



wwPDB X-ray Structure Validation Summary Report

Oct 7, 2023 – 01:55 PM EDT

PDB ID : 4PY3
Title : Crystal Structure of the N-terminal FIC domain of Bep8 protein (VirB-translocated Bartonella effector protein) from Bartonella sp. 1-1C
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2014-03-25
Resolution : 2.35 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  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

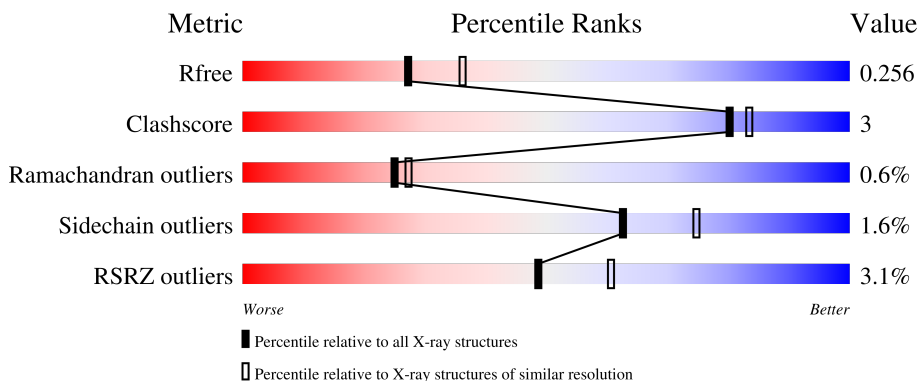
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 $\leq 5\%$. 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	241	 3% 82% 6% 12%
1	B	241	 3% 84% 12%
1	C	241	 81% 8% 10%
1	D	241	 5% 87% 10%
1	E	241	 80% 7% 11%

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Mol	Chain	Length	Quality of chain
1	F	241	 5% 82% 5% • 12%
1	G	241	 4% 83% 5% • 10%
1	H	241	 2% 83% 6% • 10%
1	I	241	 % 79% 9% 12%
1	J	241	 % 81% 6% 12%

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	EDO	I	301	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16715 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 Bartonella effector protein (Bep) substrate of VirB T4SS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	Total 1639	C 1043	N 282	O 302	S 12	0	0	0
1	B	213	Total 1650	C 1057	N 274	O 308	S 11	0	0	0
1	C	216	Total 1677	C 1071	N 281	O 313	S 12	0	0	0
1	D	216	Total 1563	C 1006	N 261	O 288	S 8	0	0	0
1	E	215	Total 1739	C 1112	N 295	O 319	S 13	0	1	0
1	F	211	Total 1549	C 986	N 261	O 294	S 8	0	0	0
1	G	217	Total 1667	C 1068	N 281	O 308	S 10	0	0	0
1	H	216	Total 1610	C 1025	N 270	O 306	S 9	0	0	0
1	I	213	Total 1701	C 1086	N 287	O 316	S 12	0	0	0
1	J	212	Total 1645	C 1051	N 277	O 306	S 11	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP E6YV77
A	2	ALA	-	expression tag	UNP E6YV77
A	3	HIS	-	expression tag	UNP E6YV77
A	4	HIS	-	expression tag	UNP E6YV77
A	5	HIS	-	expression tag	UNP E6YV77
A	6	HIS	-	expression tag	UNP E6YV77
A	7	HIS	-	expression tag	UNP E6YV77
A	8	HIS	-	expression tag	UNP E6YV77
A	9	MET	-	expression tag	UNP E6YV77

