



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:15 AM GMT

PDB ID : 2CEA  
Title : CELL DIVISION PROTEIN FTSH  
Authors : Bieniossek, C.; Baumann, U.  
Deposited on : 2006-02-03  
Resolution : 2.75 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

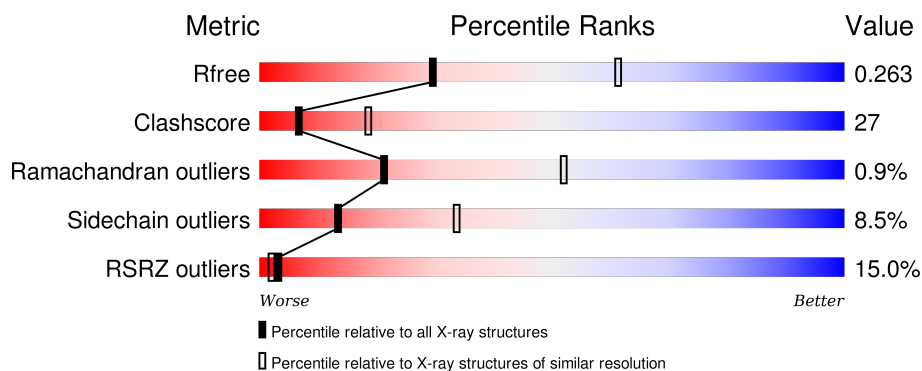
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	<div> <div>5%</div> <div>59% 22% • 14%</div> </div>
1	B	476	<div> <div>8%</div> <div>56% 27% • 14%</div> </div>
1	C	476	<div> <div>16%</div> <div>50% 33% 6% 12%</div> </div>
1	D	476	<div> <div>8%</div> <div>63% 21% • 13%</div> </div>
1	E	476	<div> <div>7%</div> <div>55% 26% • 15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	476	

