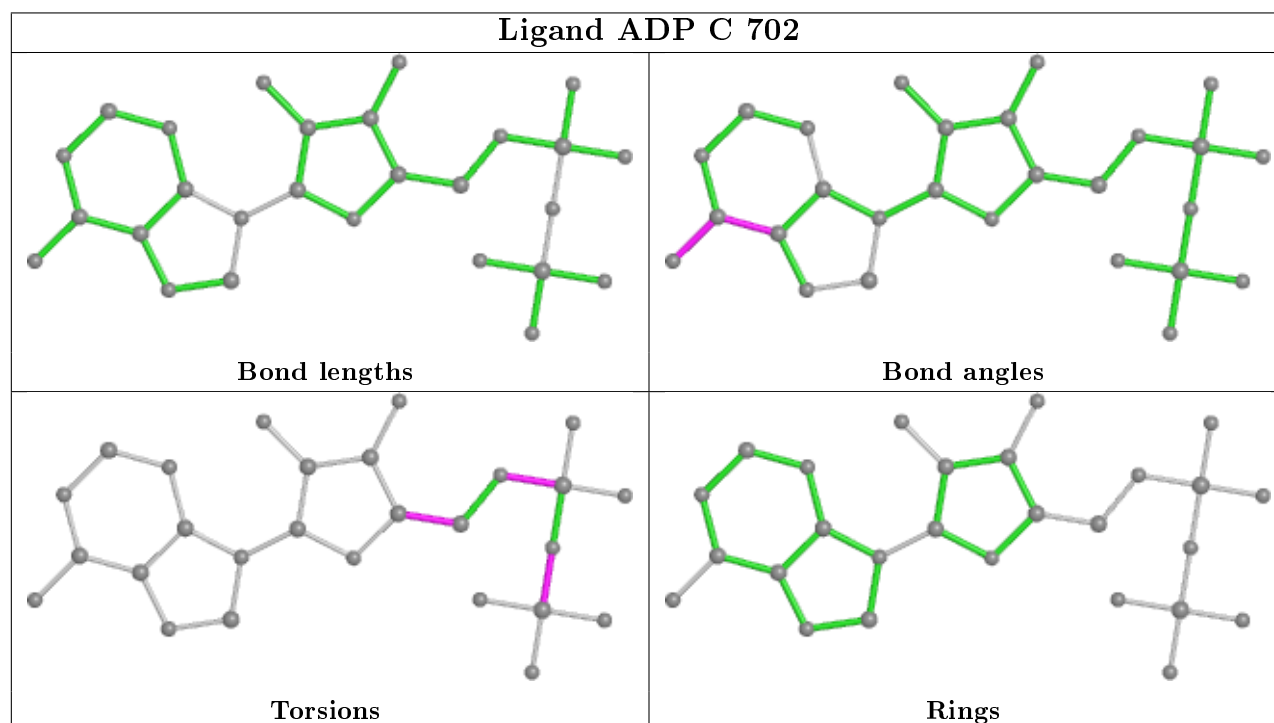
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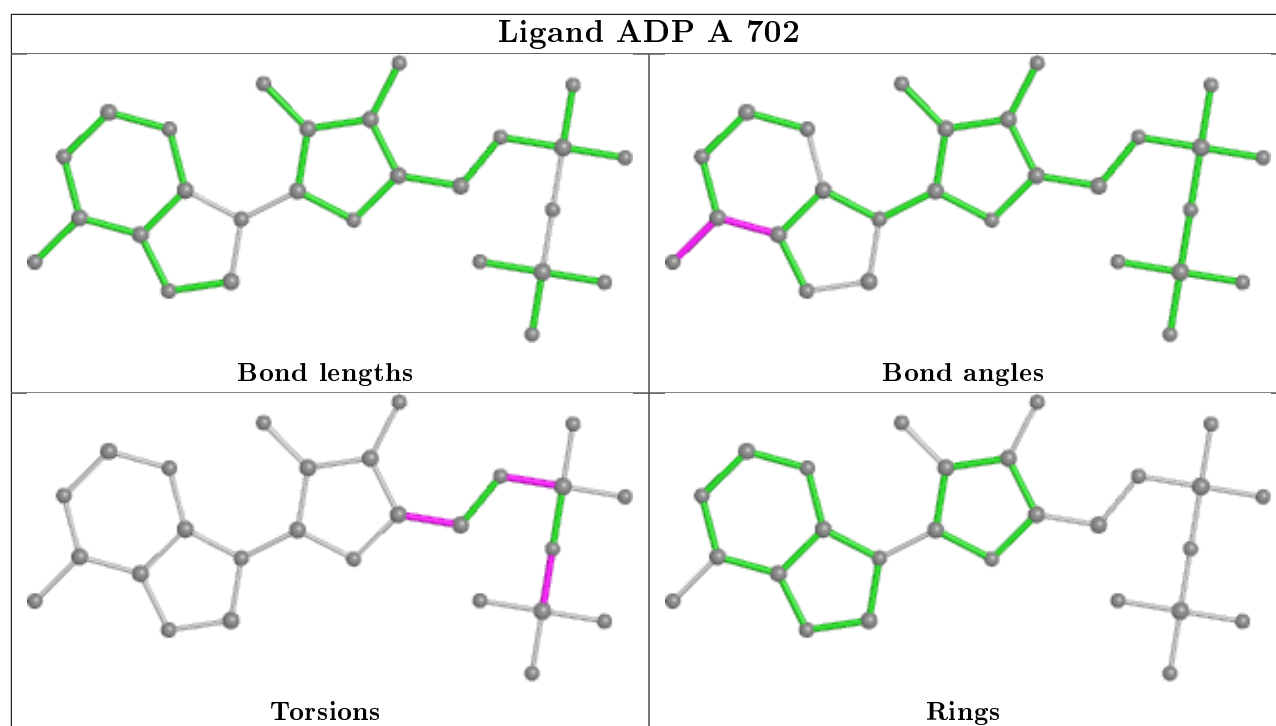
Mol	Chain	Res	Type	Atoms
3	A	702	ADP	C5'-O5'-PA-O3A
3	C	702	ADP	PA-O3A-PB-O3B
3	C	702	ADP	C5'-O5'-PA-O1A
3	C	702	ADP	C5'-O5'-PA-O2A
3	C	702	ADP	C5'-O5'-PA-O3A
3	A	702	ADP	O4'-C4'-C5'-O5'
3	A	702	ADP	C3'-C4'-C5'-O5'
3	C	702	ADP	O4'-C4'-C5'-O5'
3	C	702	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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	425/497 (85%)	2.91	184 (43%) 0 0	86, 270, 297, 299	0
1	B	425/497 (85%)	2.54	165 (38%) 0 0	85, 266, 296, 299	0
1	C	423/497 (85%)	2.83	174 (41%) 0 0	95, 273, 295, 298	0
All	All	1273/1491 (85%)	2.76	523 (41%) 0 0	85, 270, 296, 299	0

All (523) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	371	GLU	25.1
1	C	296	ILE	24.8
1	A	296	ILE	22.9
1	C	182	LYS	21.4
1	A	230	GLY	20.3
1	A	369	LEU	20.2
1	A	344	LEU	19.3
1	B	226	GLU	19.0
1	A	229	VAL	18.1
1	A	193	LEU	16.1
1	A	185	GLY	15.8
1	A	228	PHE	15.7
1	C	368	LEU	15.2
1	A	192	LEU	15.1
1	C	382	GLU	14.8
1	C	370	ASN	14.5
1	A	295	ILE	14.1
1	B	344	LEU	13.7
1	A	191	VAL	13.3
1	C	183	LEU	13.3
1	B	293	ASP	13.3
1	B	369	LEU	13.2
1	A	294	GLY	13.1

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Mol	Chain	Res	Type	RSRZ
1	A	184	GLY	13.1
1	C	195	GLY	12.9
1	B	292	SER	12.8
1	B	297	VAL	12.7
