



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:38 PM GMT

PDB ID : 4PHX
Title : Crystal structure of AggB, the minor subunit of aggregative adherence fimbriae type I from the Escherichia coli O4H104
Authors : Pakharukova, N.A.; Tuitilla, M.; Zavialov, A.V.
Deposited on : 2014-05-07
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

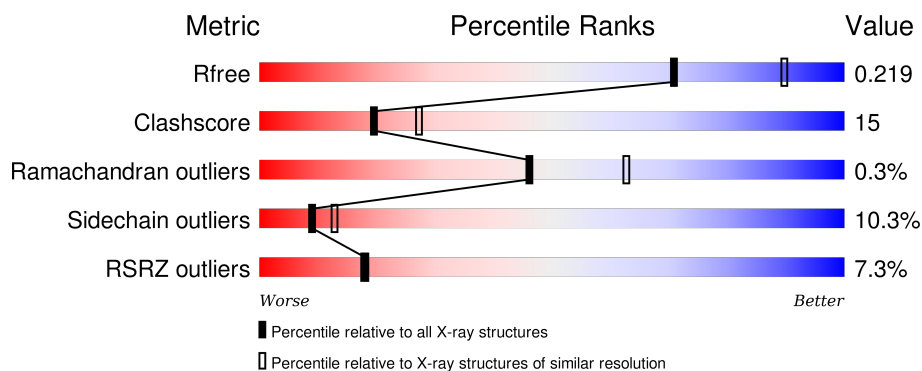
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	142	<div> <div>6%</div> <div>60% 29% 5% 6%</div> </div>
1	B	142	<div> <div>66% 25% • 8%</div> </div>
1	C	142	<div> <div>73% 19% • 7%</div> </div>
1	D	142	<div> <div>63% 27% • 7%</div> </div>
1	E	142	<div> <div>6% 57% 27% • 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	142	<div><div></div><div>9%</div><div>58%</div><div>27%</div><div>•</div><div>11%</div></div>
1	G	142	<div><div></div><div>11%</div><div>49%</div><div>38%</div><div>•</div><div>11%</div></div>
1	H	142	<div><div></div><div>25%</div><div>39%</div><div>41%</div><div>7%</div><div>13%</div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8247 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 Protein AggB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	130	Total	C	N	O	S	0	0	0
			1012	633	184	191	4			
1	A	133	Total	C	N	O	S	0	0	0
			1032	642	191	195	4			
1	C	132	Total	C	N	O	S	0	0	0
			1019	637	186	192	4			
1	D	132	Total	C	N	O	S	0	0	0
			1016	635	186	191	4			
1	E	126	Total	C	N	O	S	0	0	0
			976	610	177	185	4			
1	F	126	Total	C	N	O	S	0	0	0
			963	605	173	182	3			
1	G	126	Total	C	N	O	S	0	0	0
			976	610	177	185	4			
1	H	123	Total	C	N	O	S	0	0	0
			941	588	171	178	4			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	122	ASP	-	expression tag	UNP P46006
B	123	ASN	-	expression tag	UNP P46006
B	124	LYS	-	expression tag	UNP P46006
B	125	GLN	-	expression tag	UNP P46006
B	126	ALA	-	expression tag	UNP P46006
B	127	LEU	-	expression tag	UNP P46006
B	128	GLU	-	expression tag	UNP P46006
B	129	ARG	-	expression tag	UNP P46006
B	130	PRO	-	expression tag	UNP P46006
B	131	PRO	-	expression tag	UNP P46006
B	132	ILE	-	expression tag	UNP P46006
B	133	LYS	-	expression tag	UNP P46006
B	134	ALA	-	expression tag	UNP P46006