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
3	ADP	C	1608	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19564 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 CELL DIVISION PROTEIN FTSH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	1
			3160	1996	559	595	10			
1	B	411	Total	C	N	O	S	0	0	0
			3191	2017	560	604	10			
1	C	421	Total	C	N	O	S	0	0	0
			3280	2076	573	621	10			
1	D	413	Total	C	N	O	S	0	0	0
			3212	2032	562	608	10			
1	E	406	Total	C	N	O	S	0	0	1
			3144	1986	557	591	10			
1	F	412	Total	C	N	O	S	0	0	0
			3204	2024	564	606	10			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	-	EXPRESSION TAG	UNP Q9WZ49
A	611	ALA	-	EXPRESSION TAG	UNP Q9WZ49
A	612	ALA	-	EXPRESSION TAG	UNP Q9WZ49
A	613	ALA	-	EXPRESSION TAG	UNP Q9WZ49
A	614	LEU	-	EXPRESSION TAG	UNP Q9WZ49
A	615	GLU	-	EXPRESSION TAG	UNP Q9WZ49
A	616	HIS	-	EXPRESSION TAG	UNP Q9WZ49
A	617	HIS	-	EXPRESSION TAG	UNP Q9WZ49
A	618	HIS	-	EXPRESSION TAG	UNP Q9WZ49
A	619	HIS	-	EXPRESSION TAG	UNP Q9WZ49
A	620	HIS	-	EXPRESSION TAG	UNP Q9WZ49
A	621	HIS	-	EXPRESSION TAG	UNP Q9WZ49
A	410	LEU	LYS	ENGINEERED MUTATION	UNP Q9WZ49
A	415	ALA	LYS	ENGINEERED MUTATION	UNP Q9WZ49
B	146	MET	-	EXPRESSION TAG	UNP Q9WZ49
B	611	ALA	-	EXPRESSION TAG	UNP Q9WZ49
B	612	ALA	-	EXPRESSION TAG	UNP Q9WZ49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	613	ALA	-	EXPRESSION TAG	UNP Q9WZ49
B	614	LEU	-	EXPRESSION TAG	UNP Q9WZ49
B	615	GLU	-	EXPRESSION TAG	UNP Q9WZ49
B	616	HIS	-	EXPRESSION TAG	UNP Q9WZ49
B	617	HIS	-	EXPRESSION TAG	UNP Q9WZ49
B	618	HIS	-	EXPRESSION TAG	UNP Q9WZ49
B	619	HIS	-	EXPRESSION TAG	UNP Q9WZ49
B	620	HIS	-	EXPRESSION TAG	UNP Q9WZ49
B	621	HIS	-	EXPRESSION TAG	UNP Q9WZ49
B	410	LEU	LYS	ENGINEERED MUTATION	UNP Q9WZ49
B	415	ALA	LYS	ENGINEERED MUTATION	UNP Q9WZ49
C	146	MET	-	EXPRESSION TAG	UNP Q9WZ49
C	611	ALA	-	EXPRESSION TAG	UNP Q9WZ49
C	612	ALA	-	EXPRESSION TAG	UNP Q9WZ49
C	613	ALA	-	EXPRESSION TAG	UNP Q9WZ49
C	614	LEU	-	EXPRESSION TAG	UNP Q9WZ49
C	615	GLU	-	EXPRESSION TAG	UNP Q9WZ49
C	616	HIS	-	EXPRESSION TAG	UNP Q9WZ49
C	617	HIS	-	EXPRESSION TAG	UNP Q9WZ49
C	618	HIS	-	EXPRESSION TAG	UNP Q9WZ49
C	619	HIS	-	EXPRESSION TAG	UNP Q9WZ49
C	620	HIS	-	EXPRESSION TAG	UNP Q9WZ49
C	621	HIS	-	EXPRESSION TAG	UNP Q9WZ49
C	410	LEU	LYS	ENGINEERED MUTATION	UNP Q9WZ49
C	415	ALA	LYS	ENGINEERED MUTATION	UNP Q9WZ49
D	146	MET	-	EXPRESSION TAG	UNP Q9WZ49
D	611	ALA	-	EXPRESSION TAG	UNP Q9WZ49
D	612	ALA	-	EXPRESSION TAG	UNP Q9WZ49
D	613	ALA	-	EXPRESSION TAG	UNP Q9WZ49
D	614	LEU	-	EXPRESSION TAG	UNP Q9WZ49
D	615	GLU	-	EXPRESSION TAG	UNP Q9WZ49
D	616	HIS	-	EXPRESSION TAG	UNP Q9WZ49
D	617	HIS	-	EXPRESSION TAG	UNP Q9WZ49
D	618	HIS	-	EXPRESSION TAG	UNP Q9WZ49
D	619	HIS	-	EXPRESSION TAG	UNP Q9WZ49
D	620	HIS	-	EXPRESSION TAG	UNP Q9WZ49
D	621	HIS	-	EXPRESSION TAG	UNP Q9WZ49
D	410	LEU	LYS	ENGINEERED MUTATION	UNP Q9WZ49
D	415	ALA	LYS	ENGINEERED MUTATION	UNP Q9WZ49
E	146	MET	-	EXPRESSION TAG	UNP Q9WZ49
E	611	ALA	-	EXPRESSION TAG	UNP Q9WZ49
E	612	ALA	-	EXPRESSION TAG	UNP Q9WZ49

