wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:22 PM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

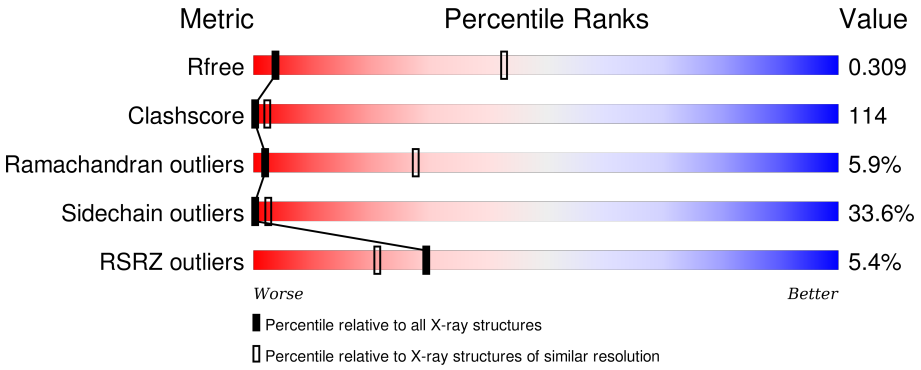
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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. 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 <=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	508	4% 16% 49% 23% • 10%
1	B	508	5% 9% 53% 22% • 12%
1	C	508	6% 16% 49% 21% • 10%
1	D	508	4% 9% 52% 23% • 12%
1	E	508	6% 17% 49% 22% • 10%

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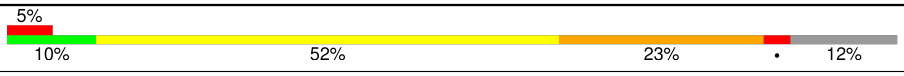
Mol	Chain	Length	Quality of chain
1	F	508	

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 criteria:

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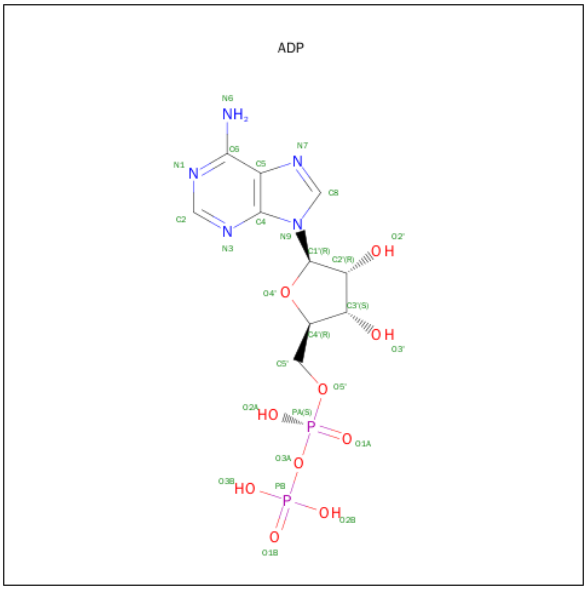
Chain	Residue	Modelled	Actual	Comment	Reference
F	399	LEU	GLY	ENGINEERED MUTATION	UNP Q5SI82

