Full wwPDB X-ray Structure Validation Report (i)

Mar 27, 2023 – 01:07 pm BST

PDB ID	:	7ZBH
Title	:	ATP-dependent zinc metalloprotease FtsH (BB0789) from Borrelia burgdorferi
Authors	:	Brangulis, K.
Deposited on	:	2022-03-23
Resolution	:	3.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

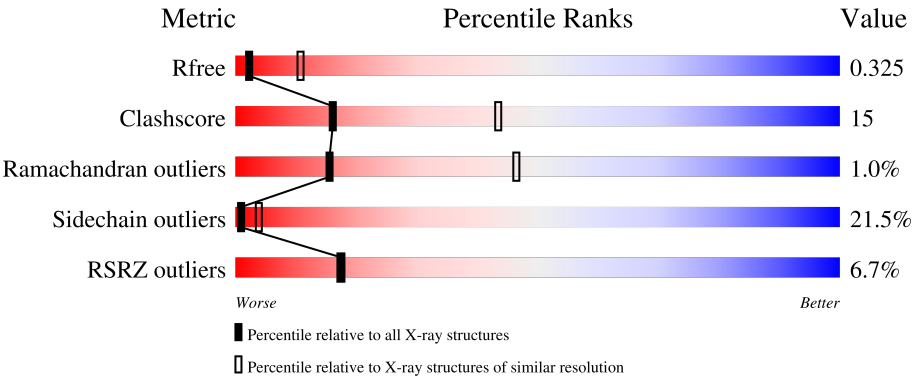
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	453	3% 47% 30% · 19%
1	B	453	6% 49% 28% 6% 17%
1	D	453	5% 49% 27% 5% 19%
1	F	453	8% 51% 26% 5% 19%
1	I	453	6% 46% 32% · 19%

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Mol	Chain	Length	Quality of chain
1	K	453	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16396 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	368	Total	C	N	O	S	0	0	0
			2703	1722	463	510	8			
1	B	374	Total	C	N	O	S	0	0	0
			2752	1748	473	523	8			
1	D	366	Total	C	N	O	S	0	0	0
			2678	1704	456	510	8			
1	F	367	Total	C	N	O	S	0	0	0
			2692	1712	461	511	8			
1	I	367	Total	C	N	O	S	0	0	0
			2701	1716	466	511	8			
1	K	368	Total	C	N	O	S	0	0	0
			2702	1718	464	512	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	GLY	-	expression tag	UNP O51729
A	163	ALA	-	expression tag	UNP O51729
A	164	MET	-	expression tag	UNP O51729
B	162	GLY	-	expression tag	UNP O51729
B	163	ALA	-	expression tag	UNP O51729
B	164	MET	-	expression tag	UNP O51729
D	162	GLY	-	expression tag	UNP O51729
D	163	ALA	-	expression tag	UNP O51729
D	164	MET	-	expression tag	UNP O51729
F	162	GLY	-	expression tag	UNP O51729
F	163	ALA	-	expression tag	UNP O51729
F	164	MET	-	expression tag	UNP O51729
I	162	GLY	-	expression tag	UNP O51729
I	163	ALA	-	expression tag	UNP O51729
I	164	MET	-	expression tag	UNP O51729
K	162	GLY	-	expression tag	UNP O51729
K	163	ALA	-	expression tag	UNP O51729

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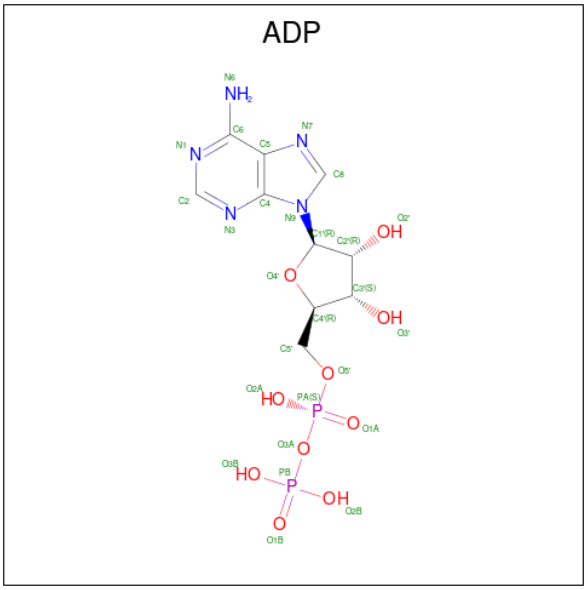
Chain	Residue	Modelled	Actual	Comment	Reference
K	164	MET	-	expression tag	UNP O51729

- 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	27	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	27	0
			27	10	5	10	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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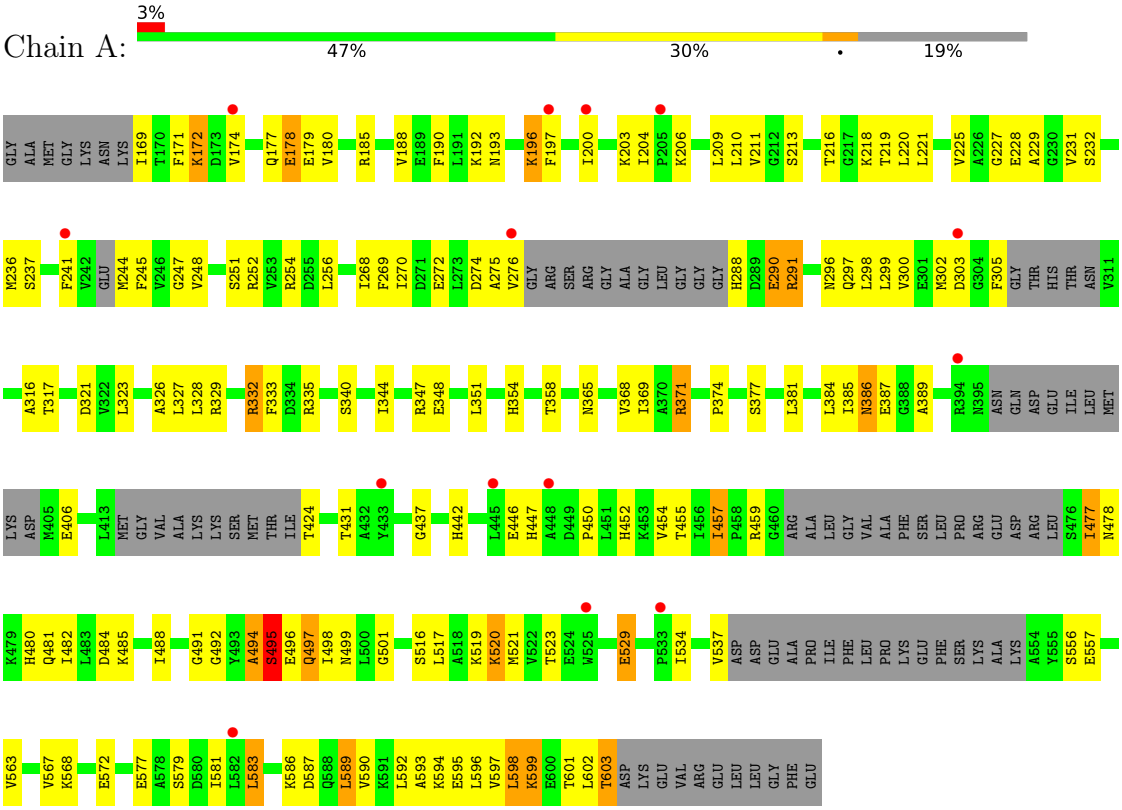
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	1	0
3	F	1	Total Zn 1 1	1	0
3	I	1	Total Zn 1 1	1	0
3	K	1	Total Zn 1 1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

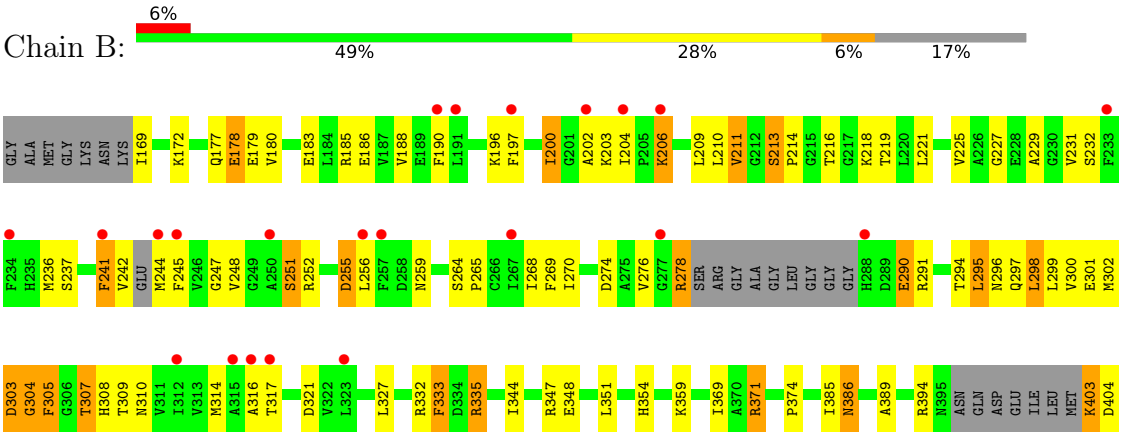
• Molecule 1: ATP-dependent zinc metalloprotease FtsH

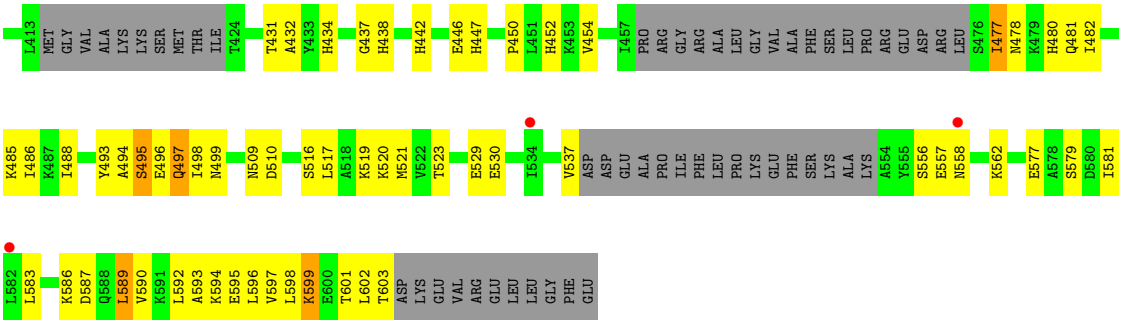
Chain A:



• Molecule 1: ATP-dependent zinc metalloprotease FtsH

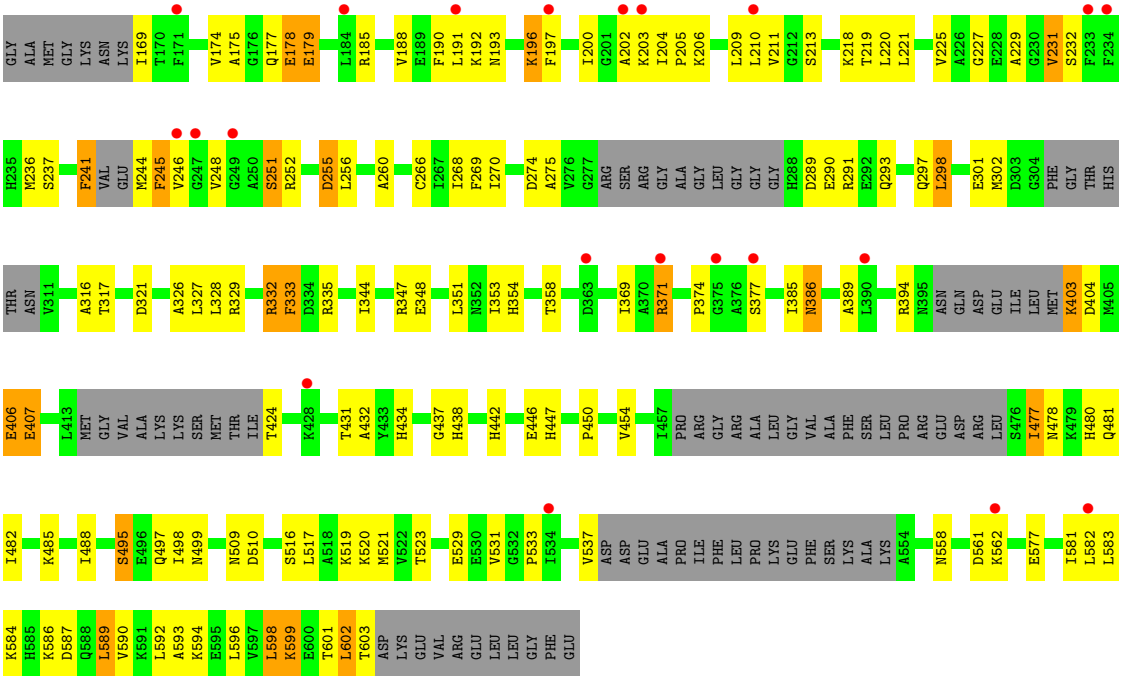
Chain B:





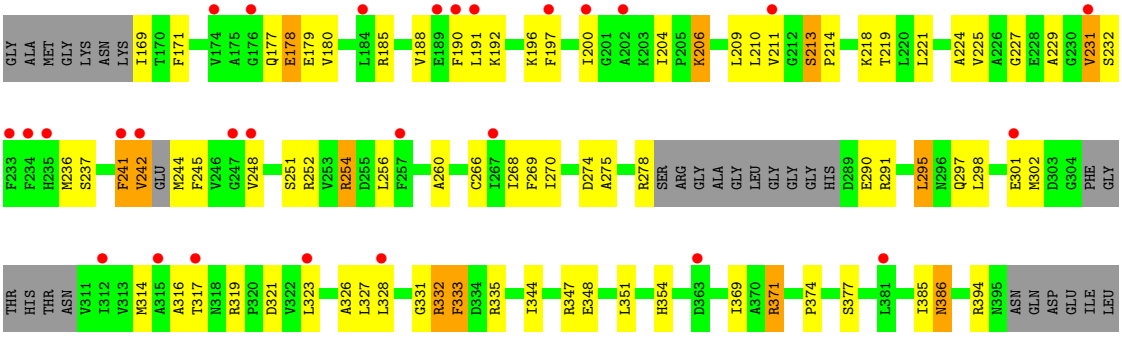
• Molecule 1: ATP-dependent zinc metalloprotease FtsH

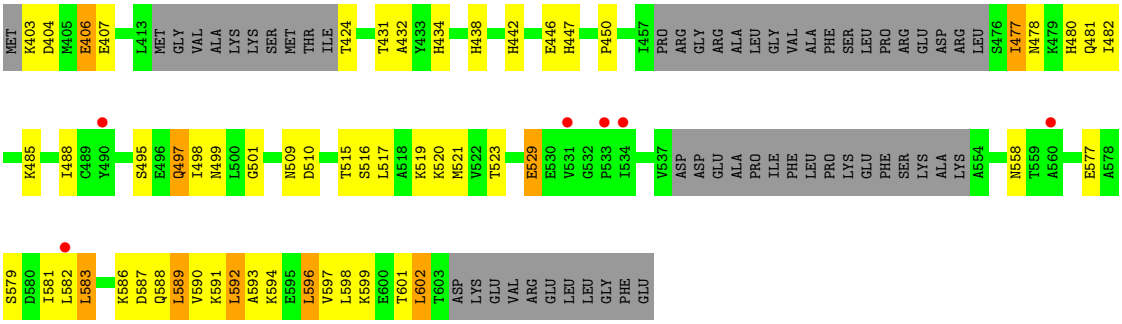
Chain D:



• Molecule 1: ATP-dependent zinc metalloprotease FtsH

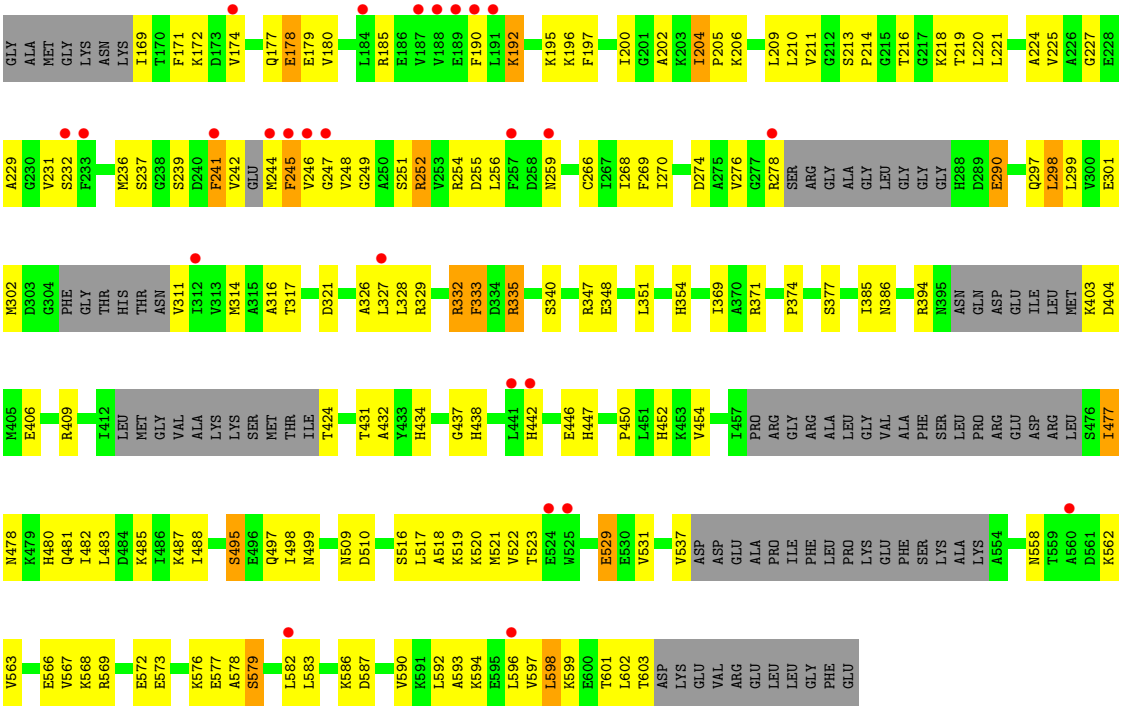
Chain F:





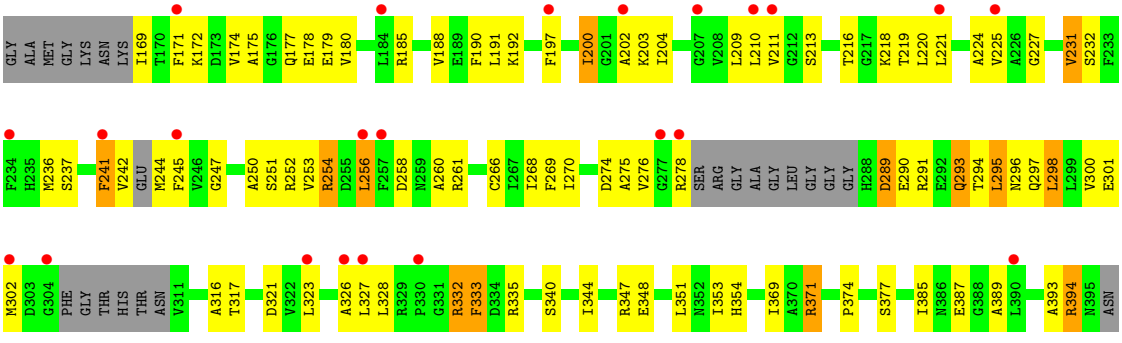
• Molecule 1: ATP-dependent zinc metalloprotease FtsH

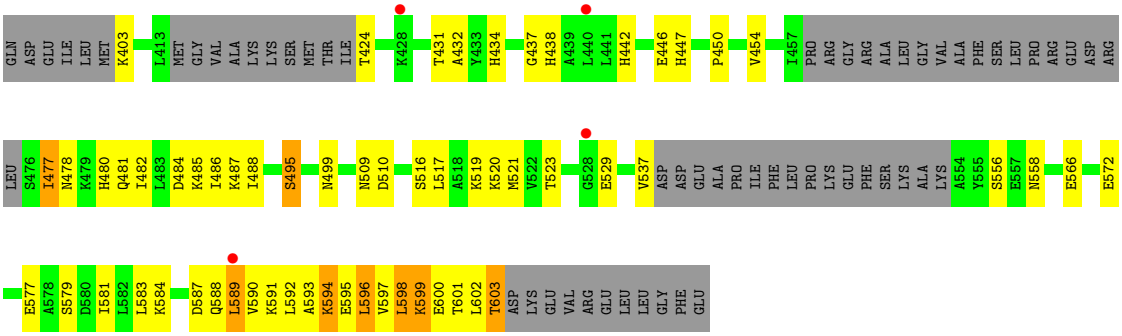
Chain I:



• Molecule 1: ATP-dependent zinc metalloprotease FtsH

Chain K:




GLN ASP GLU ILE LEU MET K403 L413 MET GLY VAL ALA LYS LYS SER MET THR ILE T424 K428 T431 A432 Y433 H434 G437 H438 A439 L440 L441 H442 E446 H447 P450 V454 I457 PRO ARG GLY ARG ALA LEU GLY VAL ALA PHE SER LEU PRO ARG GLU ASP ARG
LEU S476 I477 N478 K479 H480 Q481 I482 L483 D484 K485 I486 K487 I488 S496 N499 N509 D510 S516 L517 A518 K519 K520 M521 V522 T523 G528 E529 V537 ASP ASP GLU ALA PRO ILE PHE LEU PRO LYS GLU PHE SER LYS ALA LYS A554 Y555 S556 E557 N558 E566 E572
E577 A578 S579 D580 T581 L582 L583 K584 D587 Q588 L589 V590 K591 L592 A593 K594 E595 L596 V597 L598 K599 E600 T601 L602 T603 ASP LYS GLU VAL ARG GLU LEU LEU GLY PHE GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.81Å 192.80Å 114.13Å 90.00° 124.31° 90.00°	Depositor
Resolution (Å)	96.75 – 3.30 96.56 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (96.75-3.30) 97.8 (96.56-3.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.279 , 0.332 0.279 , 0.325	Depositor DCC
R_{free} test set	2048 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	106.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 121.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16396	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.77	0/2736	0.84	0/3687
1	B	0.77	1/2786 (0.0%)	0.84	0/3755
1	D	0.76	0/2709	0.85	0/3650
1	F	0.77	0/2722	0.83	0/3666
1	I	0.79	1/2732 (0.0%)	0.85	0/3679
1	K	0.79	1/2733 (0.0%)	0.83	0/3681
All	All	0.77	3/16418 (0.0%)	0.84	0/22118

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	572	GLU	CD-OE2	9.29	1.35	1.25
1	I	452	HIS	CG-CD2	6.62	1.47	1.35
1	B	530	GLU	CD-OE1	5.35	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2703	0	2588	77	0
1	B	2752	0	2631	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2678	0	2556	78	0
1	F	2692	0	2582	73	0
1	I	2701	0	2594	75	0
1	K	2702	0	2589	89	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	D	27	0	12	0	0
2	F	27	0	12	0	0
2	I	27	0	12	0	0
2	K	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
All	All	16396	0	15612	461	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 15.