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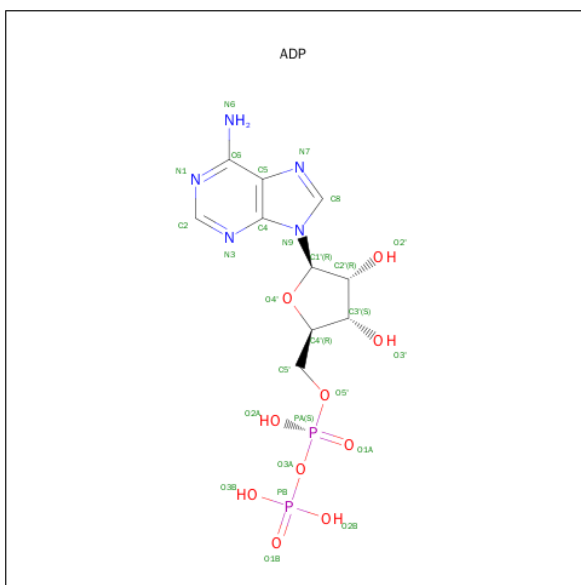
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Chain	Residue	Modelled	Actual	Comment	Reference
E	613	ALA	-	EXPRESSION TAG	UNP Q9WZ49
E	614	LEU	-	EXPRESSION TAG	UNP Q9WZ49
E	615	GLU	-	EXPRESSION TAG	UNP Q9WZ49
E	616	HIS	-	EXPRESSION TAG	UNP Q9WZ49
E	617	HIS	-	EXPRESSION TAG	UNP Q9WZ49
E	618	HIS	-	EXPRESSION TAG	UNP Q9WZ49
E	619	HIS	-	EXPRESSION TAG	UNP Q9WZ49
E	620	HIS	-	EXPRESSION TAG	UNP Q9WZ49
E	621	HIS	-	EXPRESSION TAG	UNP Q9WZ49
E	410	LEU	LYS	ENGINEERED MUTATION	UNP Q9WZ49
E	415	ALA	LYS	ENGINEERED MUTATION	UNP Q9WZ49
F	146	MET	-	EXPRESSION TAG	UNP Q9WZ49
F	611	ALA	-	EXPRESSION TAG	UNP Q9WZ49
F	612	ALA	-	EXPRESSION TAG	UNP Q9WZ49
F	613	ALA	-	EXPRESSION TAG	UNP Q9WZ49
F	614	LEU	-	EXPRESSION TAG	UNP Q9WZ49
F	615	GLU	-	EXPRESSION TAG	UNP Q9WZ49
F	616	HIS	-	EXPRESSION TAG	UNP Q9WZ49
F	617	HIS	-	EXPRESSION TAG	UNP Q9WZ49
F	618	HIS	-	EXPRESSION TAG	UNP Q9WZ49
F	619	HIS	-	EXPRESSION TAG	UNP Q9WZ49
F	620	HIS	-	EXPRESSION TAG	UNP Q9WZ49
F	621	HIS	-	EXPRESSION TAG	UNP Q9WZ49

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

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

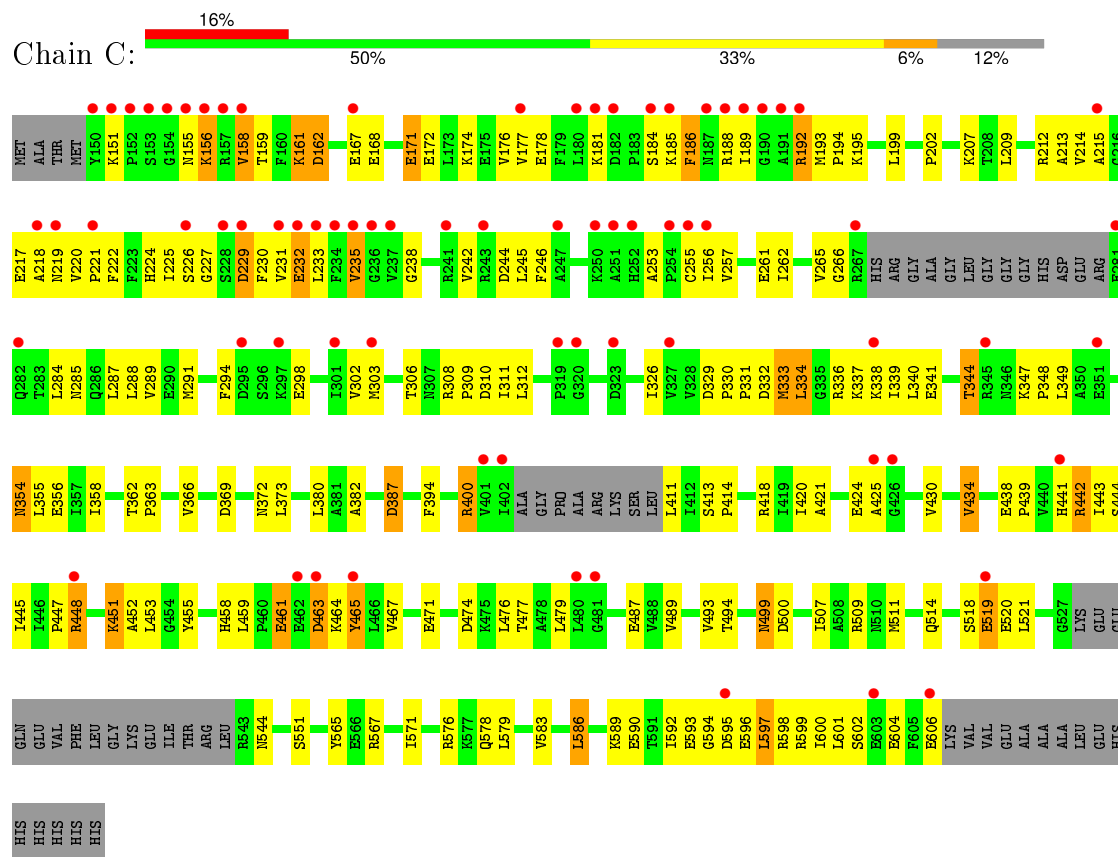
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total 46	O 46	0	0
5	B	35	Total 35	O 35	0	0
5	C	26	Total 26	O 26	0	0
5	D	34	Total 34	O 34	0	0
5	E	34	Total 34	O 34	0	0
5	F	24	Total 24	O 24	0	0