1	B	372	ALA	12.6
1	B	191	VAL	12.6
1	B	368	LEU	12.6
1	C	228	PHE	12.3
1	A	227	MET	12.0
1	C	372	ALA	11.8
1	C	143	LYS	11.8
1	C	157	VAL	11.8
1	A	250	MET	11.6
1	B	227	MET	11.4
1	B	144	VAL	11.4
1	C	250	MET	11.3
1	C	208	ILE	11.3
1	C	184	GLY	11.2
1	B	365	LEU	11.0
1	C	375	LEU	11.0
1	A	343	LYS	11.0
1	A	248	PRO	10.9
1	A	226	GLU	10.9
1	B	192	LEU	10.8
1	B	193	LEU	10.7
1	A	208	ILE	10.7
1	C	191	VAL	10.7
1	C	376	ALA	10.7
1	B	208	ILE	10.6
1	C	212	ALA	10.6
1	A	372	ALA	10.5
1	C	343	LYS	10.5
1	C	273	ASP	10.4
1	C	180	PHE	10.4
1	A	376	ALA	10.4
1	B	228	PHE	10.2
1	B	370	ASN	10.2
1	B	157	VAL	10.0
1	A	180	PHE	10.0
1	A	292	SER	9.9
1	A	297	VAL	9.8
1	A	380	GLY	9.8

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Mol	Chain	Res	Type	RSRZ
1	B	194	TYR	9.8
1	B	383	GLU	9.8
1	A	317	PHE	9.8
1	C	380	GLY	9.8
1	A	368	LEU	9.5
1	A	247	ALA	9.4
1	C	365	LEU	9.4
1	C	261	ARG	9.3
1	B	296	ILE	9.3
1	B	170	ILE	9.2
1	C	297	VAL	9.2
1	B	222	SER	9.1
1	B	185	GLY	9.1
1	A	342	LYS	9.0
1	C	374	LEU	9.0
1	C	175	LYS	8.9
1	A	167	VAL	8.8
1	A	307	LEU	8.8
1	C	383	GLU	8.7
1	C	185	GLY	8.7
1	C	369	LEU	8.7
1	C	179	LYS	8.7
1	A	183	LEU	8.6
1	B	151	LYS	8.6
1	C	339	ALA	8.6
1	C	210	GLY	8.6
1	A	365	LEU	8.5
1	B	295	ILE	8.4
1	C	232	GLY	8.4
1	A	231	VAL	8.4
1	A	171	ILE	8.3
1	A	147	GLU	8.3
1	C	295	ILE	8.2
1	B	147	GLU	8.2
1	B	180	PHE	8.2
1	A	157	VAL	8.2
1	B	176	ASP	8.1
