



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 26, 2022 – 12:13 pm GMT

PDB ID : 6Z3D  
Title : L-FerritinMSA  
Authors : Davidov, G.; Zarivach, R.  
Deposited on : 2020-05-20  
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

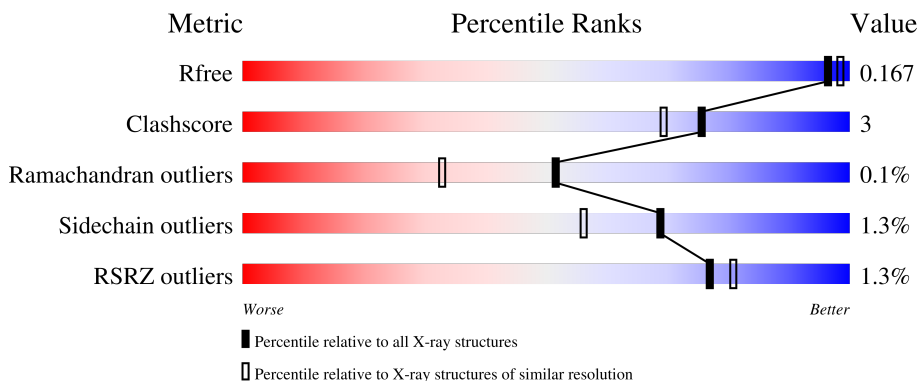
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	216	 73% 5% 22%
1	B	216	 71% 6% 21%
1	C	216	 75% 2% 21%
1	D	216	 72% 6% 21%
1	E	216	 74% 2% 21%

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Mol	Chain	Length	Quality of chain
1	F	216	 % 73% 5% 21%

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	ACT	A	201	-	-	X	-
2	ACT	A	202	-	-	X	-
2	ACT	C	201	-	-	X	-
2	ACT	D	201	-	-	X	-
2	ACT	E	201	-	-	X	-
2	ACT	E	202	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9643 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	169	1409	889	255	259	6	0	6	0
1	B	170	1412	888	254	264	6	0	5	0
1	C	170	1411	889	254	262	6	0	5	0
1	D	170	1416	891	258	261	6	0	5	0
1	E	170	1427	898	259	264	6	0	7	0
1	F	170	1407	883	258	261	5	0	4	0