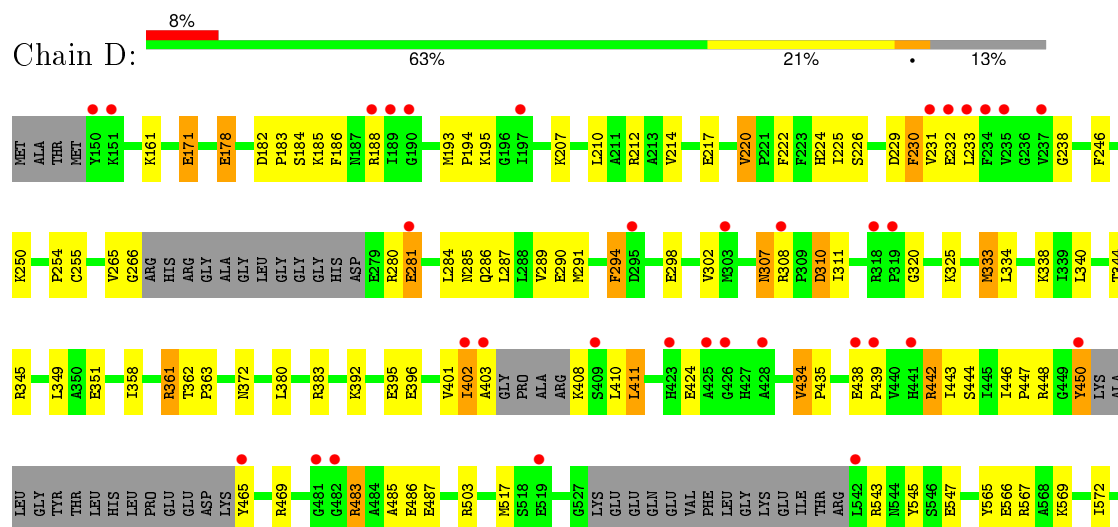




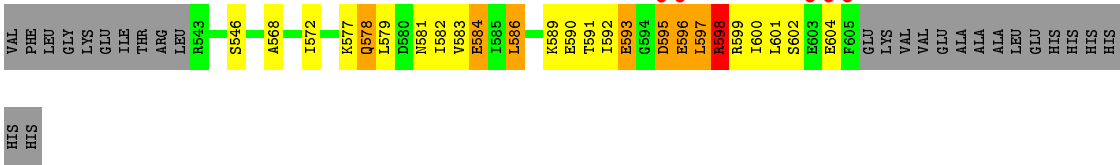
- Molecule 1: CELL DIVISION PROTEIN FTSH



