



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:53 pm BST

PDB ID : 3B8N
Title : Structure of FepE- Bacterial Polysaccharide Co-polymerase
Authors : Tocilj, A.; Matte, A.; Cygler, M.
Deposited on : 2007-11-01
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

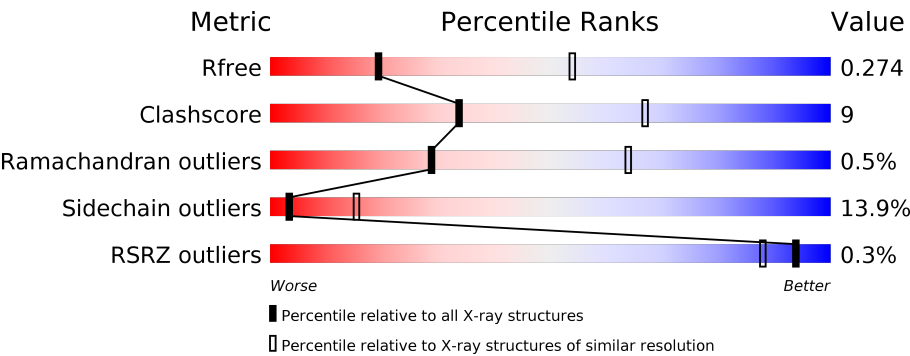
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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	279	<div><div></div><div>62%20%•14%</div></div>
1	B	279	<div>%<div></div><div>59%23%•14%</div></div>
1	C	279	<div><div></div><div>67%16%•14%</div></div>
1	D	279	<div><div></div><div>65%17%•14%</div></div>
1	E	279	<div><div></div><div>64%19%•14%</div></div>
1	F	279	<div><div></div><div>63%18%5%14%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	279	<div><div>%</div><div><div></div><div>63%</div><div>20%</div><div>•</div><div>14%</div></div></div>
1	H	279	<div><div></div><div>63%</div><div>19%</div><div>•</div><div>14%</div></div>
1	I	279	<div><div></div><div>64%</div><div>18%</div><div>5%</div><div>14%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17478 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 Ferric enterobactin (Enterochelin) transport.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0
1	B	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0
1	C	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0
1	D	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0
1	E	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0
1	F	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0
1	G	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0
1	H	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0
1	I	241	Total 1942	C 1241	N 320	O 378	S 3	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
A	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
A	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
A	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
A	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
B	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
B	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
B	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
B	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
B	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
B	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
C	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
C	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
C	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
C	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
C	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
C	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
D	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
D	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
D	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
D	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
D	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
D	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
E	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
E	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
E	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
E	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
E	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
E	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
F	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
F	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
F	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
F	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
F	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
F	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
G	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
G	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
G	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
G	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
G	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
G	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
H	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
H	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
H	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
H	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
H	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8

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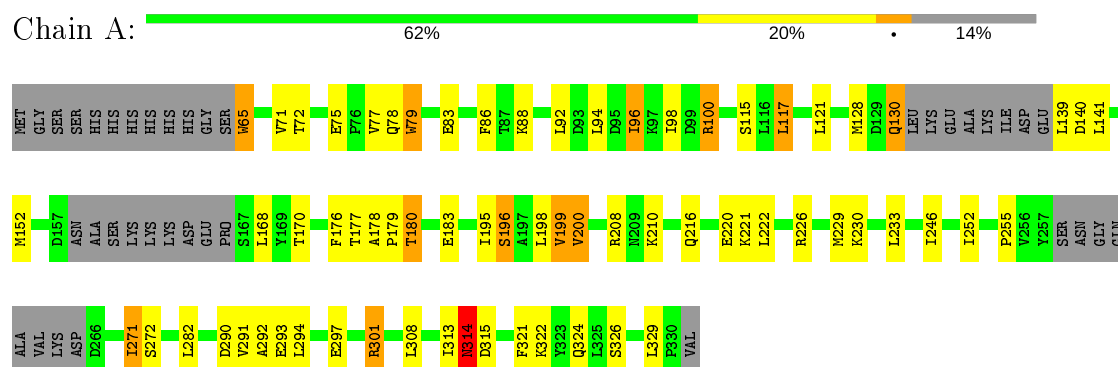
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Chain	Residue	Modelled	Actual	Comment	Reference
H	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
I	53	MET	-	EXPRESSION TAG	UNP Q8XBV8
I	54	GLY	-	EXPRESSION TAG	UNP Q8XBV8
I	55	SER	-	EXPRESSION TAG	UNP Q8XBV8
I	56	SER	-	EXPRESSION TAG	UNP Q8XBV8
I	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
I	64	SER	-	EXPRESSION TAG	UNP Q8XBV8

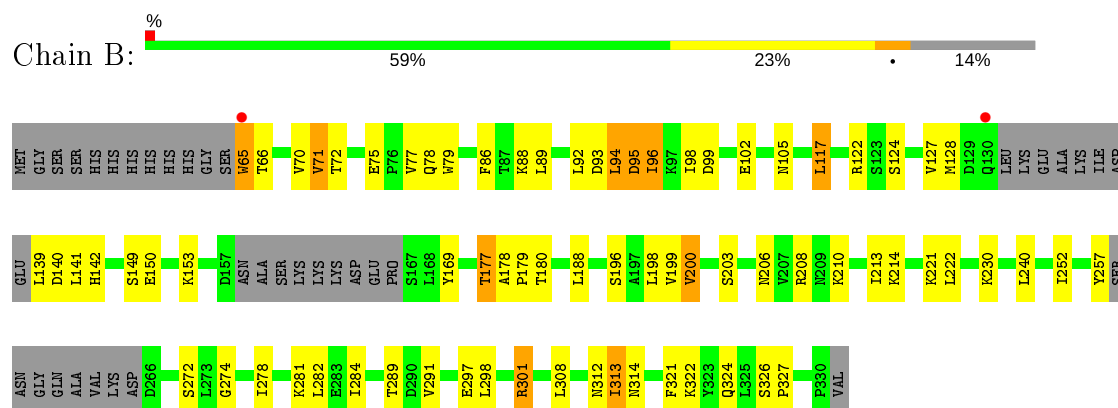
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

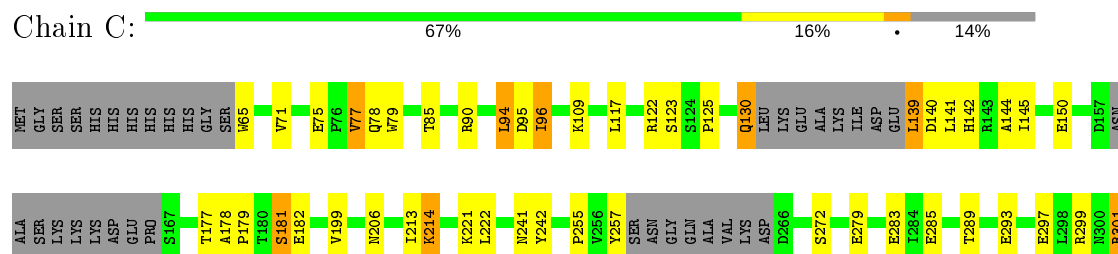
- Molecule 1: Ferric enterobactin (Enterochelin) transport



