wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2021 – 07:41 PM EDT

PDB ID	:	3D19
Title	:	Crystal structure of a conserved metalloprotein from Bacillus cereus
Authors	:	Bonanno, J.B.; Patskovsky, Y.; Freeman, J.; Bain, K.T.; Chang, S.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-05-05
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

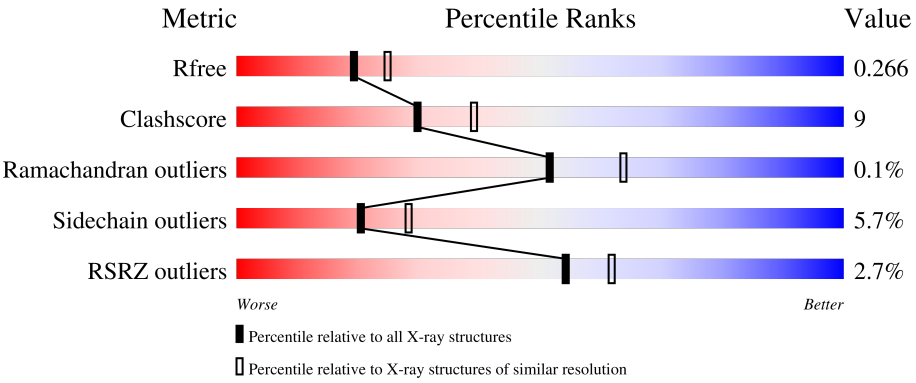
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	283	76% 15% • 7%
1	B	283	73% 18% • 7%
1	C	283	75% 14% • 9%
1	D	283	2% 65% 24% • 8%
1	E	283	7% 67% 22% • 9%

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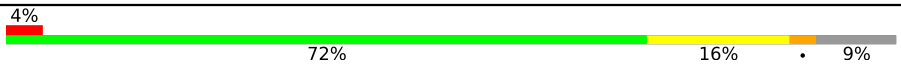
Mol	Chain	Length	Quality of chain
1	F	283	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13109 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 Conserved metalloprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2183	1393	381	400	9			
1	B	262	Total	C	N	O	S	0	3	0
			2181	1396	379	395	11			
1	C	258	Total	C	N	O	S	0	2	0
			2156	1380	375	391	10			
1	D	260	Total	C	N	O	S	0	1	0
			2160	1382	377	392	9			
1	E	257	Total	C	N	O	S	0	1	0
			2142	1371	374	388	9			
1	F	257	Total	C	N	O	S	0	1	0
			2146	1374	374	389	9			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP Q4MW04
A	9	SER	-	expression tag	UNP Q4MW04
A	10	LEU	-	expression tag	UNP Q4MW04
A	39	PHE	LEU	engineered mutation	UNP Q4MW04
A	137	ILE	MET	engineered mutation	UNP Q4MW04
A	138	GLN	GLU	engineered mutation	UNP Q4MW04
A	193	GLU	ALA	engineered mutation	UNP Q4MW04
A	211	ALA	VAL	engineered mutation	UNP Q4MW04
A	283	GLU	-	expression tag	UNP Q4MW04
A	284	GLY	-	expression tag	UNP Q4MW04
A	285	HIS	-	expression tag	UNP Q4MW04
A	286	HIS	-	expression tag	UNP Q4MW04
A	287	HIS	-	expression tag	UNP Q4MW04
A	288	HIS	-	expression tag	UNP Q4MW04
A	289	HIS	-	expression tag	UNP Q4MW04
A	290	HIS	-	expression tag	UNP Q4MW04
B	8	MET	-	expression tag	UNP Q4MW04