All (461) 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:D:403:LYS:O	1:D:406:GLU:CD	1.92	1.06
1:B:305:PHE:HB3	1:B:307:THR:HG23	1.62	0.82
1:A:599:LYS:HD3	1:A:602:LEU:HB2	1.61	0.82
1:D:403:LYS:O	1:D:406:GLU:OE2	1.98	0.82
1:K:599:LYS:HD3	1:K:602:LEU:HB2	1.64	0.80
1:I:190:PHE:CD1	1:I:204:ILE:HG21	2.19	0.77
1:D:244:MET:O	1:D:290:GLU:OE2	2.04	0.76
1:A:437:GLY:HA3	1:A:491:GLY:O	1.86	0.76
1:F:438:HIS:CE1	1:F:510:ASP:OD2	2.40	0.74
1:I:438:HIS:CE1	1:I:510:ASP:OD2	2.41	0.72
1:A:387:GLU:OE2	1:B:335:ARG:NH2	2.22	0.72
1:I:438:HIS:NE2	1:I:510:ASP:OD2	2.23	0.72
1:D:406:GLU:N	1:D:406:GLU:OE1	2.23	0.72
1:D:438:HIS:CE1	1:D:510:ASP:OD2	2.42	0.72
1:F:438:HIS:NE2	1:F:510:ASP:OD2	2.23	0.71
1:A:241:PHE:HZ	1:A:256:LEU:HD22	1.53	0.71
1:K:438:HIS:CE1	1:K:510:ASP:OD2	2.43	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:438:HIS:NE2	1:K:510:ASP:OD2	2.23	0.70
1:A:499:ASN:HD21	1:A:589:LEU:HD21	1.56	0.70
1:K:291:ARG:HA	1:K:294:THR:HB	1.73	0.70
1:F:592:LEU:HD11	1:F:602:LEU:HD11	1.73	0.69
1:K:293:GLN:HG2	1:K:294:THR:N	2.07	0.69
1:K:477:ILE:HG22	1:K:481:GLN:HB2	1.75	0.69
1:F:206:LYS:NZ	1:F:332:ARG:HG3	2.08	0.69
1:I:477:ILE:HG22	1:I:481:GLN:HB2	1.75	0.69
1:I:195:LYS:CG	1:I:196:LYS:NZ	2.56	0.68
1:D:244:MET:HB3	1:D:248:VAL:HB	1.75	0.68
1:K:434:HIS:NE2	1:K:438:HIS:NE2	2.42	0.68
1:I:202:ALA:HB2	1:K:389:ALA:HB1	1.76	0.68
1:A:358:THR:HA	1:B:200:ILE:O	1.93	0.67
1:D:245:PHE:CD2	1:D:246:VAL:HG12	2.30	0.67
1:B:302:MET:C	1:B:304:GLY:H	1.98	0.67
1:B:477:ILE:HG22	1:B:481:GLN:HB2	1.77	0.67
1:D:477:ILE:HG22	1:D:481:GLN:HB2	1.78	0.66
1:B:244:MET:HB3	1:B:248:VAL:HB	1.78	0.65
1:I:244:MET:HB3	1:I:248:VAL:HB	1.79	0.65
1:A:244:MET:HB3	1:A:248:VAL:HB	1.77	0.65
1:F:477:ILE:HG22	1:F:481:GLN:HB2	1.79	0.65
1:B:209:LEU:HD11	1:B:317:THR:HG22	1.79	0.64
1:F:218:LYS:HE2	1:F:316:ALA:HB1	1.79	0.64
1:F:434:HIS:NE2	1:F:438:HIS:NE2	2.43	0.64
1:F:209:LEU:HD11	1:F:317:THR:HG22	1.80	0.64
1:K:209:LEU:HD11	1:K:317:THR:HG22	1.80	0.63
1:A:477:ILE:HG22	1:A:481:GLN:HB2	1.80	0.63
1:I:209:LEU:HD11	1:I:317:THR:HG22	1.79	0.63
1:B:386:ASN:HD21	1:D:203:LYS:HG2	1.64	0.63
1:F:499:ASN:HD21	1:F:589:LEU:HD21	1.63	0.63
1:D:245:PHE:CE2	1:D:246:VAL:HG12	2.34	0.62
1:B:296:ASN:O	1:B:300:VAL:HG23	1.99	0.62
1:K:499:ASN:HD21	1:K:589:LEU:HD21	1.65	0.62
1:B:499:ASN:HD21	1:B:589:LEU:HD21	1.64	0.62
1:B:495:SER:HB3	1:B:589:LEU:HD11	1.81	0.61
1:I:195:LYS:CG	1:I:196:LYS:HZ2	2.13	0.61
1:D:218:LYS:HE2	1:D:316:ALA:HB1	1.83	0.61
1:D:326:ALA:O	1:D:332:ARG:NH1	2.34	0.61
1:I:434:HIS:NE2	1:I:438:HIS:NE2	2.43	0.61
1:A:209:LEU:HD11	1:A:317:THR:HG22	1.83	0.61
1:D:602:LEU:HG	1:D:603:THR:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASN:HD21	1:B:203:LYS:HG2	1.65	0.60
1:D:598:LEU:HG	1:D:599:LYS:N	2.16	0.60
1:D:209:LEU:HD11	1:D:317:THR:HG22	1.82	0.60
1:B:304:GLY:O	1:B:305:PHE:HB2	2.02	0.60
1:B:298:LEU:O	1:B:302:MET:HG2	2.01	0.59
1:B:595:GLU:HA	1:B:598:LEU:HD12	1.83	0.59
1:B:297:GLN:HE21	1:B:301:GLU:HG2	1.68	0.59
1:D:403:LYS:O	1:D:406:GLU:OE1	2.19	0.59
1:K:290:GLU:HA	1:K:293:GLN:CD	2.23	0.59
1:K:484:ASP:HA	1:K:487:LYS:HD2	1.83	0.59
1:D:358:THR:HA	1:K:200:ILE:O	2.03	0.59
1:A:347:ARG:CZ	1:A:374:PRO:HA	2.33	0.59
1:F:347:ARG:CZ	1:F:374:PRO:HA	2.33	0.58
1:I:566:GLU:O	1:I:569:ARG:HB3	2.04	0.58
1:K:347:ARG:CZ	1:K:374:PRO:HA	2.33	0.58
1:A:484:ASP:O	1:A:488:ILE:HG13	2.03	0.58
1:I:406:GLU:O	1:I:409:ARG:HB3	2.03	0.58
1:B:347:ARG:CZ	1:B:374:PRO:HA	2.34	0.58
1:D:175:ALA:HB2	1:D:353:ILE:HD11	1.85	0.58
1:I:598:LEU:HG	1:I:599:LYS:N	2.19	0.58
1:D:499:ASN:HD21	1:D:589:LEU:HD21	1.69	0.58
1:I:347:ARG:CZ	1:I:374:PRO:HA	2.33	0.58
1:B:264:SER:OG	1:B:310:ASN:HB3	2.03	0.58
1:B:495:SER:O	1:B:499:ASN:ND2	2.34	0.58
1:I:247:GLY:N	1:I:290:GLU:OE1	2.36	0.58
1:D:347:ARG:CZ	1:D:374:PRO:HA	2.33	0.57
1:I:299:LEU:HD22	1:I:332:ARG:NH1	2.17	0.57
1:K:256:LEU:HD21	1:K:268:ILE:HG21	1.84	0.57
1:A:389:ALA:HB1	1:B:202:ALA:HB2	1.85	0.57
1:B:303:ASP:O	1:B:304:GLY:C	2.42	0.57
1:A:169:ILE:O	1:A:227:GLY:HA3	2.05	0.57
1:D:193:ASN:CG	1:D:196:LYS:HD2	2.25	0.57
1:B:432:ALA:HB1	1:B:593:ALA:HA	1.86	0.57
1:B:305:PHE:HB3	1:B:307:THR:CG2	2.33	0.57
1:B:294:THR:O	1:B:297:GLN:HB3	2.05	0.56
1:F:169:ILE:O	1:F:227:GLY:HA3	2.06	0.56
1:F:326:ALA:O	1:F:332:ARG:NH1	2.38	0.56
1:I:169:ILE:O	1:I:227:GLY:HA3	2.06	0.56
1:D:495:SER:O	1:D:499:ASN:ND2	2.39	0.56
1:B:190:PHE:HA	1:B:197:PHE:CE2	2.41	0.55
1:B:302:MET:C	1:B:304:GLY:N	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:568:LYS:O	1:I:572:GLU:HG3	2.06	0.55
1:F:495:SER:O	1:F:499:ASN:ND2	2.39	0.55
1:B:169:ILE:O	1:B:227:GLY:HA3	2.06	0.55
1:B:298:LEU:O	1:B:298:LEU:HD12	2.07	0.55
1:D:169:ILE:O	1:D:227:GLY:HA3	2.06	0.55
1:K:290:GLU:HG3	1:K:294:THR:OG1	2.06	0.55
1:I:190:PHE:HA	1:I:197:PHE:CE2	2.40	0.55
1:I:516:SER:O	1:I:520:LYS:HG3	2.07	0.55
1:A:193:ASN:HB3	1:A:196:LYS:HD2	1.88	0.55
1:D:561:ASP:OD2	1:K:558:ASN:OD1	2.25	0.54
1:D:177:GLN:O	1:D:178:GLU:C	2.45	0.54
1:K:190:PHE:HA	1:K:197:PHE:CE2	2.42	0.54
1:F:256:LEU:HD21	1:F:268:ILE:HG21	1.90	0.54
1:K:169:ILE:O	1:K:227:GLY:HA3	2.07	0.54
1:D:386:ASN:HD21	1:K:203:LYS:HG2	1.73	0.54
1:K:295:LEU:O	1:K:296:ASN:C	2.45	0.54
1:A:595:GLU:O	1:A:599:LYS:HG2	2.07	0.53
1:D:406:GLU:OE1	1:D:407:GLU:N	2.39	0.53
1:A:494:ALA:O	1:A:496:GLU:N	2.41	0.53
1:I:249:GLY:HA2	1:I:252:ARG:HG3	1.89	0.53
1:K:247:GLY:H	1:K:293:GLN:NE2	2.06	0.53
1:I:434:HIS:CE1	1:I:510:ASP:OD1	2.62	0.53
1:K:434:HIS:CE1	1:K:510:ASP:OD1	2.62	0.53
1:D:404:ASP:O	1:D:407:GLU:HG2	2.09	0.53
1:F:434:HIS:CE1	1:F:510:ASP:OD1	2.62	0.53
1:D:434:HIS:CE1	1:D:510:ASP:OD1	2.62	0.53
1:A:516:SER:O	1:A:520:LYS:HG3	2.08	0.53
1:K:247:GLY:H	1:K:293:GLN:HE21	1.55	0.53
1:F:241:PHE:O	1:F:244:MET:N	2.42	0.52
1:A:299:LEU:HD22	1:A:332:ARG:NH2	2.24	0.52
1:B:434:HIS:CE1	1:B:510:ASP:OD1	2.63	0.52
1:A:256:LEU:HD21	1:A:268:ILE:HG21	1.90	0.52
1:A:326:ALA:O	1:A:332:ARG:NH1	2.43	0.52
1:F:206:LYS:HZ1	1:F:332:ARG:HG3	1.75	0.52
1:F:434:HIS:CD2	1:F:438:HIS:CD2	2.98	0.52
1:B:354:HIS:HB2	1:B:385:ILE:HD12	1.92	0.51
1:F:206:LYS:HE2	1:F:331:GLY:C	2.29	0.51
1:F:354:HIS:HB2	1:F:385:ILE:HD12	1.92	0.51
1:K:593:ALA:O	1:K:597:VAL:HG23	2.10	0.51
1:A:497:GLN:O	1:A:498:ILE:C	2.46	0.51
1:I:576:LYS:O	1:I:577:GLU:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:290:GLU:HA	1:K:293:GLN:NE2	2.25	0.51
1:K:326:ALA:O	1:K:332:ARG:NH1	2.42	0.51
1:B:256:LEU:HD21	1:B:268:ILE:HG21	1.92	0.51
1:I:442:HIS:HB3	1:I:450:PRO:HA	1.92	0.51
1:A:387:GLU:OE1	1:B:335:ARG:NH1	2.43	0.51
1:B:599:LYS:C	1:B:601:THR:H	2.14	0.51
1:K:190:PHE:CD1	1:K:204:ILE:HG12	2.46	0.51
1:I:326:ALA:O	1:I:332:ARG:NH1	2.43	0.51
1:K:495:SER:O	1:K:499:ASN:ND2	2.43	0.51
1:K:602:LEU:HG	1:K:603:THR:N	2.25	0.51
1:I:434:HIS:CD2	1:I:438:HIS:CD2	2.99	0.51
1:K:434:HIS:CD2	1:K:438:HIS:CD2	2.98	0.51
1:F:190:PHE:HA	1:F:197:PHE:CE1	2.46	0.51
1:F:298:LEU:O	1:F:302:MET:HG3	2.11	0.50