- Molecule 1: Ferric enterobactin (Enterochelin) transport



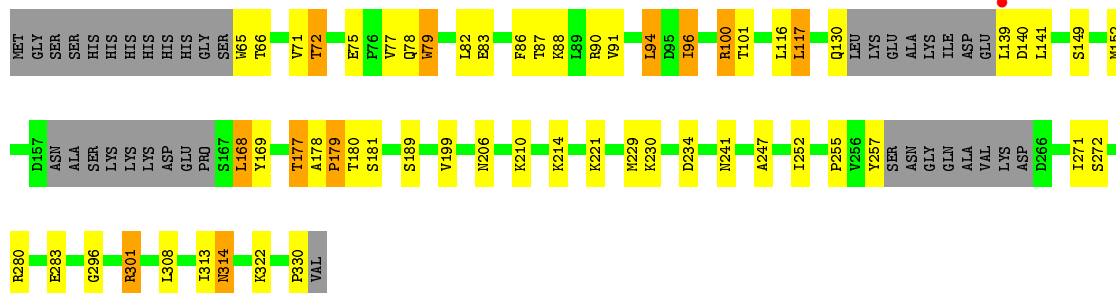
- Molecule 1: Ferric enterobactin (Enterochelin) transport





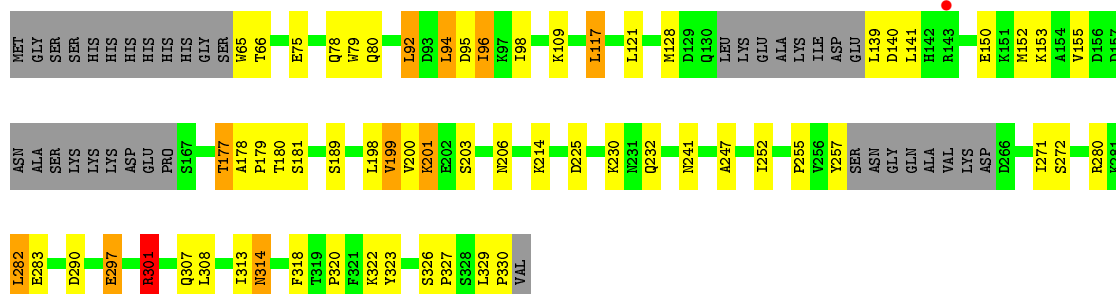
- Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain D: 65% 17% 14%



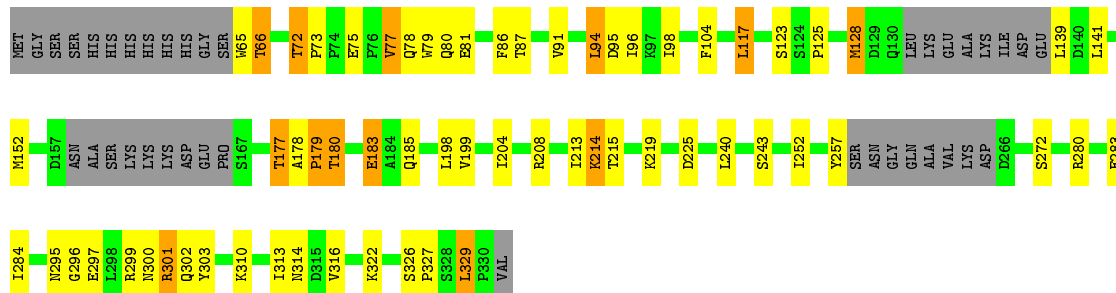
- Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain E: 64% 19% 14%



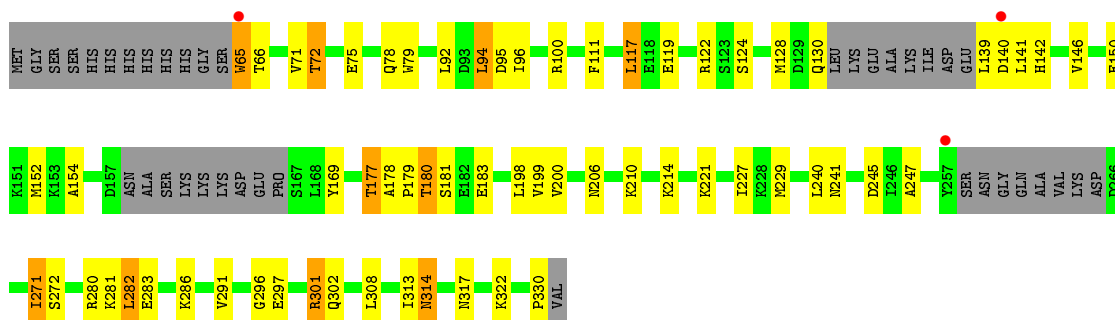
- Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain F: 63% 18% 5% 14%



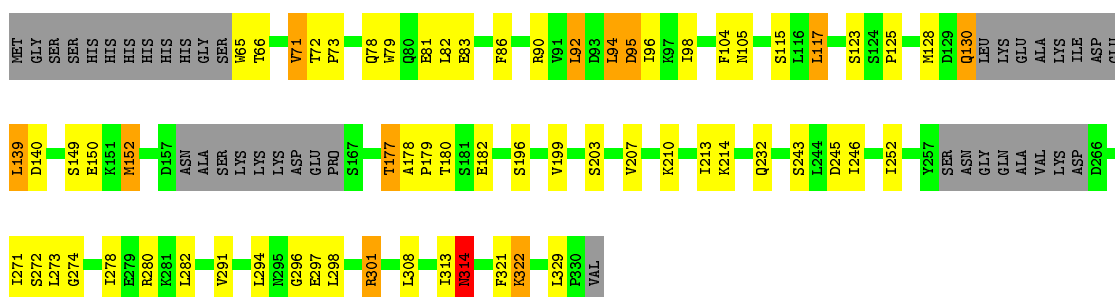
- Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain G: 63% 20% 14%