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



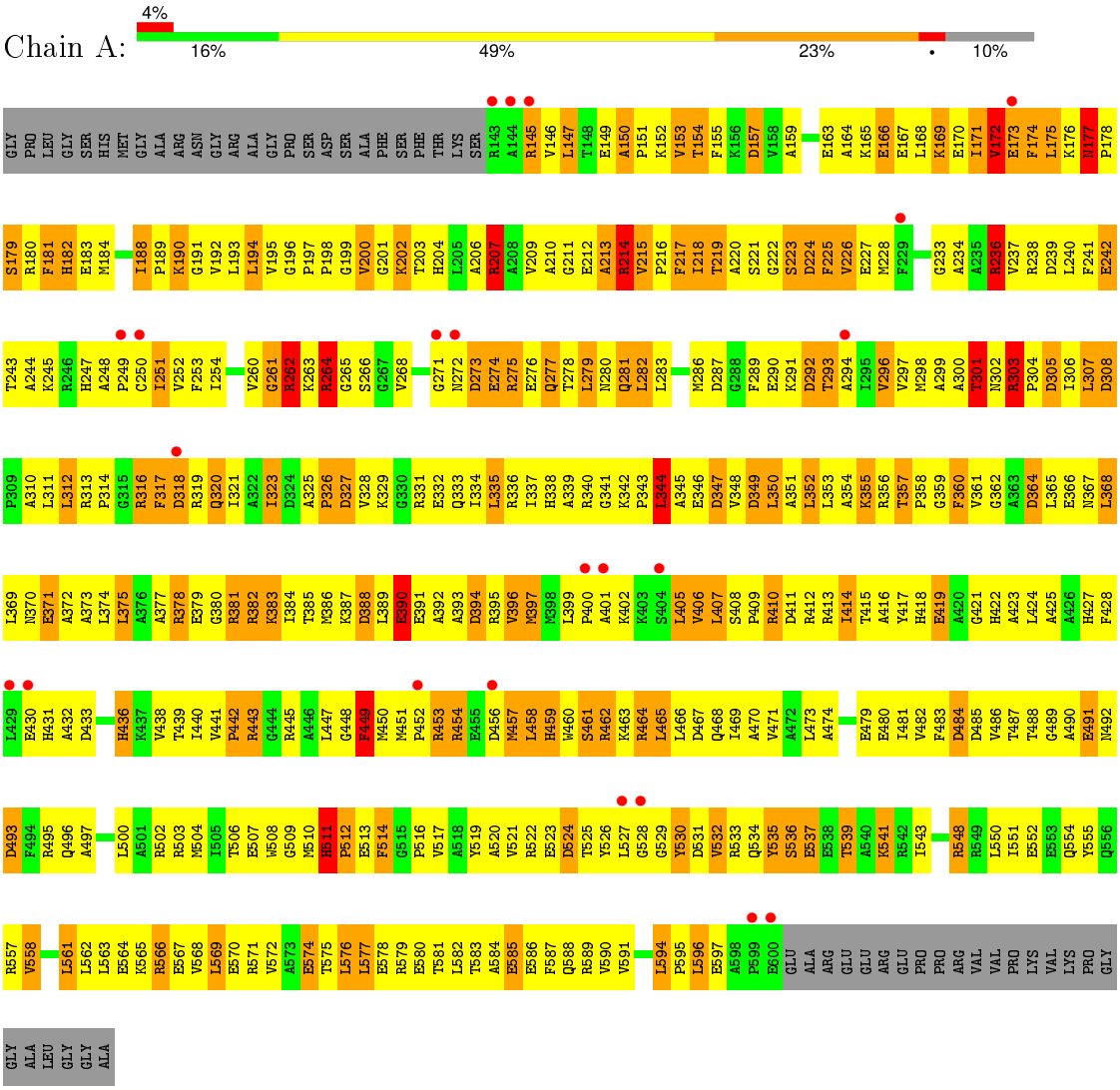
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