1:A:478:ASN:O	1:A:482:ILE:HG12	2.11	0.50
1:B:493:TYR:HE2	1:D:533:PRO:HB3	1.77	0.50
1:B:389:ALA:HB1	1:D:202:ALA:HB2	1.93	0.50
1:D:297:GLN:HE21	1:D:301:GLU:HG2	1.77	0.50
1:F:478:ASN:O	1:F:482:ILE:HG12	2.12	0.50
1:B:434:HIS:CD2	1:B:438:HIS:CD2	2.99	0.50
1:A:602:LEU:HG	1:A:603:THR:N	2.26	0.50
1:B:190:PHE:CD1	1:B:204:ILE:HG12	2.47	0.50
1:D:434:HIS:CD2	1:D:438:HIS:CD2	2.99	0.50
1:K:241:PHE:O	1:K:244:MET:HB2	2.11	0.50
1:D:256:LEU:HD21	1:D:268:ILE:HG21	1.94	0.49
1:I:245:PHE:HB3	1:I:248:VAL:HG21	1.93	0.49
1:A:497:GLN:HG3	1:A:501:GLY:O	2.11	0.49
1:I:599:LYS:C	1:I:601:THR:H	2.14	0.49
1:A:557:GLU:OE2	1:B:557:GLU:N	2.40	0.49
1:D:190:PHE:CD1	1:D:204:ILE:HG12	2.48	0.49
1:D:447:HIS:CE1	1:D:480:HIS:HB3	2.47	0.49
1:I:213:SER:HB3	1:I:214:PRO:HD2	1.94	0.49
1:D:290:GLU:O	1:D:290:GLU:HG2	2.12	0.49
1:B:437:GLY:HA3	1:B:495:SER:OG	2.13	0.49
1:K:254:ARG:CZ	1:K:254:ARG:HB2	2.42	0.49
1:A:534:ILE:HG13	1:F:515:THR:HG23	1.94	0.49
1:B:265:PRO:HA	1:B:310:ASN:O	2.13	0.49
1:D:602:LEU:HG	1:D:603:THR:H	1.77	0.49
1:A:593:ALA:O	1:A:597:VAL:HG23	2.13	0.48
1:B:478:ASN:O	1:B:482:ILE:HG12	2.12	0.48
1:D:478:ASN:O	1:D:482:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:LYS:C	1:D:601:THR:H	2.17	0.48
1:K:434:HIS:CD2	1:K:438:HIS:NE2	2.81	0.48
1:A:190:PHE:HA	1:A:197:PHE:CE1	2.48	0.48
1:I:478:ASN:O	1:I:482:ILE:HG12	2.13	0.48
1:K:447:HIS:CE1	1:K:480:HIS:HB3	2.48	0.48
1:K:291:ARG:O	1:K:295:LEU:HB3	2.13	0.48
1:B:403:LYS:HD2	1:B:403:LYS:N	2.28	0.48
1:I:437:GLY:HA3	1:I:495:SER:OG	2.13	0.48
1:K:188:VAL:HG12	1:K:192:LYS:HD2	1.95	0.48
1:A:354:HIS:HB2	1:A:385:ILE:HD12	1.95	0.48
1:A:497:GLN:HG3	1:A:501:GLY:C	2.34	0.48
1:A:599:LYS:C	1:A:601:THR:H	2.16	0.48
1:A:296:ASN:HA	1:A:299:LEU:HD12	1.94	0.48
1:D:437:GLY:HA3	1:D:495:SER:OG	2.13	0.48
1:I:432:ALA:HB1	1:I:593:ALA:HA	1.94	0.48
1:I:586:LYS:O	1:I:590:VAL:HG23	2.14	0.48
1:K:298:LEU:O	1:K:302:MET:HG3	2.12	0.48
1:D:389:ALA:HB1	1:K:202:ALA:HB2	1.95	0.48
1:D:599:LYS:HE3	1:D:599:LYS:HB3	1.63	0.48
1:K:295:LEU:O	1:K:298:LEU:N	2.47	0.48
1:K:296:ASN:O	1:K:300:VAL:HG23	2.14	0.48
1:K:590:VAL:O	1:K:594:LYS:HE3	2.14	0.48
1:K:595:GLU:O	1:K:599:LYS:HG2	2.13	0.48
1:B:302:MET:O	1:B:304:GLY:N	2.47	0.48
1:D:354:HIS:HB2	1:D:385:ILE:HD12	1.94	0.48
1:F:236:MET:O	1:F:270:ILE:HA	2.14	0.48
1:K:432:ALA:HB1	1:K:593:ALA:HA	1.95	0.48
1:F:593:ALA:O	1:F:597:VAL:HG23	2.14	0.48
1:K:478:ASN:O	1:K:482:ILE:HG12	2.13	0.48
1:I:531:VAL:HG23	1:I:566:GLU:HG3	1.94	0.47
1:K:485:LYS:HA	1:K:488:ILE:HD12	1.96	0.47
1:A:190:PHE:CD1	1:A:204:ILE:HG12	2.48	0.47
1:B:295:LEU:HG	1:B:296:ASN:N	2.29	0.47
1:A:177:GLN:O	1:A:180:VAL:N	2.47	0.47
1:B:442:HIS:HB3	1:B:450:PRO:HA	1.97	0.47
1:D:485:LYS:HA	1:D:488:ILE:HD12	1.96	0.47
1:B:255:ASP:O	1:B:259:ASN:OD1	2.32	0.47
1:I:177:GLN:O	1:I:180:VAL:N	2.48	0.47
1:I:354:HIS:HB2	1:I:385:ILE:HD12	1.96	0.47
1:F:206:LYS:HZ3	1:F:332:ARG:HG3	1.78	0.47
1:A:236:MET:O	1:A:270:ILE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:LYS:HA	1:B:488:ILE:HD12	1.95	0.47
1:F:344:ILE:HD13	1:F:371:ARG:HB3	1.97	0.47
1:F:434:HIS:CD2	1:F:438:HIS:NE2	2.83	0.47
1:K:437:GLY:HA3	1:K:495:SER:OG	2.15	0.47
1:F:447:HIS:CE1	1:F:480:HIS:HB3	2.50	0.47
1:B:447:HIS:CE1	1:B:480:HIS:HB3	2.50	0.47
1:I:434:HIS:CD2	1:I:438:HIS:NE2	2.83	0.47
1:K:236:MET:O	1:K:270:ILE:HA	2.13	0.47
1:A:583:LEU:HD13	1:A:583:LEU:HA	1.82	0.46
1:B:190:PHE:CD1	1:B:204:ILE:HG21	2.49	0.46
1:B:236:MET:O	1:B:270:ILE:HA	2.14	0.46
1:K:595:GLU:CG	1:K:599:LYS:HD2	2.45	0.46
1:B:344:ILE:HD13	1:B:371:ARG:HB3	1.97	0.46
1:F:177:GLN:O	1:F:180:VAL:N	2.48	0.46
1:F:442:HIS:HB3	1:F:450:PRO:HA	1.98	0.46
1:F:485:LYS:HA	1:F:488:ILE:HD12	1.97	0.46
1:D:236:MET:O	1:D:270:ILE:HA	2.15	0.46
1:K:177:GLN:O	1:K:180:VAL:N	2.48	0.46
1:B:177:GLN:O	1:B:180:VAL:N	2.48	0.46
1:B:296:ASN:HA	1:B:299:LEU:HD12	1.97	0.46
1:B:593:ALA:O	1:B:597:VAL:HG23	2.14	0.46
1:D:432:ALA:HB1	1:D:593:ALA:HA	1.97	0.46
1:F:171:PHE:HD1	1:F:224:ALA:HB1	1.81	0.46
1:I:593:ALA:O	1:I:597:VAL:HG23	2.15	0.46
1:K:219:THR:HG23	1:K:269:PHE:CE2	2.50	0.46
1:K:297:GLN:HE21	1:K:301:GLU:HG2	1.80	0.46
1:K:588:GLN:O	1:K:591:LYS:HB2	2.14	0.46
1:K:442:HIS:HB3	1:K:450:PRO:HA	1.97	0.46
1:D:298:LEU:O	1:D:302:MET:HG3	2.16	0.46
1:I:216:THR:OG1	1:I:218:LYS:HE2	2.15	0.46
1:A:216:THR:OG1	1:A:218:LYS:HE2	2.15	0.46
1:B:216:THR:OG1	1:B:218:LYS:HE2	2.16	0.46
1:B:295:LEU:O	1:B:299:LEU:HG	2.14	0.46
1:B:586:LYS:O	1:B:590:VAL:HG23	2.15	0.46
1:F:516:SER:O	1:F:520:LYS:HG3	2.15	0.46
1:I:335:ARG:NH1	1:K:387:GLU:OE1	2.49	0.46
1:K:216:THR:OG1	1:K:218:LYS:HE2	2.15	0.46
1:A:188:VAL:HG13	1:A:229:ALA:HB2	1.96	0.46
1:D:219:THR:HG23	1:D:269:PHE:CE2	2.49	0.46
1:D:260:ALA:O	1:D:266:CYS:SG	2.74	0.46
1:K:599:LYS:CD	1:K:602:LEU:HB2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:GLU:OE2	1:B:178:GLU:HA	2.16	0.46
1:B:206:LYS:HD2	1:B:302:MET:O	2.16	0.46
1:I:204:ILE:HG22	1:I:205:PRO:HD2	1.98	0.46
1:F:297:GLN:HE21	1:F:301:GLU:HG2	1.80	0.46
1:I:297:GLN:HE21	1:I:301:GLU:HG2	1.81	0.46
1:A:327:LEU:O	1:A:333:PHE:HB2	2.16	0.45
1:A:203:LYS:HG2	1:F:386:ASN:HD21	1.80	0.45
1:K:495:SER:HB3	1:K:589:LEU:HD11	1.99	0.45
1:A:247:GLY:N	1:A:290:GLU:OE1	2.44	0.45
1:F:519:LYS:O	1:F:523:THR:OG1	2.27	0.45
1:I:236:MET:O	1:I:270:ILE:HA	2.15	0.45
1:A:190:PHE:CD1	1:A:204:ILE:HG21	2.51	0.45
1:A:219:THR:HG23	1:A:269:PHE:CE2	2.51	0.45
1:A:447:HIS:CE1	1:A:480:HIS:HB3	2.50	0.45
1:B:327:LEU:O	1:B:333:PHE:HB2	2.17	0.45
1:D:190:PHE:HA	1:D:197:PHE:CE1	2.51	0.45
1:D:577:GLU:O	1:D:581:ILE:HG13	2.17	0.45
1:F:583:LEU:HD13	1:F:583:LEU:HA	1.82	0.45
1:I:519:LYS:O	1:I:523:THR:OG1	2.27	0.45
1:K:599:LYS:O	1:K:601:THR:N	2.46	0.45
1:A:519:LYS:O	1:A:523:THR:OG1	2.27	0.45
1:B:308:HIS:O	1:B:309:THR:HB	2.17	0.45
1:D:251:SER:O	1:D:255:ASP:HB3	2.17	0.45
1:D:516:SER:O	1:D:520:LYS:HG3	2.17	0.45
1:I:298:LEU:O	1:I:302:MET:HG3	2.15	0.45
1:K:344:ILE:HD13	1:K:371:ARG:HB3	1.98	0.45
1:B:213:SER:HB3	1:B:214:PRO:HD2	1.98	0.45
1:B:251:SER:O	1:B:255:ASP:HB3	2.17	0.45
1:F:221:LEU:O	1:F:225:VAL:HG23	2.17	0.45
1:I:447:HIS:CE1	1:I:480:HIS:HB3	2.51	0.45
1:K:596:LEU:C	1:K:598:LEU:N	2.68	0.45
1:A:494:ALA:C	1:A:496:GLU:H	2.20	0.45
1:B:247:GLY:N	1:B:290:GLU:OE1	2.43	0.45
1:B:278:ARG:HD2	1:B:291:ARG:HD2	1.99	0.45
1:D:221:LEU:O	1:D:225:VAL:HG23	2.17	0.45
1:F:432:ALA:HB1	1:F:593:ALA:HA	1.97	0.45
1:F:586:LYS:O	1:F:590:VAL:HG23	2.16	0.45
1:I:327:LEU:O	1:I:333:PHE:HB2	2.17	0.45
1:B:221:LEU:O	1:B:225:VAL:HG23	2.17	0.45
1:F:327:LEU:O	1:F:333:PHE:HB2	2.16	0.45
1:I:485:LYS:HA	1:I:488:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:HB2	1:A:172:LYS:HE3	1.70	0.44
1:D:531:VAL:HA	1:D:562:LYS:HD3	1.98	0.44
1:A:492:GLY:O	1:A:496:GLU:HB2	2.18	0.44
1:D:344:ILE:HD13	1:D:371:ARG:HB3	1.98	0.44
1:D:519:LYS:O	1:D:523:THR:OG1	2.26	0.44
1:I:221:LEU:O	1:I:225:VAL:HG23	2.17	0.44
1:I:248:VAL:O	1:I:252:ARG:HG2	2.17	0.44
1:K:577:GLU:O	1:K:581:ILE:HG13	2.16	0.44