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9CPX4
A	-18	GLY	-	expression tag	UNP Q9CPX4
A	-17	SER	-	expression tag	UNP Q9CPX4
A	-16	SER	-	expression tag	UNP Q9CPX4
A	-15	HIS	-	expression tag	UNP Q9CPX4
A	-14	HIS	-	expression tag	UNP Q9CPX4
A	-13	HIS	-	expression tag	UNP Q9CPX4
A	-12	HIS	-	expression tag	UNP Q9CPX4
A	-11	HIS	-	expression tag	UNP Q9CPX4
A	-10	HIS	-	expression tag	UNP Q9CPX4
A	-9	SER	-	expression tag	UNP Q9CPX4
A	-8	SER	-	expression tag	UNP Q9CPX4
A	-7	GLY	-	expression tag	UNP Q9CPX4
A	-6	LEU	-	expression tag	UNP Q9CPX4
A	-5	VAL	-	expression tag	UNP Q9CPX4
A	-4	PRO	-	expression tag	UNP Q9CPX4
A	-3	ARG	-	expression tag	UNP Q9CPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9CPX4
A	-1	SER	-	expression tag	UNP Q9CPX4
A	0	HIS	-	expression tag	UNP Q9CPX4
A	184	GLY	-	expression tag	UNP Q9CPX4
A	185	ASP	-	expression tag	UNP Q9CPX4
A	186	ILE	-	expression tag	UNP Q9CPX4
A	187	GLU	-	expression tag	UNP Q9CPX4
A	188	SER	-	expression tag	UNP Q9CPX4
A	189	ALA	-	expression tag	UNP Q9CPX4
A	190	GLN	-	expression tag	UNP Q9CPX4
A	191	SER	-	expression tag	UNP Q9CPX4
A	192	ASP	-	expression tag	UNP Q9CPX4
A	193	GLU	-	expression tag	UNP Q9CPX4
A	194	GLU	-	expression tag	UNP Q9CPX4
A	195	VAL	-	expression tag	UNP Q9CPX4
A	196	GLU	-	expression tag	UNP Q9CPX4
B	-19	MET	-	initiating methionine	UNP Q9CPX4
B	-18	GLY	-	expression tag	UNP Q9CPX4
B	-17	SER	-	expression tag	UNP Q9CPX4
B	-16	SER	-	expression tag	UNP Q9CPX4
B	-15	HIS	-	expression tag	UNP Q9CPX4
B	-14	HIS	-	expression tag	UNP Q9CPX4
B	-13	HIS	-	expression tag	UNP Q9CPX4
B	-12	HIS	-	expression tag	UNP Q9CPX4
B	-11	HIS	-	expression tag	UNP Q9CPX4
B	-10	HIS	-	expression tag	UNP Q9CPX4
B	-9	SER	-	expression tag	UNP Q9CPX4
B	-8	SER	-	expression tag	UNP Q9CPX4
B	-7	GLY	-	expression tag	UNP Q9CPX4
B	-6	LEU	-	expression tag	UNP Q9CPX4
B	-5	VAL	-	expression tag	UNP Q9CPX4
B	-4	PRO	-	expression tag	UNP Q9CPX4
B	-3	ARG	-	expression tag	UNP Q9CPX4
B	-2	GLY	-	expression tag	UNP Q9CPX4
B	-1	SER	-	expression tag	UNP Q9CPX4
B	0	HIS	-	expression tag	UNP Q9CPX4
B	184	GLY	-	expression tag	UNP Q9CPX4
B	185	ASP	-	expression tag	UNP Q9CPX4
B	186	ILE	-	expression tag	UNP Q9CPX4
B	187	GLU	-	expression tag	UNP Q9CPX4
B	188	SER	-	expression tag	UNP Q9CPX4
B	189	ALA	-	expression tag	UNP Q9CPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	190	GLN	-	expression tag	UNP Q9CPX4
B	191	SER	-	expression tag	UNP Q9CPX4
B	192	ASP	-	expression tag	UNP Q9CPX4
B	193	GLU	-	expression tag	UNP Q9CPX4
B	194	GLU	-	expression tag	UNP Q9CPX4
B	195	VAL	-	expression tag	UNP Q9CPX4
B	196	GLU	-	expression tag	UNP Q9CPX4
C	-19	MET	-	initiating methionine	UNP Q9CPX4
C	-18	GLY	-	expression tag	UNP Q9CPX4
C	-17	SER	-	expression tag	UNP Q9CPX4
C	-16	SER	-	expression tag	UNP Q9CPX4
C	-15	HIS	-	expression tag	UNP Q9CPX4
C	-14	HIS	-	expression tag	UNP Q9CPX4
C	-13	HIS	-	expression tag	UNP Q9CPX4
C	-12	HIS	-	expression tag	UNP Q9CPX4
C	-11	HIS	-	expression tag	UNP Q9CPX4
C	-10	HIS	-	expression tag	UNP Q9CPX4
C	-9	SER	-	expression tag	UNP Q9CPX4
C	-8	SER	-	expression tag	UNP Q9CPX4
C	-7	GLY	-	expression tag	UNP Q9CPX4
C	-6	LEU	-	expression tag	UNP Q9CPX4
C	-5	VAL	-	expression tag	UNP Q9CPX4
C	-4	PRO	-	expression tag	UNP Q9CPX4
C	-3	ARG	-	expression tag	UNP Q9CPX4
C	-2	GLY	-	expression tag	UNP Q9CPX4
C	-1	SER	-	expression tag	UNP Q9CPX4
C	0	HIS	-	expression tag	UNP Q9CPX4
C	184	GLY	-	expression tag	UNP Q9CPX4
C	185	ASP	-	expression tag	UNP Q9CPX4
C	186	ILE	-	expression tag	UNP Q9CPX4
C	187	GLU	-	expression tag	UNP Q9CPX4
C	188	SER	-	expression tag	UNP Q9CPX4
C	189	ALA	-	expression tag	UNP Q9CPX4
