



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 02:17 am BST

PDB ID : 4EIW  
Title : Whole cytosolic region of atp-dependent metalloprotease FtsH (G399L)  
Authors : Suno, R.; Niwa, H.; Tsuchiya, D.; Yoshida, M.; Morikawa, K.  
Deposited on : 2012-04-06  
Resolution : 3.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

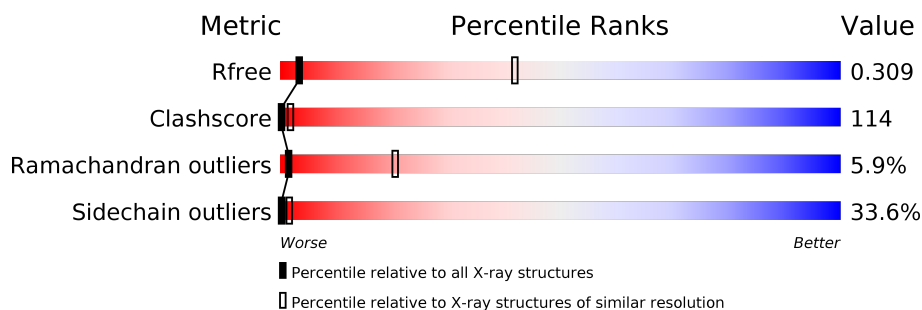
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	508	
1	B	508	
1	C	508	
1	D	508	
1	E	508	
1	F	508	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	B	2001	-	-	X	-
2	ADP	C	1001	-	-	X	-
2	ADP	D	2001	-	-	X	-
2	ADP	E	1001	-	-	X	-
2	ADP	F	2001	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21429 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	458	Total	C	N	O	S	0	0	0
			3578	2245	658	662	13			
1	B	446	Total	C	N	O	S	0	0	0
			3511	2206	641	651	13			
1	C	458	Total	C	N	O	S	0	0	0
			3578	2245	658	662	13			
1	D	446	Total	C	N	O	S	0	0	0
			3511	2206	641	651	13			
1	E	458	Total	C	N	O	S	0	0	0
			3578	2245	658	662	13			
1	F	446	Total	C	N	O	S	0	0	0
			3511	2206	641	651	13			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
A	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
A	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
A	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
A	121	SER	-	EXPRESSION TAG	UNP Q5SI82
A	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
A	123	MET	-	EXPRESSION TAG	UNP Q5SI82
A	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
A	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
A	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
B	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
B	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
B	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
B	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
B	121	SER	-	EXPRESSION TAG	UNP Q5SI82
B	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
B	123	MET	-	EXPRESSION TAG	UNP Q5SI82

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Chain	Residue	Modelled	Actual	Comment	Reference
B	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
B	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
B	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
C	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
C	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
C	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
C	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
C	121	SER	-	EXPRESSION TAG	UNP Q5SI82
C	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
C	123	MET	-	EXPRESSION TAG	UNP Q5SI82
C	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
C	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
C	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
D	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
D	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
D	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
D	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
D	121	SER	-	EXPRESSION TAG	UNP Q5SI82
D	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
D	123	MET	-	EXPRESSION TAG	UNP Q5SI82
D	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
D	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
D	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
E	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
E	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
E	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
E	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
E	121	SER	-	EXPRESSION TAG	UNP Q5SI82
E	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
E	123	MET	-	EXPRESSION TAG	UNP Q5SI82
E	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
E	125	ALA	-	EXPRESSION TAG	UNP Q5SI82
E	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82
F	117	GLY	-	EXPRESSION TAG	UNP Q5SI82
F	118	PRO	-	EXPRESSION TAG	UNP Q5SI82
F	119	LEU	-	EXPRESSION TAG	UNP Q5SI82
F	120	GLY	-	EXPRESSION TAG	UNP Q5SI82
F	121	SER	-	EXPRESSION TAG	UNP Q5SI82
F	122	HIS	-	EXPRESSION TAG	UNP Q5SI82
F	123	MET	-	EXPRESSION TAG	UNP Q5SI82
F	124	GLY	-	EXPRESSION TAG	UNP Q5SI82
F	125	ALA	-	EXPRESSION TAG	UNP Q5SI82

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Chain	Residue	Modelled	Actual	Comment	Reference
F	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82

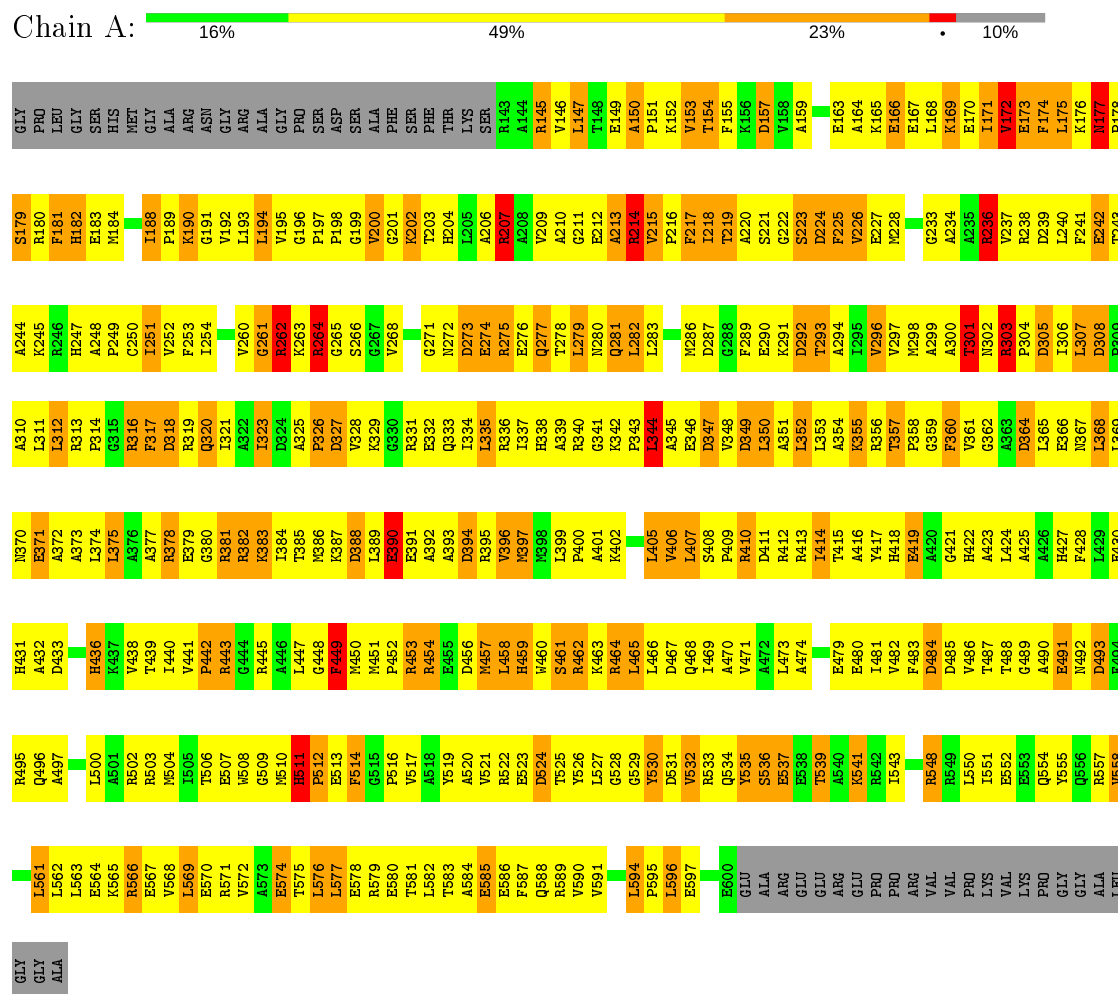
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10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