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP E6YV77
B	2	ALA	-	expression tag	UNP E6YV77
B	3	HIS	-	expression tag	UNP E6YV77
B	4	HIS	-	expression tag	UNP E6YV77
B	5	HIS	-	expression tag	UNP E6YV77
B	6	HIS	-	expression tag	UNP E6YV77
B	7	HIS	-	expression tag	UNP E6YV77
B	8	HIS	-	expression tag	UNP E6YV77
B	9	MET	-	expression tag	UNP E6YV77
C	1	MET	-	initiating methionine	UNP E6YV77
C	2	ALA	-	expression tag	UNP E6YV77
C	3	HIS	-	expression tag	UNP E6YV77
C	4	HIS	-	expression tag	UNP E6YV77
C	5	HIS	-	expression tag	UNP E6YV77
C	6	HIS	-	expression tag	UNP E6YV77
C	7	HIS	-	expression tag	UNP E6YV77
C	8	HIS	-	expression tag	UNP E6YV77
C	9	MET	-	expression tag	UNP E6YV77
D	1	MET	-	initiating methionine	UNP E6YV77
D	2	ALA	-	expression tag	UNP E6YV77
D	3	HIS	-	expression tag	UNP E6YV77
D	4	HIS	-	expression tag	UNP E6YV77
D	5	HIS	-	expression tag	UNP E6YV77
D	6	HIS	-	expression tag	UNP E6YV77
D	7	HIS	-	expression tag	UNP E6YV77
D	8	HIS	-	expression tag	UNP E6YV77
D	9	MET	-	expression tag	UNP E6YV77
E	1	MET	-	initiating methionine	UNP E6YV77
E	2	ALA	-	expression tag	UNP E6YV77
E	3	HIS	-	expression tag	UNP E6YV77
E	4	HIS	-	expression tag	UNP E6YV77
E	5	HIS	-	expression tag	UNP E6YV77
E	6	HIS	-	expression tag	UNP E6YV77
E	7	HIS	-	expression tag	UNP E6YV77
E	8	HIS	-	expression tag	UNP E6YV77
E	9	MET	-	expression tag	UNP E6YV77
F	1	MET	-	initiating methionine	UNP E6YV77
F	2	ALA	-	expression tag	UNP E6YV77
F	3	HIS	-	expression tag	UNP E6YV77
F	4	HIS	-	expression tag	UNP E6YV77
F	5	HIS	-	expression tag	UNP E6YV77
F	6	HIS	-	expression tag	UNP E6YV77

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Chain	Residue	Modelled	Actual	Comment	Reference
F	7	HIS	-	expression tag	UNP E6YV77
F	8	HIS	-	expression tag	UNP E6YV77
F	9	MET	-	expression tag	UNP E6YV77
G	1	MET	-	initiating methionine	UNP E6YV77
G	2	ALA	-	expression tag	UNP E6YV77
G	3	HIS	-	expression tag	UNP E6YV77
G	4	HIS	-	expression tag	UNP E6YV77
G	5	HIS	-	expression tag	UNP E6YV77
G	6	HIS	-	expression tag	UNP E6YV77
G	7	HIS	-	expression tag	UNP E6YV77
G	8	HIS	-	expression tag	UNP E6YV77
G	9	MET	-	expression tag	UNP E6YV77
H	1	MET	-	initiating methionine	UNP E6YV77
H	2	ALA	-	expression tag	UNP E6YV77
H	3	HIS	-	expression tag	UNP E6YV77
H	4	HIS	-	expression tag	UNP E6YV77
H	5	HIS	-	expression tag	UNP E6YV77
H	6	HIS	-	expression tag	UNP E6YV77
H	7	HIS	-	expression tag	UNP E6YV77
H	8	HIS	-	expression tag	UNP E6YV77
H	9	MET	-	expression tag	UNP E6YV77
I	1	MET	-	initiating methionine	UNP E6YV77
I	2	ALA	-	expression tag	UNP E6YV77
I	3	HIS	-	expression tag	UNP E6YV77
I	4	HIS	-	expression tag	UNP E6YV77
I	5	HIS	-	expression tag	UNP E6YV77
I	6	HIS	-	expression tag	UNP E6YV77
I	7	HIS	-	expression tag	UNP E6YV77
I	8	HIS	-	expression tag	UNP E6YV77
I	9	MET	-	expression tag	UNP E6YV77
J	1	MET	-	initiating methionine	UNP E6YV77
J	2	ALA	-	expression tag	UNP E6YV77
J	3	HIS	-	expression tag	UNP E6YV77
J	4	HIS	-	expression tag	UNP E6YV77
J	5	HIS	-	expression tag	UNP E6YV77
J	6	HIS	-	expression tag	UNP E6YV77
J	7	HIS	-	expression tag	UNP E6YV77
J	8	HIS	-	expression tag	UNP E6YV77
J	9	MET	-	expression tag	UNP E6YV77