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Chain	Residue	Modelled	Actual	Comment	Reference
B	135	THR	-	expression tag	UNP P46006
B	136	GLU	-	expression tag	UNP P46006
B	137	THR	-	expression tag	UNP P46006
B	138	ILE	-	expression tag	UNP P46006
B	139	ARG	-	expression tag	UNP P46006
B	140	LEU	-	expression tag	UNP P46006
B	141	THR	-	expression tag	UNP P46006
B	142	VAL	-	expression tag	UNP P46006
A	122	ASP	-	expression tag	UNP P46006
A	123	ASN	-	expression tag	UNP P46006
A	124	LYS	-	expression tag	UNP P46006
A	125	GLN	-	expression tag	UNP P46006
A	126	ALA	-	expression tag	UNP P46006
A	127	LEU	-	expression tag	UNP P46006
A	128	GLU	-	expression tag	UNP P46006
A	129	ARG	-	expression tag	UNP P46006
A	130	PRO	-	expression tag	UNP P46006
A	131	PRO	-	expression tag	UNP P46006
A	132	ILE	-	expression tag	UNP P46006
A	133	LYS	-	expression tag	UNP P46006
A	134	ALA	-	expression tag	UNP P46006
A	135	THR	-	expression tag	UNP P46006
A	136	GLU	-	expression tag	UNP P46006
A	137	THR	-	expression tag	UNP P46006
A	138	ILE	-	expression tag	UNP P46006
A	139	ARG	-	expression tag	UNP P46006
A	140	LEU	-	expression tag	UNP P46006
A	141	THR	-	expression tag	UNP P46006
A	142	VAL	-	expression tag	UNP P46006
C	122	ASP	-	expression tag	UNP P46006
C	123	ASN	-	expression tag	UNP P46006
C	124	LYS	-	expression tag	UNP P46006
C	125	GLN	-	expression tag	UNP P46006
C	126	ALA	-	expression tag	UNP P46006
C	127	LEU	-	expression tag	UNP P46006
C	128	GLU	-	expression tag	UNP P46006
C	129	ARG	-	expression tag	UNP P46006
C	130	PRO	-	expression tag	UNP P46006
C	131	PRO	-	expression tag	UNP P46006
C	132	ILE	-	expression tag	UNP P46006
C	133	LYS	-	expression tag	UNP P46006
C	134	ALA	-	expression tag	UNP P46006

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Chain	Residue	Modelled	Actual	Comment	Reference
C	135	THR	-	expression tag	UNP P46006
C	136	GLU	-	expression tag	UNP P46006
C	137	THR	-	expression tag	UNP P46006
C	138	ILE	-	expression tag	UNP P46006
C	139	ARG	-	expression tag	UNP P46006
C	140	LEU	-	expression tag	UNP P46006
C	141	THR	-	expression tag	UNP P46006
C	142	VAL	-	expression tag	UNP P46006
D	122	ASP	-	expression tag	UNP P46006
D	123	ASN	-	expression tag	UNP P46006
D	124	LYS	-	expression tag	UNP P46006
D	125	GLN	-	expression tag	UNP P46006
D	126	ALA	-	expression tag	UNP P46006
D	127	LEU	-	expression tag	UNP P46006
D	128	GLU	-	expression tag	UNP P46006
D	129	ARG	-	expression tag	UNP P46006
D	130	PRO	-	expression tag	UNP P46006
D	131	PRO	-	expression tag	UNP P46006
D	132	ILE	-	expression tag	UNP P46006
D	133	LYS	-	expression tag	UNP P46006
D	134	ALA	-	expression tag	UNP P46006
D	135	THR	-	expression tag	UNP P46006
D	136	GLU	-	expression tag	UNP P46006
D	137	THR	-	expression tag	UNP P46006
D	138	ILE	-	expression tag	UNP P46006
D	139	ARG	-	expression tag	UNP P46006
D	140	LEU	-	expression tag	UNP P46006
D	141	THR	-	expression tag	UNP P46006
D	142	VAL	-	expression tag	UNP P46006
E	122	ASP	-	expression tag	UNP P46006
E	123	ASN	-	expression tag	UNP P46006
E	124	LYS	-	expression tag	UNP P46006
E	125	GLN	-	expression tag	UNP P46006
E	126	ALA	-	expression tag	UNP P46006
E	127	LEU	-	expression tag	UNP P46006
E	128	GLU	-	expression tag	UNP P46006
E	129	ARG	-	expression tag	UNP P46006
E	130	PRO	-	expression tag	UNP P46006
E	131	PRO	-	expression tag	UNP P46006
E	132	ILE	-	expression tag	UNP P46006
E	133	LYS	-	expression tag	UNP P46006
E	134	ALA	-	expression tag	UNP P46006