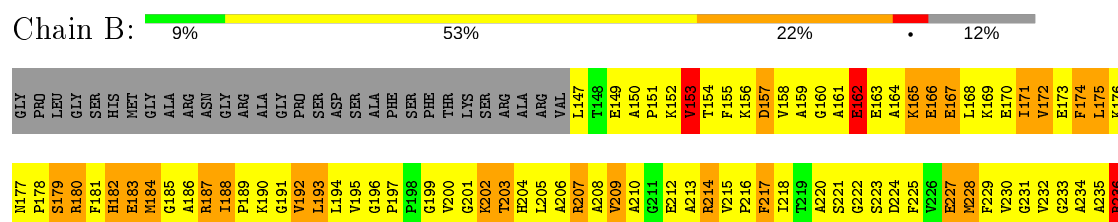
### 3 Residue-property plots

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. 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. 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

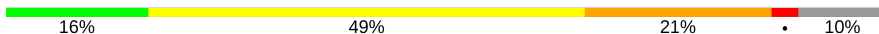


- Molecule 1: ATP-dependent zinc metalloprotease FtsH



V237	V287	T357	H418	E479	K541	GLU
R238	M298	P368	E419	E480	R542	GLU
D239	A299	I543	A420	I481	D644	ARG
L240	A300	F360	G421	V482	D644	GLU
F241	T301	G362	H422	F483	V547	PRO
E242	N302	D362	A423	D484	R548	PRO
T243	R303	A363	L424	D485	R549	ARG
K244	F304	D364	H427	V486	R550	VAL
K245	L365	D365	H427	T487	L550	VAL
R246	I306	E366	F428	T488	F551	PRO
H247	L307	E367	L429	G489	E552	LVS
L248	N308	L368	E430	A490	E553	VAL
A249	P309	L369	H431	E491	E554	LVS
C250	A310	N370	A432	N492	F555	PRO
	L311	E371	D433	D493	G556	GLY
	L251	A372	G434	F494	E557	GLY
	F252	A373	V435	R495	E558	ALA
	F253	L374	H436	Q496	K559	LEU
	I254	L375	K437	A497	A560	GLY
	D255	A376	V438	L500	L561	GLY
	E256	A377	T439	A501	L562	ALA
	I257	R378	V441	R502	E564	
	D258	R319	V441	R503	E565	
	V260	G320	P442	M504	R566	
	G261	I321	R443	I505	E567	
	G262	A322	G444	T506	E568	
	R263	I323	R445	E507	L569	
	ARG	D324	A446	W508	E570	
	GLY	A325	L447	G509	R571	
	SER	P326	G448	V146	V572	
	GLY	D327	F449	M510		
	VAL	V328	M450	B511		
	GLY	K329	M451	P512	L576	
	GLY	G330	R453	F514	L577	
	GLY	R331	R454		R579	
	I272	E332	R455	V517	E580	
	D273	Q333	D456	A518	T581	
	E274	I334	M457	F519	L582	
	R275	L335	L458	A520	T583	
	E276	R336	H459	V521	E584	
	Q277	R337	R460	R522	E585	
	L278	R338	S461	E523	E586	
	L279	A339	P462	D524	F587	
	I280	R340	R463	T525	Q588	
	Q281	G341	R464	V526	R589	
	L282	R342	V471	R532	L596	
	L283	P343	A472	R533	E597	
	V284	L344	L465	Q534	A598	
	E285	A345	L466	V591	E599	
	M286	A346	D467	G529	F174	
	M287	E346	Q468	F530	L175	
	D287	D347	I469	L594	K176	
	G288	V348	V532	P595	E242	
	F289	D349	A470	L596	T243	
	E290	L350	R410	E533		
	K291	A351	D411	Q534		
	D292	L352	R412	F535		
	T293	L353	R413	S536		
	A294	K354	R414	E537		
	K295	A355	I414	E600		
	V296	R356	A476	GLU		
			A477	ALA		
			A478	ARG		

• Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain C: 

GLY	S179	A244	A310	E371	A432	L561
PRO	R180	K245	L311	A372	D433	L562
LEU	F181	R246	L312	A373	H436	L563
ARG	H182	H247	R313	L374	K437	E564
SER	E183	A248	R316	I375	V438	E565
PRO	M184	C250	F317	A376	T439	E566
ARG		I188	D318	A377	L440	E567
VAL		P189	R319	R378	V441	E568
VAL		K190	Q320	E379	P442	L569
VAL		G191	I321	G380	R443	E570
LVS		V192	A322	R381	E444	E571
LVS		L193	E323	R382	R445	E572
PRO		L194	D324	I384	R446	E573
GLY		V195	A325	T385	L447	E574
GLY		G196	P326	K386	G448	T575
PRO		K197	D327	K387	F449	L576
ALA		P198	V328	D388	E450	L577
ASP		G199	K329	L389	M451	E578
SER		V200	G330	E390	P452	E579
ALA		A206	R336	E391	R453	E580
SER		R143	I337	R392	L458	E581
R143		A208	R338	K393	H459	E582
A144		E276	R339	M398	W460	Q583
R145		Q277	A339	L399	E461	F584
V146		T278	R340	P400	R462	E585
L147		G211	G341	A401	K463	E586
T148		E212	K342	K402	R464	E587
E149		A213	F343	L405	L465	E588
A150		R214	A344	V406	D466	E589
K152		V215	E346	L407	D467	E590
V153		P216	R347	S408	Q468	E591
T154		I218	V348	P409	L469	E592
F155		T219	D349	R410	A472	E593
R156		A220	L350	D411	L473	E594
D157		S221	A351	R412	F482	E595
V158		G222	L352	R413	E483	E596
A159		S223	L353	I414	D484	E597
		D224	A354	T415	A420	E598
		F225	K355	A416	G421	E599
		V226	R356	Y417	H422	E600
		E227	T357	H418	T483	
		M228	P358	E419	L424	
		G233	G359	D485	A425	
		A234	F360	D486	A426	
		E235	V361	D487	R427	
		R236	G362	L488	F428	
		V237	A363	E490	L429	
		R238	D364	A491	D493	
		D239	L365	E492	F494	
		L240	R366	E493	R495	
		F241	N367	E494		
		E242	L368	E495		
		T243	N370	E496		