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	SER	-	expression tag	UNP Q4MW04
B	10	LEU	-	expression tag	UNP Q4MW04
B	39	PHE	LEU	engineered mutation	UNP Q4MW04
B	137	ILE	MET	engineered mutation	UNP Q4MW04
B	138	GLN	GLU	engineered mutation	UNP Q4MW04
B	193	GLU	ALA	engineered mutation	UNP Q4MW04
B	211	ALA	VAL	engineered mutation	UNP Q4MW04
B	283	GLU	-	expression tag	UNP Q4MW04
B	284	GLY	-	expression tag	UNP Q4MW04
B	285	HIS	-	expression tag	UNP Q4MW04
B	286	HIS	-	expression tag	UNP Q4MW04
B	287	HIS	-	expression tag	UNP Q4MW04
B	288	HIS	-	expression tag	UNP Q4MW04
B	289	HIS	-	expression tag	UNP Q4MW04
B	290	HIS	-	expression tag	UNP Q4MW04
C	8	MET	-	expression tag	UNP Q4MW04
C	9	SER	-	expression tag	UNP Q4MW04
C	10	LEU	-	expression tag	UNP Q4MW04
C	39	PHE	LEU	engineered mutation	UNP Q4MW04
C	137	ILE	MET	engineered mutation	UNP Q4MW04
C	138	GLN	GLU	engineered mutation	UNP Q4MW04
C	193	GLU	ALA	engineered mutation	UNP Q4MW04
C	211	ALA	VAL	engineered mutation	UNP Q4MW04
C	283	GLU	-	expression tag	UNP Q4MW04
C	284	GLY	-	expression tag	UNP Q4MW04
C	285	HIS	-	expression tag	UNP Q4MW04
C	286	HIS	-	expression tag	UNP Q4MW04
C	287	HIS	-	expression tag	UNP Q4MW04
C	288	HIS	-	expression tag	UNP Q4MW04
C	289	HIS	-	expression tag	UNP Q4MW04
C	290	HIS	-	expression tag	UNP Q4MW04
D	8	MET	-	expression tag	UNP Q4MW04
D	9	SER	-	expression tag	UNP Q4MW04
D	10	LEU	-	expression tag	UNP Q4MW04
D	39	PHE	LEU	engineered mutation	UNP Q4MW04
D	137	ILE	MET	engineered mutation	UNP Q4MW04
D	138	GLN	GLU	engineered mutation	UNP Q4MW04
D	193	GLU	ALA	engineered mutation	UNP Q4MW04
D	211	ALA	VAL	engineered mutation	UNP Q4MW04
D	283	GLU	-	expression tag	UNP Q4MW04
D	284	GLY	-	expression tag	UNP Q4MW04
D	285	HIS	-	expression tag	UNP Q4MW04

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Chain	Residue	Modelled	Actual	Comment	Reference
D	286	HIS	-	expression tag	UNP Q4MW04
D	287	HIS	-	expression tag	UNP Q4MW04
D	288	HIS	-	expression tag	UNP Q4MW04
D	289	HIS	-	expression tag	UNP Q4MW04
D	290	HIS	-	expression tag	UNP Q4MW04
E	8	MET	-	expression tag	UNP Q4MW04
E	9	SER	-	expression tag	UNP Q4MW04
E	10	LEU	-	expression tag	UNP Q4MW04
E	39	PHE	LEU	engineered mutation	UNP Q4MW04
E	137	ILE	MET	engineered mutation	UNP Q4MW04
E	138	GLN	GLU	engineered mutation	UNP Q4MW04
E	193	GLU	ALA	engineered mutation	UNP Q4MW04
E	211	ALA	VAL	engineered mutation	UNP Q4MW04
E	283	GLU	-	expression tag	UNP Q4MW04
E	284	GLY	-	expression tag	UNP Q4MW04
E	285	HIS	-	expression tag	UNP Q4MW04
E	286	HIS	-	expression tag	UNP Q4MW04
E	287	HIS	-	expression tag	UNP Q4MW04
E	288	HIS	-	expression tag	UNP Q4MW04
E	289	HIS	-	expression tag	UNP Q4MW04
E	290	HIS	-	expression tag	UNP Q4MW04
F	8	MET	-	expression tag	UNP Q4MW04
F	9	SER	-	expression tag	UNP Q4MW04
F	10	LEU	-	expression tag	UNP Q4MW04
F	39	PHE	LEU	engineered mutation	UNP Q4MW04
F	137	ILE	MET	engineered mutation	UNP Q4MW04
F	138	GLN	GLU	engineered mutation	UNP Q4MW04
F	193	GLU	ALA	engineered mutation	UNP Q4MW04
F	211	ALA	VAL	engineered mutation	UNP Q4MW04
F	283	GLU	-	expression tag	UNP Q4MW04
F	284	GLY	-	expression tag	UNP Q4MW04
F	285	HIS	-	expression tag	UNP Q4MW04
F	286	HIS	-	expression tag	UNP Q4MW04
F	287	HIS	-	expression tag	UNP Q4MW04
F	288	HIS	-	expression tag	UNP Q4MW04
F	289	HIS	-	expression tag	UNP Q4MW04
F	290	HIS	-	expression tag	UNP Q4MW04