C	190	GLN	-	expression tag	UNP Q9CPX4
C	191	SER	-	expression tag	UNP Q9CPX4
C	192	ASP	-	expression tag	UNP Q9CPX4
C	193	GLU	-	expression tag	UNP Q9CPX4
C	194	GLU	-	expression tag	UNP Q9CPX4
C	195	VAL	-	expression tag	UNP Q9CPX4
C	196	GLU	-	expression tag	UNP Q9CPX4
D	-19	MET	-	initiating methionine	UNP Q9CPX4
D	-18	GLY	-	expression tag	UNP Q9CPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP Q9CPX4
D	-16	SER	-	expression tag	UNP Q9CPX4
D	-15	HIS	-	expression tag	UNP Q9CPX4
D	-14	HIS	-	expression tag	UNP Q9CPX4
D	-13	HIS	-	expression tag	UNP Q9CPX4
D	-12	HIS	-	expression tag	UNP Q9CPX4
D	-11	HIS	-	expression tag	UNP Q9CPX4
D	-10	HIS	-	expression tag	UNP Q9CPX4
D	-9	SER	-	expression tag	UNP Q9CPX4
D	-8	SER	-	expression tag	UNP Q9CPX4
D	-7	GLY	-	expression tag	UNP Q9CPX4
D	-6	LEU	-	expression tag	UNP Q9CPX4
D	-5	VAL	-	expression tag	UNP Q9CPX4
D	-4	PRO	-	expression tag	UNP Q9CPX4
D	-3	ARG	-	expression tag	UNP Q9CPX4
D	-2	GLY	-	expression tag	UNP Q9CPX4
D	-1	SER	-	expression tag	UNP Q9CPX4
D	0	HIS	-	expression tag	UNP Q9CPX4
D	184	GLY	-	expression tag	UNP Q9CPX4
D	185	ASP	-	expression tag	UNP Q9CPX4
D	186	ILE	-	expression tag	UNP Q9CPX4
D	187	GLU	-	expression tag	UNP Q9CPX4
D	188	SER	-	expression tag	UNP Q9CPX4
D	189	ALA	-	expression tag	UNP Q9CPX4
D	190	GLN	-	expression tag	UNP Q9CPX4
D	191	SER	-	expression tag	UNP Q9CPX4
D	192	ASP	-	expression tag	UNP Q9CPX4
D	193	GLU	-	expression tag	UNP Q9CPX4
D	194	GLU	-	expression tag	UNP Q9CPX4
D	195	VAL	-	expression tag	UNP Q9CPX4
D	196	GLU	-	expression tag	UNP Q9CPX4
E	-19	MET	-	initiating methionine	UNP Q9CPX4
E	-18	GLY	-	expression tag	UNP Q9CPX4
E	-17	SER	-	expression tag	UNP Q9CPX4
E	-16	SER	-	expression tag	UNP Q9CPX4
E	-15	HIS	-	expression tag	UNP Q9CPX4
E	-14	HIS	-	expression tag	UNP Q9CPX4
E	-13	HIS	-	expression tag	UNP Q9CPX4
E	-12	HIS	-	expression tag	UNP Q9CPX4
E	-11	HIS	-	expression tag	UNP Q9CPX4
E	-10	HIS	-	expression tag	UNP Q9CPX4
E	-9	SER	-	expression tag	UNP Q9CPX4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	SER	-	expression tag	UNP Q9CPX4
E	-7	GLY	-	expression tag	UNP Q9CPX4
E	-6	LEU	-	expression tag	UNP Q9CPX4
E	-5	VAL	-	expression tag	UNP Q9CPX4
E	-4	PRO	-	expression tag	UNP Q9CPX4
E	-3	ARG	-	expression tag	UNP Q9CPX4
E	-2	GLY	-	expression tag	UNP Q9CPX4
E	-1	SER	-	expression tag	UNP Q9CPX4
E	0	HIS	-	expression tag	UNP Q9CPX4
E	184	GLY	-	expression tag	UNP Q9CPX4
E	185	ASP	-	expression tag	UNP Q9CPX4
E	186	ILE	-	expression tag	UNP Q9CPX4
E	187	GLU	-	expression tag	UNP Q9CPX4
E	188	SER	-	expression tag	UNP Q9CPX4
E	189	ALA	-	expression tag	UNP Q9CPX4
E	190	GLN	-	expression tag	UNP Q9CPX4
E	191	SER	-	expression tag	UNP Q9CPX4
E	192	ASP	-	expression tag	UNP Q9CPX4
E	193	GLU	-	expression tag	UNP Q9CPX4
E	194	GLU	-	expression tag	UNP Q9CPX4
E	195	VAL	-	expression tag	UNP Q9CPX4
E	196	GLU	-	expression tag	UNP Q9CPX4
F	-19	MET	-	initiating methionine	UNP Q9CPX4
F	-18	GLY	-	expression tag	UNP Q9CPX4
F	-17	SER	-	expression tag	UNP Q9CPX4
F	-16	SER	-	expression tag	UNP Q9CPX4
F	-15	HIS	-	expression tag	UNP Q9CPX4
F	-14	HIS	-	expression tag	UNP Q9CPX4
F	-13	HIS	-	expression tag	UNP Q9CPX4
F	-12	HIS	-	expression tag	UNP Q9CPX4
F	-11	HIS	-	expression tag	UNP Q9CPX4
F	-10	HIS	-	expression tag	UNP Q9CPX4
F	-9	SER	-	expression tag	UNP Q9CPX4
F	-8	SER	-	expression tag	UNP Q9CPX4
F	-7	GLY	-	expression tag	UNP Q9CPX4
F	-6	LEU	-	expression tag	UNP Q9CPX4
F	-5	VAL	-	expression tag	UNP Q9CPX4
F	-4	PRO	-	expression tag	UNP Q9CPX4
F	-3	ARG	-	expression tag	UNP Q9CPX4
F	-2	GLY	-	expression tag	UNP Q9CPX4
F	-1	SER	-	expression tag	UNP Q9CPX4
F	0	HIS	-	expression tag	UNP Q9CPX4