GLY  
ALA

- Molecule 1: ATP-dependent zinc metalloprotease FtsH

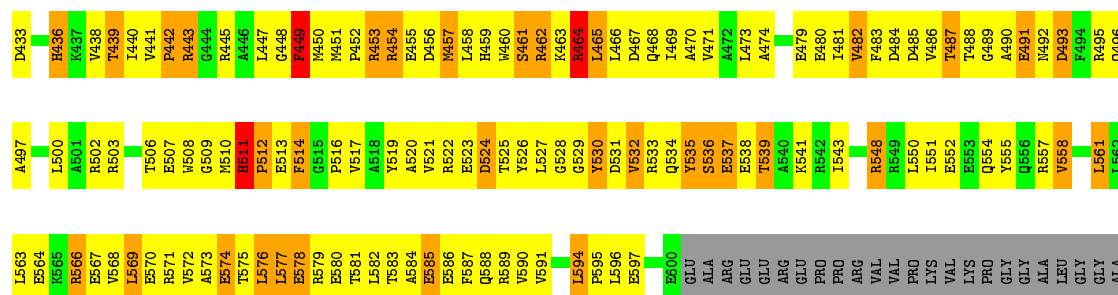
Chain D:  9% 52% 23% 12%

GLU	GLU	ARG	GLU	PRO	ARG	VAL	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GL
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- Molecule 1: ATP-dependent zinc metalloprotease FtsH

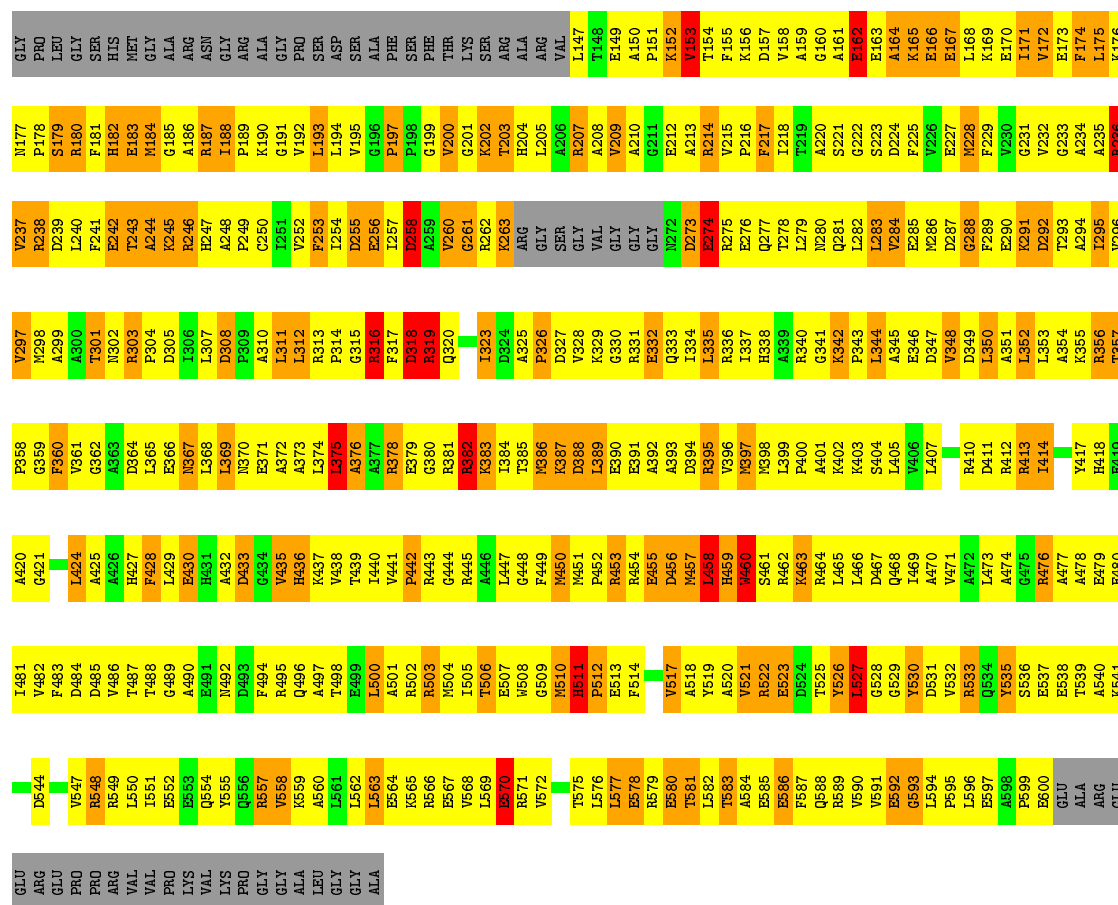
Chain E:  17% 49% 22% 10%

GLY	PRO	LEU	GLY	SER	HIS	MET	GLY	ALA	ARG	ASN	GLY	ARG	ALA	GLY	PRO	SER	ASP	ASP	SER	ALA	PHE	PHE	THR	LYS	SER	ARG	ALA	VAL	L147	T148	E149	A150	P151	K152	V153	T154	F155	K156	D157	V158	A159	E163	A164	E165	E166	E167	L168	K169	E170	V171	R172	F173	L174	L175	K176	A177	P178
S179	R180	F181	H182	E183	M184	I188	P189	K190	G191	V192	L193	L194	V195	G196	R261	K262	P197	K263	G199	V200	G201	T202	H204	L205	A206	D207	A208	V209	E270	A210	G211	P216	F217	I218	T219	A220	S221	G222	V226	E227	M228	G233	A234	A235	A300	T301	R238	D239	L240	F241	E242	T243					
A244	K245	E246	R247	L248	P249	C250	L251	V252	F253	L254	D255	E256	V260	G261	K262	P197	K263	G199	V200	G201	T202	H204	L205	A206	D207	A208	V209	E270	A210	G211	P216	F217	I218	T219	A220	S221	G222	V226	E227	M228	G233	A234	A235	A300	T301	R238	D239	L240	F241	E242	T243						
D308	P309	A310	L311	L312	R313	R316	F317	D318	R319	Q320	L321	A322	I323	G324	A325	P326	D327	V328	K329	E330	R331	E332	Q333	I334	L335	R336	H338	A339	R340	G341	K342	P343	L344	A345	E346	D347	V348	D349	L350	G351	T357	P358	G359	F360	V361	D364	L365	E366	N367	L368	L369						
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
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N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374	L375	A376	A377	V378	E379	G380	R381	R382	K383	I384	T385	K386	P387	D388	L389	E390	L391	A392	D393	R394	R395	V396	P397	E398	E399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424			
N370	E371	A372	A373	L374																																																					



• Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain F: 10% 52% 23% 12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.15Å 146.15Å 349.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.53 – 3.90 71.53 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (71.53-3.90) 97.1 (71.53-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.46 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.299 , 0.312 0.298 , 0.309	Depositor DCC
$R_{free}$ test set	1967 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.1	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 19.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.27$ , $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.237 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	21429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.60	3/3636 (0.1%)	0.95	16/4906 (0.3%)
1	B	0.63	3/3568 (0.1%)	1.01	18/4815 (0.4%)
1	C	0.59	2/3636 (0.1%)	1.03	24/4906 (0.5%)
1	D	0.60	2/3568 (0.1%)	0.98	17/4815 (0.4%)
1	E	0.61	6/3636 (0.2%)	0.96	13/4906 (0.3%)
1	F	0.58	2/3568 (0.1%)	0.96	12/4815 (0.2%)
All	All	0.60	18/21612 (0.1%)	0.98	100/29163 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
1	C	0	1
1	D	0	6
1	E	0	1
1	F	0	5
All	All	0	20

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	GLU	CD-OE1	-12.04	1.12	1.25
1	C	214	ARG	CZ-NH2	8.16	1.43	1.33
1	E	214	ARG	CZ-NH2	-8.12	1.22	1.33
1	E	319	ARG	CZ-NH1	-7.39	1.23	1.33
1	D	586	GLU	CD-OE1	-6.72	1.18	1.25

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	319	ARG	NE-CZ-NH2	18.11	129.36	120.30
1	C	207	ARG	NE-CZ-NH1	-15.37	112.61	120.30
1	A	316	ARG	NE-CZ-NH1	-15.14	112.73	120.30
1	B	236	ARG	NE-CZ-NH1	-14.64	112.98	120.30
1	C	207	ARG	NE-CZ-NH2	13.93	127.26	120.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	ALA	Peptide
1	A	532	VAL	Peptide
1	B	244	ALA	Peptide
1	B	288	GLY	Peptide
1	B	382	ARG	Peptide

## 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	3578	0	3623	862	5
1	B	3511	0	3556	851	3
1	C	3578	0	3623	815	0
1	D	3511	0	3556	851	3
1	E	3578	0	3623	805	3
1	F	3511	0	3556	857	2
2	A	27	0	12	8	0
2	B	27	0	12	9	0
2	C	27	0	12	10	0
2	D	27	0	12	9	0
2	E	27	0	12	11	0
2	F	27	0	12	10	0
All	All	21429	0	21609	4895	8

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 114.

The worst 5 of 4895 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:E:416:ALA:CB	1:E:577:LEU:HD23	1.18	1.63
1:A:416:ALA:HB3	1:A:577:LEU:CD2	1.33	1.58
1:A:416:ALA:CB	1:A:577:LEU:HD23	1.15	1.55
1:F:376:ALA:CA	1:F:381:ARG:HD2	1.31	1.55
1:E:416:ALA:HB3	1:E:577:LEU:CD2	1.35	1.55

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLU:CG	1:D:382:ARG:NH2[3_564]	1.61	0.59
1:A:417:TYR:OH	1:D:382:ARG:NE[3_564]	1.74	0.46
1:A:177:ASN:OD1	1:E:214:ARG:NH2[6_665]	1.85	0.35
1:B:238:ARG:NE	1:F:378:ARG:NH2[6_665]	1.91	0.29
1:A:570:GLU:CB	1:D:382:ARG:NH2[3_564]	2.08	0.12

## 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	456/508 (90%)	323 (71%)	111 (24%)	22 (5%)	2	24
1	B	442/508 (87%)	289 (65%)	125 (28%)	28 (6%)	1	19
1	C	456/508 (90%)	323 (71%)	112 (25%)	21 (5%)	2	25
1	D	442/508 (87%)	288 (65%)	121 (27%)	33 (8%)	1	16
1	E	456/508 (90%)	324 (71%)	110 (24%)	22 (5%)	2	24
1	F	442/508 (87%)	288 (65%)	120 (27%)	34 (8%)	1	16
All	All	2694/3048 (88%)	1835 (68%)	699 (26%)	160 (6%)	1	20

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	VAL
1	A	511	HIS
1	B	153	VAL
1	B	274	GLU
1	B	379	GLU

### 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	365/402 (91%)	240 (66%)	125 (34%)	0	1
1	B	361/402 (90%)	242 (67%)	119 (33%)	0	1
1	C	365/402 (91%)	240 (66%)	125 (34%)	0	1
1	D	361/402 (90%)	241 (67%)	120 (33%)	0	1
1	E	365/402 (91%)	244 (67%)	121 (33%)	0	1
1	F	361/402 (90%)	240 (66%)	121 (34%)	0	1
All	All	2178/2412 (90%)	1447 (66%)	731 (34%)	0	1

5 of 731 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	443	ARG
1	D	284	VAL
1	F	360	PHE
1	C	482	VAL
1	D	162	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	468	GLN
1	D	281	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	333	GLN
1	C	496	GLN
1	D	204	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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	D	2001	-	24,29,29	1.03	3 (12%)	29,45,45	1.45	5 (17%)
2	ADP	C	1001	-	24,29,29	1.10	3 (12%)	29,45,45	1.56	4 (13%)
2	ADP	E	1001	-	24,29,29	1.06	2 (8%)	29,45,45	1.45	4 (13%)
2	ADP	B	2001	-	24,29,29	1.05	2 (8%)	29,45,45	1.49	4 (13%)
2	ADP	A	1001	-	24,29,29	1.10	2 (8%)	29,45,45	1.50	4 (13%)
2	ADP	F	2001	-	24,29,29	1.01	1 (4%)	29,45,45	1.52	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the



Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	D	2001	-	-	2/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	E	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	B	2001	-	-	3/12/32/32	0/3/3/3
2	ADP	A	1001	-	-	2/12/32/32	0/3/3/3
2	ADP	F	2001	-	-	2/12/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ADP	C5-C4	2.78	1.48	1.40
2	F	2001	ADP	C5-C4	2.76	1.48	1.40
2	E	1001	ADP	C5-C4	2.73	1.48	1.40
2	C	1001	ADP	C5-C4	2.62	1.47	1.40
2	B	2001	ADP	C5-C4	2.59	1.47	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ADP	PA-O3A-PB	-4.26	118.21	132.83
2	C	1001	ADP	PA-O3A-PB	-4.20	118.40	132.83
2	E	1001	ADP	PA-O3A-PB	-4.05	118.92	132.83
2	B	2001	ADP	PA-O3A-PB	-3.99	119.13	132.83
2	C	1001	ADP	N3-C2-N1	-3.72	122.86	128.68