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

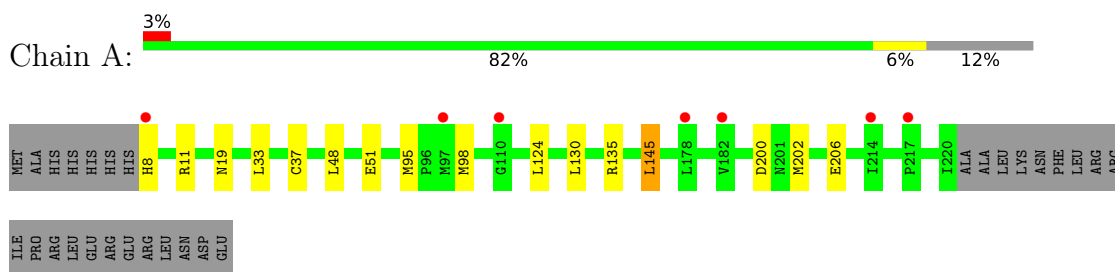
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	14	Total O 14 14	0	0
3	B	32	Total O 32 32	0	0
3	C	25	Total O 25 25	0	0
3	D	8	Total O 8 8	0	0
3	E	56	Total O 56 56	0	0
3	F	2	Total O 2 2	0	0
3	G	20	Total O 20 20	0	0
3	H	5	Total O 5 5	0	0
3	I	70	Total O 70 70	0	0
3	J	35	Total O 35 35	0	0

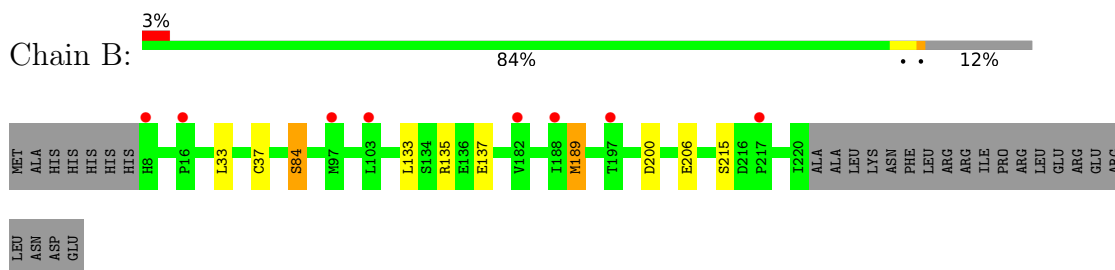
3 Residue-property plots [i](#)

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.

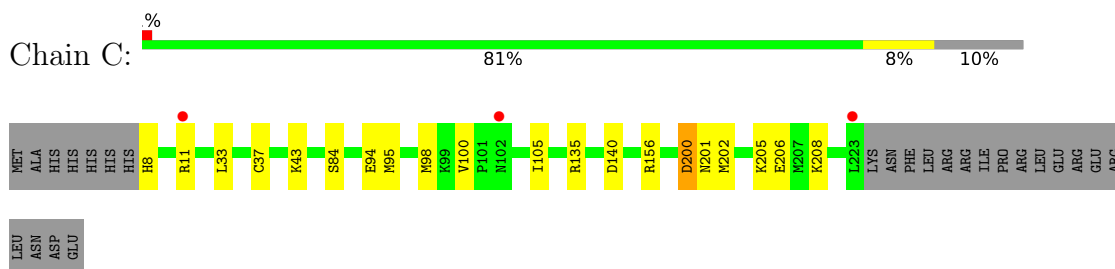
- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS



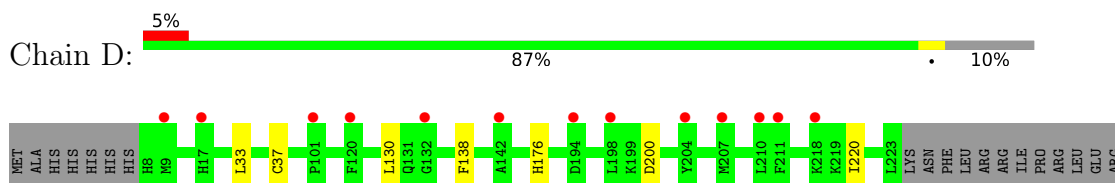
- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS



- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS




- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS



GLU
ARG
LEU
ASN
ASP
GLU


- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain E:  80% 7% 11%

MET ALA HIS HIS HIS HIS H7 H8 R11 M19 L33 C37 I45 L48 E51 Q67 R68 L69 F70 E71 P96 K99 V100 P101 N102 L103 D104 I105 M128 R135 M189 D200 N201 I220 A221 ALA LEU LYS ASN PHE LEU ARG ARG ARG ILE PRO

ARG
LEU
GLU
ARG
GLU
ARG
LEU
ASP
GLU


- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain F:  5% 82% 5% 12%

MET ALA HIS HIS HIS HIS M9 A10 Y13 H17 T20 L33 C37 Y40 I45 F74 D89 V92 M95 M98 P101 R135 R156 N159 Q163 F167 S181 V182 D200 I214 S215 K219 ILE ALA ALA LEU