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Chain	Residue	Modelled	Actual	Comment	Reference
E	135	THR	-	expression tag	UNP P46006
E	136	GLU	-	expression tag	UNP P46006
E	137	THR	-	expression tag	UNP P46006
E	138	ILE	-	expression tag	UNP P46006
E	139	ARG	-	expression tag	UNP P46006
E	140	LEU	-	expression tag	UNP P46006
E	141	THR	-	expression tag	UNP P46006
E	142	VAL	-	expression tag	UNP P46006
F	122	ASP	-	expression tag	UNP P46006
F	123	ASN	-	expression tag	UNP P46006
F	124	LYS	-	expression tag	UNP P46006
F	125	GLN	-	expression tag	UNP P46006
F	126	ALA	-	expression tag	UNP P46006
F	127	LEU	-	expression tag	UNP P46006
F	128	GLU	-	expression tag	UNP P46006
F	129	ARG	-	expression tag	UNP P46006
F	130	PRO	-	expression tag	UNP P46006
F	131	PRO	-	expression tag	UNP P46006
F	132	ILE	-	expression tag	UNP P46006
F	133	LYS	-	expression tag	UNP P46006
F	134	ALA	-	expression tag	UNP P46006
F	135	THR	-	expression tag	UNP P46006
F	136	GLU	-	expression tag	UNP P46006
F	137	THR	-	expression tag	UNP P46006
F	138	ILE	-	expression tag	UNP P46006
F	139	ARG	-	expression tag	UNP P46006
F	140	LEU	-	expression tag	UNP P46006
F	141	THR	-	expression tag	UNP P46006
F	142	VAL	-	expression tag	UNP P46006
G	122	ASP	-	expression tag	UNP P46006
G	123	ASN	-	expression tag	UNP P46006
G	124	LYS	-	expression tag	UNP P46006
G	125	GLN	-	expression tag	UNP P46006
G	126	ALA	-	expression tag	UNP P46006
G	127	LEU	-	expression tag	UNP P46006
G	128	GLU	-	expression tag	UNP P46006
G	129	ARG	-	expression tag	UNP P46006
G	130	PRO	-	expression tag	UNP P46006
G	131	PRO	-	expression tag	UNP P46006
G	132	ILE	-	expression tag	UNP P46006
G	133	LYS	-	expression tag	UNP P46006
G	134	ALA	-	expression tag	UNP P46006

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Chain	Residue	Modelled	Actual	Comment	Reference
G	135	THR	-	expression tag	UNP P46006
G	136	GLU	-	expression tag	UNP P46006
G	137	THR	-	expression tag	UNP P46006
G	138	ILE	-	expression tag	UNP P46006
G	139	ARG	-	expression tag	UNP P46006
G	140	LEU	-	expression tag	UNP P46006
G	141	THR	-	expression tag	UNP P46006
G	142	VAL	-	expression tag	UNP P46006
H	122	ASP	-	expression tag	UNP P46006
H	123	ASN	-	expression tag	UNP P46006
H	124	LYS	-	expression tag	UNP P46006
H	125	GLN	-	expression tag	UNP P46006
H	126	ALA	-	expression tag	UNP P46006
H	127	LEU	-	expression tag	UNP P46006
H	128	GLU	-	expression tag	UNP P46006
H	129	ARG	-	expression tag	UNP P46006
H	130	PRO	-	expression tag	UNP P46006
H	131	PRO	-	expression tag	UNP P46006
H	132	ILE	-	expression tag	UNP P46006
H	133	LYS	-	expression tag	UNP P46006
H	134	ALA	-	expression tag	UNP P46006
H	135	THR	-	expression tag	UNP P46006
H	136	GLU	-	expression tag	UNP P46006
H	137	THR	-	expression tag	UNP P46006
H	138	ILE	-	expression tag	UNP P46006
H	139	ARG	-	expression tag	UNP P46006
H	140	LEU	-	expression tag	UNP P46006
H	141	THR	-	expression tag	UNP P46006
H	142	VAL	-	expression tag	UNP P46006

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	43	Total O 43 43	0	0
2	A	31	Total O 31 31	0	0
2	C	57	Total O 57 57	0	0
2	D	48	Total O 48 48	0	0
2	E	54	Total O 54 54	0	0