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

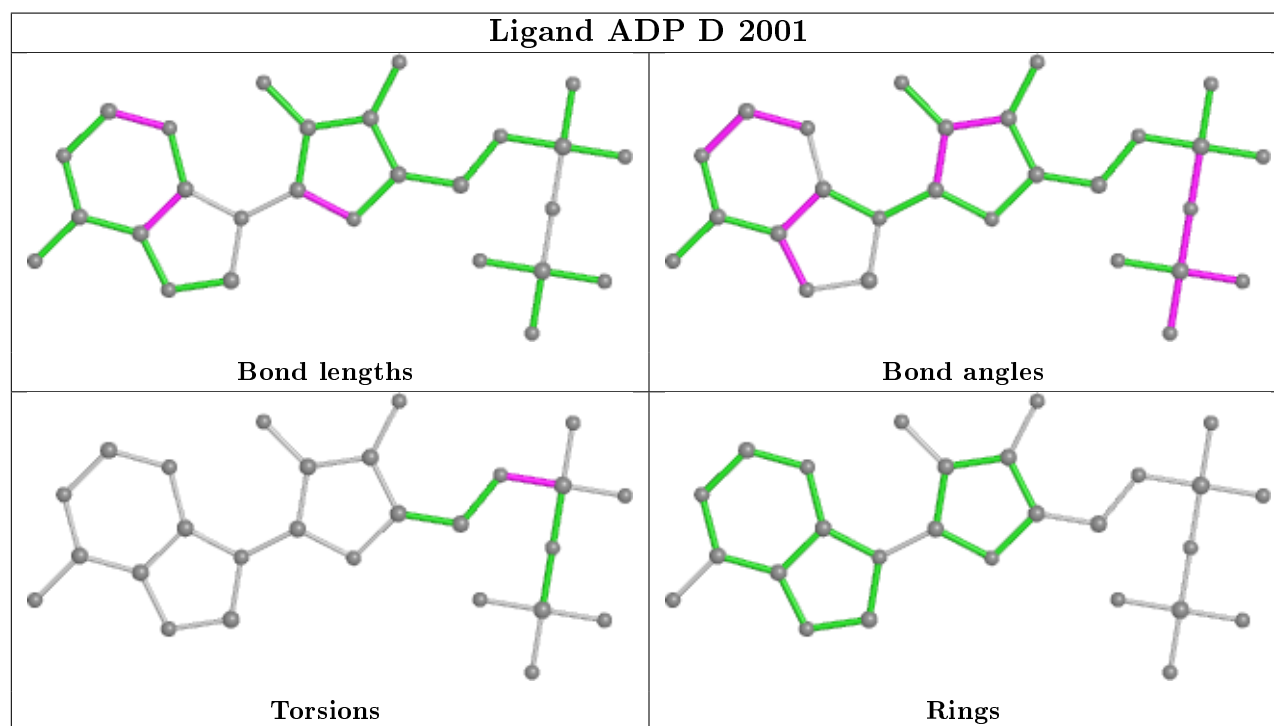
Mol	Chain	Res	Type	Atoms
2	D	2001	ADP	C5'-O5'-PA-O3A
2	C	1001	ADP	C5'-O5'-PA-O1A
2	C	1001	ADP	C5'-O5'-PA-O3A
2	E	1001	ADP	C5'-O5'-PA-O1A
2	B	2001	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

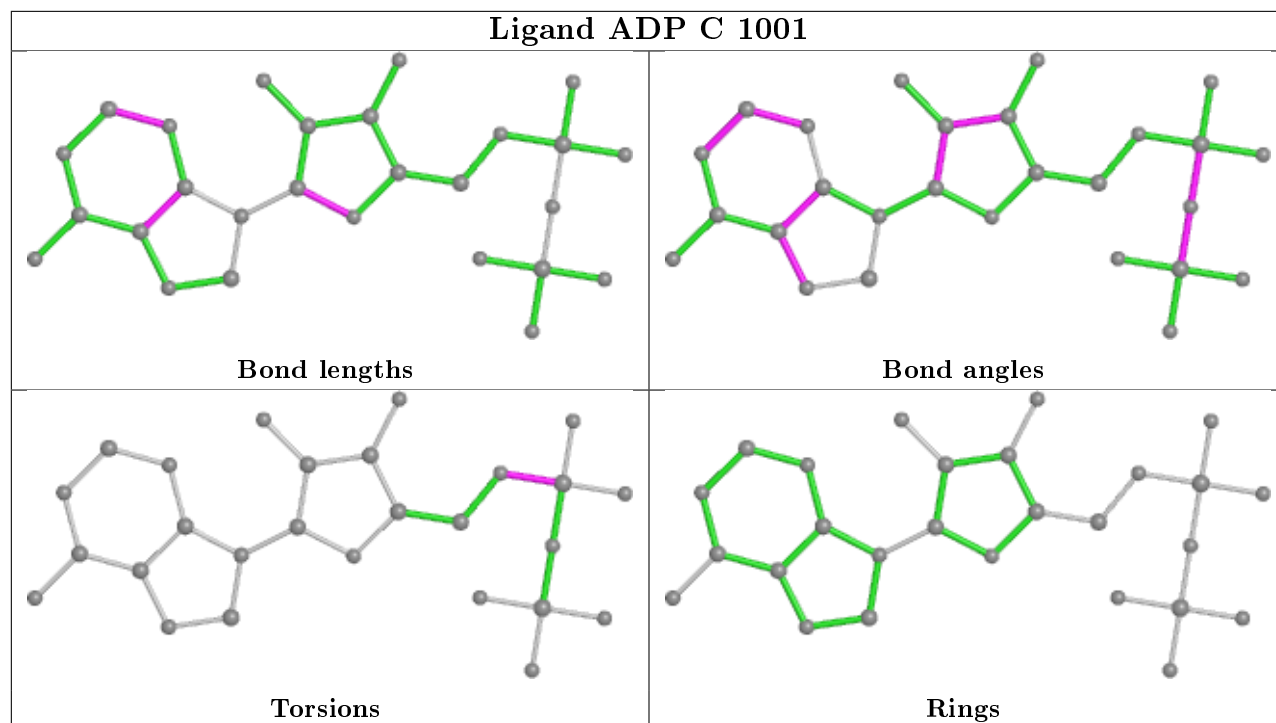
6 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2001	ADP	9	0
2	C	1001	ADP	10	0
2	E	1001	ADP	11	0
2	B	2001	ADP	9	0
2	A	1001	ADP	8	0
2	F	2001	ADP	10	0