1	C	239	LEU	8.0
1	C	193	LEU	8.0
1	C	240	PHE	7.9
1	A	332	TYR	7.9
1	A	375	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	194	TYR	7.9
1	C	229	VAL	7.9
1	A	220	SER	7.9
1	A	179	LYS	7.8
1	C	328	VAL	7.8
1	C	241	GLU	7.7
1	C	294	GLY	7.7
1	A	389	ILE	7.7
1	B	182	LYS	7.6
1	A	212	ALA	7.6
1	A	195	GLY	7.6
1	C	344	LEU	7.6
1	C	292	SER	7.6
1	A	170	ILE	7.6
1	B	286	MET	7.5
1	A	383	GLU	7.4
1	B	261	ARG	7.4
1	C	211	GLU	7.4
1	C	373	ALA	7.4
1	A	370	ASN	7.3
1	A	215	PRO	7.3
1	B	145	TYR	7.3
1	A	239	LEU	7.2
1	C	384	ILE	7.2
1	B	294	GLY	7.1
1	C	317	PHE	7.1
1	A	175	LYS	7.1
1	A	246	HIS	7.1
1	C	192	LEU	7.1
1	B	351	GLU	6.9
1	C	215	PRO	6.9
1	B	291	THR	6.8
1	C	377	ALA	6.8
1	C	147	GLU	6.8
1	A	345	ALA	6.8
1	B	343	LYS	6.7
1	C	176	ASP	6.7
1	C	396	ILE	6.6
1	C	155	LYS	6.6
1	C	150	PRO	6.5
1	B	163	VAL	6.5
1	B	317	PHE	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	350	LEU	6.5
1	B	154	PHE	6.5
1	A	174	LEU	6.4
1	B	375	LEU	6.4
1	A	252	PHE	6.4
1	B	183	LEU	6.3
1	B	273	ASP	6.3
1	C	170	ILE	6.3
1	C	348	VAL	6.2
1	C	602	LEU	6.2
1	B	237	ARG	6.1
1	C	142	ALA	6.1
1	B	240	PHE	6.1
1	C	148	GLU	6.1
1	A	384	ILE	6.1
1	B	239	LEU	6.1
1	C	174	LEU	6.0
1	C	227	MET	6.0
1	B	241	GLU	6.0
1	B	167	VAL	5.9
1	C	286	MET	5.9
1	B	179	LYS	5.9
1	A	173	TYR	5.9
1	A	306	ILE	5.9
1	B	376	ALA	5.9
1	A	143	LYS	5.8
1	B	336	LYS	5.8
1	A	361	THR	5.8
1	A	144	VAL	5.8
1	B	216	PHE	5.8