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

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

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	E	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	39	Total O 39 39	0	0
4	C	37	Total O 37 37	0	0
4	D	8	Total O 8 8	0	0

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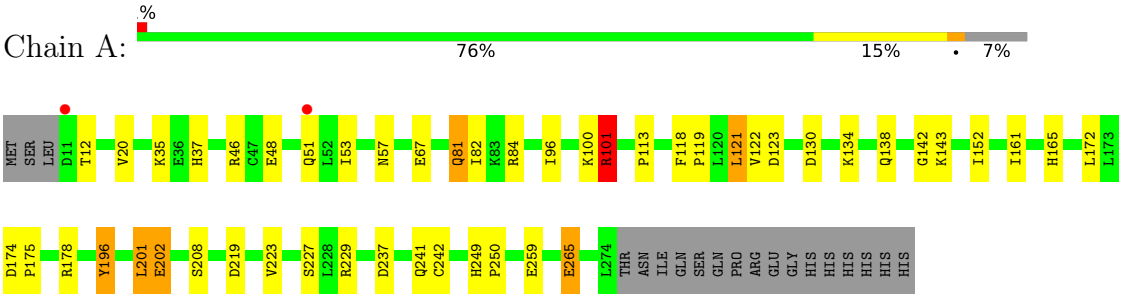
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	6	Total O 6 6	0	0
4	F	14	Total O 14 14	0	0

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.

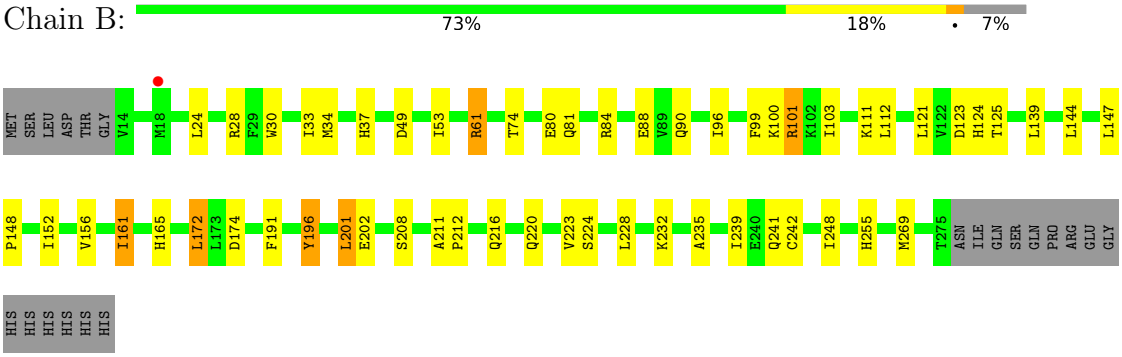
• Molecule 1: Conserved metalloprotein

Chain A:



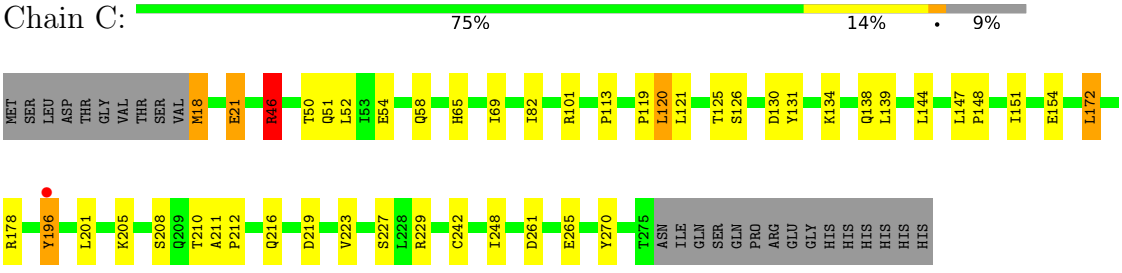
• Molecule 1: Conserved metalloprotein

Chain B:



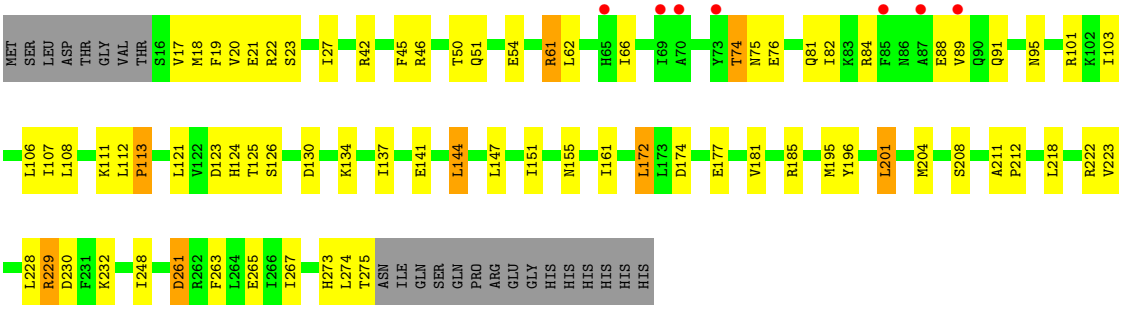
• Molecule 1: Conserved metalloprotein

Chain C:

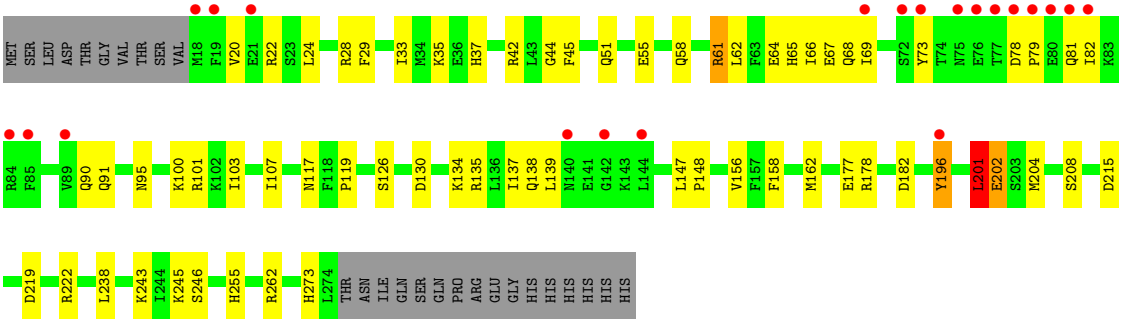


• Molecule 1: Conserved metalloprotein

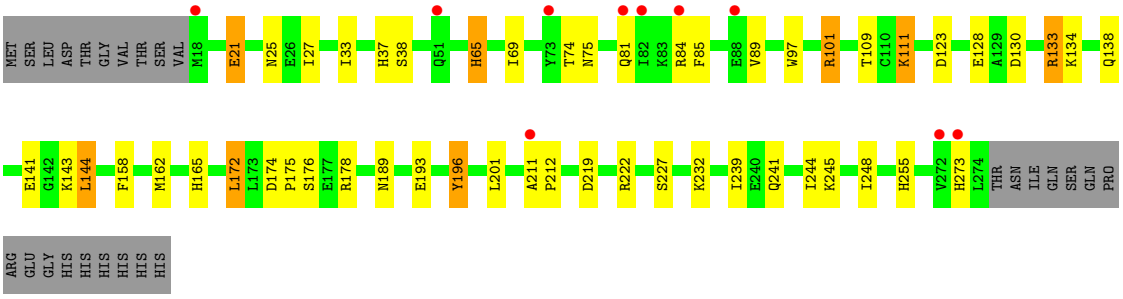
Chain D:



• Molecule 1: Conserved metalloprotein



• Molecule 1: Conserved metalloprotein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.83Å 136.38Å 87.06Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 40.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 99.2 (40.07-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.268 0.206 , 0.266	Depositor DCC
R_{free} test set	3758 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13109	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: FE, MG

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	0.83	0/2228	0.83	3/3004 (0.1%)
1	B	0.88	1/2236 (0.0%)	0.83	2/3014 (0.1%)
1	C	0.92	1/2208 (0.0%)	0.87	4/2976 (0.1%)
1	D	0.77	0/2209	0.77	0/2978
1	E	0.70	0/2191	0.76	3/2954 (0.1%)
1	F	0.75	0/2195	0.75	0/2958
All	All	0.81	2/13267 (0.0%)	0.80	12/17884 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	CYS	CB-SG	-6.69	1.70	1.82
1	B	88	GLU	CB-CG	5.27	1.62	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	101	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	101	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	E	222	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	C	178	ARG	NE-CZ-NH2	-5.93	117.33	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	2183	0	2161	33	0
1	B	2181	0	2148	44	0
1	C	2156	0	2131	30	0
1	D	2160	0	2135	59	0
1	E	2142	0	2117	46	0
1	F	2146	0	2125	45	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	25	0	0	1	0
4	B	39	0	0	0	0
4	C	37	0	0	0	0
4	D	8	0	0	0	0
4	E	6	0	0	1	0
4	F	14	0	0	1	0
All	All	13109	0	12817	242	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 9.

