Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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:

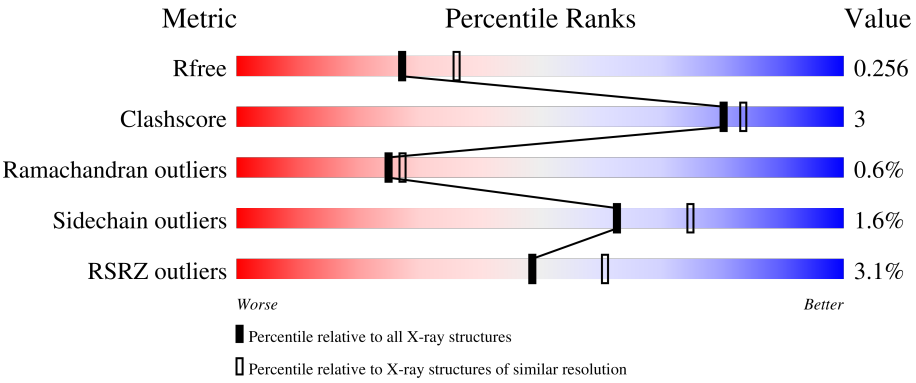
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

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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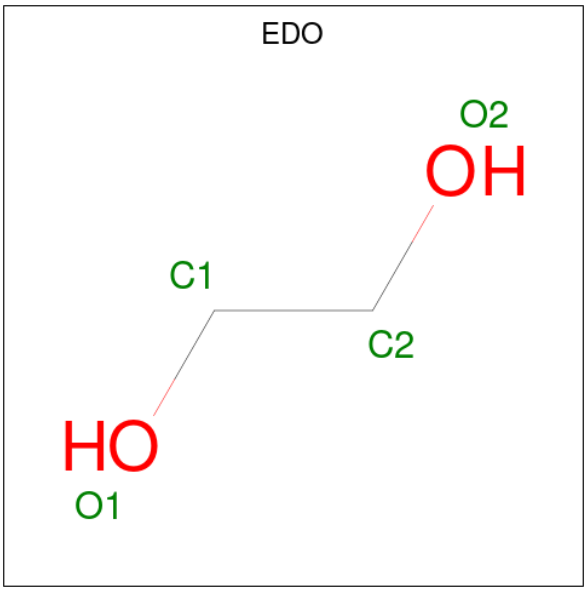
Chain	Residue	Modelled	Actual	Comment	Reference
F	7	HIS	-	expression tag	UNP E6YV77
F	8	HIS	-	expression tag	UNP E6YV77
F	9	MET	-	expression tag	UNP E6YV77
G	1	MET	-	initiating methionine	UNP E6YV77
G	2	ALA	-	expression tag	UNP E6YV77
G	3	HIS	-	expression tag	UNP E6YV77
G	4	HIS	-	expression tag	UNP E6YV77
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: $C_2H_6O_2$).



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

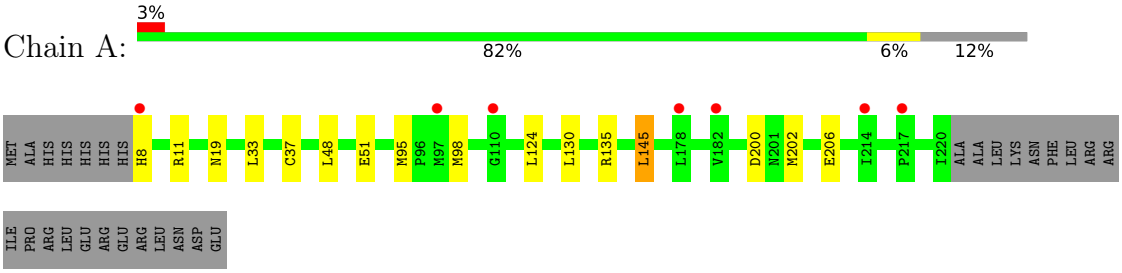
- Molecule 3 is water.

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

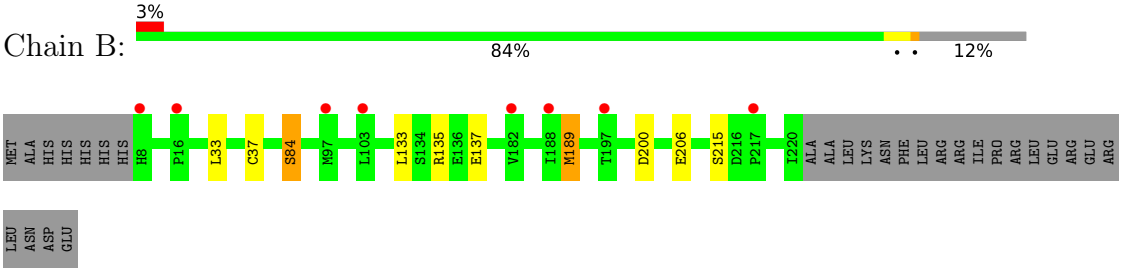
3 Residue-property plots (i)

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.