1	A	176	ASP	5.8
1	B	299	ALA	5.7
1	C	299	ALA	5.7
1	B	173	TYR	5.7
1	B	225	VAL	5.7
1	C	154	PHE	5.7
1	C	251	ILE	5.7
1	A	293	ASP	5.7
1	B	243	ALA	5.7
1	C	222	SER	5.6
1	A	182	LYS	5.5
1	A	150	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	311	LEU	5.5
1	C	338	HIS	5.5
1	A	280	ASN	5.5
1	A	275	ARG	5.5
1	C	181	GLN	5.5
1	C	275	ARG	5.5
1	B	171	ILE	5.4
1	A	273	ASP	5.4
1	A	241	GLU	5.4
1	C	167	VAL	5.3
1	A	381	LYS	5.3
1	A	142	ALA	5.3
1	A	232	GLY	5.2
1	B	388	GLU	5.2
1	C	293	ASP	5.2
1	A	238	ASP	5.2
1	B	607	LYS	5.2
1	B	275	ARG	5.2
1	A	349	ASP	5.1
1	C	291	THR	5.1
1	B	352	PHE	5.1
1	A	289	PHE	5.1
1	B	143	LYS	5.0
1	C	307	LEU	5.0
1	A	163	VAL	5.0
1	A	211	GLU	4.9
1	A	199	VAL	4.9
1	B	389	ILE	4.9
1	C	385	THR	4.9
1	B	373	ALA	4.9
1	C	237	ARG	4.9
1	B	169	GLU	4.8
1	A	298	ILE	4.7
1	B	386	MET	4.7
1	A	251	ILE	4.7
1	B	229	VAL	4.7
1	A	350	LEU	4.7
1	A	245	LYS	4.7
1	B	319	ARG	4.7
1	C	156	ASP	4.7
1	A	249	CYS	4.7
1	B	298	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	379	LYS	4.6
1	B	244	LYS	4.6
1	C	298	ILE	4.5
1	B	339	ALA	4.5
1	A	196	GLU	4.5
1	C	216	PHE	4.5
1	B	320	GLN	4.5
1	B	236	VAL	4.5
1	B	307	LEU	4.5
1	C	252	PHE	4.5
1	A	217	ILE	4.5
1	B	337	VAL	4.4
1	C	248	PRO	4.4
1	B	335	LEU	4.4
1	B	308	ASP	4.4
1	C	350	LEU	4.4
1	C	361	THR	4.4
1	A	286	MET	4.3
1	B	342	LYS	4.3
1	C	279	LEU	4.3
1	B	328	VAL	4.3
1	B	384	ILE	4.3
1	A	237	ARG	4.2
1	C	213	HIS	4.2