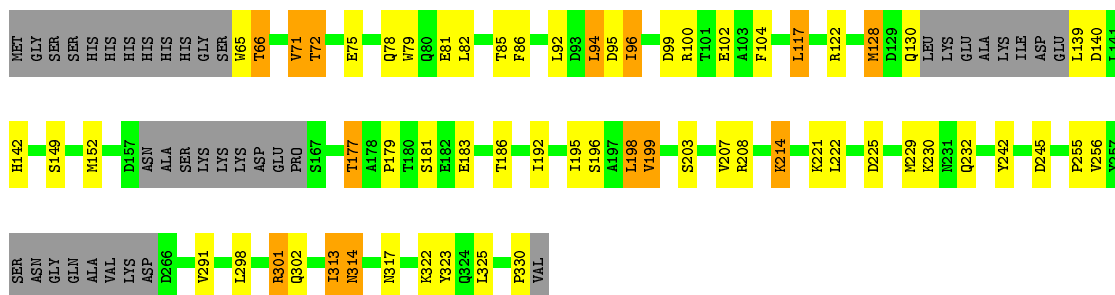
• Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain H: 63% 19% 14%



• Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain I: 64% 18% 5% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.67Å 160.67Å 276.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.10) 99.7 (19.88-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.98Å)	Xtriage
Refinement program	REFMAC refmac _5.2.0019	Depositor
R, R_{free}	0.254 , 0.282 0.241 , 0.274	Depositor DCC
R_{free} test set	4150 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 11.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17478	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.63	0/1973	0.76	2/2669 (0.1%)
1	B	0.63	0/1973	0.79	2/2669 (0.1%)
1	C	0.62	0/1973	0.75	2/2669 (0.1%)
1	D	0.61	0/1973	0.75	2/2669 (0.1%)
1	E	0.59	0/1973	0.76	3/2669 (0.1%)
1	F	0.65	0/1973	0.79	2/2669 (0.1%)
1	G	0.59	0/1973	0.74	1/2669 (0.0%)
1	H	0.58	0/1973	0.72	3/2669 (0.1%)
1	I	0.60	0/1973	0.74	2/2669 (0.1%)
All	All	0.61	0/17757	0.76	19/24021 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	314	ASN	N-CA-CB	-12.69	87.76	110.60
1	G	313	ILE	N-CA-C	-10.75	81.98	111.00
1	I	313	ILE	N-CA-C	-10.37	83.00	111.00
1	A	313	ILE	N-CA-C	-10.37	83.02	111.00
1	H	314	ASN	N-CA-CB	-10.23	92.18	110.60
1	E	313	ILE	N-CA-C	-10.21	83.44	111.00
1	C	313	ILE	N-CA-C	-10.18	83.53	111.00
1	B	313	ILE	N-CA-C	-10.02	83.95	111.00
1	D	313	ILE	N-CA-C	-9.98	84.05	111.00
1	H	313	ILE	N-CA-C	-9.89	84.30	111.00
1	F	313	ILE	N-CA-C	-9.71	84.78	111.00
1	E	313	ILE	CB-CA-C	-8.74	94.13	111.60
1	F	313	ILE	CB-CA-C	-8.61	94.37	111.60
1	C	314	ASN	N-CA-CB	-8.38	95.51	110.60
1	A	314	ASN	N-CA-CB	-7.57	96.97	110.60
1	I	313	ILE	CB-CA-C	-6.48	98.63	111.60
1	D	139	LEU	CA-CB-CG	6.15	129.44	115.30
1	E	301	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	139	LEU	CA-CB-CG	5.31	127.52	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1942	0	1964	38	0
1	B	1942	0	1964	42	0
1	C	1942	0	1964	35	0
1	D	1942	0	1964	34	0
1	E	1942	0	1964	36	0
1	F	1942	0	1964	35	0
1	G	1942	0	1964	37	0
1	H	1942	0	1964	38	0
1	I	1942	0	1964	35	0
All	All	17478	0	17676	300	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.