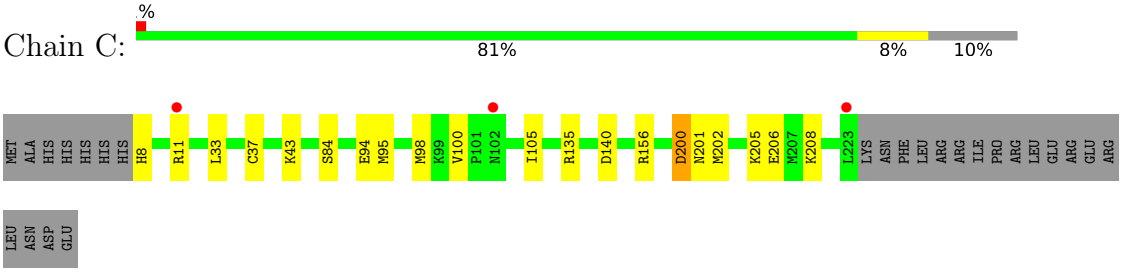
• Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS



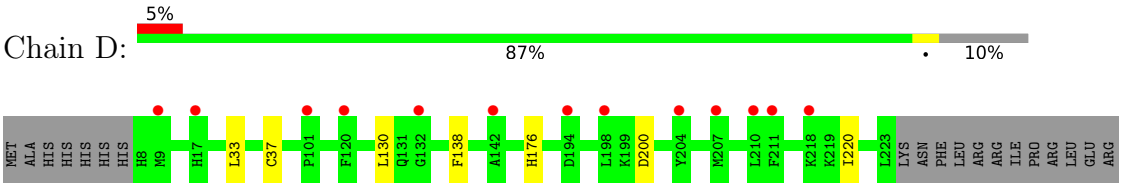
• Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS



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

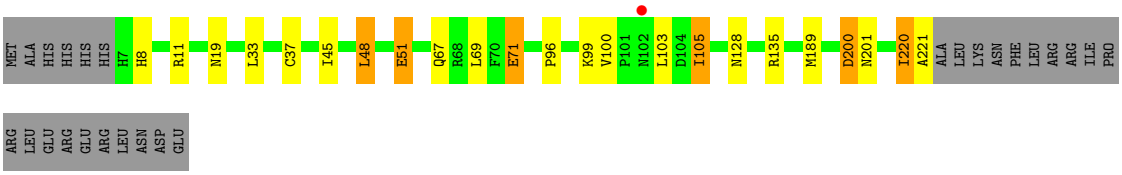


• Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS



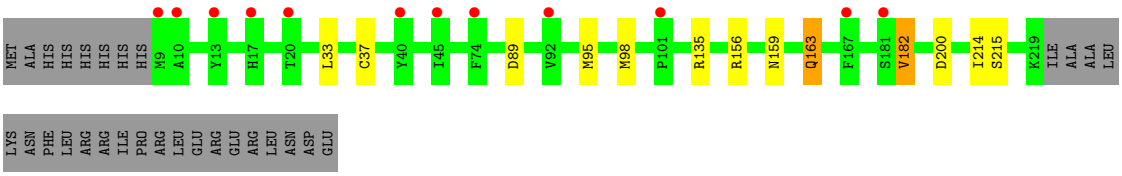
• Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain E:



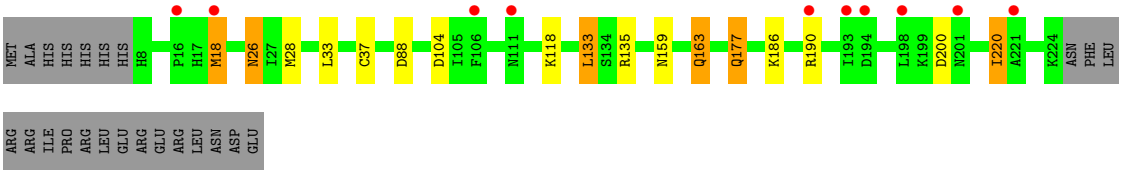
• Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain F:



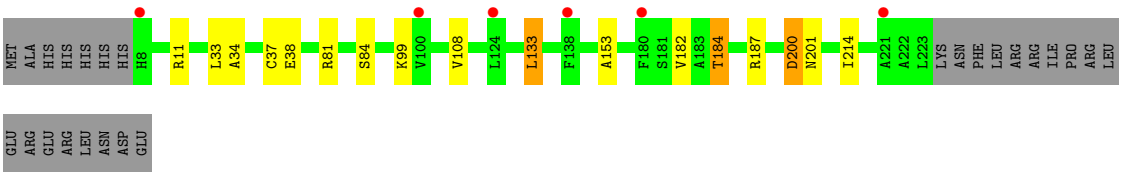
• Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain G:



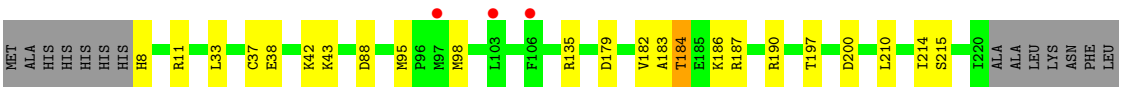
• Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain H:

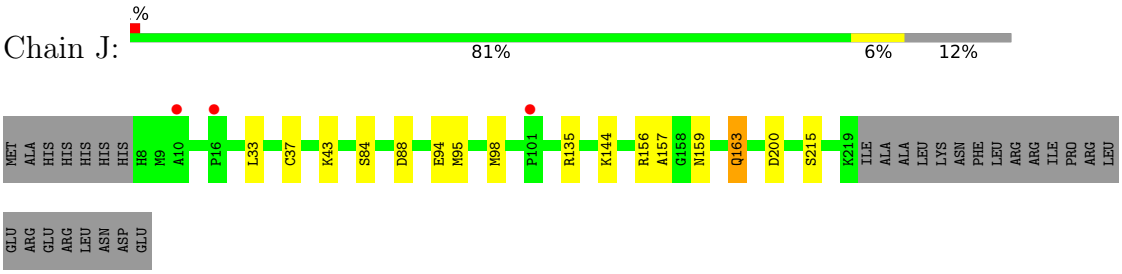


• Molecule 1: Bartonella effector protein (Bep) substrate of VirB T4SS

Chain I:



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



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
$< I/\sigma(I) >$ [1]	2.53 (at 2.34Å)	Xtriage
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	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 23.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.206 for h,-k,-h-l	Xtriage
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

Xtriage'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.*

[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: 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

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	D	130	LEU	CA-CB-CG	7.23	131.92	115.30
1	A	130	LEU	CA-CB-CG	7.22	131.92	115.30
1	E	19	ASN	CB-CA-C	-7.12	96.16	110.40
1	A	145	LEU	CB-CG-CD2	6.97	122.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	48	LEU	CB-CG-CD2	-6.65	99.69	111.00
1	A	19	ASN	CB-CA-C	-6.38	97.64	110.40
1	H	11	ARG	N-CA-CB	-6.18	99.47	110.60
1	A	145	LEU	CA-CB-CG	5.88	128.83	115.30
1	J	163	GLN	CA-CB-CG	5.56	125.63	113.40
1	F	163	GLN	CA-CB-CG	5.47	125.43	113.40
1	E	48	LEU	CA-CB-CG	5.43	127.78	115.30
1	G	163	GLN	CA-CB-CG	5.27	124.98	113.40
1	E	71	GLU	CA-CB-CG	5.21	124.87	113.40
1	B	189	MET	CG-SD-CE	-5.20	91.88	100.20
1	E	71	GLU	CB-CA-C	-5.19	100.03	110.40
1	E	103	LEU	CA-CB-CG	5.18	127.22	115.30