1	B	306	ILE	4.2
1	A	209	ALA	4.2
1	A	308	ASP	4.2
1	A	388	GLU	4.2
1	C	346	LYS	4.2
1	A	154	PHE	4.2
1	C	276	GLU	4.2
1	A	216	PHE	4.2
1	A	189	LYS	4.2
1	A	377	ALA	4.1
1	B	250	MET	4.1
1	A	360	LEU	4.1
1	B	175	LYS	4.1
1	C	173	TYR	4.1
1	C	308	ASP	4.1
1	A	152	VAL	4.0
1	C	223	ASP	4.0
1	B	247	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	156	ASP	4.0
1	B	211	GLU	4.0
1	A	223	ASP	4.0
1	C	364	ASP	4.0
1	C	381	LYS	4.0
1	A	214	VAL	4.0
1	A	240	PHE	3.9
1	A	315	GLY	3.9
1	B	382	GLU	3.9
1	C	209	ALA	3.9
1	C	389	ILE	3.9
1	C	280	ASN	3.9
1	C	367	ASN	3.9
1	C	591	PHE	3.8
1	B	204	LEU	3.8
1	C	217	ILE	3.8
1	C	204	LEU	3.8
1	C	412	LYS	3.7
1	A	319	ARG	3.7
1	C	388	GLU	3.7
1	A	158	ALA	3.7
1	A	328	VAL	3.7
1	B	152	VAL	3.7
1	A	323	ILE	3.6
1	A	385	THR	3.6
1	C	417	ILE	3.6
1	A	393	LEU	3.6
1	B	341	ASN	3.6
1	A	304	PRO	3.5
1	A	225	VAL	3.5
1	A	181	GLN	3.5
1	B	249	CYS	3.5
1	C	194	TYR	3.5
1	C	342	LYS	3.5
1	C	258	ALA	3.4
1	A	172	GLU	3.4
1	B	602	LEU	3.4
1	A	224	PHE	3.4
1	B	246	HIS	3.4
1	B	349	ASP	3.4
1	A	291	THR	3.4
1	A	186	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	431	ASP	3.3
1	A	382	GLU	3.3
1	A	390	GLU	3.3
1	A	145	TYR	3.3
1	C	319	ARG	3.3
1	B	280	ASN	3.3
1	B	371	GLU	3.3
1	C	151	LYS	3.3
1	C	474	LEU	3.3
1	B	199	VAL	3.3
1	C	583	LYS	3.3
1	A	396	ILE	3.2
1	C	427	LEU	3.2
1	C	507	MET	3.2
1	A	206	LYS	3.2
1	B	361	THR	3.2
1	A	407	ILE	3.2