All (300) 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:301:ARG:HH11	1:B:301:ARG:HG2	1.10	1.06
1:E:301:ARG:HG2	1:E:301:ARG:HH11	1.28	0.97
1:C:221:LYS:HB3	1:C:301:ARG:HH12	1.30	0.96
1:I:128:MET:HE2	1:I:128:MET:HA	1.47	0.93
1:I:128:MET:HA	1:I:128:MET:CE	1.97	0.93
1:I:301:ARG:HH21	1:I:301:ARG:HG2	1.37	0.88
1:G:301:ARG:HH11	1:G:301:ARG:HB3	1.39	0.88
1:A:314:ASN:C	1:A:314:ASN:HD22	1.78	0.87
1:B:94:LEU:HD22	1:B:96:ILE:HG12	1.55	0.86
1:A:252:ILE:HD11	1:I:255:PRO:HG2	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ASN:HD22	1:C:314:ASN:C	1.82	0.84
1:F:94:LEU:HG	1:F:214:LYS:HG3	1.60	0.82
1:A:226:ARG:NH2	1:A:290:ASP:OD1	2.12	0.81
1:B:301:ARG:HH11	1:B:301:ARG:CG	1.94	0.81
1:H:66:THR:OG1	1:H:177:THR:HB	1.82	0.80
1:B:222:LEU:HD13	1:B:301:ARG:HB3	1.62	0.80
1:B:75:GLU:OE2	1:C:109:LYS:NZ	2.16	0.79
1:C:94:LEU:HG	1:C:214:LYS:HG3	1.63	0.79
1:G:301:ARG:CB	1:G:301:ARG:HH11	1.97	0.78
1:B:301:ARG:HG2	1:B:301:ARG:NH1	1.91	0.77
1:E:94:LEU:HG	1:E:214:LYS:HG3	1.67	0.77
1:G:301:ARG:CG	1:G:301:ARG:HH11	2.01	0.73
1:F:75:GLU:H	1:F:78:GLN:HE21	1.37	0.73
1:G:314:ASN:C	1:G:314:ASN:HD22	1.92	0.72
1:D:314:ASN:C	1:D:314:ASN:HD22	1.93	0.71
1:B:94:LEU:HG	1:B:214:LYS:HG3	1.72	0.71
1:F:66:THR:OG1	1:F:177:THR:HB	1.91	0.70
1:G:65:TRP:HB2	1:G:178:ALA:O	1.91	0.70
1:H:94:LEU:HD22	1:H:96:ILE:HG12	1.74	0.70
1:I:94:LEU:HG	1:I:214:LYS:HG3	1.72	0.70
1:D:94:LEU:HG	1:D:214:LYS:HG3	1.74	0.70
1:B:66:THR:OG1	1:B:177:THR:HB	1.91	0.69
1:C:75:GLU:H	1:C:78:GLN:NE2	1.90	0.68
1:G:122:ARG:NH2	1:G:142:HIS:HD2	1.92	0.68
1:G:296:GLY:HA3	1:H:232:GLN:HE21	1.58	0.68
1:E:95:ASP:O	1:E:96:ILE:HD13	1.93	0.68
1:H:314:ASN:HD22	1:H:314:ASN:C	1.98	0.67
1:B:65:TRP:HB2	1:B:178:ALA:O	1.95	0.67
1:H:86:PHE:HZ	1:H:98:ILE:HG13	1.60	0.67
1:G:122:ARG:HH21	1:G:142:HIS:HD2	1.41	0.67
1:G:301:ARG:HB3	1:G:301:ARG:NH1	2.10	0.67
1:B:75:GLU:H	1:B:78:GLN:NE2	1.93	0.66
1:B:75:GLU:H	1:B:78:GLN:HE21	1.42	0.66
1:F:280:ARG:O	1:F:284:ILE:HG12	1.96	0.65
1:D:301:ARG:HB3	1:D:301:ARG:HH11	1.62	0.65
1:H:94:LEU:HG	1:H:214:LYS:HG3	1.77	0.65
1:G:240:LEU:HD21	1:G:281:LYS:HG2	1.79	0.64
1:I:66:THR:OG1	1:I:177:THR:HB	1.97	0.64
1:B:122:ARG:HH22	1:B:142:HIS:CD2	2.15	0.64
1:E:128:MET:HE2	1:E:128:MET:HA	1.79	0.64
1:C:314:ASN:C	1:C:314:ASN:ND2	2.48	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:301:ARG:NH2	1:I:301:ARG:HG2	2.08	0.63
1:I:72:THR:HG22	1:I:322:LYS:HB3	1.80	0.63
1:C:301:ARG:CG	1:C:301:ARG:HH21	2.11	0.63
1:D:86:PHE:CD2	1:D:96:ILE:HG22	2.34	0.62
1:D:75:GLU:H	1:D:78:GLN:NE2	1.98	0.62
1:G:72:THR:HG22	1:G:322:LYS:HB3	1.82	0.62
1:D:66:THR:OG1	1:D:177:THR:HB	2.00	0.62
1:E:301:ARG:HH11	1:E:301:ARG:CG	2.08	0.61
1:F:86:PHE:HZ	1:F:98:ILE:HG13	1.65	0.61
1:D:65:TRP:HB2	1:D:178:ALA:O	1.99	0.61
1:G:247:ALA:N	1:G:271:ILE:HD11	2.15	0.61
1:G:66:THR:OG1	1:G:177:THR:HB	2.00	0.61
1:H:117:LEU:HD13	1:H:149:SER:HB2	1.83	0.61
1:A:128:MET:HA	1:A:128:MET:CE	2.31	0.61
1:A:314:ASN:ND2	1:A:314:ASN:C	2.53	0.60
1:B:128:MET:CE	1:B:128:MET:HA	2.31	0.60
1:D:87:THR:O	1:D:91:VAL:HG23	2.01	0.60
1:B:86:PHE:CZ	1:B:98:ILE:HG13	2.36	0.60
1:D:72:THR:HG22	1:D:322:LYS:HB3	1.84	0.60
1:G:75:GLU:H	1:G:78:GLN:HE21	1.49	0.60
1:H:301:ARG:HB3	1:H:301:ARG:HH11	1.67	0.60
1:I:117:LEU:HD13	1:I:149:SER:HB2	1.83	0.60
1:I:229:MET:HG3	1:I:298:LEU:HD11	1.83	0.60
1:E:80:GLN:HE22	1:F:213:ILE:HD13	1.67	0.59
1:D:82:LEU:HB3	1:D:86:PHE:CE1	2.37	0.59
1:F:128:MET:CE	1:F:128:MET:HA	2.32	0.59
1:I:181:SER:HB2	1:I:330:PRO:HG2	1.83	0.59
1:E:314:ASN:C	1:E:314:ASN:HD22	2.06	0.58
1:F:91:VAL:HG13	1:G:221:LYS:HG2	1.83	0.58
1:A:117:LEU:HD22	1:A:121:LEU:HD11	1.86	0.58
1:E:94:LEU:HD22	1:E:96:ILE:HG12	1.85	0.58
1:F:180:THR:OG1	1:F:183:GLU:HB2	2.04	0.58
1:C:122:ARG:HH21	1:C:142:HIS:HD2	1.52	0.58
1:D:96:ILE:CD1	1:D:210:LYS:HD3	2.34	0.58
1:E:128:MET:CE	1:E:128:MET:HA	2.33	0.58
1:H:314:ASN:ND2	1:H:314:ASN:C	2.57	0.58
1:H:274:GLY:O	1:H:278:ILE:HG12	2.04	0.57
1:E:65:TRP:HB2	1:E:178:ALA:O	2.04	0.57
1:F:123:SER:O	1:F:125:PRO:HD3	2.05	0.56
1:H:65:TRP:HB2	1:H:178:ALA:O	2.06	0.56
1:C:122:ARG:NH2	1:C:142:HIS:HD2	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:VAL:HG12	1:D:206:ASN:HD21	1.70	0.56
1:H:81:GLU:OE1	1:H:81:GLU:HA	2.04	0.56
1:C:181:SER:HB2	1:C:330:PRO:HG2	1.88	0.56
1:E:301:ARG:HG2	1:E:301:ARG:NH1	2.07	0.56
1:I:208:ARG:HG2	1:I:313:ILE:HG13	1.87	0.56
1:G:117:LEU:HD11	1:G:152:MET:HB2	1.89	0.55
1:H:71:VAL:HG13	1:H:104:PHE:HE1	1.72	0.55
1:G:128:MET:HA	1:G:128:MET:CE	2.36	0.55
1:G:301:ARG:HG2	1:G:301:ARG:HH11	1.71	0.55
1:E:117:LEU:HD22	1:E:121:LEU:HD11	1.87	0.54
1:H:123:SER:O	1:H:125:PRO:HD3	2.07	0.54
1:A:117:LEU:HD11	1:A:152:MET:HB2	1.88	0.54