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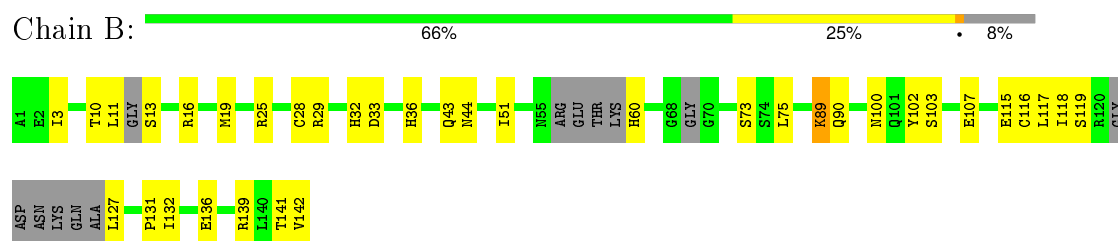
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	32	Total 32	O 32	0	0
2	G	18	Total 18	O 18	0	0
2	H	29	Total 29	O 29	0	0

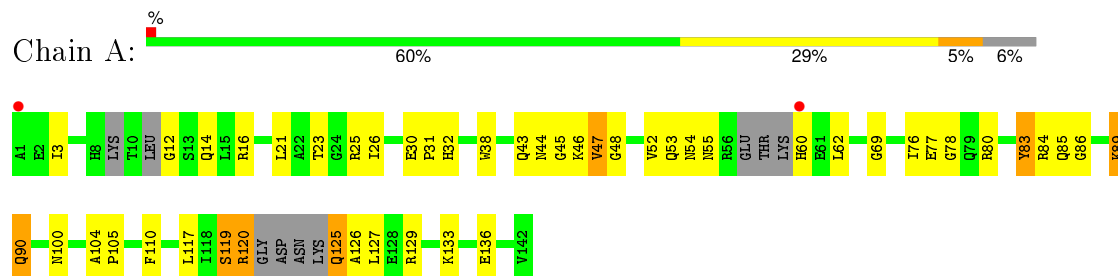
3 Residue-property plots

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

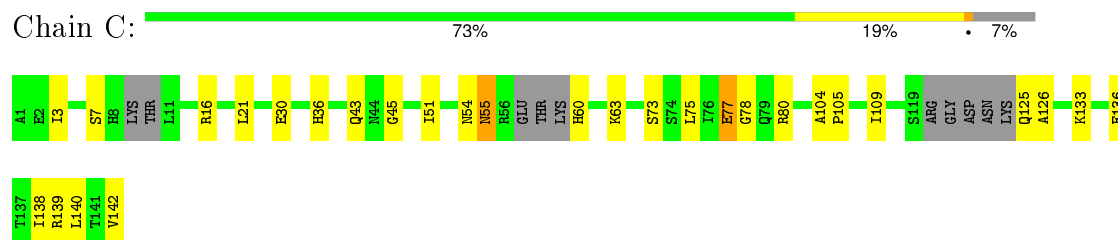
• Molecule 1: Protein AggB



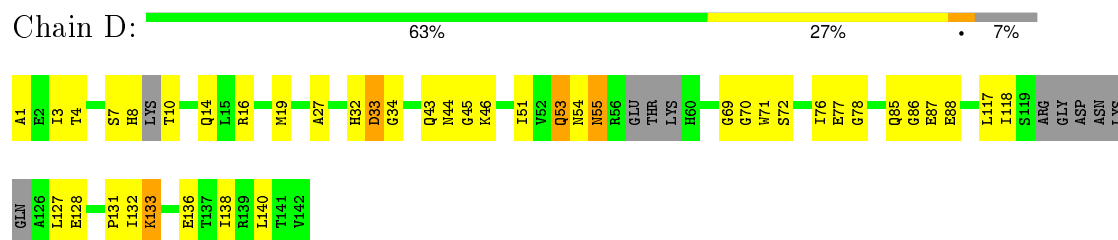
• Molecule 1: Protein AggB



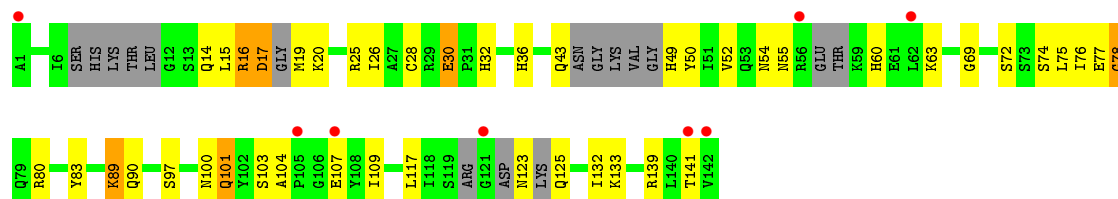
• Molecule 1: Protein AggB



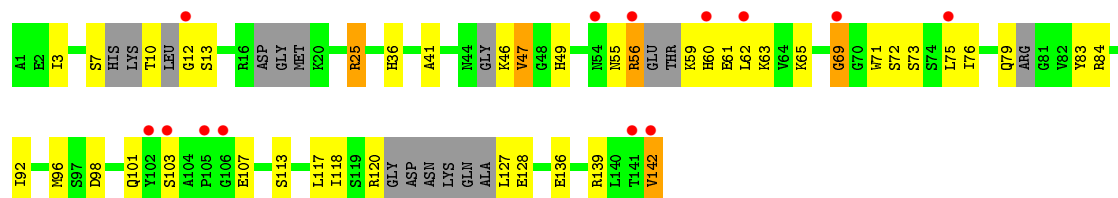
• Molecule 1: Protein AggB



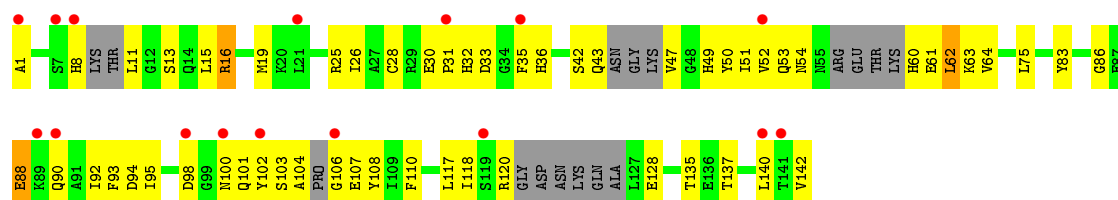
- Molecule 1: Protein AggB



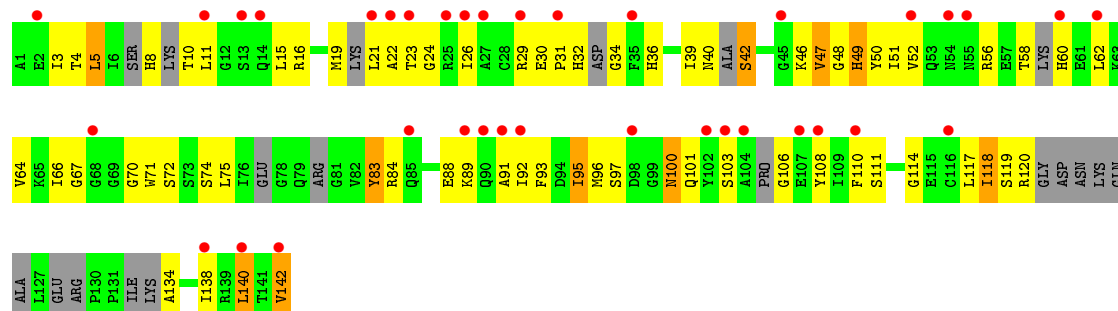
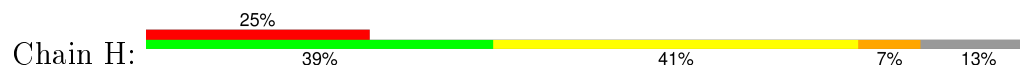
- Molecule 1: Protein AggB



- Molecule 1: Protein AggB



- Molecule 1: Protein AggB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	130.80Å 163.97Å 58.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.63 – 2.40 58.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.63-2.40) 96.0 (58.63-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.228 , 0.273 0.227 , 0.219	Depositor DCC
R_{free} test set	2381 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50155 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8247	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.46	0/1047	0.66	0/1403
1	B	0.48	0/1027	0.67	0/1378
1	C	0.50	0/1035	0.67	1/1389 (0.1%)
1	D	0.48	0/1032	0.67	0/1386
1	E	0.47	0/987	0.75	1/1319 (0.1%)
1	F	0.42	0/974	0.65	0/1303
1	G	0.36	0/989	0.59	0/1325
1	H	0.36	0/947	0.59	0/1258
All	All	0.45	0/8038	0.66	2/10761 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	GLY	N-CA-C	-5.54	99.26	113.10
1	C	78	GLY	N-CA-C	-5.41	99.58	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	77	GLU	Peptide
1	D	76	ILE	Peptide
1	E	69	GLY	Peptide
1	E	78	GLY	Peptide
1	F	69	GLY	Peptide