- Molecule 1: CELL DIVISION PROTEIN FTSH







HIS  
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.32Å 165.32Å 234.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.75 19.98 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.75) 97.8 (19.98-2.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.216 , 0.262 0.215 , 0.263	Depositor DCC
$R_{free}$ test set	1283 reflections (1.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 77.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 82694 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 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	0.79	2/3202 (0.1%)	0.57	0/4314
1	B	0.76	2/3233 (0.1%)	0.56	1/4356 (0.0%)
1	C	0.59	0/3328	0.49	0/4488
1	D	0.68	0/3256	0.52	0/4388
1	E	0.72	1/3185 (0.0%)	0.54	0/4291
1	F	0.55	1/3248 (0.0%)	0.47	0/4376
All	All	0.68	6/19452 (0.0%)	0.53	1/26213 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	513	CYS	CB-SG	-7.17	1.70	1.82
1	A	519	GLU	CG-CD	6.13	1.61	1.51
1	F	513	CYS	CB-SG	-6.08	1.72	1.82
1	B	506	GLU	CG-CD	5.75	1.60	1.51
1	B	172	GLU	CG-CD	5.48	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	PRO	N-CA-CB	6.36	110.93	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3160	0	3240	119	0
1	B	3191	0	3261	143	0
1	C	3280	0	3346	199	0
1	D	3212	0	3283	121	0
1	E	3144	0	3231	172	0
1	F	3204	0	3270	301	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	7	0
3	C	27	0	12	10	0
3	D	27	0	12	6	0
3	E	27	0	12	7	0
3	F	27	0	12	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	46	0	0	5	0
5	B	35	0	0	13	0
5	C	26	0	0	9	0
5	D	34	0	0	11	0
5	E	34	0	0	6	0
5	F	24	0	0	9	0
All	All	19564	0	19703	1053	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 27.

The worst 5 of 1053 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:GLU:HA	5:C:2018:HOH:O	1.15	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:VAL:HG12	1:E:232:GLU:OE2	1.11	1.27
1:E:231:VAL:CG1	1:E:232:GLU:OE2	1.84	1.24
1:C:340:LEU:O	1:C:344:THR:HG22	1.38	1.20
1:C:594:GLY:N	5:C:2024:HOH:O	1.74	1.19

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	397/476 (83%)	379 (96%)	13 (3%)	5 (1%)	15	40
1	B	401/476 (84%)	378 (94%)	20 (5%)	3 (1%)	26	59
1	C	413/476 (87%)	393 (95%)	18 (4%)	2 (0%)	34	67
1	D	403/476 (85%)	383 (95%)	19 (5%)	1 (0%)	52	83
1	E	396/476 (83%)	376 (95%)	13 (3%)	7 (2%)	11	30
1	F	402/476 (84%)	372 (92%)	26 (6%)	4 (1%)	19	48
All	All	2412/2856 (84%)	2281 (95%)	109 (4%)	22 (1%)	21	52

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
1	A	602	SER
1	B	595	ASP
1	D	402	ILE
1	F	450	TYR



### 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	337/390 (86%)	308 (91%)	29 (9%)	13	33
1	B	339/390 (87%)	317 (94%)	22 (6%)	21	48
1	C	349/390 (90%)	312 (89%)	37 (11%)	8	22
1	D	342/390 (88%)	318 (93%)	24 (7%)	19	44
1	E	335/390 (86%)	308 (92%)	27 (8%)	15	36
1	F	340/390 (87%)	305 (90%)	35 (10%)	9	23
All	All	2042/2340 (87%)	1868 (92%)	174 (8%)	13	34