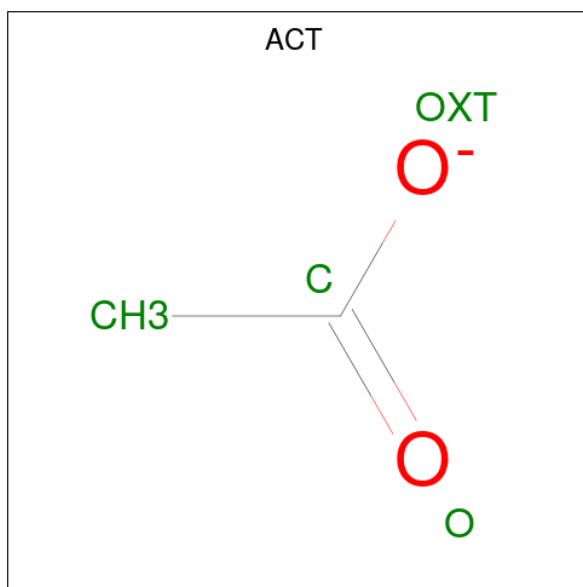
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Chain	Residue	Modelled	Actual	Comment	Reference
F	184	GLY	-	expression tag	UNP Q9CPX4
F	185	ASP	-	expression tag	UNP Q9CPX4
F	186	ILE	-	expression tag	UNP Q9CPX4
F	187	GLU	-	expression tag	UNP Q9CPX4
F	188	SER	-	expression tag	UNP Q9CPX4
F	189	ALA	-	expression tag	UNP Q9CPX4
F	190	GLN	-	expression tag	UNP Q9CPX4
F	191	SER	-	expression tag	UNP Q9CPX4
F	192	ASP	-	expression tag	UNP Q9CPX4
F	193	GLU	-	expression tag	UNP Q9CPX4
F	194	GLU	-	expression tag	UNP Q9CPX4
F	195	VAL	-	expression tag	UNP Q9CPX4
F	196	GLU	-	expression tag	UNP Q9CPX4