1:B:219:THR:HG23	1:B:269:PHE:CE2	2.52	0.44
1:F:191:LEU:HB3	1:F:231:VAL:HG21	2.00	0.44
1:I:219:THR:HG23	1:I:269:PHE:CE2	2.52	0.44
1:F:260:ALA:O	1:F:266:CYS:SG	2.75	0.44
1:F:406:GLU:N	1:F:406:GLU:OE1	2.51	0.44
1:I:498:ILE:HD12	1:I:582:LEU:HB3	1.99	0.44
1:K:327:LEU:O	1:K:333:PHE:HB2	2.17	0.44
1:A:221:LEU:O	1:A:225:VAL:HG23	2.17	0.44
1:A:442:HIS:HB3	1:A:450:PRO:HA	1.99	0.44
1:A:485:LYS:HA	1:A:488:ILE:HD12	2.00	0.44
1:D:289:ASP:OD1	1:D:291:ARG:HB3	2.17	0.44
1:I:348:GLU:HA	1:I:351:LEU:HD12	1.99	0.44
1:A:381:LEU:O	1:A:384:LEU:HB3	2.18	0.44
1:D:586:LYS:O	1:D:590:VAL:HG23	2.18	0.44
1:I:434:HIS:CD2	1:I:438:HIS:HE2	2.34	0.44
1:D:193:ASN:O	1:D:196:LYS:HG2	2.18	0.44
1:D:348:GLU:HA	1:D:351:LEU:HD12	2.00	0.44
1:D:442:HIS:HB3	1:D:450:PRO:HA	1.99	0.44
1:K:221:LEU:O	1:K:225:VAL:HG23	2.17	0.44
1:I:190:PHE:CG	1:I:204:ILE:HG21	2.53	0.43
1:I:483:LEU:O	1:I:487:LYS:HG3	2.17	0.43
1:A:188:VAL:HG12	1:A:192:LYS:HD2	2.00	0.43
1:I:529:GLU:HG2	1:I:569:ARG:NH2	2.33	0.43
1:K:210:LEU:O	1:K:316:ALA:HA	2.19	0.43
1:K:519:LYS:O	1:K:523:THR:OG1	2.29	0.43
1:D:188:VAL:HG12	1:D:192:LYS:HD2	2.00	0.43
1:B:188:VAL:HG13	1:B:229:ALA:HB2	2.00	0.43
1:F:434:HIS:CD2	1:F:438:HIS:HE2	2.34	0.43
1:I:446:GLU:CG	1:I:447:HIS:CE1	3.02	0.43
1:A:494:ALA:C	1:A:496:GLU:N	2.72	0.43
1:B:519:LYS:O	1:B:523:THR:OG1	2.27	0.43
1:D:275:ALA:O	1:D:291:ARG:NH1	2.50	0.43
1:A:586:LYS:O	1:A:590:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:GLU:CG	1:D:447:HIS:CE1	3.02	0.43
1:F:295:LEU:O	1:F:298:LEU:HB3	2.18	0.43
1:F:348:GLU:HA	1:F:351:LEU:HD12	2.00	0.43
1:I:192:LYS:HD2	1:I:229:ALA:HA	2.01	0.43
1:D:178:GLU:OE2	1:D:179:GLU:HG3	2.18	0.43
1:F:219:THR:HG23	1:F:269:PHE:CE2	2.54	0.43
1:F:517:LEU:O	1:F:521:MET:HG3	2.19	0.43
1:F:577:GLU:O	1:F:581:ILE:HG13	2.19	0.43
1:F:592:LEU:HD13	1:F:592:LEU:HA	1.93	0.43
1:I:602:LEU:HD12	1:I:603:THR:H	1.82	0.43
1:K:290:GLU:O	1:K:293:GLN:HG2	2.18	0.43
1:K:446:GLU:CG	1:K:447:HIS:CE1	3.02	0.43
1:K:477:ILE:HB	1:K:482:ILE:HD11	2.01	0.43
1:A:348:GLU:HA	1:A:351:LEU:HD12	2.01	0.43
1:A:446:GLU:CG	1:A:447:HIS:CE1	3.02	0.43
1:I:495:SER:O	1:I:499:ASN:ND2	2.38	0.43
1:K:275:ALA:O	1:K:291:ARG:NH1	2.51	0.43
1:K:516:SER:O	1:K:520:LYS:HG3	2.18	0.43
1:D:327:LEU:O	1:D:333:PHE:HB2	2.17	0.43
1:I:256:LEU:HD21	1:I:268:ILE:HG21	2.00	0.43
1:I:302:MET:HE2	1:I:302:MET:HB3	1.96	0.43
1:F:242:VAL:O	1:F:244:MET:HA	2.19	0.42
1:K:190:PHE:CD1	1:K:204:ILE:HG21	2.54	0.42
1:A:344:ILE:HD13	1:A:371:ARG:HB3	2.02	0.42
1:D:517:LEU:O	1:D:521:MET:HG3	2.19	0.42
1:A:499:ASN:ND2	1:A:589:LEU:HD21	2.30	0.42
1:B:295:LEU:O	1:B:296:ASN:C	2.57	0.42
1:D:191:LEU:HB3	1:D:231:VAL:HG21	2.01	0.42
1:F:446:GLU:CG	1:F:447:HIS:CE1	3.02	0.42
1:D:190:PHE:CD1	1:D:204:ILE:HG21	2.55	0.42
1:I:578:ALA:O	1:I:579:SER:C	2.58	0.42
1:B:303:ASP:O	1:B:305:PHE:N	2.53	0.42
1:B:497:GLN:O	1:B:498:ILE:C	2.58	0.42
1:B:516:SER:O	1:B:520:LYS:HG3	2.18	0.42
1:F:188:VAL:HG13	1:F:229:ALA:HB2	2.01	0.42
1:F:599:LYS:C	1:F:601:THR:H	2.22	0.42
1:K:348:GLU:HA	1:K:351:LEU:HD12	2.00	0.42
1:A:210:LEU:O	1:A:316:ALA:HA	2.19	0.42
1:D:236:MET:HB3	1:D:241:PHE:CZ	2.55	0.42
1:K:260:ALA:O	1:K:266:CYS:SG	2.74	0.42
1:A:365:ASN:ND2	1:A:368:VAL:H	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LEU:O	1:A:521:MET:HG3	2.19	0.42
1:I:236:MET:HB3	1:I:241:PHE:CZ	2.55	0.42
1:K:354:HIS:HB2	1:K:385:ILE:HD12	2.00	0.42
1:A:317:THR:HG21	1:A:323:LEU:HD11	2.01	0.42
1:D:188:VAL:HG13	1:D:229:ALA:HB2	2.01	0.42
1:K:191:LEU:HB3	1:K:231:VAL:HG21	2.01	0.42
1:B:210:LEU:O	1:B:316:ALA:HA	2.20	0.42
1:F:210:LEU:O	1:F:316:ALA:HA	2.20	0.42
1:F:498:ILE:HD12	1:F:582:LEU:HB3	2.02	0.42
1:K:599:LYS:C	1:K:601:THR:H	2.22	0.42
1:B:577:GLU:O	1:B:581:ILE:HG13	2.20	0.41
1:I:602:LEU:HG	1:I:603:THR:N	2.35	0.41
1:K:596:LEU:C	1:K:598:LEU:H	2.23	0.41
1:A:241:PHE:CZ	1:A:256:LEU:HD22	2.44	0.41
1:A:529:GLU:H	1:A:529:GLU:HG2	1.70	0.41
1:B:236:MET:HB3	1:B:241:PHE:CZ	2.55	0.41
1:B:454:VAL:O	1:B:601:THR:HA	2.20	0.41
1:K:478:ASN:HB2	1:K:481:GLN:HG3	2.03	0.41
1:B:183:GLU:O	1:B:186:GLU:HG2	2.20	0.41
1:B:494:ALA:O	1:B:496:GLU:N	2.53	0.41
1:K:171:PHE:HD1	1:K:224:ALA:HB1	1.84	0.41
1:A:297:GLN:O	1:A:300:VAL:HB	2.20	0.41
1:B:437:GLY:HA3	1:B:495:SER:HG	1.86	0.41
1:F:190:PHE:CD1	1:F:204:ILE:HG21	2.56	0.41
1:F:317:THR:HG21	1:F:323:LEU:HD11	2.03	0.41
1:B:348:GLU:HA	1:B:351:LEU:HD12	2.01	0.41
1:I:210:LEU:O	1:I:316:ALA:HA	2.20	0.41
1:I:517:LEU:O	1:I:521:MET:HG3	2.20	0.41
1:K:517:LEU:O	1:K:521:MET:HG3	2.20	0.41
1:B:211:VAL:HG13	1:B:317:THR:HG23	2.03	0.41
1:A:275:ALA:O	1:A:291:ARG:NH1	2.54	0.41
1:A:296:ASN:O	1:A:300:VAL:HG23	2.21	0.41
1:A:457:ILE:HD13	1:A:457:ILE:O	2.21	0.41
1:A:598:LEU:HG	1:A:599:LYS:N	2.35	0.41
1:F:236:MET:HB3	1:F:241:PHE:CZ	2.56	0.41
1:F:596:LEU:HD13	1:F:596:LEU:HA	1.89	0.41
1:F:213:SER:HB3	1:F:214:PRO:HD2	2.02	0.41
1:F:275:ALA:O	1:F:291:ARG:NH1	2.51	0.41
1:I:518:ALA:O	1:I:522:VAL:HG23	2.20	0.41
1:K:596:LEU:O	1:K:600:GLU:N	2.49	0.41
1:A:577:GLU:O	1:A:581:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LYS:CG	1:B:359:LYS:O	2.69	0.41
1:B:517:LEU:O	1:B:521:MET:HG3	2.19	0.41
1:D:204:ILE:HG23	1:D:205:PRO:HD2	2.02	0.41
1:F:529:GLU:H	1:F:529:GLU:HG2	1.69	0.41
1:I:558:ASN:O	1:I:562:LYS:HG3	2.21	0.41
1:B:482:ILE:O	1:B:486:ILE:HG13	2.21	0.41
1:D:210:LEU:O	1:D:316:ALA:HA	2.20	0.41
1:F:478:ASN:HB2	1:F:481:GLN:HG3	2.03	0.41
1:I:266:CYS:SG	1:I:311:VAL:HG12	2.62	0.41
1:K:317:THR:HG21	1:K:323:LEU:HD11	2.02	0.41
1:B:269:PHE:HA	1:B:314:MET:O	2.22	0.40
1:I:569:ARG:O	1:I:573:GLU:HG3	2.21	0.40
1:K:596:LEU:HD12	1:K:596:LEU:HA	1.71	0.40
1:A:495:SER:HB3	1:A:589:LEU:HD11	2.03	0.40
1:A:568:LYS:O	1:A:572:GLU:HG3	2.22	0.40
1:D:498:ILE:HD12	1:D:582:LEU:HB3	2.03	0.40
1:F:269:PHE:HA	1:F:314:MET:O	2.21	0.40
1:F:497:GLN:O	1:F:501:GLY:HA2	2.21	0.40
1:I:269:PHE:HA	1:I:314:MET:O	2.21	0.40
1:D:478:ASN:HB2	1:D:481:GLN:HG3	2.04	0.40
1:F:477:ILE:HB	1:F:482:ILE:HD11	2.03	0.40
1:K:250:ALA:O	1:K:253:VAL:HB	2.21	0.40
1:K:258:ASP:O	1:K:261:ARG:CG	2.69	0.40
1:K:323:LEU:HB3	1:K:327:LEU:HD12	2.03	0.40
1:D:406:GLU:OE1	1:D:407:GLU:HG2	2.21	0.40
1:I:171:PHE:HD1	1:I:224:ALA:HB1	1.87	0.40
1:I:563:VAL:O	1:I:567:VAL:HG23	2.20	0.40
1:A:171:PHE:H	1:A:228:GLU:CD	2.25	0.40
1:A:563:VAL:O	1:A:567:VAL:HG23	2.22	0.40
1:F:254:ARG:HE	1:F:297:GLN:CD	2.24	0.40
1:F:434:HIS:HE1	1:F:510:ASP:OD1	2.05	0.40
1:F:588:GLN:O	1:F:591:LYS:HB2	2.22	0.40
1:K:175:ALA:HB2	1:K:353:ILE:HD11	2.04	0.40
1:K:393:ALA:HB3	1:K:394:ARG:HH12	1.85	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	352/453 (78%)	325 (92%)	23 (6%)	4 (1%)	14	45
1	B	360/453 (80%)	331 (92%)	23 (6%)	6 (2%)	9	35
1	D	350/453 (77%)	325 (93%)	23 (7%)	2 (1%)	25	57
1	F	351/453 (78%)	327 (93%)	21 (6%)	3 (1%)	17	48
1	I	351/453 (78%)	326 (93%)	22 (6%)	3 (1%)	17	48
1	K	352/453 (78%)	325 (92%)	23 (6%)	4 (1%)	14	45
All	All	2116/2718 (78%)	1959 (93%)	135 (6%)	22 (1%)	15	46