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:G:177:GLN:HG2	1:G:220:ILE:HD13	1.78	0.66
1:I:183:ALA:CB	1:I:214:ILE:HD11	2.26	0.66
1:E:96:PRO:HD2	3:E:322:HOH:O	1.96	0.65
1:I:182:VAL:HG22	1:I:214:ILE:HG12	1.81	0.63
1:E:220:ILE:O	1:E:221:ALA:HB2	1.99	0.62
1:H:81:ARG:NH2	1:H:108:VAL:O	2.33	0.62
1:C:202:MET:HA	1:C:205:LYS:HG3	1.84	0.59
1:J:135:ARG:NH1	1:J:215:SER:OG	2.36	0.59
1:J:95:MET:SD	1:J:98:MET:HE3	2.43	0.58
1:G:159:ASN:O	1:G:163:GLN:HG3	2.04	0.58
1:C:95:MET:SD	1:C:98:MET:HE3	2.43	0.58
1:A:95:MET:SD	1:A:98:MET:HE3	2.43	0.58
1:H:182:VAL:HG22	1:H:214:ILE:HG22	1.86	0.58
1:B:135:ARG:NH1	1:B:215:SER:OG	2.37	0.57
1:B:133:LEU:HD22	1:B:137:GLU:HG2	1.85	0.57
1:J:159:ASN:O	1:J:163:GLN:HG3	2.05	0.57
1:I:95:MET:SD	1:I:98:MET:HE3	2.44	0.56
1:F:159:ASN:O	1:F:163:GLN:HG3	2.06	0.55
1:I:210:LEU:CD1	1:I:214:ILE:HD12	2.36	0.55
1:C:95:MET:SD	1:C:98:MET:CE	2.96	0.54
1:A:95:MET:SD	1:A:98:MET:CE	2.96	0.54
1:I:95:MET:SD	1:I:98:MET:CE	2.96	0.54
1:C:200:ASP:OD1	1:C:201:ASN:N	2.41	0.53
1:J:95:MET:SD	1:J:98:MET:CE	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:GLN:O	1:E:71:GLU:HG3	2.09	0.52
1:F:95:MET:SD	1:F:98:MET:CE	2.97	0.52
1:H:182:VAL:CG2	1:H:214:ILE:HG22	2.39	0.52
1:E:8:HIS:O	1:E:11:ARG:HG2	2.10	0.51
1:E:200:ASP:OD1	1:E:201:ASN:N	2.41	0.51
1:H:200:ASP:OD1	1:H:201:ASN:N	2.41	0.51
1:I:8:HIS:O	1:I:11:ARG:HG2	2.10	0.51
1:G:177:GLN:HG2	1:G:220:ILE:CD1	2.40	0.51
1:A:8:HIS:O	1:A:11:ARG:HG2	2.11	0.50
1:J:84:SER:HB2	1:J:94:GLU:OE2	2.11	0.50
1:C:8:HIS:O	1:C:11:ARG:HG2	2.12	0.49
1:F:135:ARG:NH1	1:F:215:SER:OG	2.46	0.49
1:F:182:VAL:HG12	1:F:214:ILE:HG22	1.95	0.48
1:E:45:ILE:HD11	1:E:69:LEU:HD21	1.96	0.48
1:F:98:MET:HE1	1:F:156:ARG:HD2	1.96	0.47
1:E:220:ILE:O	1:E:221:ALA:CB	2.61	0.47
1:C:140:ASP:OD1	1:C:208:LYS:HD3	2.14	0.47
1:G:186:LYS:O	1:G:190:ARG:HG3	2.15	0.47
1:C:8:HIS:O	1:C:11:ARG:NH1	2.48	0.46
1:I:88:ASP:OD1	1:J:43:LYS:HE3	2.15	0.46
1:E:48:LEU:O	1:E:51:GLU:HG2	2.16	0.45
1:I:38:GLU:HG2	1:I:42:LYS:HE2	1.98	0.45
1:I:210:LEU:HD11	1:I:214:ILE:HD12	1.98	0.45
1:G:33:LEU:O	1:G:37:CYS:HB2	2.17	0.45
1:A:124:LEU:CD2	1:A:145:LEU:CD2	2.95	0.45
1:I:210:LEU:HD11	1:I:214:ILE:CD1	2.46	0.45
1:H:34:ALA:O	1:H:38:GLU:HG3	2.16	0.44
1:I:186:LYS:O	1:I:190:ARG:HG3	2.16	0.44
1:F:95:MET:SD	1:F:98:MET:HE3	2.56	0.44
1:I:135:ARG:HH11	1:I:215:SER:HB3	1.83	0.44
1:J:33:LEU:O	1:J:37:CYS:HB2	2.17	0.44
1:J:84:SER:HA	1:J:94:GLU:CG	2.47	0.44
1:A:202:MET:HE3	1:I:197:THR:HG22	2.00	0.43
1:D:33:LEU:O	1:D:37:CYS:HB2	2.18	0.43
1:J:157:ALA:HB1	3:J:307:HOH:O	2.18	0.43
1:D:138:PHE:HB2	1:D:176:HIS:CE1	2.53	0.43
1:H:184:THR:HG23	1:H:187:ARG:H	1.84	0.43
1:J:84:SER:CB	1:J:94:GLU:OE2	2.67	0.43
1:I:184:THR:HG23	1:I:187:ARG:H	1.84	0.43
1:B:33:LEU:O	1:B:37:CYS:HB2	2.19	0.43
1:J:98:MET:CE	1:J:156:ARG:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LEU:O	1:E:37:CYS:HB2	2.19	0.42
1:C:33:LEU:O	1:C:37:CYS:HB2	2.19	0.42
1:I:33:LEU:O	1:I:37:CYS:HB2	2.19	0.42
1:C:100:VAL:CG2	1:C:105:ILE:HG23	2.49	0.42
1:F:98:MET:CE	1:F:156:ARG:HD2	2.49	0.42
1:I:179:ASP:H	1:I:214:ILE:HG23	1.84	0.42
1:F:95:MET:SD	1:F:98:MET:HE2	2.60	0.42
1:A:33:LEU:O	1:A:37:CYS:HB2	2.20	0.42
1:F:33:LEU:O	1:F:37:CYS:HB2	2.18	0.41
1:F:98:MET:HE1	1:F:156:ARG:HA	2.01	0.41
1:C:43:LYS:HE3	1:G:88:ASP:OD1	2.20	0.41
1:G:18:MET:CE	1:G:28:MET:O	2.69	0.41
1:H:33:LEU:O	1:H:37:CYS:HB2	2.19	0.41
1:A:48:LEU:O	1:A:51:GLU:HG2	2.21	0.41
1:E:100:VAL:CG2	1:E:105:ILE:HG23	2.51	0.40
1:C:98:MET:CE	1:C:156:ARG:HD2	2.51	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