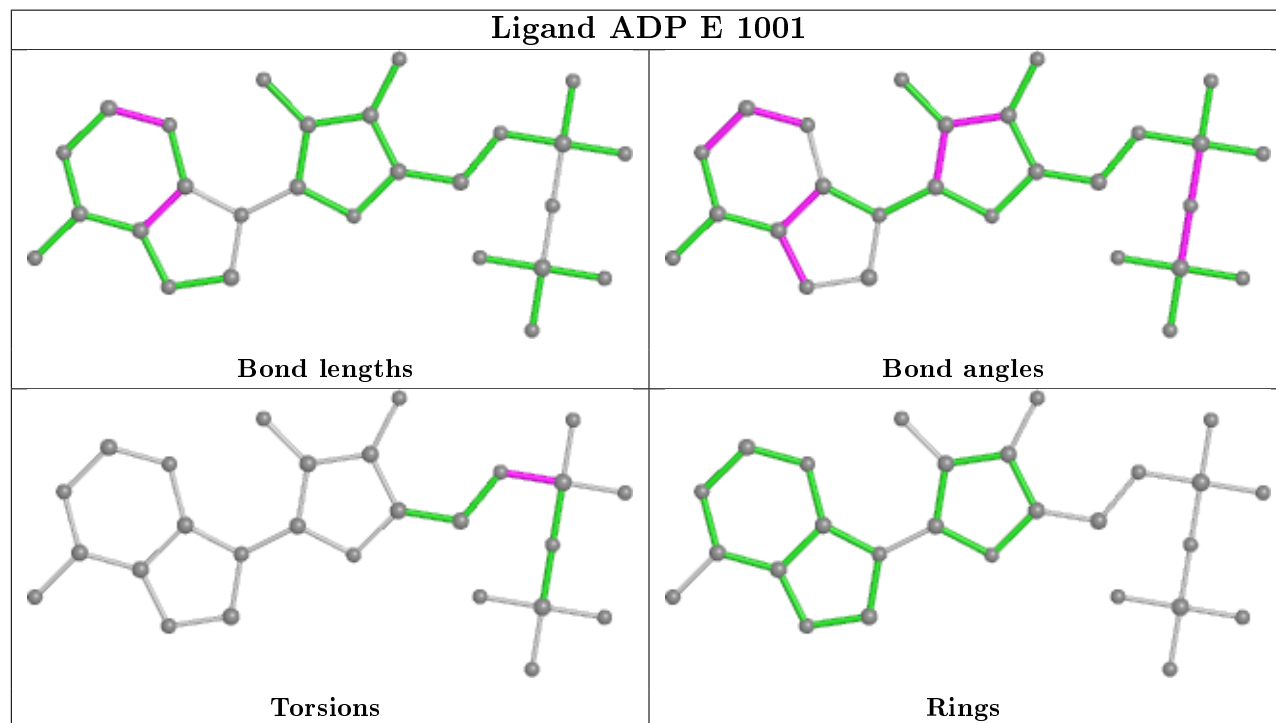
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