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	476	LEU
1	D	310	ASP
1	F	487	GLU
1	C	514	GLN
1	D	171	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	307	ASN
1	D	510	ASN
1	F	510	ASN
1	D	499	ASN
1	D	578	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 18 ligands modelled in this entry, 12 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	$\# Z  > 2$
3	ADP	A	1604	4	22,29,29	1.17	2 (9%)	27,45,45	2.40	6 (22%)
3	ADP	B	1607	4	22,29,29	0.96	0	27,45,45	2.34	6 (22%)
3	ADP	C	1608	4	22,29,29	1.09	2 (9%)	27,45,45	2.13	4 (14%)
3	ADP	D	1608	4	22,29,29	1.03	2 (9%)	27,45,45	2.30	4 (14%)
3	ADP	E	1604	4	22,29,29	0.98	2 (9%)	27,45,45	2.34	4 (14%)
3	ADP	F	1607	4	22,29,29	1.11	3 (13%)	27,45,45	2.01	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
3	ADP	A	1604	4	-	0/12/32/32	0/3/3/3
3	ADP	B	1607	4	-	0/12/32/32	0/3/3/3
3	ADP	C	1608	4	-	0/12/32/32	0/3/3/3
3	ADP	D	1608	4	-	0/12/32/32	0/3/3/3
3	ADP	E	1604	4	-	0/12/32/32	0/3/3/3
3	ADP	F	1607	4	-	0/12/32/32	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1608	ADP	C5-C4	2.02	1.45	1.40
3	F	1607	ADP	C2-N3	2.10	1.35	1.32
3	E	1604	ADP	C5-C4	2.10	1.45	1.40
3	E	1604	ADP	C2-N3	2.10	1.35	1.32
3	D	1608	ADP	C2-N3	2.21	1.36	1.32

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1608	ADP	N3-C2-N1	-8.26	122.57	128.89
3	A	1604	ADP	N3-C2-N1	-8.05	122.73	128.89
3	B	1607	ADP	N3-C2-N1	-8.03	122.75	128.89
3	C	1608	ADP	N3-C2-N1	-8.02	122.76	128.89
3	F	1607	ADP	N3-C2-N1	-7.80	122.92	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1604	ADP	1	0
3	B	1607	ADP	7	0
3	C	1608	ADP	10	0
3	D	1608	ADP	6	0
3	E	1604	ADP	7	0
3	F	1607	ADP	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/476 (85%)	0.38	23 (5%) 27 21	35, 44, 54, 66	0
1	B	411/476 (86%)	0.44	36 (8%) 12 8	34, 44, 54, 74	0
1	C	421/476 (88%)	0.99	74 (17%) 2 1	36, 43, 57, 86	0
1	D	413/476 (86%)	0.55	36 (8%) 13 8	35, 44, 56, 78	0
1	E	406/476 (85%)	0.44	31 (7%) 17 11	35, 44, 55, 84	0
1	F	412/476 (86%)	2.38	171 (41%) 0 0	34, 43, 56, 90	0
All	All	2470/2856 (86%)	0.86	371 (15%) 3 2	34, 43, 55, 90	0

The worst 5 of 371 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	236	GLY	28.0
1	F	235	VAL	20.5
1	F	230	PHE	15.1
1	C	235	VAL	11.6
1	F	153	SER	11.3

### 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ADP	C	1608	27/27	0.93	0.24	1.35	54,57,59,61	0
2	ZN	B	1606	1/1	0.97	0.23	0.10	64,64,64,64	0
3	ADP	A	1604	27/27	0.97	0.19	-0.16	32,34,39,41	0
2	ZN	A	1603	1/1	0.97	0.16	-0.56	63,63,63,63	0
3	ADP	F	1607	27/27	0.92	0.23	-0.69	72,79,80,81	0
3	ADP	D	1608	27/27	0.97	0.14	-1.02	21,25,30,31	0
4	MG	C	1609	1/1	0.68	0.14	-1.03	60,60,60,60	0
3	ADP	B	1607	27/27	0.97	0.14	-1.07	20,26,33,37	0
3	ADP	E	1604	27/27	0.97	0.14	-1.13	34,38,42,48	0
2	ZN	D	1607	1/1	0.97	0.27	-	79,79,79,79	0
4	MG	A	1605	1/1	0.93	0.12	-	47,47,47,47	0
4	MG	F	1608	1/1	0.95	0.10	-	68,68,68,68	0
4	MG	E	1605	1/1	0.89	0.20	-	53,53,53,53	0
2	ZN	F	1606	1/1	0.98	0.13	-	69,69,69,69	0
4	MG	B	1608	1/1	0.88	0.16	-	44,44,44,44	0
4	MG	D	1609	1/1	0.91	0.20	-	41,41,41,41	0
2	ZN	E	1603	1/1	0.98	0.15	-	63,63,63,63	0
2	ZN	C	1607	1/1	0.98	0.15	-	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.