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0

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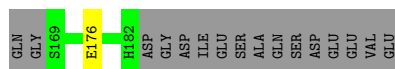
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			4	2	2		

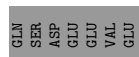
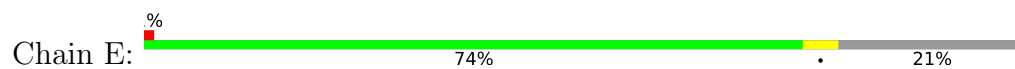
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		
3	B	221	Total	O	0	0
			221	221		
3	C	173	Total	O	0	0
			173	173		
3	D	198	Total	O	0	0
			198	198		
3	E	163	Total	O	0	0
			163	163		
3	F	168	Total	O	0	0
			168	168		

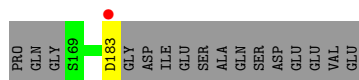
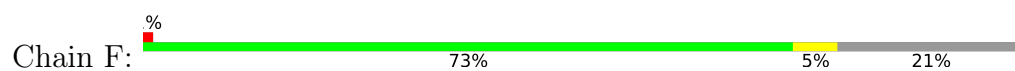




- Molecule 1: Ferritin



- Molecule 1: Ferritin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.30Å 134.30Å 166.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	166.85 – 1.70 48.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (166.85-1.70) 100.0 (48.74-1.70)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.155 , 0.176 0.168 , 0.167	Depositor DCC
$R_{free}$ test set	8447 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9643	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.85	1/1447 (0.1%)	0.91	4/1941 (0.2%)
1	B	0.87	4/1447 (0.3%)	0.96	8/1940 (0.4%)
1	C	0.80	0/1446	0.85	1/1939 (0.1%)
1	D	0.86	3/1448 (0.2%)	0.89	1/1941 (0.1%)
1	E	0.77	0/1468	0.85	3/1968 (0.2%)
1	F	0.78	0/1442	0.91	3/1934 (0.2%)
All	All	0.82	8/8698 (0.1%)	0.90	20/11663 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	GLU	CD-OE2	7.29	1.33	1.25
1	D	12	GLU	CD-OE2	5.89	1.32	1.25
1	B	12	GLU	CD-OE1	5.79	1.32	1.25
1	D	176	GLU	CD-OE1	5.19	1.31	1.25
1	B	58[A]	GLU	CD-OE2	5.17	1.31	1.25

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	B	154	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	154	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	C	154	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	E	154	ARG	NE-CZ-NH2	-8.02	116.29	120.30

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	1409	0	1403	10	0
1	B	1412	0	1397	11	0
1	C	1411	0	1400	6	0
1	D	1416	0	1409	8	0
1	E	1427	0	1421	4	0
1	F	1407	0	1391	7	0
2	A	8	0	6	3	0
2	C	4	0	3	2	0
2	D	4	0	3	2	0
2	E	8	0	6	4	0
3	A	214	0	0	3	1
3	B	221	0	0	5	1
3	C	173	0	0	3	0
3	D	198	0	0	4	0
3	E	163	0	0	0	0
3	F	168	0	0	2	0
All	All	9643	0	8439	52	1

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 3.