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	245	PHE
1	B	245	PHE
1	B	304	GLY
1	D	245	PHE
1	F	178	GLU
1	F	245	PHE
1	I	178	GLU
1	I	245	PHE
1	K	178	GLU
1	K	245	PHE
1	A	494	ALA
1	B	303	ASP
1	B	305	PHE
1	A	495	SER
1	I	333	PHE
1	K	289	ASP
1	B	178	GLU
1	B	333	PHE
1	D	333	PHE

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Mol	Chain	Res	Type
1	F	333	PHE
1	K	333	PHE

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	259/375 (69%)	197 (76%)	62 (24%)	0	2
1	B	263/375 (70%)	209 (80%)	54 (20%)	1	4
1	D	256/375 (68%)	203 (79%)	53 (21%)	1	4
1	F	257/375 (68%)	205 (80%)	52 (20%)	1	5
1	I	260/375 (69%)	203 (78%)	57 (22%)	1	3
1	K	259/375 (69%)	203 (78%)	56 (22%)	1	4
All	All	1554/2250 (69%)	1220 (78%)	334 (22%)	1	4

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	174	VAL
1	A	178	GLU
1	A	179	GLU
1	A	185	ARG
1	A	196	LYS
1	A	200	ILE
1	A	206	LYS
1	A	211	VAL
1	A	213	SER
1	A	220	LEU
1	A	231	VAL
1	A	232	SER
1	A	237	SER
1	A	251	SER
1	A	252	ARG

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Mol	Chain	Res	Type
1	A	254	ARG
1	A	272	GLU
1	A	274	ASP
1	A	276	VAL
1	A	288	HIS
1	A	290	GLU
1	A	291	ARG
1	A	298	LEU
1	A	302	MET
1	A	303	ASP
1	A	305	PHE
1	A	321	ASP
1	A	328	LEU
1	A	329	ARG
1	A	332	ARG
1	A	335	ARG
1	A	340	SER
1	A	369	ILE
1	A	371	ARG
1	A	377	SER
1	A	386	ASN
1	A	406	GLU
1	A	424	THR
1	A	431	THR
1	A	452	HIS
1	A	454	VAL
1	A	455	THR
1	A	457	ILE
1	A	459	ARG
1	A	477	ILE
1	A	495	SER
1	A	497	GLN
1	A	520	LYS
1	A	529	GLU
1	A	537	VAL
1	A	556	SER
1	A	579	SER
1	A	583	LEU
1	A	587	ASP
1	A	589	LEU
1	A	592	LEU
1	A	594	LYS

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Mol	Chain	Res	Type
1	A	596	LEU
1	A	598	LEU
1	A	599	LYS
1	A	603	THR
1	B	172	LYS
1	B	179	GLU
1	B	185	ARG
1	B	196	LYS
1	B	200	ILE
1	B	206	LYS
1	B	211	VAL
1	B	213	SER
1	B	231	VAL
1	B	232	SER
1	B	237	SER
1	B	241	PHE
1	B	242	VAL
1	B	251	SER
1	B	252	ARG
1	B	255	ASP
1	B	274	ASP
1	B	276	VAL
1	B	278	ARG
1	B	290	GLU
1	B	295	LEU
1	B	298	LEU
1	B	307	THR
1	B	321	ASP
1	B	332	ARG
1	B	335	ARG
1	B	369	ILE
1	B	371	ARG
1	B	386	ASN
1	B	394	ARG
1	B	403	LYS
1	B	404	ASP
1	B	431	THR
1	B	446	GLU
1	B	452	HIS
1	B	477	ILE
1	B	495	SER
1	B	497	GLN

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Mol	Chain	Res	Type
1	B	509	ASN
1	B	529	GLU
1	B	537	VAL
1	B	556	SER
1	B	558	ASN
1	B	562	LYS
1	B	579	SER
1	B	583	LEU
1	B	587	ASP
1	B	589	LEU
1	B	592	LEU
1	B	594	LYS
1	B	596	LEU
1	B	599	LYS
1	B	602	LEU
1	B	603	THR
1	D	174	VAL
1	D	178	GLU
1	D	179	GLU
1	D	185	ARG
1	D	196	LYS
1	D	200	ILE
1	D	206	LYS
1	D	211	VAL
1	D	213	SER
1	D	220	LEU
1	D	231	VAL
1	D	232	SER
1	D	237	SER
1	D	241	PHE
1	D	251	SER
1	D	252	ARG
1	D	255	ASP
1	D	274	ASP
1	D	293	GLN
1	D	298	LEU
1	D	321	ASP
1	D	328	LEU
1	D	329	ARG
1	D	332	ARG
1	D	335	ARG
1	D	369	ILE

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Mol	Chain	Res	Type
1	D	371	ARG
1	D	377	SER
1	D	386	ASN
1	D	394	ARG
1	D	403	LYS
1	D	406	GLU
1	D	407	GLU
1	D	424	THR
1	D	431	THR
1	D	454	VAL
1	D	477	ILE
1	D	495	SER
1	D	497	GLN
1	D	509	ASN
1	D	529	GLU
1	D	537	VAL
1	D	558	ASN
1	D	583	LEU
1	D	584	LYS
1	D	587	ASP
1	D	589	LEU
1	D	592	LEU
1	D	594	LYS
1	D	596	LEU
1	D	598	LEU
1	D	599	LYS
1	D	602	LEU
1	F	178	GLU
1	F	179	GLU
1	F	185	ARG
1	F	192	LYS
1	F	196	LYS
1	F	200	ILE
1	F	206	LYS
1	F	211	VAL
1	F	213	SER
1	F	231	VAL
1	F	232	SER
1	F	237	SER
1	F	241	PHE
1	F	242	VAL
1	F	248	VAL

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Mol	Chain	Res	Type
1	F	251	SER
1	F	252	ARG
1	F	254	ARG
1	F	274	ASP
1	F	278	ARG
1	F	290	GLU
1	F	295	LEU
1	F	319	ARG
1	F	321	ASP
1	F	328	LEU
1	F	332	ARG
1	F	335	ARG
1	F	369	ILE
1	F	371	ARG
1	F	377	SER
1	F	386	ASN
1	F	394	ARG
1	F	403	LYS
1	F	404	ASP
1	F	406	GLU
1	F	407	GLU
1	F	424	THR
1	F	431	THR
1	F	477	ILE
1	F	497	GLN
1	F	509	ASN
1	F	529	GLU
1	F	558	ASN
1	F	579	SER
1	F	583	LEU
1	F	587	ASP
1	F	589	LEU
1	F	592	LEU
1	F	594	LYS
1	F	596	LEU
1	F	598	LEU
1	F	602	LEU
1	I	172	LYS
1	I	174	VAL
1	I	178	GLU
1	I	179	GLU
1	I	185	ARG

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Mol	Chain	Res	Type
1	I	192	LYS
1	I	200	ILE
1	I	204	ILE
1	I	206	LYS
1	I	211	VAL
1	I	220	LEU
1	I	231	VAL
1	I	232	SER
1	I	237	SER
1	I	239	SER
1	I	241	PHE
1	I	242	VAL
1	I	246	VAL
1	I	251	SER
1	I	252	ARG
1	I	254	ARG
1	I	255	ASP
1	I	259	ASN
1	I	274	ASP
1	I	276	VAL
1	I	278	ARG
1	I	290	GLU
1	I	298	LEU
1	I	321	ASP
1	I	328	LEU
1	I	329	ARG
1	I	332	ARG
1	I	335	ARG
1	I	340	SER
1	I	369	ILE
1	I	371	ARG
1	I	377	SER
1	I	386	ASN
1	I	394	ARG
1	I	403	LYS
1	I	404	ASP
1	I	424	THR
1	I	431	THR
1	I	454	VAL
1	I	477	ILE
1	I	495	SER
1	I	497	GLN

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Mol	Chain	Res	Type
1	I	509	ASN
1	I	529	GLU
1	I	537	VAL
1	I	579	SER
1	I	583	LEU
1	I	587	ASP
1	I	592	LEU
1	I	594	LYS
1	I	596	LEU
1	I	598	LEU
1	K	172	LYS
1	K	174	VAL
1	K	179	GLU
1	K	185	ARG
1	K	200	ILE
1	K	211	VAL
1	K	213	SER
1	K	220	LEU
1	K	231	VAL
1	K	232	SER
1	K	237	SER
1	K	241	PHE
1	K	242	VAL
1	K	251	SER
1	K	252	ARG
1	K	254	ARG
1	K	256	LEU
1	K	274	ASP
1	K	276	VAL
1	K	278	ARG
1	K	289	ASP
1	K	293	GLN
1	K	295	LEU
1	K	298	LEU
1	K	321	ASP
1	K	328	LEU
1	K	332	ARG
1	K	335	ARG
1	K	340	SER
1	K	369	ILE
1	K	371	ARG
1	K	377	SER

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Mol	Chain	Res	Type
1	K	394	ARG
1	K	403	LYS
1	K	424	THR
1	K	431	THR
1	K	454	VAL
1	K	477	ILE
1	K	486	ILE
1	K	495	SER
1	K	509	ASN
1	K	529	GLU
1	K	537	VAL
1	K	556	SER
1	K	566	GLU
1	K	579	SER
1	K	583	LEU
1	K	584	LYS
1	K	587	ASP
1	K	589	LEU
1	K	592	LEU
1	K	594	LYS
1	K	596	LEU
1	K	598	LEU
1	K	599	LYS
1	K	603	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	ASN
1	A	383	ASN
1	A	478	ASN
1	A	499	ASN
1	B	296	ASN
1	B	297	GLN
1	B	383	ASN
1	B	478	ASN
1	B	558	ASN
1	D	297	GLN
1	D	318	ASN
1	D	478	ASN
1	F	383	ASN
1	F	478	ASN

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Mol	Chain	Res	Type
1	F	499	ASN
1	I	297	GLN
1	I	383	ASN
1	I	478	ASN
1	K	293	GLN
1	K	297	GLN
1	K	383	ASN
1	K	478	ASN
1	K	558	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
2	ADP	B	701	-	24,29,29	0.77	0	29,45,45	1.01	2 (6%)
2	ADP	K	701	-	24,29,29	0.87	1 (4%)	29,45,45	1.07	2 (6%)
2	ADP	F	701	-	24,29,29	0.99	1 (4%)	29,45,45	1.32	3 (10%)
2	ADP	I	701	-	24,29,29	0.84	1 (4%)	29,45,45	1.02	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ADP	A	701	-	24,29,29	0.71	1 (4%)	29,45,45	1.03	2 (6%)
2	ADP	D	701	-	24,29,29	0.74	0	29,45,45	1.01	3 (10%)

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	B	701	-	-	2/12/32/32	0/3/3/3
2	ADP	K	701	-	-	1/12/32/32	0/3/3/3
2	ADP	F	701	-	-	1/12/32/32	0/3/3/3
2	ADP	I	701	-	-	0/12/32/32	0/3/3/3
2	ADP	A	701	-	-	2/12/32/32	0/3/3/3
2	ADP	D	701	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	ADP	C8-N7	-2.79	1.29	1.34
2	K	701	ADP	C4-N3	-2.48	1.32	1.35
2	I	701	ADP	C4-N3	-2.38	1.32	1.35
2	A	701	ADP	C8-N7	-2.01	1.31	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	701	ADP	C5-C6-N6	4.53	127.24	120.35
2	A	701	ADP	C5-C6-N6	3.00	124.92	120.35
2	D	701	ADP	C5-C6-N6	2.97	124.87	120.35
2	K	701	ADP	PA-O3A-PB	-2.92	122.81	132.83
2	B	701	ADP	C5-C6-N6	2.65	124.38	120.35
2	F	701	ADP	PA-O3A-PB	-2.64	123.78	132.83
2	I	701	ADP	PA-O3A-PB	-2.59	123.94	132.83
2	A	701	ADP	PA-O3A-PB	-2.55	124.07	132.83
2	B	701	ADP	PA-O3A-PB	-2.50	124.25	132.83
2	I	701	ADP	C5-C6-N6	2.47	124.11	120.35
2	F	701	ADP	C5-C6-N1	-2.44	114.82	120.35
2	K	701	ADP	C5-C6-N6	2.38	123.97	120.35
2	D	701	ADP	PA-O3A-PB	-2.30	124.95	132.83
2	D	701	ADP	C5-C6-N1	-2.03	115.76	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