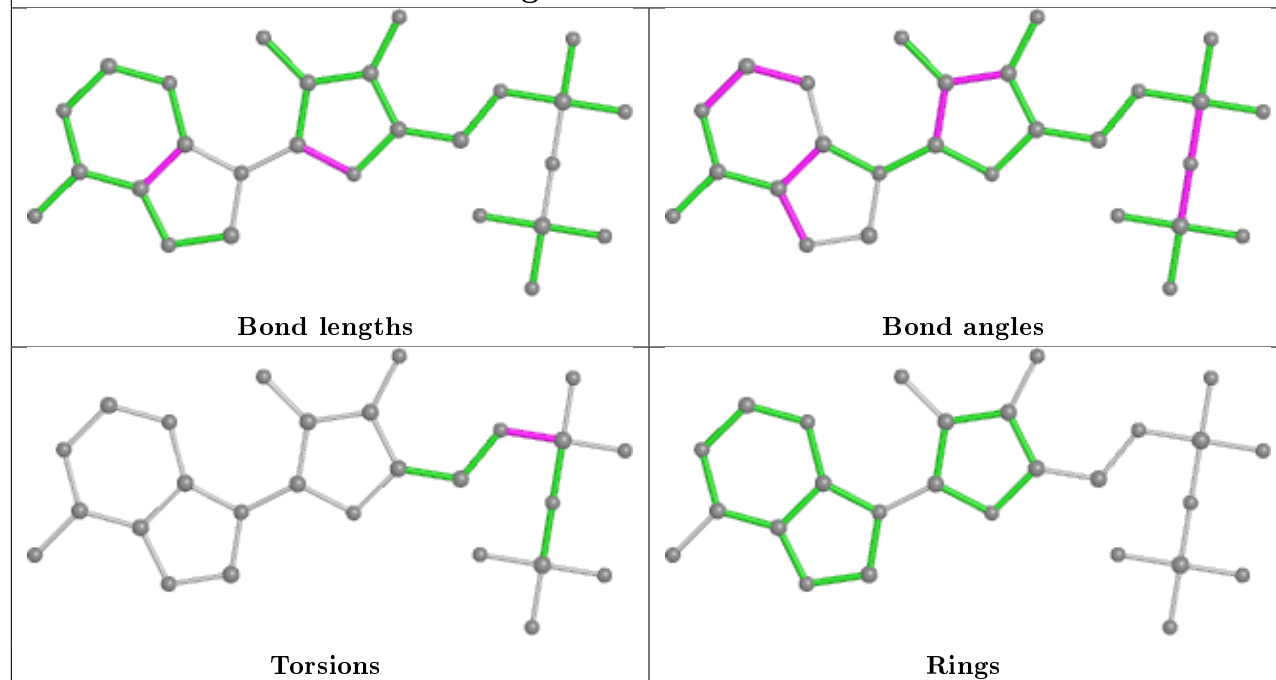
## Ligand ADP C 1001



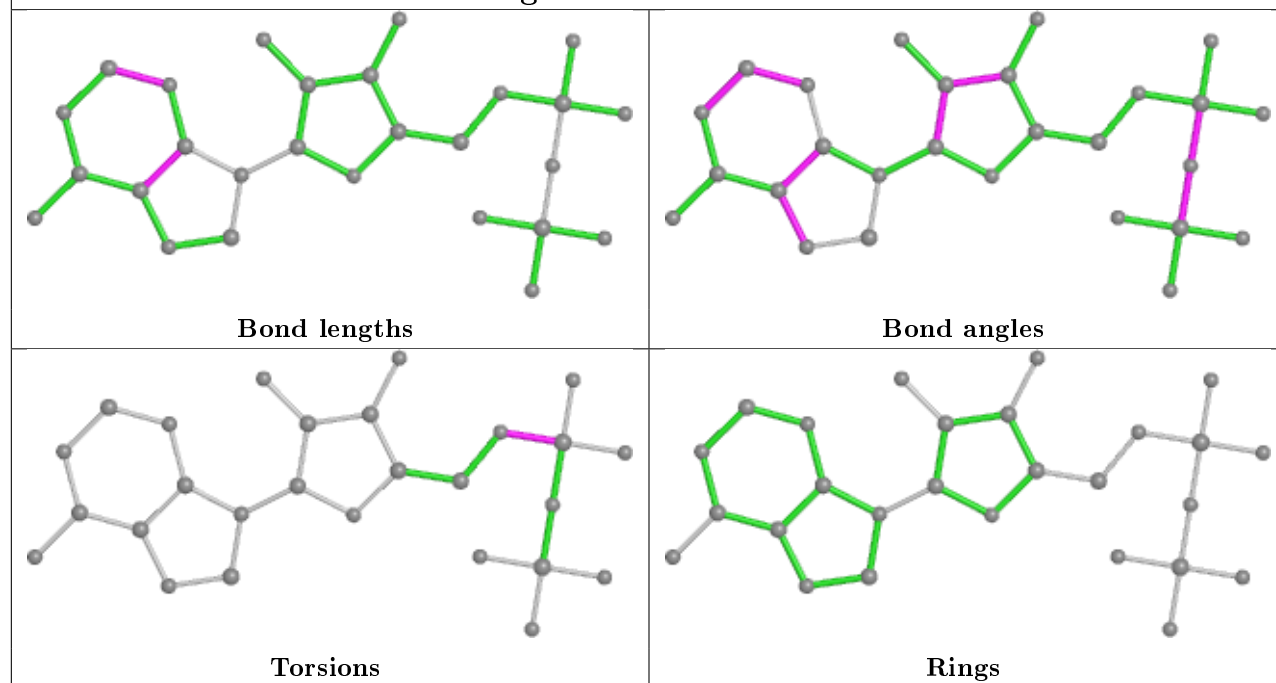
## Ligand ADP E 1001

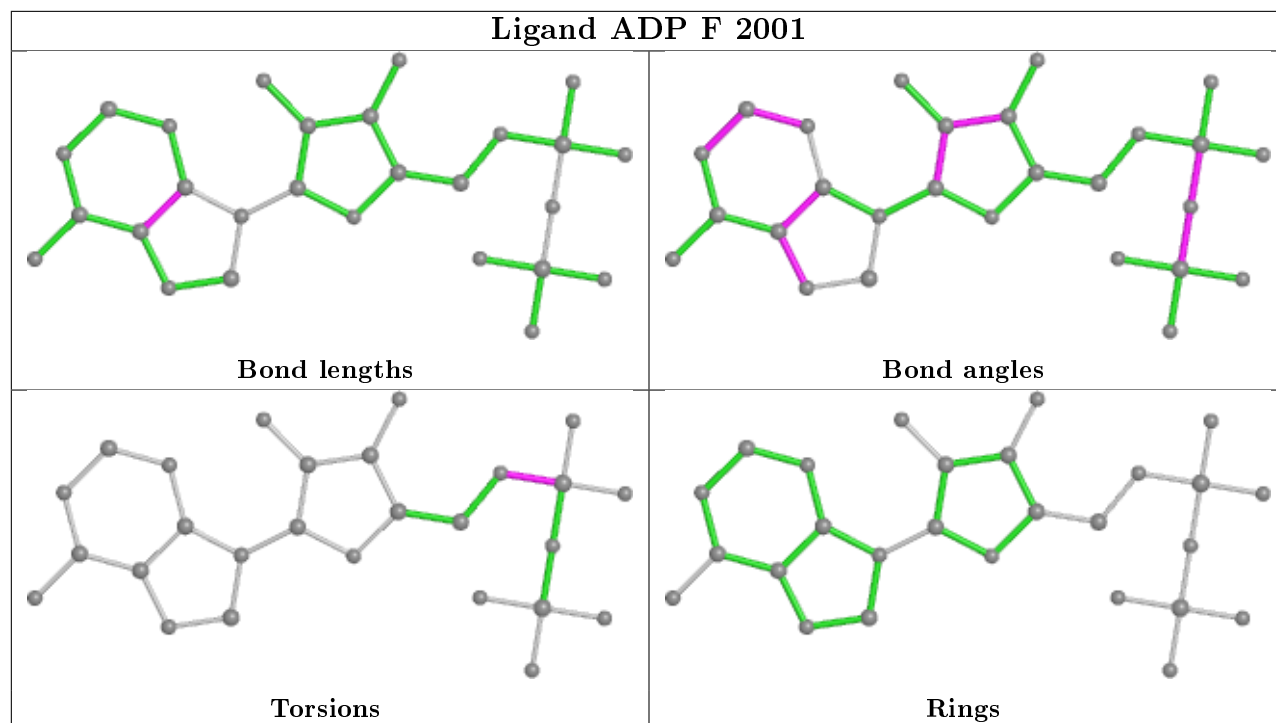


## Ligand ADP B 2001



## Ligand ADP A 1001





## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

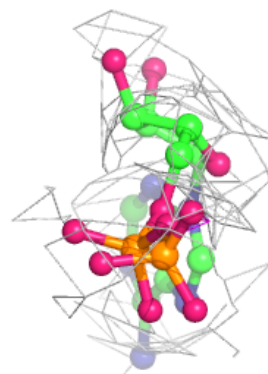
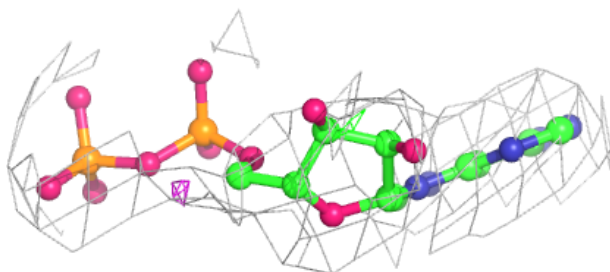
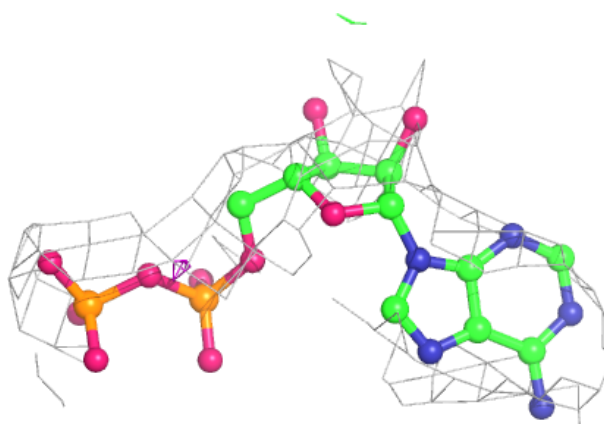
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

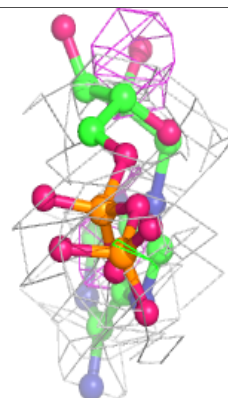
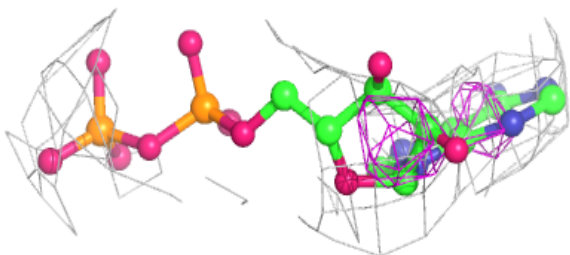
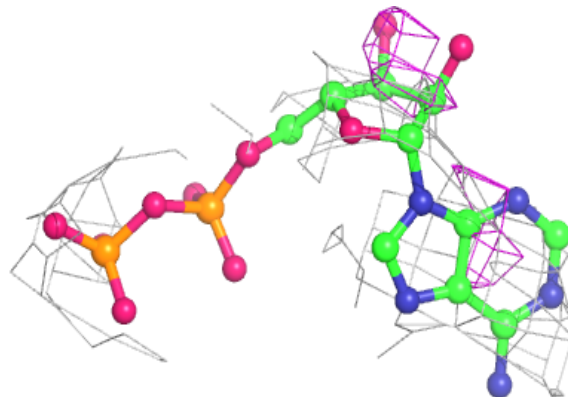
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ADP D 2001:**