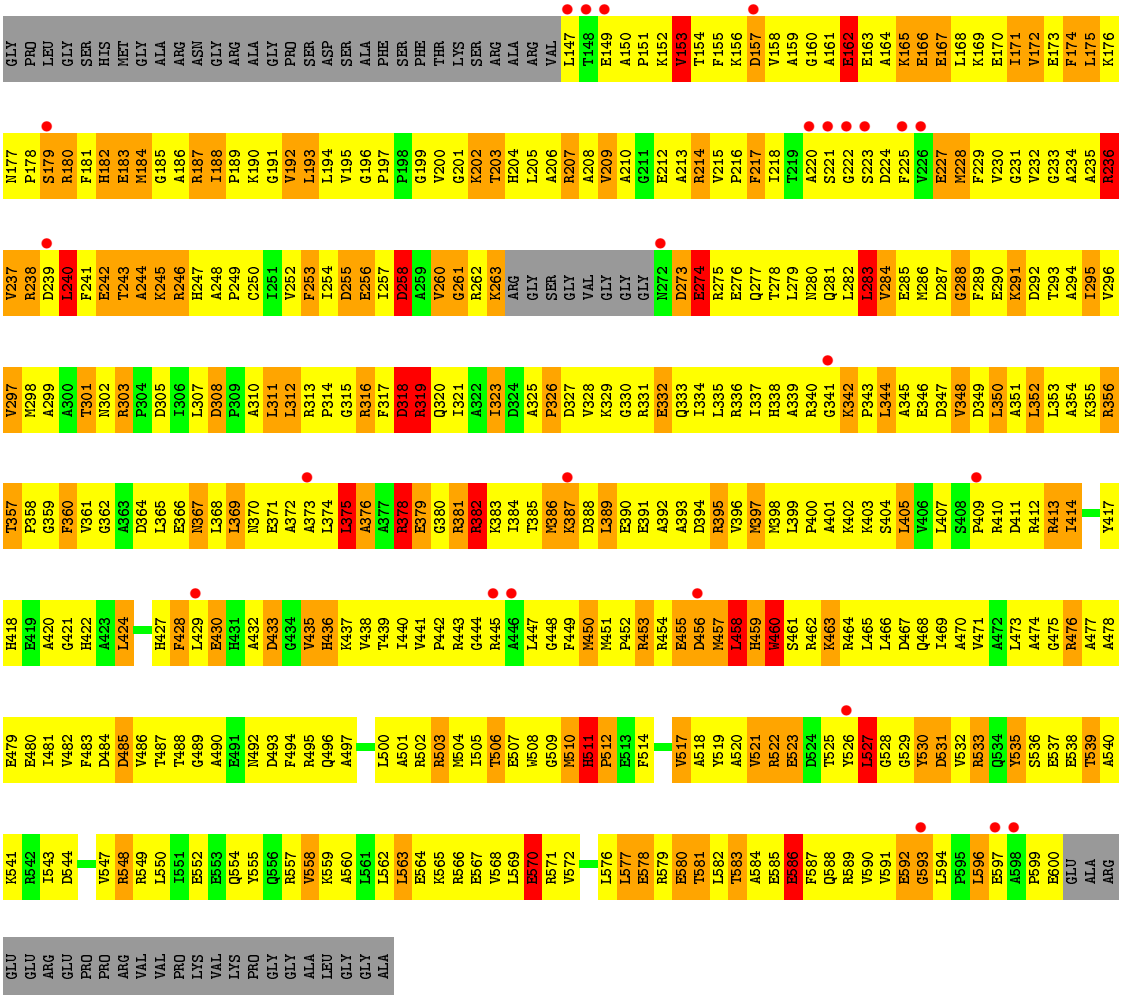
- Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain A:



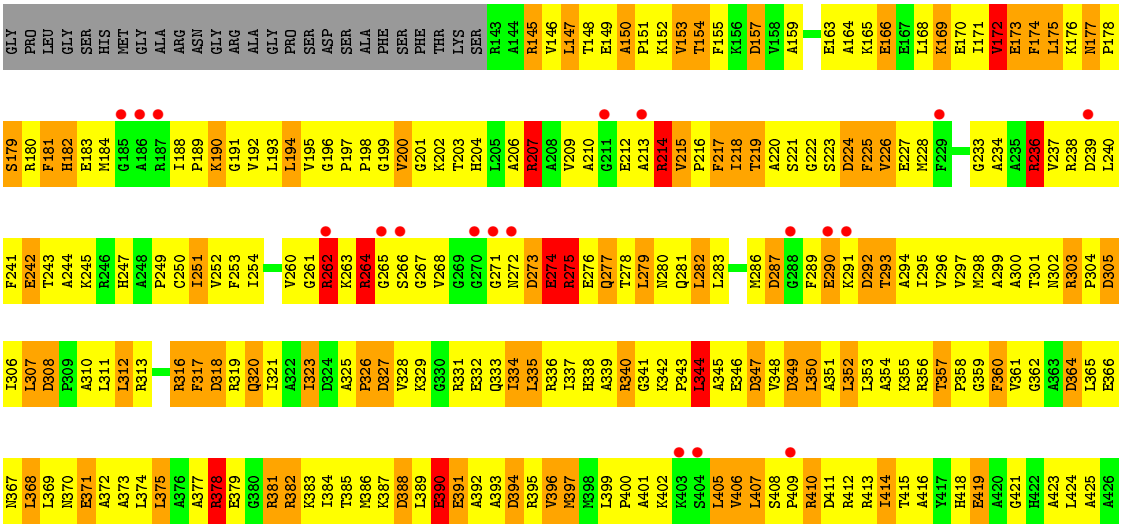
- Molecule 1: ATP-dependent zinc metalloprotease FtsH