1:D:314:ASN:C	1:D:314:ASN:ND2	2.60	0.54
1:B:77:VAL:HG13	1:C:206:ASN:HD21	1.72	0.54
1:C:75:GLU:H	1:C:78:GLN:HE21	1.55	0.54
1:C:301:ARG:O	1:C:305:VAL:HG23	2.07	0.54
1:E:66:THR:HG23	1:E:177:THR:HG22	1.90	0.54
1:G:180:THR:HB	1:G:183:GLU:H	1.73	0.54
1:D:247:ALA:N	1:D:271:ILE:HD11	2.22	0.54
1:C:293:GLU:HA	1:C:299:ARG:HH21	1.73	0.53
1:C:255:PRO:HG2	1:D:252:ILE:HD11	1.90	0.53
1:I:94:LEU:HD22	1:I:96:ILE:HG12	1.90	0.53
1:A:196:SER:O	1:A:200:VAL:HG12	2.09	0.53
1:I:208:ARG:HH21	1:I:314:ASN:HA	1.74	0.53
1:E:117:LEU:HD11	1:E:152:MET:HB2	1.90	0.53
1:E:75:GLU:H	1:E:78:GLN:HE21	1.57	0.53
1:B:196:SER:O	1:B:200:VAL:HG12	2.10	0.52
1:F:86:PHE:CE2	1:F:96:ILE:HG22	2.44	0.52
1:B:96:ILE:HD11	1:B:210:LYS:HD3	1.91	0.52
1:A:195:ILE:O	1:A:199:VAL:HG12	2.10	0.52
1:A:86:PHE:HZ	1:A:98:ILE:HG13	1.74	0.52
1:B:70:VAL:HG12	1:B:324:GLN:HB2	1.92	0.52
1:G:296:GLY:HA3	1:H:232:GLN:NE2	2.25	0.51
1:B:77:VAL:HG13	1:C:206:ASN:ND2	2.26	0.51
1:D:65:TRP:CE3	1:D:65:TRP:N	2.79	0.51
1:F:75:GLU:H	1:F:78:GLN:NE2	2.05	0.51
1:I:71:VAL:HG13	1:I:104:PHE:HE1	1.75	0.51
1:A:216:GLN:O	1:A:220:GLU:HG3	2.10	0.51
1:G:122:ARG:NH2	1:G:142:HIS:CD2	2.77	0.51
1:C:123:SER:O	1:C:125:PRO:HD3	2.11	0.51
1:F:204:ILE:HG22	1:F:208:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD11	1:B:313:ILE:HD11	1.93	0.51
1:C:65:TRP:HB2	1:C:178:ALA:O	2.10	0.51
1:A:75:GLU:H	1:A:78:GLN:NE2	2.09	0.51
1:D:296:GLY:HA3	1:E:232:GLN:NE2	2.26	0.51
1:E:75:GLU:H	1:E:78:GLN:NE2	2.09	0.51
1:B:99:ASP:HB3	1:B:102:GLU:HB2	1.92	0.50
1:G:146:VAL:O	1:G:150:GLU:HG3	2.11	0.50
1:D:96:ILE:HD11	1:D:210:LYS:HD3	1.93	0.50
1:F:225:ASP:OD2	1:F:301:ARG:NH1	2.44	0.50
1:B:188:LEU:HD23	1:B:327:PRO:HB3	1.94	0.50
1:H:95:ASP:O	1:H:96:ILE:HD13	2.11	0.50
1:B:86:PHE:HZ	1:B:98:ILE:HG13	1.77	0.50
1:E:290:ASP:C	1:E:290:ASP:OD1	2.48	0.50
1:I:82:LEU:HB3	1:I:86:PHE:CE1	2.47	0.50
1:D:117:LEU:HD11	1:D:152:MET:HB2	1.93	0.50
1:F:326:SER:HB2	1:F:327:PRO:HD2	1.93	0.50
1:B:72:THR:HG22	1:B:322:LYS:O	2.11	0.49
1:F:296:GLY:HA2	1:F:299:ARG:HD2	1.94	0.49
1:H:86:PHE:CZ	1:H:98:ILE:HG13	2.45	0.49
1:D:255:PRO:HG2	1:E:252:ILE:HD11	1.95	0.49
1:F:295:ASN:O	1:F:299:ARG:HG3	2.12	0.49
1:G:314:ASN:ND2	1:G:314:ASN:C	2.64	0.49
1:B:124:SER:OG	1:B:127:VAL:HG23	2.13	0.49
1:G:282:LEU:HD22	1:G:286:LYS:HD2	1.93	0.49
1:A:222:LEU:HD13	1:A:301:ARG:HB3	1.93	0.49
1:I:225:ASP:OD2	1:I:301:ARG:NH1	2.46	0.49
1:B:95:ASP:O	1:B:96:ILE:HD13	2.12	0.49
1:F:72:THR:HG22	1:F:322:LYS:HB3	1.95	0.49
1:I:203:SER:O	1:I:207:VAL:HG23	2.13	0.49
1:A:72:THR:HG22	1:A:322:LYS:O	2.13	0.49
1:G:301:ARG:CG	1:G:301:ARG:NH1	2.69	0.49
1:H:128:MET:CE	1:H:128:MET:HA	2.43	0.48
1:C:314:ASN:O	1:C:314:ASN:ND2	2.46	0.48
1:F:65:TRP:HB2	1:F:178:ALA:O	2.13	0.48
1:E:225:ASP:OD2	1:E:301:ARG:NH2	2.36	0.48
1:E:181:SER:OG	1:E:330:PRO:HD2	2.14	0.48
1:F:300:ASN:O	1:F:303:TYR:HB3	2.14	0.48
1:C:222:LEU:HD13	1:C:301:ARG:HB3	1.95	0.47
1:H:96:ILE:HD12	1:H:210:LYS:HD3	1.96	0.47
1:A:255:PRO:HG3	1:B:252:ILE:HD11	1.95	0.47
1:D:86:PHE:CE2	1:D:96:ILE:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:GLN:OE1	1:F:329:LEU:HB2	2.15	0.47
1:G:96:ILE:CD1	1:G:210:LYS:HD3	2.44	0.47
1:C:94:LEU:HD22	1:C:96:ILE:HG12	1.96	0.47
1:A:96:ILE:HG13	1:A:210:LYS:HD3	1.97	0.47
1:F:128:MET:HE2	1:F:128:MET:HA	1.96	0.47
1:A:96:ILE:HD13	1:A:96:ILE:HA	1.67	0.47
1:F:117:LEU:HD11	1:F:152:MET:HB2	1.95	0.47
1:A:117:LEU:O	1:A:121:LEU:HG	2.15	0.47
1:E:247:ALA:N	1:E:271:ILE:HD11	2.30	0.47
1:E:255:PRO:HG2	1:F:252:ILE:HD11	1.97	0.47
1:I:75:GLU:H	1:I:78:GLN:HE21	1.61	0.47
1:G:280:ARG:HE	1:H:245:ASP:HB3	1.80	0.46
1:D:117:LEU:HD13	1:D:149:SER:HB2	1.97	0.46
1:A:314:ASN:ND2	1:A:314:ASN:O	2.46	0.46
1:A:180:THR:HB	1:A:183:GLU:H	1.81	0.46
1:C:130:GLN:HG2	1:C:130:GLN:H	1.34	0.46
1:C:122:ARG:HG3	1:C:145:ILE:CD1	2.46	0.46
1:D:75:GLU:H	1:D:78:GLN:HE21	1.63	0.46
1:I:128:MET:CA	1:I:128:MET:CE	2.82	0.46
1:C:279:GLU:O	1:C:283:GLU:HG2	2.16	0.45
1:E:201:LYS:HE2	1:E:201:LYS:HB3	1.68	0.45
1:H:273:LEU:HD23	1:H:278:ILE:HD13	1.97	0.45
1:A:115:SER:OG	1:I:325:LEU:HA	2.16	0.45
1:D:280:ARG:HH11	1:D:283:GLU:HG3	1.80	0.45
1:E:280:ARG:HH11	1:E:283:GLU:HG3	1.82	0.45
1:F:87:THR:O	1:F:91:VAL:HG23	2.17	0.45
1:E:200:VAL:HB	1:E:318:PHE:CE2	2.52	0.45
1:E:241:ASN:HD22	1:E:282:LEU:HD11	1.82	0.45
1:I:195:ILE:O	1:I:199:VAL:HG12	2.16	0.45
1:A:324:GLN:NE2	1:A:324:GLN:HA	2.31	0.45
1:G:301:ARG:HG2	1:G:301:ARG:NH1	2.30	0.45
1:G:181:SER:HB2	1:G:330:PRO:HG2	1.99	0.45
1:G:94:LEU:HG	1:G:214:LYS:HG3	1.99	0.45
1:H:294:LEU:HD21	1:I:242:TYR:CE1	2.52	0.45
1:B:117:LEU:HD13	1:B:149:SER:HB2	1.99	0.45
1:G:96:ILE:HD12	1:G:210:LYS:HD3	1.99	0.45