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	1032	0	1016	35	0
1	B	1012	0	997	29	0
1	C	1019	0	1004	22	0
1	D	1016	0	1003	33	0
1	E	976	0	951	27	0
1	F	963	0	937	23	0
1	G	976	0	953	38	0
1	H	941	0	908	44	0
2	A	31	0	0	4	0
2	B	43	0	0	10	0
2	C	57	0	0	6	0
2	D	48	0	0	8	0
2	E	54	0	0	4	0
2	F	32	0	0	5	0
2	G	18	0	0	4	0
2	H	29	0	0	3	0
All	All	8247	0	7769	236	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.

The worst 5 of 236 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:60:HIS:N	2:C:253:HOH:O	1.95	0.97
1:C:125:GLN:N	2:C:232:HOH:O	2.00	0.92
1:B:10:THR:HG23	1:B:11:LEU:HB2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ILE:HD11	1:G:120:ARG:HH11	1.40	0.85
1:E:89:LYS:HD2	1:E:90:GLN:HG3	1.58	0.84

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	124/142 (87%)	114 (92%)	8 (6%)	2 (2%)	12	16
1	B	120/142 (84%)	116 (97%)	4 (3%)	0	100	100
1	C	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
1	D	124/142 (87%)	115 (93%)	9 (7%)	0	100	100
1	E	112/142 (79%)	104 (93%)	8 (7%)	0	100	100
1	F	111/142 (78%)	108 (97%)	2 (2%)	1 (1%)	21	30
1	G	114/142 (80%)	102 (90%)	12 (10%)	0	100	100
1	H	99/142 (70%)	85 (86%)	14 (14%)	0	100	100
All	All	928/1136 (82%)	863 (93%)	62 (7%)	3 (0%)	46	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	SER
1	F	41	ALA
1	A	69	GLY

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	109/117 (93%)	100 (92%)	9 (8%)	14	21
1	B	108/117 (92%)	103 (95%)	5 (5%)	33	51
1	C	107/117 (92%)	103 (96%)	4 (4%)	41	62
1	D	107/117 (92%)	101 (94%)	6 (6%)	26	41
1	E	102/117 (87%)	89 (87%)	13 (13%)	5	6
1	F	101/117 (86%)	84 (83%)	17 (17%)	2	3
1	G	103/117 (88%)	92 (89%)	11 (11%)	8	11
1	H	99/117 (85%)	78 (79%)	21 (21%)	1	1
All	All	836/936 (89%)	750 (90%)	86 (10%)	9	13

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	10	THR
1	F	84	ARG
1	H	96	MET
1	F	25	ARG
1	F	59	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	D	44	ASN
1	E	101	GLN
1	G	60	HIS

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](#)

There are no ligands in this entry.

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, 95th 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	133/142 (93%)	0.03	2 (1%) 76 75	31, 48, 72, 82	0
1	B	130/142 (91%)	0.12	0 100 100	29, 47, 68, 83	0
1	C	132/142 (92%)	0.14	0 100 100	27, 41, 56, 69	0
1	D	132/142 (92%)	0.14	0 100 100	29, 45, 65, 84	0
1	E	126/142 (88%)	0.27	8 (6%) 23 24	28, 51, 99, 107	0
1	F	126/142 (88%)	0.49	13 (10%) 9 8	34, 56, 100, 113	0
1	G	126/142 (88%)	0.92	16 (12%) 5 5	44, 75, 105, 108	0
1	H	123/142 (86%)	1.75	36 (29%) 1 1	53, 85, 113, 124	0
All	All	1028/1136 (90%)	0.47	75 (7%) 18 18	27, 52, 100, 124	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	68	GLY	9.8
1	H	14	GLN	8.6
1	H	35	PHE	8.3
1	H	90	GLN	7.9
1	H	21	LEU	7.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.