1	B	289	PHE	3.2
1	C	505	TYR	3.2
1	C	332	TYR	3.2
1	A	204	LEU	3.1
1	C	331	ARG	3.1
1	A	221	GLY	3.1
1	B	287	ASP	3.1
1	A	379	LYS	3.1
1	B	397	THR	3.1
1	B	258	ALA	3.1
1	C	196	GLU	3.1
1	C	345	ALA	3.1
1	B	217	ILE	3.1
1	A	213	HIS	3.1
1	B	284	VAL	3.1
1	C	386	MET	3.0
1	B	435	VAL	3.0
1	B	150	PRO	3.0
1	C	366	GLU	3.0
1	C	483	PHE	3.0
1	A	543	LEU	3.0
1	B	190	GLY	3.0
1	B	252	PHE	3.0
1	C	177	PRO	3.0
1	A	346	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	189	LYS	2.9
1	C	260	GLY	2.9
1	C	246	HIS	2.9
1	B	539	THR	2.9
1	B	230	GLY	2.9
1	C	349	ASP	2.9
1	B	209	ALA	2.9
1	C	242	THR	2.9
1	C	360	LEU	2.9
1	C	455	ILE	2.9
1	B	196	GLU	2.9
1	B	184	GLY	2.9
1	A	312	LEU	2.9
1	A	156	ASP	2.9
1	A	282	LEU	2.9
1	B	332	TYR	2.8
1	B	374	LEU	2.8
1	C	566	VAL	2.8
1	C	397	THR	2.8
1	C	311	LEU	2.8
1	B	407	ILE	2.8
1	B	153	THR	2.8
1	B	215	PRO	2.8
1	A	438	ILE	2.8
1	C	316	ARG	2.7
1	A	335	LEU	2.7
1	A	299	ALA	2.7
1	A	522	ILE	2.7
1	B	311	LEU	2.7
1	B	466	LEU	2.7
1	C	519	PRO	2.7
1	B	543	LEU	2.7
1	A	222	SER	2.7
1	A	440	ILE	2.7
1	C	543	LEU	2.6
1	A	338	HIS	2.6
1	A	573	LEU	2.6
1	B	390	GLU	2.6
1	C	440	ILE	2.6
1	C	595	PHE	2.6
1	B	218	SER	2.6
1	C	255	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	580	LEU	2.6
1	C	172	GLU	2.6
1	A	151	LYS	2.6
1	A	358	PRO	2.6
1	C	517	VAL	2.5
1	B	146	ILE	2.5
1	C	378	ARG	2.5
1	A	316	ARG	2.5
1	A	539	THR	2.5
1	A	508	VAL	2.5