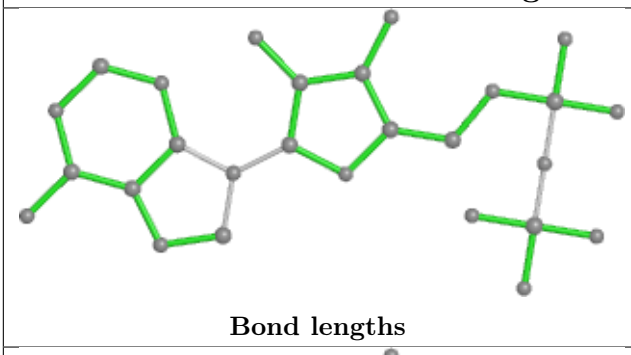
Mol	Chain	Res	Type	Atoms
2	A	701	ADP	PA-O3A-PB-O2B
2	B	701	ADP	PA-O3A-PB-O2B
2	D	701	ADP	PA-O3A-PB-O2B
2	F	701	ADP	PA-O3A-PB-O2B
2	K	701	ADP	PA-O3A-PB-O2B
2	A	701	ADP	C5'-O5'-PA-O1A
2	B	701	ADP	C5'-O5'-PA-O1A
2	D	701	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

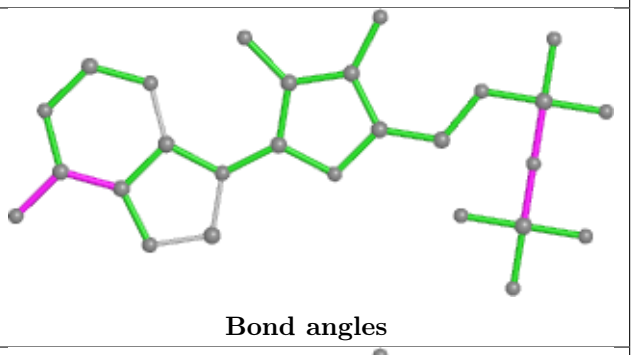
No monomer is involved in short contacts.

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 then 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.