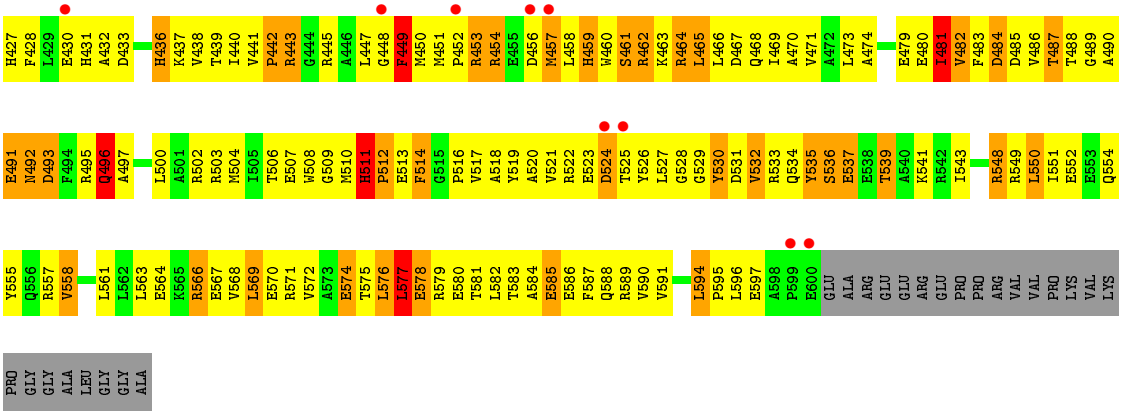
Chain B:



• Molecule 1: ATP-dependent zinc metalloprotease FtsH

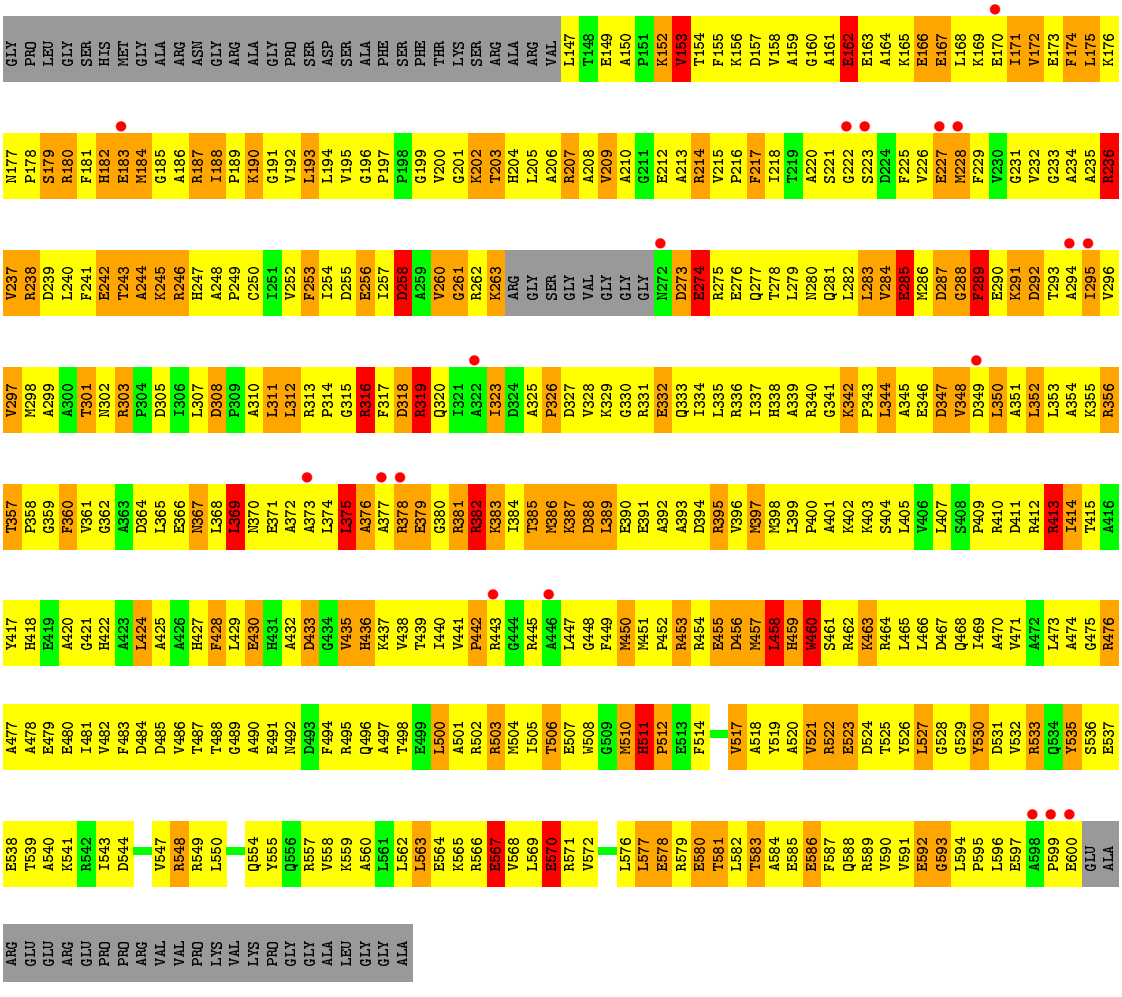
Chain C:





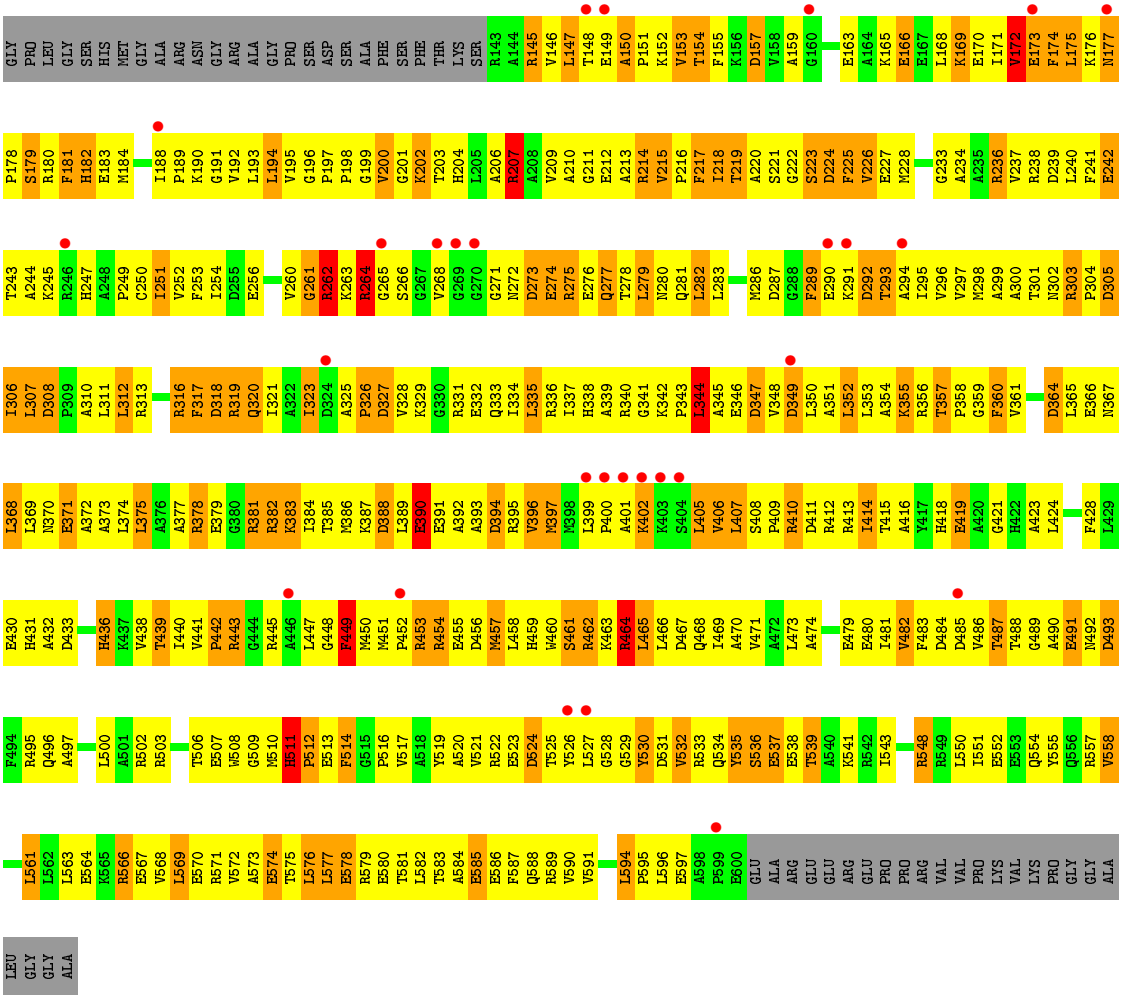
• Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain D:



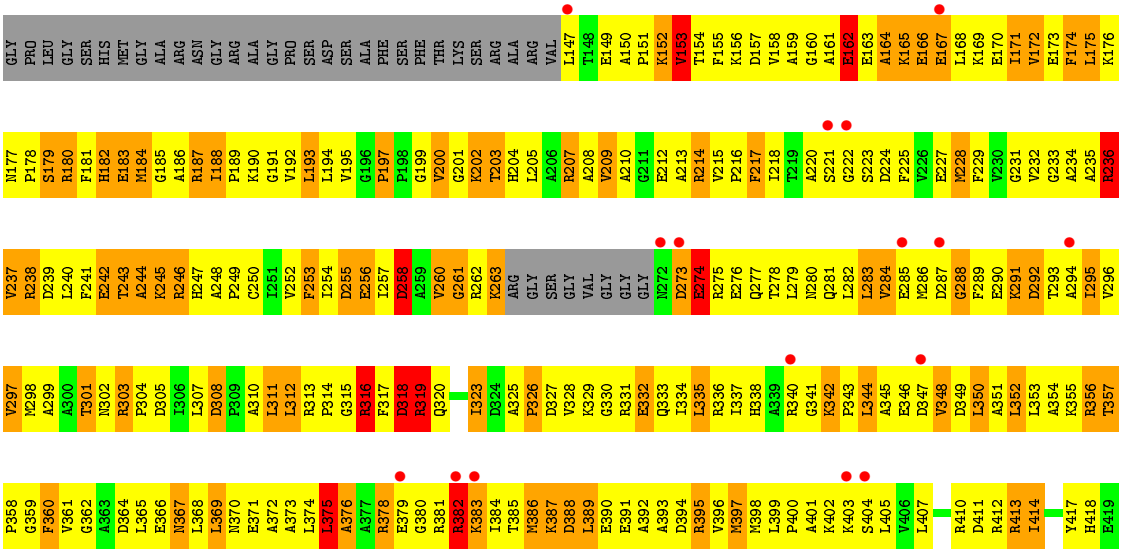
• Molecule 1: ATP-dependent zinc metalloprotease FtsH