All (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
1	E	200	ASP
1	F	200	ASP
1	G	200	ASP
1	H	200	ASP
1	I	200	ASP
1	J	200	ASP
1	G	220	ILE
1	E	220	ILE

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ARG
1	A	206	GLU
1	B	84	SER
1	B	189	MET
1	B	206	GLU
1	C	135	ARG
1	C	206	GLU
1	E	99	LYS
1	E	105	ILE
1	E	128	ASN
1	E	135	ARG
1	E	189	MET
1	F	182	VAL
1	G	18	MET
1	G	26	ASN
1	G	104	ASP
1	G	118	LYS
1	G	133	LEU
1	G	135	ARG
1	G	177	GLN
1	H	84	SER
1	H	99	LYS
1	H	133	LEU
1	H	184	THR
1	I	184	THR
1	J	144	LYS

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

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	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

All (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
1	F	9	MET	3.8
1	D	142	ALA	3.7
1	B	8	HIS	3.6
1	B	16	PRO	3.6
1	G	190	ARG	3.4
1	I	103	LEU	3.1
1	D	9	MET	3.1
1	D	120	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	17	HIS	3.0
1	A	97	MET	3.0
1	E	102	ASN	3.0
1	F	20	THR	2.8
1	B	103	LEU	2.8
1	G	194	ASP	2.7
1	G	18	MET	2.7
1	D	17	HIS	2.7
1	D	132	GLY	2.7
1	B	182	VAL	2.7
1	C	223	LEU	2.7
1	F	92	VAL	2.7
1	G	111	ASN	2.6
1	A	182	VAL	2.6
1	H	180	PHE	2.6
1	B	197	THR	2.5
1	A	217	PRO	2.5
1	G	16	PRO	2.5
1	F	10	ALA	2.5
1	D	194	ASP	2.4
1	D	218	LYS	2.4
1	H	8	HIS	2.4
1	F	167	PHE	2.4
1	D	204	TYR	2.4
1	G	221	ALA	2.4
1	J	101	PRO	2.4
1	G	198	LEU	2.3
1	F	74	PHE	2.3
1	F	181	SER	2.3
1	G	193	ILE	2.3
1	F	101	PRO	2.3
1	J	10	ALA	2.3
1	H	124	LEU	2.3
1	A	214	ILE	2.3
1	D	210	LEU	2.2
1	D	101	PRO	2.2
1	B	217	PRO	2.2
1	F	13	TYR	2.2
1	C	11	ARG	2.1
1	H	100	VAL	2.1
1	F	45	ILE	2.1
1	B	188	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLY	2.1
1	F	40	TYR	2.1
1	D	211	PHE	2.1
1	I	97	MET	2.0
1	H	221	ALA	2.0
1	H	138	PHE	2.0
1	I	106	PHE	2.0
1	A	178	LEU	2.0
1	C	102	ASN	2.0
1	D	207	MET	2.0
1	B	97	MET	2.0

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^{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	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.