1:D:88:LYS:HB3	1:D:88:LYS:HE2	1.45	0.44
1:H:72:THR:OG1	1:H:73:PRO:HD2	2.17	0.44
1:I:99:ASP:HB3	1:I:102:GLU:HB2	1.99	0.44
1:E:199:VAL:HG11	1:E:320:PRO:HG3	1.98	0.44
1:F:215:THR:O	1:F:219:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG12	1:B:206:ASN:ND2	2.31	0.44
1:C:301:ARG:HG3	1:C:301:ARG:HH21	1.81	0.44
1:B:208:ARG:HE	1:B:313:ILE:HB	1.83	0.44
1:G:111:PHE:CE2	1:G:154:ALA:HB2	2.53	0.44
1:B:284:ILE:HD13	1:C:242:TYR:HB3	2.00	0.44
1:F:95:ASP:O	1:F:96:ILE:HD13	2.18	0.44
1:H:314:ASN:ND2	1:H:314:ASN:O	2.51	0.44
1:G:128:MET:HA	1:G:128:MET:HE2	1.98	0.44
1:H:96:ILE:CD1	1:H:210:LYS:HD3	2.47	0.44
1:C:139:LEU:O	1:C:139:LEU:HD23	2.18	0.44
1:C:222:LEU:HD21	1:C:302:GLN:HG2	1.99	0.44
1:F:178:ALA:HB1	1:F:179:PRO:HD2	2.00	0.44
1:A:128:MET:HA	1:A:128:MET:HE2	2.00	0.43
1:F:77:VAL:HG13	1:G:206:ASN:ND2	2.33	0.43
1:H:82:LEU:HD22	1:H:98:ILE:HD12	2.00	0.43
1:F:240:LEU:O	1:F:243:SER:HB2	2.18	0.43
1:H:130:GLN:H	1:H:130:GLN:HG2	1.40	0.43
1:D:96:ILE:HA	1:D:96:ILE:HD13	1.66	0.43
1:I:222:LEU:HD13	1:I:301:ARG:HB3	2.00	0.43
1:A:152:MET:HE1	1:A:176:PHE:HB2	2.00	0.43
1:C:77:VAL:HG12	1:D:206:ASN:ND2	2.33	0.43
1:E:199:VAL:CG1	1:E:320:PRO:HG3	2.48	0.43
1:E:323:TYR:CZ	1:E:327:PRO:HD3	2.53	0.43
1:I:96:ILE:HA	1:I:96:ILE:HD13	1.82	0.43
1:I:117:LEU:HD11	1:I:152:MET:HB2	2.01	0.43
1:H:117:LEU:HD11	1:H:152:MET:HB2	2.01	0.43
1:F:73:PRO:HA	1:F:104:PHE:CD1	2.54	0.43
1:A:65:TRP:HB2	1:A:178:ALA:O	2.18	0.43
1:A:246:ILE:HB	1:A:271:ILE:HD11	2.00	0.43
1:E:314:ASN:ND2	1:E:314:ASN:C	2.72	0.43
1:A:168:LEU:HD21	1:B:105:ASN:HB3	2.01	0.43
1:F:96:ILE:HA	1:F:96:ILE:HD13	1.87	0.43
1:H:246:ILE:HB	1:H:271:ILE:HD11	2.00	0.43
1:I:130:GLN:HE22	1:I:183:GLU:HG3	1.84	0.43
1:A:321:PHE:CD1	1:A:321:PHE:C	2.93	0.42
1:B:274:GLY:O	1:B:278:ILE:HG12	2.19	0.42
1:B:96:ILE:HA	1:B:96:ILE:HD13	1.72	0.42
1:D:79:TRP:CE2	1:D:100:ARG:HG3	2.54	0.42
1:H:252:ILE:HG22	1:H:274:GLY:HA2	2.02	0.42
1:A:79:TRP:CE2	1:A:100:ARG:HG3	2.54	0.42
1:A:77:VAL:CG1	1:B:206:ASN:HD21	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:TYR:CE1	1:G:227:ILE:HG21	2.53	0.42
1:I:122:ARG:NH2	1:I:142:HIS:CD2	2.87	0.42
1:D:66:THR:O	1:D:330:PRO:HG3	2.19	0.42
1:C:141:LEU:O	1:C:144:ALA:HB3	2.20	0.42
1:B:169:TYR:CE2	1:C:109:LYS:HG3	2.54	0.42
1:B:298:LEU:HD23	1:B:298:LEU:HA	1.91	0.42
1:F:80:GLN:OE1	1:F:80:GLN:HA	2.19	0.42
1:A:208:ARG:HH21	1:A:314:ASN:HA	1.84	0.42
1:G:169:TYR:N	1:G:169:TYR:CD2	2.87	0.41
1:E:98:ILE:HD13	1:E:203:SER:HB3	2.01	0.41
1:H:72:THR:HG22	1:H:322:LYS:O	2.20	0.41
1:A:226:ARG:HH12	1:A:292:ALA:HB2	1.86	0.41
1:A:88:LYS:HB3	1:A:88:LYS:HE2	1.85	0.41
1:B:98:ILE:HD13	1:B:203:SER:HB3	2.02	0.41
1:C:299:ARG:HH12	1:D:234:ASP:HB3	1.86	0.41
1:H:280:ARG:NH2	1:I:245:ASP:OD2	2.53	0.41
1:I:192:ILE:HG21	1:I:323:TYR:OH	2.20	0.41
1:F:81:GLU:OE1	1:F:316:VAL:HG13	2.21	0.41
1:H:321:PHE:CD1	1:H:321:PHE:C	2.94	0.41
1:I:198:LEU:HA	1:I:198:LEU:HD12	1.85	0.41
1:A:130:GLN:HG2	1:A:130:GLN:H	1.70	0.41
1:G:124:SER:O	1:G:128:MET:HG2	2.20	0.41
1:I:96:ILE:HG21	1:I:207:VAL:HG13	2.01	0.41
1:H:296:GLY:HA3	1:I:232:GLN:NE2	2.35	0.41
1:A:294:LEU:HD23	1:A:294:LEU:HA	1.93	0.41
1:B:128:MET:HA	1:B:128:MET:HE2	2.00	0.41
1:B:71:VAL:HG22	1:B:321:PHE:HB2	2.02	0.41
1:H:92:LEU:HA	1:H:92:LEU:HD12	1.94	0.41
1:H:96:ILE:HD13	1:H:96:ILE:HA	1.83	0.41
1:C:65:TRP:CE3	1:C:65:TRP:N	2.89	0.40
1:D:168:LEU:HB3	1:D:169:TYR:HD2	1.86	0.40
1:E:92:LEU:HD11	1:E:307:GLN:HB3	2.03	0.40
1:A:121:LEU:HG	1:A:121:LEU:H	1.75	0.40
1:E:78:GLN:HE22	1:E:322:LYS:HB2	1.86	0.40
1:I:122:ARG:NH2	1:I:142:HIS:HD2	2.19	0.40
1:A:139:LEU:O	1:A:139:LEU:HD23	2.21	0.40
1:B:240:LEU:HD21	1:B:281:LYS:HG2	2.02	0.40
1:H:78:GLN:HE22	1:H:322:LYS:HB2	1.87	0.40
1:B:169:TYR:CZ	1:C:109:LYS:HG3	2.56	0.40
1:D:178:ALA:HB1	1:D:179:PRO:HD2	2.03	0.40
1:D:72:THR:HG21	1:E:109:LYS:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:SER:O	1:H:207:VAL:HG23	2.22	0.40
1:D:116:LEU:HA	1:D:116:LEU:HD23	1.85	0.40
1:E:297:GLU:OE1	1:E:301:ARG:HD2	2.22	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	233/279 (84%)	226 (97%)	5 (2%)	2 (1%)	17	52
1	B	233/279 (84%)	226 (97%)	6 (3%)	1 (0%)	34	69
1	C	233/279 (84%)	226 (97%)	6 (3%)	1 (0%)	34	69
1	D	233/279 (84%)	225 (97%)	7 (3%)	1 (0%)	34	69
1	E	233/279 (84%)	226 (97%)	6 (3%)	1 (0%)	34	69
1	F	233/279 (84%)	228 (98%)	4 (2%)	1 (0%)	34	69
1	G	233/279 (84%)	227 (97%)	5 (2%)	1 (0%)	34	69
1	H	233/279 (84%)	229 (98%)	3 (1%)	1 (0%)	34	69
1	I	233/279 (84%)	228 (98%)	4 (2%)	1 (0%)	34	69
All	All	2097/2511 (84%)	2041 (97%)	46 (2%)	10 (0%)	29	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	179	PRO
1	G	179	PRO
1	A	179	PRO
1	D	179	PRO
1	A	315	ASP