1	B	323	ILE	2.5
1	C	464	LYS	2.5
1	C	362	GLY	2.5
1	C	282	LEU	2.5
1	A	454	PRO	2.5
1	A	190	GLY	2.5
1	A	309	PRO	2.5
1	C	207	ALA	2.5
1	A	547	ILE	2.5
1	A	210	GLY	2.5
1	A	566	VAL	2.5
1	C	586	ILE	2.5
1	B	168	LYS	2.5
1	A	441	ILE	2.5
1	B	580	LEU	2.4
1	A	177	PRO	2.4
1	B	516	LYS	2.4
1	B	474	LEU	2.4
1	C	592	VAL	2.4
1	B	174	LEU	2.4
1	B	186	ARG	2.4
1	A	155	LYS	2.4
1	B	181	GLN	2.4
1	B	177	PRO	2.4
1	A	456	GLU	2.4
1	B	333	GLU	2.4
1	A	474	LEU	2.4
1	C	340	ARG	2.3
1	B	519	PRO	2.3
1	B	316	ARG	2.3
1	B	282	LEU	2.3
1	A	243	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	212	ALA	2.3
1	C	497	LEU	2.3
1	B	505	TYR	2.3
1	A	509	SER	2.3
1	A	205	ALA	2.3
1	B	454	PRO	2.3
1	B	503	LEU	2.3
1	C	341	ASN	2.3
1	C	144	VAL	2.3
1	A	414	LYS	2.3
1	C	160	ILE	2.3
1	C	225	VAL	2.2
1	A	160	ILE	2.2
1	A	586	ILE	2.2
1	B	491	THR	2.2
1	C	323	ILE	2.2
1	C	547	ILE	2.2
1	C	576	VAL	2.2
1	A	188	PRO	2.2
1	A	551	VAL	2.2
1	A	330	GLY	2.2
1	B	356	ALA	2.2
1	B	223	ASP	2.2
1	C	491	THR	2.2
1	A	261	ARG	2.2
1	C	539	THR	2.2
1	A	146	ILE	2.2
1	B	206	LYS	2.2
1	C	573	LEU	2.2
1	A	378	ARG	2.2
1	C	164	LYS	2.2
1	C	220	SER	2.2
1	C	605	LYS	2.2
1	C	554	ILE	2.2
1	A	524	ARG	2.2
1	C	508	VAL	2.2
1	A	602	LEU	2.2
1	B	360	LEU	2.2
1	B	471	LEU	2.2
1	C	503	LEU	2.2
1	A	364	ASP	2.2
1	A	387	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	195	GLY	2.2
1	B	605	LYS	2.2
1	C	171	ILE	2.1