LYS
ASN
PHE
LEU
ARG
TLE
PRO
ARG
GLU
GLU
ARG
ASN
ASP
GLU


- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain G:  4% 83% 5% 10%

MET ALA HIS HIS HIS HIS H6 P16 H17 M18 M26 I27 M28 L33 C37 D88 I104 I105 F106 N111 K118 L133 S134 R135 M159 Q163 Q177 K186 R190 I193 D194 L198 K199 D200 N201 T220 A221 K224 ASN PHE LEU

ARG
ARG
TLE
PRO
ARG
LEU
GLU
ASP
GLU


- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain H:  2% 83% 6% 10%

MET ALA HIS HIS HIS HIS H6 R11 L33 A34 C37 E38 R81 S84 K99 V100 V108 L124 L133 F138 A153 F180 S181 V182 A183 T184 R187 D200 N201 I214 A221 A222 L223 LYS ASN PHE LEU ARG ARG ARG ILE PRO ARG LEU

GLU
ARG
GLU
ARG
LEU
ASN
ASP
GLU

- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain I:  79% 9% 12%

MET ALA HIS HIS HIS HIS H6 R11 L33 C37 E38 K42 K43 D88 M95 P96 M97 M98 L103 F106 R135 D179 V182 A183 T184 F185 K186 R187 R190 T197 D200 L210 T214 S215 I220 ALA ALA LEU LYS ASN PHE LEU

ARG
ARG
ILE
PRO
ARG
LEU
GLU
ARG
GLU
ARG
LEU
LEU
ASN
ASP
GLU

- Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain J: %
81% 6% 12%

MET
ALA
HIS
HIS
HIS
HIS
HIS
H8
M9
A10
P16
L33
C37
K43
S84
D88
E94
M95
M98
P101
R135
K144
R156
A157
G158
M159
Q163
D200
S215
K219
ILE
ALA
ALA
LEU
LEU
LYS
ASN
PHE
LEU
LEU
ARG
ARG
ILE
PRO
ARG
LEU

GLU
ARG
GLU
ARG
LEU
LEU
ASN
ASP
GLU

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.81Å 324.16Å 86.13Å 90.00° 109.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 47.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.35) 97.5 (47.50-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.242 , 0.259 0.241 , 0.256	Depositor DCC
R_{free} test set	5731 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtrriage
Anisotropy	0.678	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.206 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16715	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, 0.333 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: EDO

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	0.45	0/1678	0.68	4/2272 (0.2%)
1	B	0.47	1/1688 (0.1%)	0.61	1/2284 (0.0%)
1	C	0.44	0/1716	0.58	0/2323
1	D	0.39	0/1600	0.59	1/2182 (0.0%)
1	E	0.56	1/1780 (0.1%)	0.69	6/2398 (0.3%)
1	F	0.42	0/1585	0.78	4/2159 (0.2%)
1	G	0.45	0/1705	0.64	2/2308 (0.1%)
1	H	0.41	0/1648	0.64	2/2242 (0.1%)
1	I	0.53	0/1740	0.62	0/2346
1	J	0.47	0/1682	0.60	1/2273 (0.0%)
All	All	0.46	2/16822 (0.0%)	0.65	21/22787 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	SER	CA-CB	5.78	1.61	1.52
1	E	51	GLU	CD-OE2	-5.05	1.20	1.25

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	89	ASP	CB-CG-OD1	19.15	135.54	118.30
1	F	89	ASP	CB-CA-C	-9.90	90.59	110.40
1	H	133	LEU	CA-CB-CG	8.71	135.33	115.30
1	G	133	LEU	CA-CB-CG	8.67	135.25	115.30
1	F	89	ASP	OD1-CG-OD2	-8.05	108.01	123.30

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	1639	0	1499	7	0
1	B	1650	0	1539	3	0
1	C	1677	0	1562	12	0
1	D	1563	0	1360	2	0
1	E	1739	0	1685	10	0
1	F	1549	0	1338	10	0
1	G	1667	0	1547	8	0
1	H	1610	0	1423	8	0
1	I	1701	0	1631	18	0
1	J	1645	0	1550	12	0
2	I	8	0	12	0	0
3	A	14	0	0	0	0
3	B	32	0	0	0	0
3	C	25	0	0	0	0
3	D	8	0	0	0	0
3	E	56	0	0	1	0
3	F	2	0	0	0	0
3	G	20	0	0	0	0
3	H	5	0	0	0	0
3	I	70	0	0	0	0
3	J	35	0	0	1	0
All	All	16715	0	15146	86	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 3.