The worst 5 of 242 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:196[B]:TYR:CD2	1:C:196[B]:TYR:OH	1.66	1.46
1:D:81:GLN:OE1	1:D:84:ARG:NH2	1.66	1.27
1:E:61:ARG:HG2	1:E:61:ARG:HH11	1.00	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ARG:NH1	1:D:230:ASP:OD1	1.87	1.05
1:D:22:ARG:NH2	1:D:144:LEU:HD23	1.69	1.05

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	262/283 (93%)	255 (97%)	7 (3%)	0	100 100
1	B	263/283 (93%)	261 (99%)	2 (1%)	0	100 100
1	C	258/283 (91%)	254 (98%)	4 (2%)	0	100 100
1	D	259/283 (92%)	248 (96%)	10 (4%)	1 (0%)	34 42
1	E	256/283 (90%)	251 (98%)	5 (2%)	0	100 100
1	F	256/283 (90%)	251 (98%)	5 (2%)	0	100 100
All	All	1554/1698 (92%)	1520 (98%)	33 (2%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	113	PRO

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	239/258 (93%)	227 (95%)	12 (5%)	24	34
1	B	236/258 (92%)	227 (96%)	9 (4%)	33	47
1	C	235/258 (91%)	218 (93%)	17 (7%)	14	18
1	D	235/258 (91%)	219 (93%)	16 (7%)	16	21
1	E	233/258 (90%)	222 (95%)	11 (5%)	26	37
1	F	234/258 (91%)	214 (92%)	20 (8%)	10	13
All	All	1412/1548 (91%)	1327 (94%)	85 (6%)	20	26

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	196[A]	TYR
1	F	111	LYS
1	E	201	LEU
1	F	21	GLU
1	F	172	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	216	GLN
1	E	91	GLN
1	F	90	GLN
1	E	58	GLN
1	E	95	ASN

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 (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	264/283 (93%)	-0.12	2 (0%)	86	89	29, 40, 53, 62	0
1	B	262/283 (92%)	-0.12	1 (0%)	92	95	28, 39, 53, 60	0
1	C	258/283 (91%)	-0.26	1 (0%)	92	95	27, 37, 50, 59	0
1	D	260/283 (91%)	0.08	7 (2%)	54	62	31, 46, 62, 70	0
1	E	257/283 (90%)	0.29	21 (8%)	11	15	34, 51, 74, 86	0
1	F	257/283 (90%)	0.07	10 (3%)	39	46	29, 46, 62, 71	0
All	All	1558/1698 (91%)	-0.01	42 (2%)	54	62	27, 43, 62, 86	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	272	VAL	4.4
1	E	19	PHE	3.8
1	E	76	GLU	3.7
1	B	18[A]	MET	3.5
1	D	87	ALA	3.3

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

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

6.3 Carbohydrates

There are no 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	301	1/1	0.93	0.12	37,37,37,37	0
2	MG	E	301	1/1	0.94	0.05	40,40,40,40	0
2	MG	C	301	1/1	0.95	0.18	35,35,35,35	0
2	MG	D	301	1/1	0.96	0.07	35,35,35,35	0
2	MG	F	301	1/1	0.97	0.10	36,36,36,36	0
3	FE	E	302	1/1	0.98	0.11	53,53,53,53	0
3	FE	A	302	1/1	0.99	0.14	41,41,41,41	0
3	FE	B	302	1/1	0.99	0.12	42,42,42,42	0
3	FE	D	302	1/1	0.99	0.08	46,46,46,46	0
2	MG	A	301	1/1	0.99	0.16	31,31,31,31	0
3	FE	F	302	1/1	0.99	0.09	45,45,45,45	0
3	FE	C	302	1/1	1.00	0.12	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.