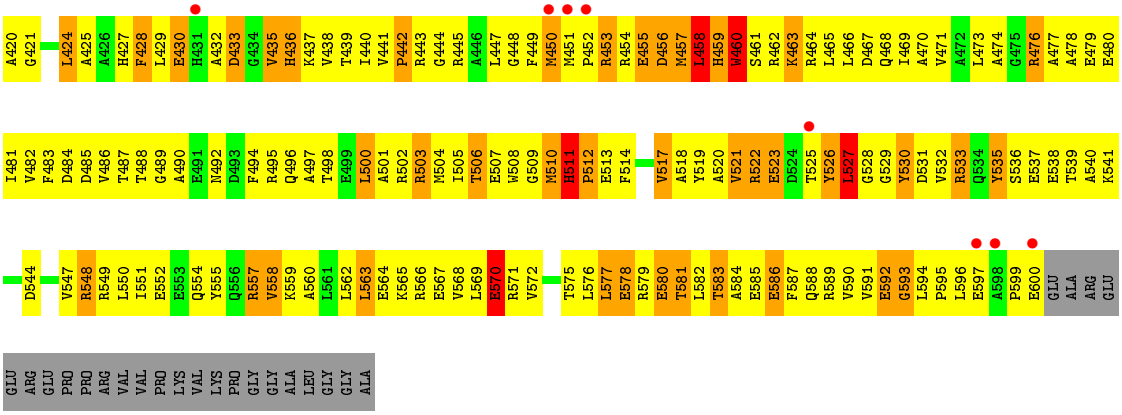
Chain E:



• Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain F:




A420 G421 L424 A425 A426 H427 F428 L429 E430 H431 A432 D433 G434 V435 H436 K437 V438 T439 I440 V441 P442 R443 G444 R445 A446 L447 G448 F449 M450 M451 P452 R453 R454 E455 D456 M457 L458 H459 W460 S461 R462 K463 R464 L465 L466 D467 Q468 I469 A470 V471 A472 L473 A474 G475 R476 A477 A478 E479 E480
I481 V482 F483 D484 D485 V486 T487 T488 G489 A490 E491 N492 D493 F494 R495 Q496 A497 T498 E499 L500 A501 R502 R503 M504 I505 T506 E507 W508 G509 M510 H511 P512 E513 F514 V517 A518 Y519 A520 V521 R522 E523 D524 T525 Y526 L527 G528 G529 Y530 D531 V532 R533 Q534 Y535 S536 E537 E538 T539 A540 K541
D544 V547 R548 R549 L550 I551 E552 E553 Q554 Y555 Q556 R557 V558 K559 A560 L561 L562 L563 E564 K565 R566 E567 V568 L569 E570 R571 V572 T575 L576 L577 E578 R579 E580 T581 L582 T583 A584 E585 E586 F587 Q588 R589 V590 V591 E592 G593 L594 P595 L596 E597 A598 P599 E600 GLU ALA ARG GLU
GLU ARG GLU PRO PRO ARG VAL VAL PRO LYS VAL LYS PRO GLY GLY ALA LEU GLY GLY ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.29%)	DCC
Wilson B-factor (Å^2)	99.1	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 17.8	EDS
Estimated twinning fraction	0.237 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.27$, $< L^2 > = 0.11$	Xtriage
Outliers	0 of 39234 reflections	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	21429	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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(^{o})	Ideal(^{o})
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 (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	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%)	3	32
1	B	442/508 (87%)	289 (65%)	125 (28%)	28 (6%)	2	26
1	C	456/508 (90%)	323 (71%)	112 (25%)	21 (5%)	3	33
1	D	442/508 (87%)	288 (65%)	121 (27%)	33 (8%)	1	21
1	E	456/508 (90%)	324 (71%)	110 (24%)	22 (5%)	3	32
1	F	442/508 (87%)	288 (65%)	120 (27%)	34 (8%)	1	20
All	All	2694/3048 (88%)	1835 (68%)	699 (26%)	160 (6%)	2	28