The worst 5 of 86 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:H:81:ARG:NH1	1:H:153:ALA:O	1.83	1.10
1:C:84:SER:OG	1:C:94:GLU:OE2	1.67	1.09
1:I:43:LYS:HD2	1:J:88:ASP:OD1	1.85	0.77
1:G:26:ASN:O	1:G:26:ASN:ND2	2.19	0.73
1:I:183:ALA:HB3	1:I:214:ILE:HD11	1.73	0.71

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	211/241 (88%)	206 (98%)	4 (2%)	1 (0%)	29	32
1	B	211/241 (88%)	206 (98%)	4 (2%)	1 (0%)	29	32
1	C	214/241 (89%)	208 (97%)	5 (2%)	1 (0%)	29	32
1	D	214/241 (89%)	208 (97%)	4 (2%)	2 (1%)	17	17
1	E	214/241 (89%)	208 (97%)	4 (2%)	2 (1%)	17	17
1	F	209/241 (87%)	205 (98%)	3 (1%)	1 (0%)	29	32
1	G	215/241 (89%)	208 (97%)	5 (2%)	2 (1%)	17	17
1	H	214/241 (89%)	208 (97%)	5 (2%)	1 (0%)	29	32
1	I	211/241 (88%)	206 (98%)	4 (2%)	1 (0%)	29	32
1	J	210/241 (87%)	206 (98%)	3 (1%)	1 (0%)	29	32
All	All	2123/2410 (88%)	2069 (98%)	41 (2%)	13 (1%)	25	27

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	220	ILE
1	A	200	ASP
1	B	200	ASP
1	C	200	ASP
1	D	200	ASP

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	160/213 (75%)	158 (99%)	2 (1%)	69	80
1	B	165/213 (78%)	162 (98%)	3 (2%)	59	70
1	C	168/213 (79%)	166 (99%)	2 (1%)	71	82
1	D	135/213 (63%)	135 (100%)	0	100	100
1	E	184/213 (86%)	179 (97%)	5 (3%)	44	55
1	F	138/213 (65%)	137 (99%)	1 (1%)	84	91
1	G	162/213 (76%)	155 (96%)	7 (4%)	29	35
1	H	150/213 (70%)	146 (97%)	4 (3%)	44	55
1	I	178/213 (84%)	177 (99%)	1 (1%)	86	93
1	J	166/213 (78%)	165 (99%)	1 (1%)	86	93
All	All	1606/2130 (75%)	1580 (98%)	26 (2%)	62	75

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	26	ASN
1	G	133	LEU
1	I	184	THR
1	G	118	LYS
1	G	135	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	163	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 [i](#)

2 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	EDO	I	301	-	3,3,3	0.65	0	2,2,2	0.16	0
2	EDO	I	302	-	3,3,3	0.44	0	2,2,2	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	I	301	-	-	0/1/1/1	-
2	EDO	I	302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	302	EDO	O1-C1-C2-O2

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 [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, 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	213/241 (88%)	0.31	7 (3%) 46 59	30, 53, 79, 96	0
1	B	213/241 (88%)	0.29	8 (3%) 40 53	21, 41, 70, 77	0
1	C	216/241 (89%)	0.15	3 (1%) 75 83	28, 46, 67, 95	0
1	D	216/241 (89%)	0.59	13 (6%) 21 32	35, 70, 102, 124	0
1	E	215/241 (89%)	0.12	1 (0%) 91 95	20, 34, 57, 67	0
1	F	211/241 (87%)	0.56	12 (5%) 23 34	45, 67, 88, 109	0
1	G	217/241 (90%)	0.47	10 (4%) 32 45	33, 58, 91, 114	0
1	H	216/241 (89%)	0.49	6 (2%) 53 64	40, 64, 88, 108	0
1	I	213/241 (88%)	0.09	3 (1%) 75 83	19, 33, 58, 70	0
1	J	212/241 (87%)	0.26	3 (1%) 75 83	22, 42, 70, 91	0
All	All	2142/2410 (88%)	0.33	66 (3%) 49 61	19, 50, 87, 124	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	HIS	5.2
1	G	201	ASN	4.6
1	G	106	PHE	4.0
1	J	16	PRO	3.8
1	D	198	LEU	3.8

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, 95th 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	EDO	I	301	4/4	0.57	0.59	58,62,63,64	0
2	EDO	I	302	4/4	0.88	0.28	57,58,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.