The worst 5 of 52 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76[A]:ARG:CG	3:B:201:HOH:O	1.96	1.12
1:B:76[A]:ARG:HG2	3:B:201:HOH:O	1.48	1.11
1:B:76[A]:ARG:NE	3:B:201:HOH:O	1.89	1.05
1:B:76[A]:ARG:CD	3:B:201:HOH:O	2.08	1.01
1:F:57:GLU:OE1	3:F:201:HOH:O	1.81	0.99

All (1) 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)
3:A:302:HOH:O	3:B:214:HOH:O[3_445]	2.18	0.02

### 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	171/216 (79%)	170 (99%)	1 (1%)	0	100	100
1	B	171/216 (79%)	170 (99%)	1 (1%)	0	100	100
1	C	171/216 (79%)	169 (99%)	2 (1%)	0	100	100
1	D	171/216 (79%)	168 (98%)	2 (1%)	1 (1%)	25	11
1	E	173/216 (80%)	171 (99%)	2 (1%)	0	100	100
1	F	170/216 (79%)	167 (98%)	3 (2%)	0	100	100
All	All	1027/1296 (79%)	1015 (99%)	11 (1%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	THR

#### 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	149/180 (83%)	147 (99%)	2 (1%)	69	56
1	B	149/180 (83%)	146 (98%)	3 (2%)	55	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	149/180 (83%)	148 (99%)	1 (1%)	84	77
1	D	149/180 (83%)	148 (99%)	1 (1%)	84	77
1	E	151/180 (84%)	148 (98%)	3 (2%)	55	38
1	F	148/180 (82%)	144 (97%)	4 (3%)	44	26
All	All	895/1080 (83%)	881 (98%)	14 (2%)	69	48

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	MET
1	E	2	THR
1	F	97[B]	MET
1	F	26	ARG
1	F	97[A]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	182	HIS
1	E	182	HIS
1	F	50	HIS
1	A	182	HIS
1	A	83	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACT	D	201	-	1,3,3	4.40	1 (100%)	0,3,3	-	-
2	ACT	A	201	-	1,3,3	4.50	1 (100%)	0,3,3	-	-
2	ACT	E	202	-	1,3,3	4.46	1 (100%)	0,3,3	-	-
2	ACT	A	202	-	1,3,3	5.54	1 (100%)	0,3,3	-	-
2	ACT	E	201	-	1,3,3	4.74	1 (100%)	0,3,3	-	-
2	ACT	C	201	-	1,3,3	3.90	1 (100%)	0,3,3	-	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	202	ACT	CH3-C	5.54	1.55	1.48
2	E	201	ACT	CH3-C	4.74	1.54	1.48
2	A	201	ACT	CH3-C	4.50	1.54	1.48
2	E	202	ACT	CH3-C	4.46	1.54	1.48
2	D	201	ACT	CH3-C	4.40	1.54	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	ACT	2	0
2	A	201	ACT	3	0
2	E	202	ACT	4	0
2	A	202	ACT	3	0
2	E	201	ACT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	ACT	2	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	169/216 (78%)	-0.16	1 (0%) 89 91	15, 21, 35, 54	0
1	B	170/216 (78%)	0.12	1 (0%) 89 91	14, 19, 31, 83	0
1	C	170/216 (78%)	-0.13	2 (1%) 79 82	20, 26, 38, 89	0
1	D	170/216 (78%)	-0.06	4 (2%) 59 63	17, 23, 38, 89	0
1	E	170/216 (78%)	-0.05	2 (1%) 79 82	23, 28, 41, 86	0
1	F	170/216 (78%)	0.12	3 (1%) 68 72	20, 27, 39, 78	0
All	All	1019/1296 (78%)	-0.03	13 (1%) 77 81	14, 25, 39, 89	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	7.7
1	C	1	MET	5.6
1	D	1	MET	5.3
1	D	2	THR	4.8
1	E	2	THR	4.7

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	D	201	4/4	0.60	0.22	52,52,56,59	0
2	ACT	E	201	4/4	0.68	0.18	61,61,63,66	0
2	ACT	A	201	4/4	0.69	0.17	45,47,49,53	0
2	ACT	A	202	4/4	0.72	0.17	39,41,44,49	0
2	ACT	E	202	4/4	0.72	0.22	55,57,58,62	0
2	ACT	C	201	4/4	0.78	0.27	51,51,54,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.