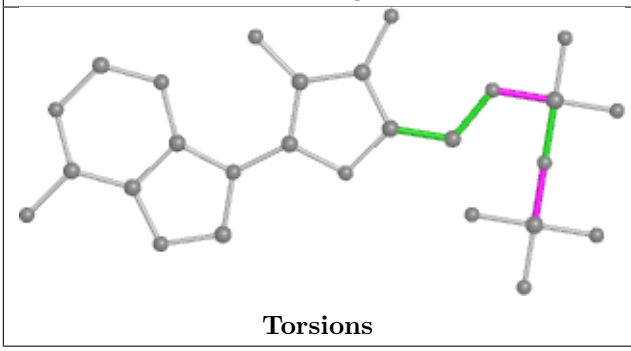
Ligand ADP B 701



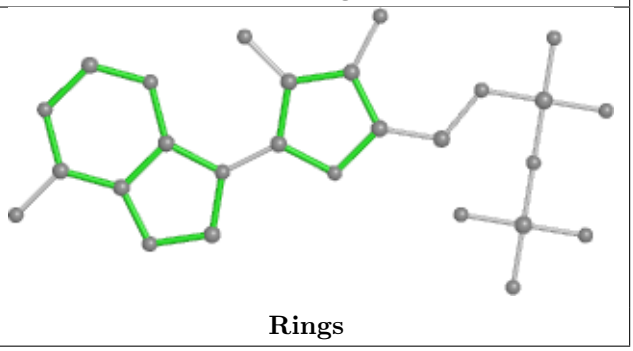
Bond lengths



Bond angles

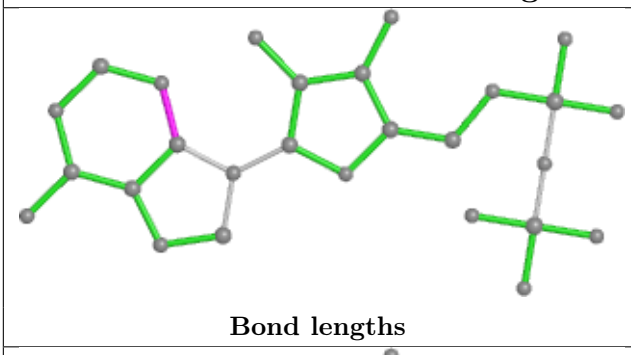


Torsions

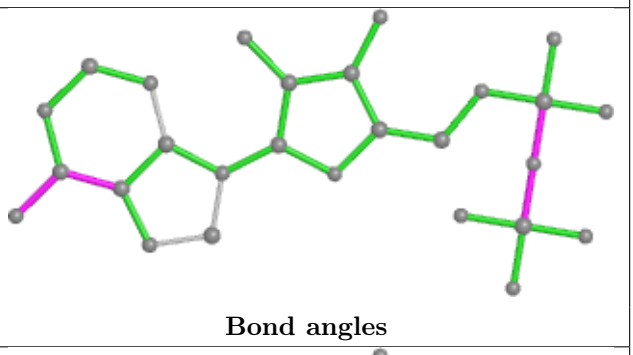


Rings

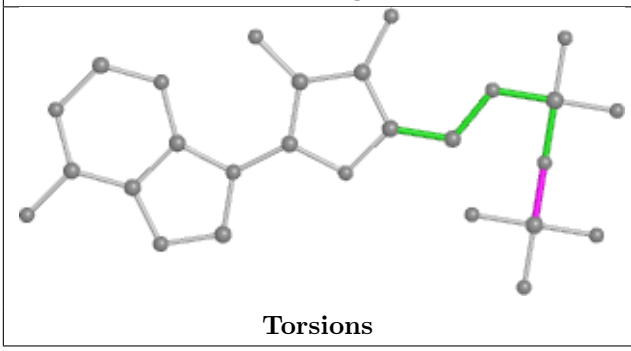
Ligand ADP K 701



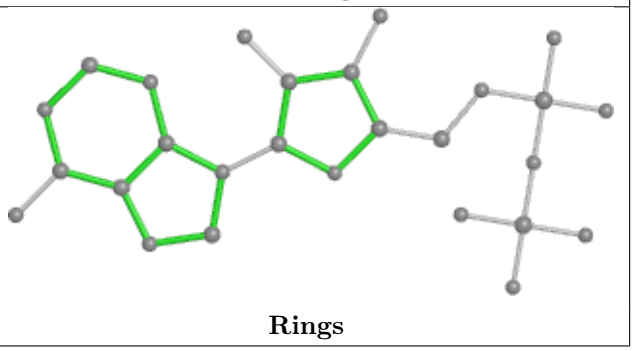
Bond lengths



Bond angles

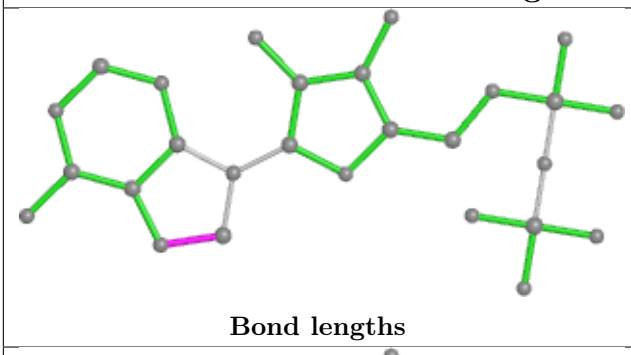


Torsions

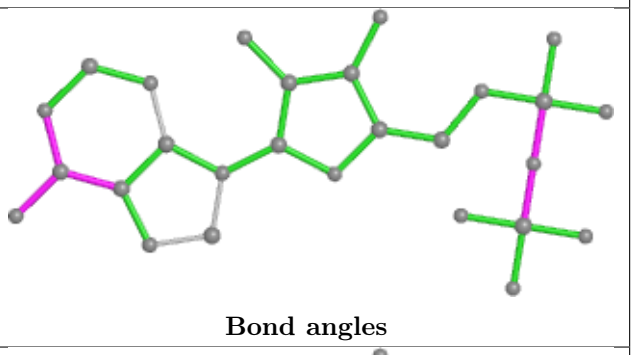


Rings

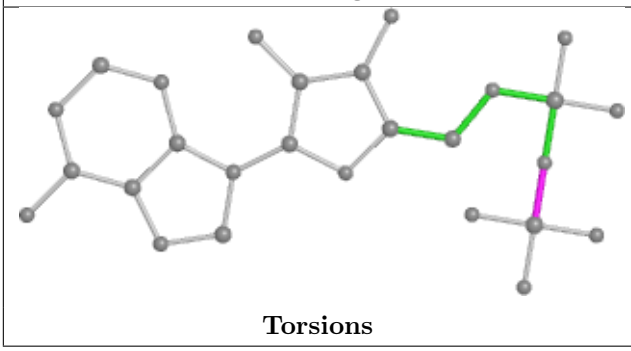
Ligand ADP F 701



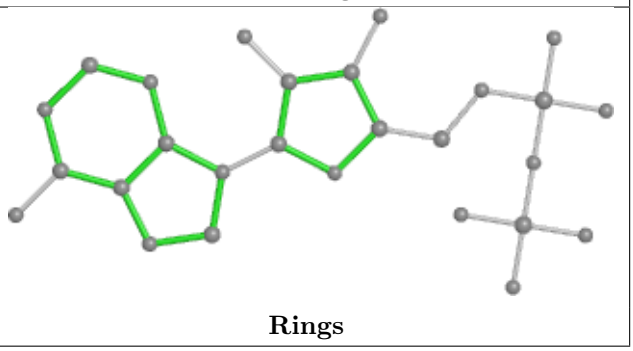
Bond lengths



Bond angles

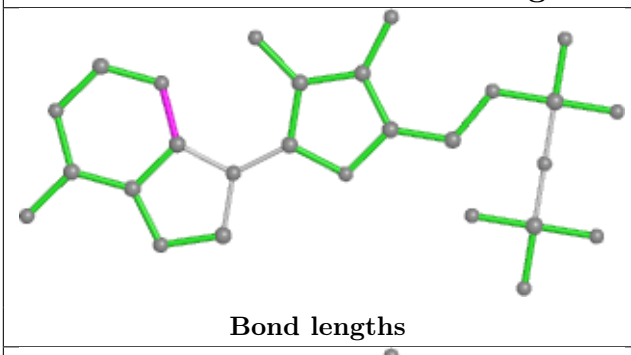


Torsions

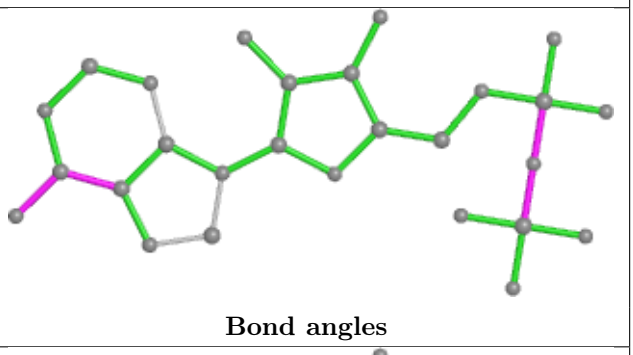


Rings

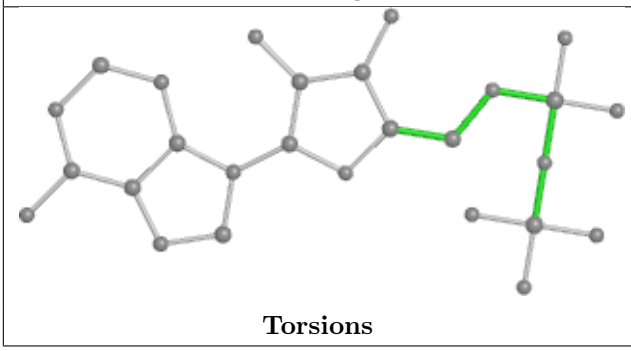
Ligand ADP I 701



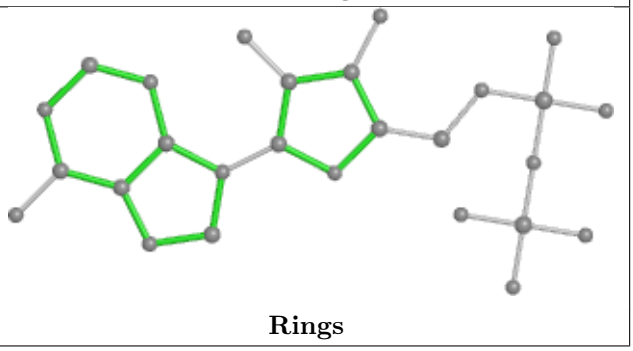
Bond lengths



Bond angles

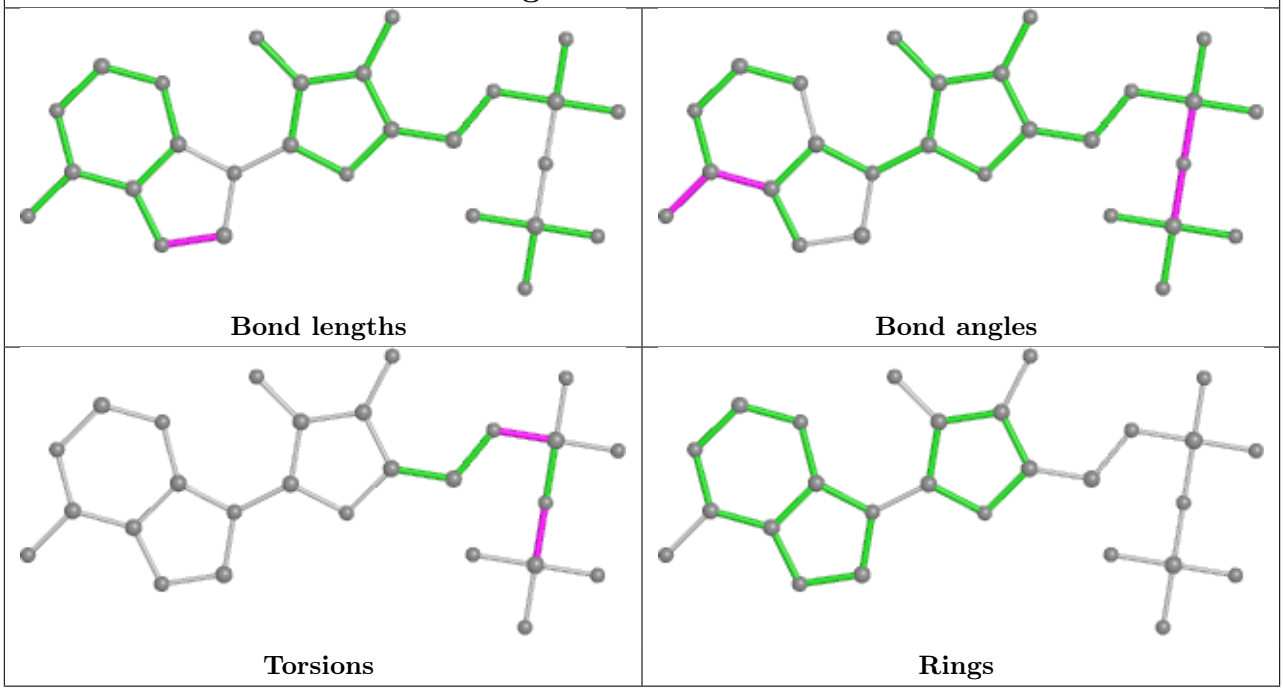


Torsions

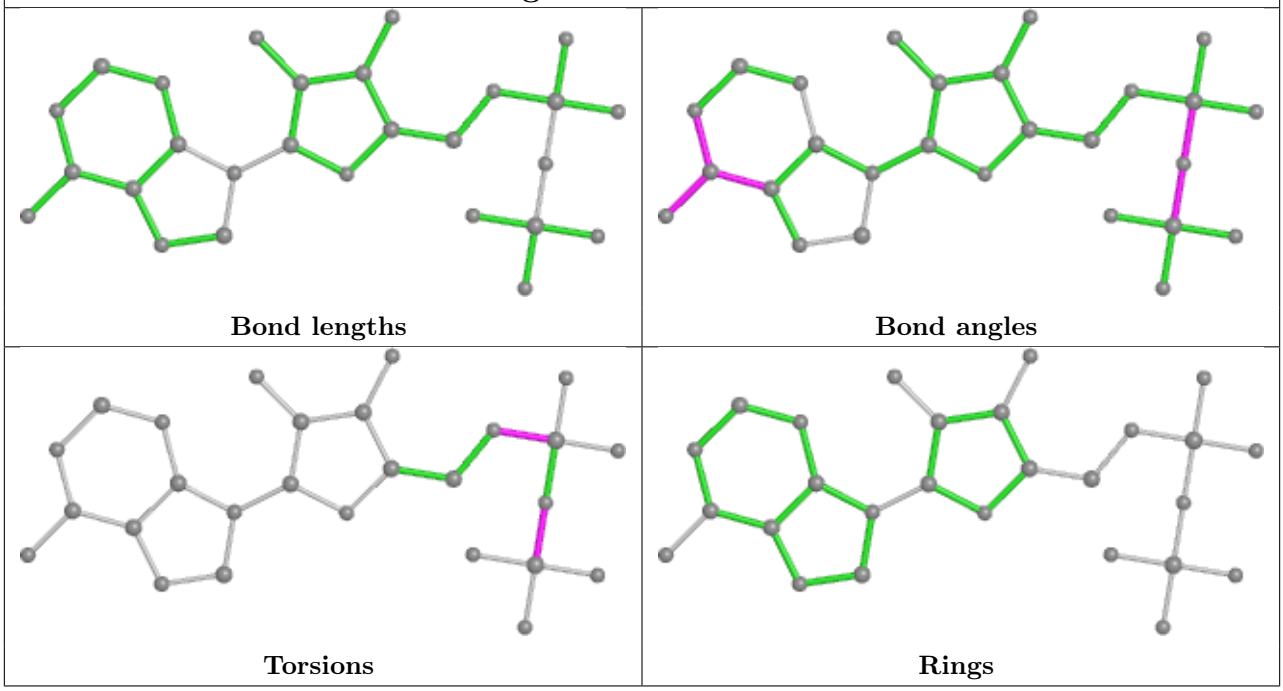


Rings

Ligand ADP A 701



Ligand ADP D 701



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	368/453 (81%)	0.24	14 (3%) 40 37	63, 122, 174, 225	0
1	B	374/453 (82%)	0.42	25 (6%) 17 17	60, 131, 191, 246	0
1	D	366/453 (80%)	0.30	21 (5%) 23 23	68, 128, 184, 256	0
1	F	367/453 (81%)	0.45	34 (9%) 8 9	63, 136, 201, 233	0
1	I	367/453 (81%)	0.38	26 (7%) 16 16	68, 133, 192, 254	0
1	K	368/453 (81%)	0.38	27 (7%) 15 15	68, 134, 189, 257	0
All	All	2210/2718 (81%)	0.36	147 (6%) 17 17	60, 131, 190, 257	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	244	MET	6.4
1	F	247	GLY	5.7
1	F	202	ALA	5.5
1	B	245	PHE	5.2
1	F	233	PHE	4.9
1	B	244	MET	4.8
1	F	312	ILE	4.6
1	B	233	PHE	4.5
1	B	317	THR	4.1
1	B	312	ILE	4.1
1	F	267	ILE	4.0
1	I	174	VAL	4.0
1	D	197	PHE	3.9
1	K	225	VAL	3.9
1	D	246	VAL	3.9
1	F	190	PHE	3.9
1	I	187	VAL	3.8
1	F	189	GLU	3.8
1	B	197	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	582	LEU	3.6
1	K	202	ALA	3.6
1	D	171	PHE	3.6
1	B	316	ALA	3.6
1	B	234	PHE	3.5
1	I	246	VAL	3.5
1	D	234	PHE	3.4
1	K	221	LEU	3.4
1	K	277	GLY	3.4
1	K	278	ARG	3.4
1	K	257	PHE	3.3
1	F	234	PHE	3.3
1	A	525	TRP	3.3
1	K	327	LEU	3.3
1	I	190	PHE	3.3
1	K	302	MET	3.3
1	I	232	SER	3.2
1	F	241	PHE	3.2
1	K	589	LEU	3.2
1	F	235	HIS	3.2
1	A	197	PHE	3.1
1	I	524	GLU	3.1
1	A	448	ALA	3.1
1	F	315	ALA	3.1
1	F	490	TYR	3.1
1	F	197	PHE	3.0
1	I	241	PHE	3.0
1	K	241	PHE	3.0
1	F	211	VAL	2.9
1	B	277	GLY	2.9
1	F	174	VAL	2.9
1	D	203	LYS	2.9
1	K	323	LEU	2.9
1	B	202	ALA	2.9
1	I	442	HIS	2.9
1	A	241	PHE	2.9
1	B	190	PHE	2.9
1	K	245	PHE	2.8
1	I	184	LEU	2.8
1	D	428	LYS	2.8
1	B	250	ALA	2.8
1	F	317	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	204	ILE	2.8
1	B	191	LEU	2.7
1	B	582	LEU	2.7
1	F	242	VAL	2.7
1	D	371	ARG	2.7
1	B	257	PHE	2.7
1	K	390	LEU	2.7
1	I	278	ARG	2.7
1	I	188	VAL	2.7
1	B	206	LYS	2.7
1	K	184	LEU	2.6
1	A	303	ASP	2.6
1	A	394	ARG	2.6
1	B	241	PHE	2.6
1	I	245	PHE	2.6
1	F	323	LEU	2.6
1	I	327	LEU	2.6
1	I	525	TRP	2.6
1	K	304	GLY	2.5
1	F	184	LEU	2.5
1	I	191	LEU	2.5
1	I	441	LEU	2.5
1	D	534	ILE	2.5
1	A	445	LEU	2.5
1	K	210	LEU	2.5
1	D	582	LEU	2.5
1	D	202	ALA	2.5
1	B	267	ILE	2.5
1	D	249	GLY	2.5
1	K	171	PHE	2.4
1	B	534	ILE	2.4
1	B	323	LEU	2.4
1	K	428	LYS	2.4
1	I	189	GLU	2.4
1	I	233	PHE	2.4
1	D	562	LYS	2.4
1	I	259	ASN	2.4
1	K	211	VAL	2.4
1	B	315	ALA	2.4
1	I	596	LEU	2.4
1	F	328	LEU	2.4
1	K	197	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	582	LEU	2.4
1	K	330	PRO	2.3
1	D	377	SER	2.3
1	F	534	ILE	2.3
1	K	207	GLY	2.3
1	D	184	LEU	2.3
1	F	257	PHE	2.3
1	A	533	PRO	2.3
1	D	375	GLY	2.3
1	K	256	LEU	2.3
1	K	234	PHE	2.3
1	I	560	ALA	2.3
1	F	176	GLY	2.2
1	F	560	ALA	2.3
1	B	256	LEU	2.2
1	I	312	ILE	2.2
1	F	363	ASP	2.2
1	K	440	LEU	2.2
1	D	390	LEU	2.2
1	A	200	ILE	2.2
1	B	558	ASN	2.2
1	F	531	VAL	2.1
1	F	301	GLU	2.1
1	F	231	VAL	2.1
1	F	381	LEU	2.1
1	K	528	GLY	2.1
1	D	233	PHE	2.1
1	F	248	VAL	2.1
1	D	363	ASP	2.1
1	D	247	GLY	2.1
1	D	191	LEU	2.1
1	I	247	GLY	2.1
1	F	200	ILE	2.1
1	F	533	PRO	2.1
1	A	205	PRO	2.0
1	B	288	HIS	2.0
1	A	174	VAL	2.0
1	A	276	VAL	2.0
1	A	433	TYR	2.0
1	F	191	LEU	2.0
1	F	582	LEU	2.0
1	I	257	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	326	ALA	2.0
1	D	210	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.