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 (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	365/402 (91%)	240 (66%)	125 (34%)	0 2
1	B	361/402 (90%)	242 (67%)	119 (33%)	0 3
1	C	365/402 (91%)	240 (66%)	125 (34%)	0 2
1	D	361/402 (90%)	241 (67%)	120 (33%)	0 3
1	E	365/402 (91%)	244 (67%)	121 (33%)	0 3
1	F	361/402 (90%)	240 (66%)	121 (34%)	0 2
All	All	2178/2412 (90%)	1447 (66%)	731 (34%)	0 2

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	A	1001	-	22,29,29	1.11	1 (4%)	27,45,45	2.06	4 (14%)
2	ADP	B	2001	-	22,29,29	1.09	2 (9%)	27,45,45	2.06	4 (14%)
2	ADP	C	1001	-	22,29,29	1.13	2 (9%)	27,45,45	2.29	5 (18%)
2	ADP	D	2001	-	22,29,29	1.06	2 (9%)	27,45,45	1.97	5 (18%)
2	ADP	E	1001	-	22,29,29	1.10	2 (9%)	27,45,45	1.86	5 (18%)
2	ADP	F	2001	-	22,29,29	1.05	1 (4%)	27,45,45	2.15	4 (14%)

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	A	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	B	2001	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	D	2001	-	-	0/12/32/32	0/3/3/3
2	ADP	E	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	F	2001	-	-	0/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	ADP	O4'-C1'	2.01	1.43	1.41
2	B	2001	ADP	O4'-C1'	2.17	1.43	1.41
2	D	2001	ADP	O4'-C1'	2.19	1.44	1.41
2	C	1001	ADP	O4'-C1'	2.32	1.44	1.41
2	D	2001	ADP	C5-C4	3.03	1.47	1.40

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	ADP	N3-C2-N1	-7.88	122.86	128.89
2	B	2001	ADP	N3-C2-N1	-6.68	123.78	128.89
2	D	2001	ADP	N3-C2-N1	-6.61	123.83	128.89
2	A	1001	ADP	N3-C2-N1	-6.53	123.89	128.89
2	F	2001	ADP	N3-C2-N1	-6.48	123.93	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 57 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	458/508 (90%)	0.04	22 (4%)	34	25	21, 118, 174, 229	0
1	B	446/508 (87%)	0.02	25 (5%)	28	20	16, 125, 176, 241	0
1	C	458/508 (90%)	0.19	28 (6%)	25	16	21, 129, 184, 237	0
1	D	446/508 (87%)	-0.08	19 (4%)	39	28	23, 103, 173, 241	0
1	E	458/508 (90%)	0.08	28 (6%)	25	16	24, 130, 179, 223	0
1	F	446/508 (87%)	0.09	24 (5%)	29	21	21, 128, 173, 261	0
All	All	2712/3048 (88%)	0.06	146 (5%)	29	21	16, 124, 177, 261	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	525	THR	6.6
1	E	404	SER	6.5
1	B	148	THR	5.8
1	B	147	LEU	5.7
1	E	269	GLY	5.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	C	1001	27/27	0.80	0.29	0.11	70,73,74,76	0
2	ADP	D	2001	27/27	0.90	0.20	0.06	58,64,74,74	0
2	ADP	F	2001	27/27	0.89	0.18	-0.39	64,69,74,74	0
2	ADP	A	1001	27/27	0.90	0.19	-0.44	63,66,70,71	0
2	ADP	E	1001	27/27	0.90	0.21	-0.95	66,70,72,73	0
2	ADP	B	2001	27/27	0.92	0.15	-1.13	65,72,75,79	0

6.5 Other polymers

There are no such residues in this entry.