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

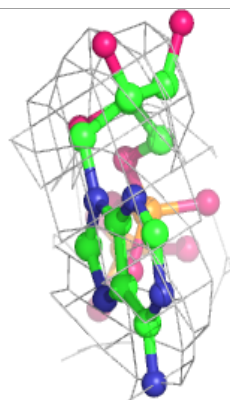
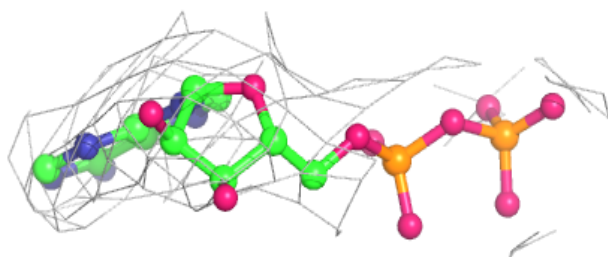
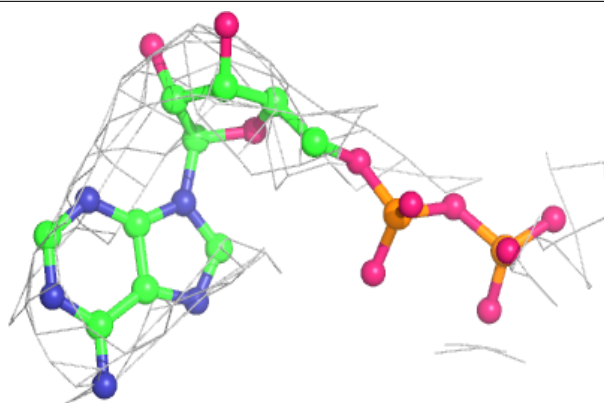
**Electron density around ADP C 1001:**

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

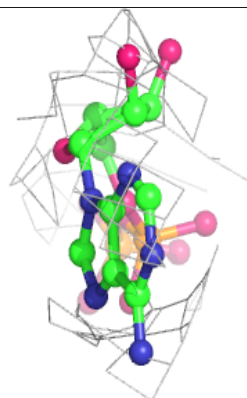
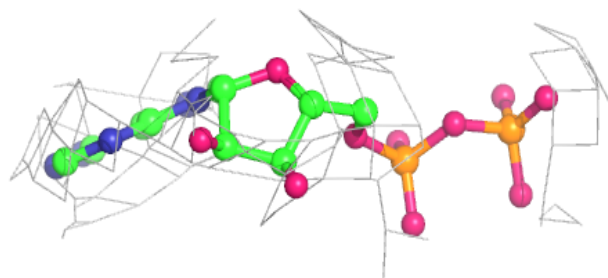
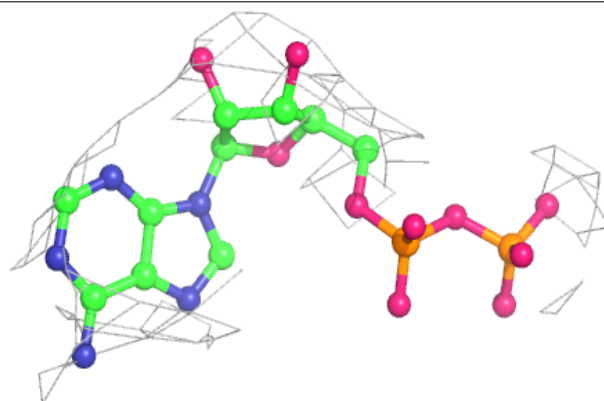


**Electron density around ADP E 1001:**

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

**Electron density around ADP B 2001:**

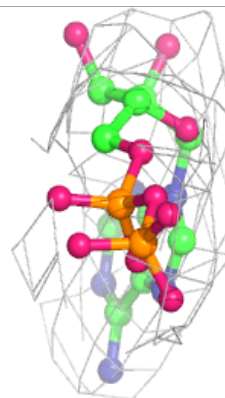
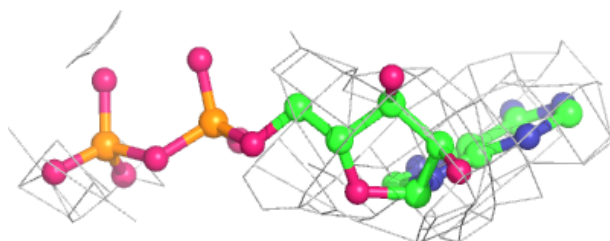
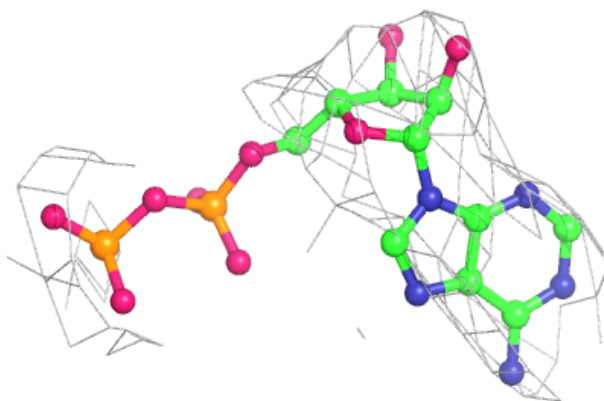
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



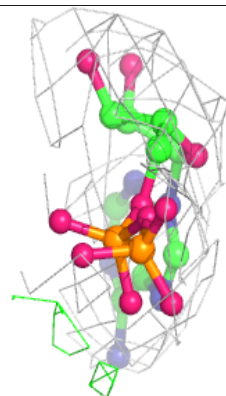
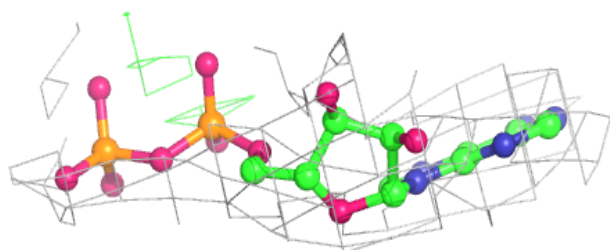
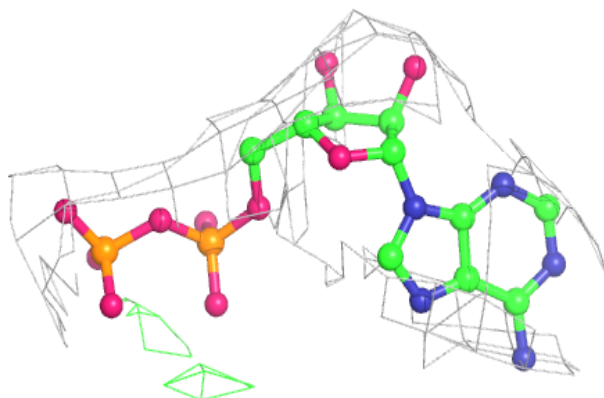


**Electron density around ADP A 1001:**

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

**Electron density around ADP F 2001:**

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



## 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.