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Mol	Chain	Res	Type
1	B	179	PRO
1	E	179	PRO
1	F	179	PRO
1	I	179	PRO
1	H	179	PRO

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	218/250 (87%)	184 (84%)	34 (16%)	2	11
1	B	218/250 (87%)	185 (85%)	33 (15%)	3	12
1	C	218/250 (87%)	189 (87%)	29 (13%)	4	16
1	D	218/250 (87%)	189 (87%)	29 (13%)	4	16
1	E	218/250 (87%)	190 (87%)	28 (13%)	4	18
1	F	218/250 (87%)	194 (89%)	24 (11%)	6	25
1	G	218/250 (87%)	185 (85%)	33 (15%)	3	12
1	H	218/250 (87%)	186 (85%)	32 (15%)	3	13
1	I	218/250 (87%)	188 (86%)	30 (14%)	3	16
All	All	1962/2250 (87%)	1690 (86%)	272 (14%)	3	15

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	TRP
1	A	71	VAL
1	A	79	TRP
1	A	83	GLU
1	A	92	LEU
1	A	94	LEU
1	A	96	ILE
1	A	100	ARG
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	130	GLN
1	A	140	ASP
1	A	141	LEU
1	A	170	THR
1	A	177	THR
1	A	180	THR
1	A	196	SER
1	A	198	LEU
1	A	199	VAL
1	A	200	VAL
1	A	221	LYS
1	A	229	MET
1	A	230	LYS
1	A	233	LEU
1	A	271	ILE
1	A	272	SER
1	A	282	LEU
1	A	291	VAL
1	A	293	GLU
1	A	297	GLU
1	A	301	ARG
1	A	308	LEU
1	A	314	ASN
1	A	326	SER
1	A	329	LEU
1	B	65	TRP
1	B	71	VAL
1	B	79	TRP
1	B	88	LYS
1	B	92	LEU
1	B	93	ASP
1	B	94	LEU
1	B	95	ASP
1	B	96	ILE
1	B	117	LEU
1	B	139	LEU
1	B	140	ASP
1	B	141	LEU
1	B	150	GLU
1	B	153	LYS
1	B	177	THR
1	B	180	THR

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Mol	Chain	Res	Type
1	B	198	LEU
1	B	199	VAL
1	B	200	VAL
1	B	213	ILE
1	B	221	LYS
1	B	230	LYS
1	B	257	TYR
1	B	272	SER
1	B	282	LEU
1	B	289	THR
1	B	291	VAL
1	B	297	GLU
1	B	301	ARG
1	B	308	LEU
1	B	312	ASN
1	B	326	SER
1	C	71	VAL
1	C	77	VAL
1	C	79	TRP
1	C	85	THR
1	C	90	ARG
1	C	94	LEU
1	C	95	ASP
1	C	96	ILE
1	C	117	LEU
1	C	130	GLN
1	C	139	LEU
1	C	140	ASP
1	C	150	GLU
1	C	177	THR
1	C	181	SER
1	C	182	GLU
1	C	199	VAL
1	C	213	ILE
1	C	214	LYS
1	C	241	ASN
1	C	257	TYR
1	C	272	SER
1	C	285	GLU
1	C	289	THR
1	C	297	GLU
1	C	301	ARG