1	B	464	LYS	2.1
1	A	373	ALA	2.1
1	B	322	PHE	2.1
1	A	520	ILE	2.1
1	C	178	VAL	2.1
1	C	356	ALA	2.1
1	A	148	GLU	2.1
1	B	380	GLY	2.1
1	B	355	ARG	2.1
1	A	424	LEU	2.1
1	B	200	GLY	2.1
1	B	279	LEU	2.1
1	C	584	GLU	2.1
1	C	320	GLN	2.1
1	A	601	GLU	2.1
1	B	414	LYS	2.1
1	A	555	ILE	2.1
1	A	165	GLU	2.1
1	B	412	LYS	2.1
1	A	519	PRO	2.1
1	B	427	LEU	2.1
1	A	546	GLU	2.0
1	A	371	GLU	2.0
1	A	341	ASN	2.0
1	A	491	THR	2.0
1	B	429	SER	2.0
1	C	429	SER	2.0
1	A	600	ILE	2.0
1	B	251	ILE	2.0
1	C	479	ALA	2.0
1	A	538	ASP	2.0
1	B	522	ILE	2.0
1	C	600	ILE	2.0
1	B	507	MET	2.0
1	C	581	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

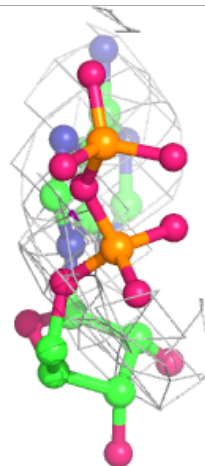
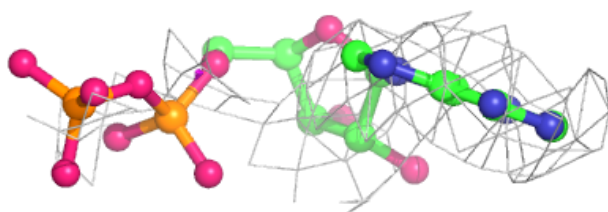
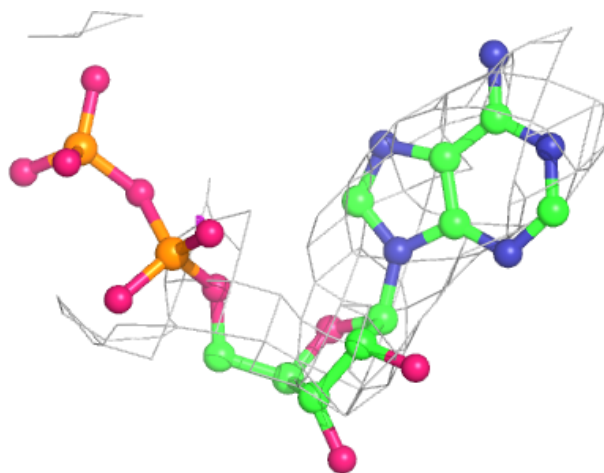
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

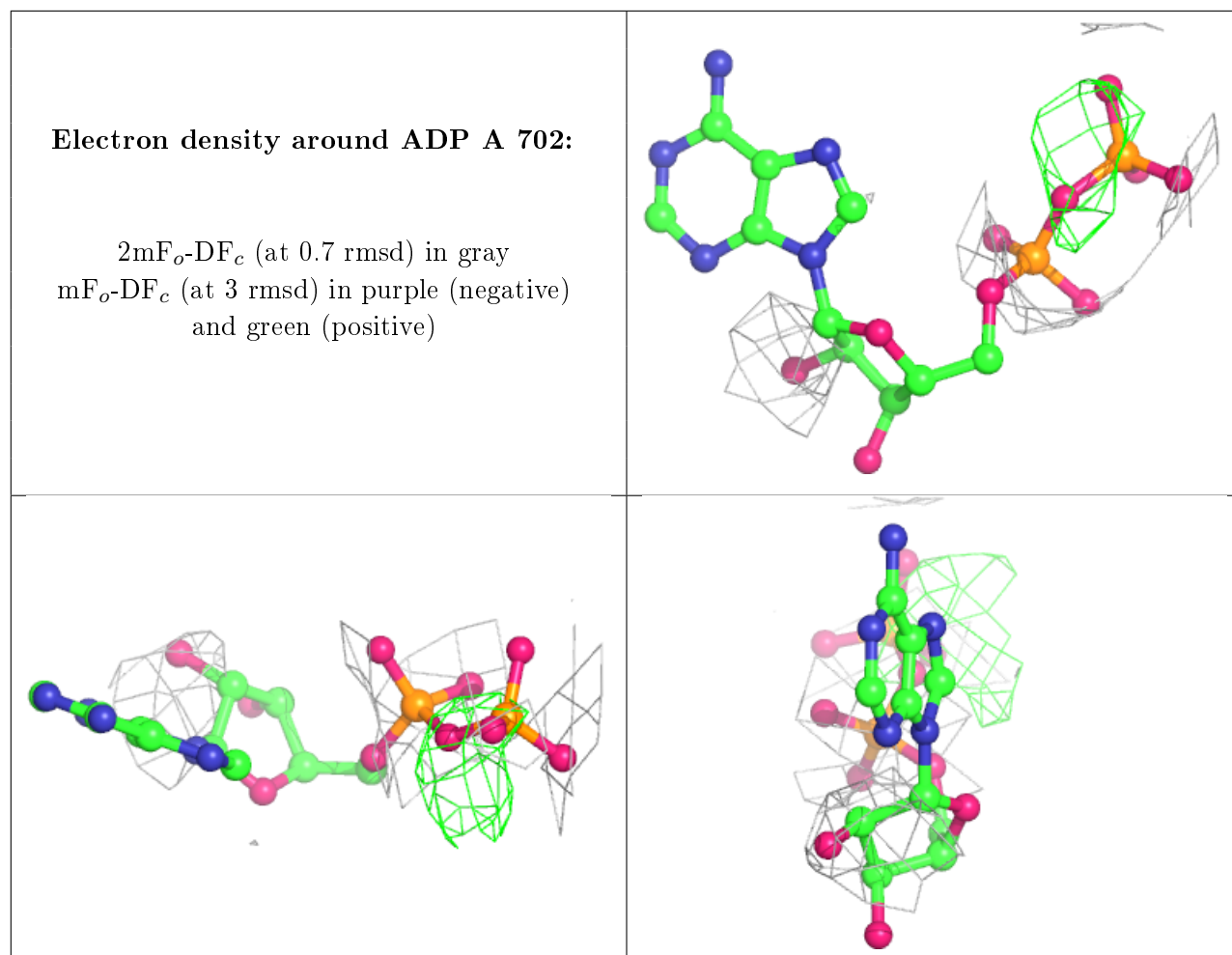
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	C	702	27/27	0.59	0.29	299,300,300,300	0
4	SO4	C	703	5/5	0.64	0.20	229,229,230,230	0
4	SO4	A	703	5/5	0.82	0.25	219,219,220,220	0
2	ZN	B	701	1/1	0.93	0.38	108,108,108,108	0
3	ADP	A	702	27/27	-	-	139,139,139,139	27
4	SO4	B	702	5/5	0.88	0.19	242,242,242,243	0
2	ZN	A	701	1/1	0.91	0.35	105,105,105,105	0
2	ZN	C	701	1/1	0.94	0.39	126,126,126,126	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 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.