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Mol	Chain	Res	Type
1	C	302	GLN
1	C	314	ASN
1	C	326	SER
1	D	71	VAL
1	D	72	THR
1	D	77	VAL
1	D	79	TRP
1	D	83	GLU
1	D	90	ARG
1	D	94	LEU
1	D	96	ILE
1	D	100	ARG
1	D	101	THR
1	D	117	LEU
1	D	130	GLN
1	D	140	ASP
1	D	141	LEU
1	D	168	LEU
1	D	177	THR
1	D	180	THR
1	D	181	SER
1	D	189	SER
1	D	199	VAL
1	D	221	LYS
1	D	229	MET
1	D	230	LYS
1	D	241	ASN
1	D	257	TYR
1	D	272	SER
1	D	301	ARG
1	D	308	LEU
1	D	314	ASN
1	E	79	TRP
1	E	92	LEU
1	E	94	LEU
1	E	96	ILE
1	E	117	LEU
1	E	139	LEU
1	E	140	ASP
1	E	141	LEU
1	E	150	GLU
1	E	153	LYS

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Mol	Chain	Res	Type
1	E	155	VAL
1	E	177	THR
1	E	180	THR
1	E	189	SER
1	E	198	LEU
1	E	199	VAL
1	E	201	LYS
1	E	206	ASN
1	E	230	LYS
1	E	257	TYR
1	E	272	SER
1	E	282	LEU
1	E	297	GLU
1	E	301	ARG
1	E	308	LEU
1	E	314	ASN
1	E	326	SER
1	E	329	LEU
1	F	66	THR
1	F	72	THR
1	F	77	VAL
1	F	79	TRP
1	F	94	LEU
1	F	117	LEU
1	F	128	MET
1	F	139	LEU
1	F	141	LEU
1	F	177	THR
1	F	180	THR
1	F	183	GLU
1	F	198	LEU
1	F	199	VAL
1	F	214	LYS
1	F	257	TYR
1	F	272	SER
1	F	283	GLU
1	F	297	GLU
1	F	301	ARG
1	F	302	GLN
1	F	310	LYS
1	F	314	ASN
1	F	329	LEU

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Mol	Chain	Res	Type
1	G	65	TRP
1	G	71	VAL
1	G	72	THR
1	G	79	TRP
1	G	92	LEU
1	G	94	LEU
1	G	95	ASP
1	G	100	ARG
1	G	117	LEU
1	G	119	GLU
1	G	130	GLN
1	G	139	LEU
1	G	140	ASP
1	G	141	LEU
1	G	177	THR
1	G	180	THR
1	G	198	LEU
1	G	199	VAL
1	G	200	VAL
1	G	229	MET
1	G	241	ASN
1	G	245	ASP
1	G	271	ILE
1	G	272	SER
1	G	282	LEU
1	G	283	GLU
1	G	291	VAL
1	G	297	GLU
1	G	301	ARG
1	G	302	GLN
1	G	308	LEU
1	G	314	ASN
1	G	317	ASN
1	H	71	VAL
1	H	79	TRP
1	H	83	GLU
1	H	90	ARG
1	H	92	LEU
1	H	94	LEU
1	H	95	ASP
1	H	105	ASN
1	H	115	SER

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Mol	Chain	Res	Type
1	H	117	LEU
1	H	130	GLN
1	H	139	LEU
1	H	140	ASP
1	H	150	GLU
1	H	152	MET
1	H	177	THR
1	H	180	THR
1	H	182	GLU
1	H	196	SER
1	H	199	VAL
1	H	213	ILE
1	H	243	SER
1	H	272	SER
1	H	282	LEU
1	H	291	VAL
1	H	297	GLU
1	H	298	LEU
1	H	301	ARG
1	H	308	LEU
1	H	314	ASN
1	H	322	LYS
1	H	329	LEU
1	I	65	TRP
1	I	66	THR
1	I	71	VAL
1	I	72	THR
1	I	79	TRP
1	I	81	GLU
1	I	85	THR
1	I	92	LEU
1	I	94	LEU
1	I	95	ASP
1	I	96	ILE
1	I	100	ARG
1	I	117	LEU
1	I	128	MET
1	I	139	LEU
1	I	140	ASP
1	I	177	THR
1	I	186	THR
1	I	196	SER

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Mol	Chain	Res	Type
1	I	198	LEU
1	I	199	VAL
1	I	214	LYS
1	I	221	LYS
1	I	230	LYS
1	I	256	VAL
1	I	291	VAL
1	I	301	ARG
1	I	302	GLN
1	I	314	ASN
1	I	317	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	105	ASN
1	A	206	ASN
1	A	216	GLN
1	A	302	GLN
1	A	314	ASN
1	A	324	GLN
1	B	78	GLN
1	B	105	ASN
1	B	142	HIS
1	B	206	ASN
1	B	216	GLN
1	B	302	GLN
1	B	312	ASN
1	B	324	GLN
1	C	78	GLN
1	C	142	HIS
1	C	206	ASN
1	C	314	ASN
1	D	78	GLN
1	D	105	ASN
1	D	206	ASN
1	D	232	GLN
1	D	312	ASN
1	D	314	ASN
1	E	78	GLN
1	E	80	GLN

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Mol	Chain	Res	Type
1	E	105	ASN
1	E	142	HIS
1	E	241	ASN
1	E	314	ASN
1	E	324	GLN
1	F	78	GLN
1	F	105	ASN
1	F	206	ASN
1	F	224	GLN
1	F	232	GLN
1	F	314	ASN
1	G	78	GLN
1	G	105	ASN
1	G	142	HIS
1	G	206	ASN
1	G	314	ASN
1	H	78	GLN
1	H	105	ASN
1	H	185	GLN
1	H	206	ASN
1	H	232	GLN
1	H	302	GLN
1	H	314	ASN
1	I	78	GLN
1	I	105	ASN
1	I	130	GLN
1	I	142	HIS
1	I	206	ASN
1	I	216	GLN
1	I	307	GLN
1	I	312	ASN
1	I	314	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	241/279 (86%)	-0.42	0 100 100	53, 59, 67, 71	0
1	B	241/279 (86%)	-0.38	2 (0%) 86 72	52, 59, 67, 73	0
1	C	241/279 (86%)	-0.42	0 100 100	53, 59, 66, 72	0
1	D	241/279 (86%)	-0.46	1 (0%) 92 84	53, 60, 66, 70	0
1	E	241/279 (86%)	-0.49	1 (0%) 92 84	55, 60, 67, 72	0
1	F	241/279 (86%)	-0.38	0 100 100	53, 60, 66, 72	0
1	G	241/279 (86%)	-0.39	3 (1%) 79 61	53, 60, 66, 72	0
1	H	241/279 (86%)	-0.48	0 100 100	54, 60, 66, 72	0
1	I	241/279 (86%)	-0.45	0 100 100	54, 60, 67, 71	0
All	All	2169/2511 (86%)	-0.43	7 (0%) 94 88	52, 60, 67, 73	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	65	TRP	3.0
1	G	140	ASP	2.8
1	D	139	LEU	2.6
1	B	65	TRP	2.4
1	G	257	TYR	2.4
1	B	130	GLN	2.1
1	E	143	ARG	2.1

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.