



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:06 AM UTC

PDB ID : 6WPY / pdb_00006wp
Title : Crystal structure of Bacillus licheniformis lipase BIEst2 in mature form
Authors : Nakamura, A.M.; Godoy, A.S.; Kadowaki, M.A.S.; Polikarpov, I.
Deposited on : 2020-04-28
Resolution : 3.60 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

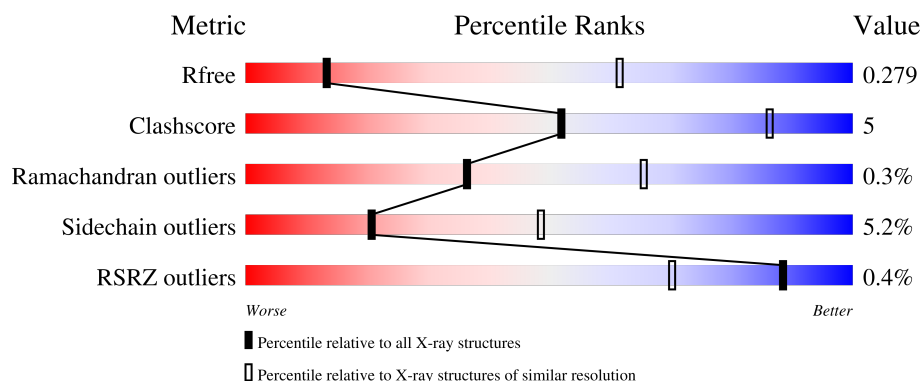
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	487	
1	B	487	
1	C	487	
1	D	487	
1	E	487	

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Mol	Chain	Length	Quality of chain
1	F	487	41%7%50%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11889 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 BIEst2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total 1935	C 1245	N 327	O 357	S 6	0	1	0
1	B	245	Total 1935	C 1245	N 327	O 357	S 6	0	1	0
1	C	245	Total 1935	C 1245	N 327	O 357	S 6	0	1	0
1	D	245	Total 1935	C 1245	N 327	O 357	S 6	0	1	0
1	E	245	Total 1935	C 1245	N 327	O 357	S 6	0	1	0
1	F	245	Total 1935	C 1245	N 327	O 357	S 6	0	1	0

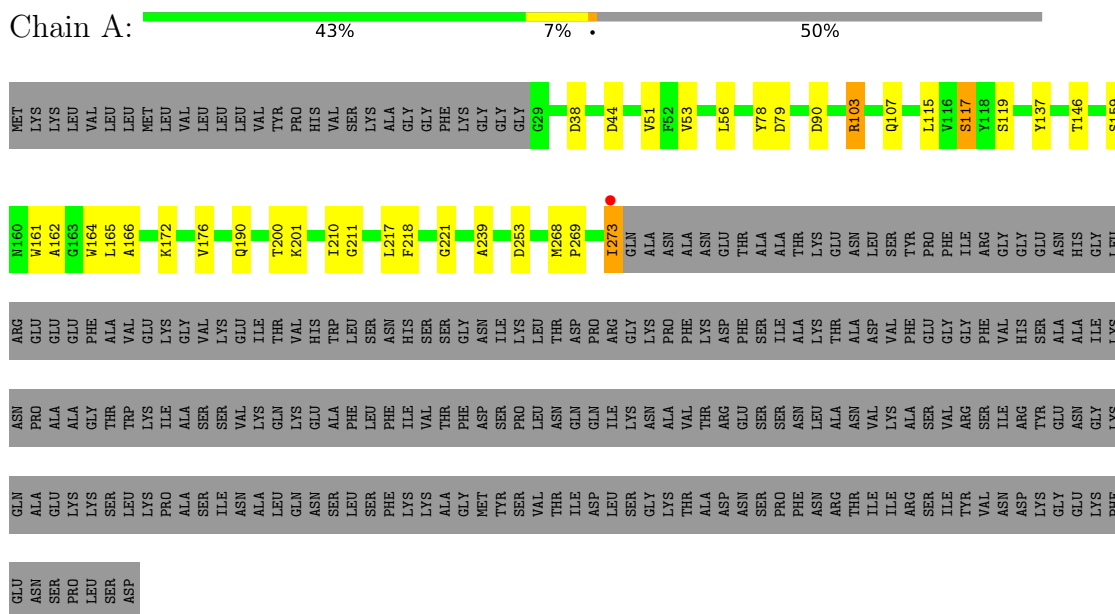
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total 59	O 59	0	0
2	B	54	Total 54	O 54	0	0
2	C	44	Total 44	O 44	0	0
2	D	45	Total 45	O 45	0	0
2	E	40	Total 40	O 40	0	0
2	F	37	Total 37	O 37	0	0

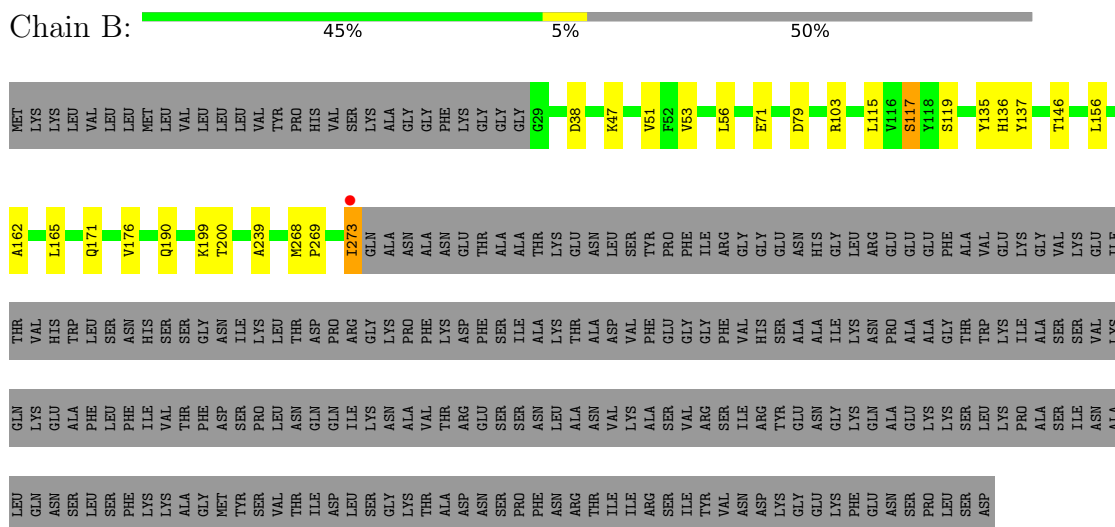
3 Residue-property plots

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: BIEst2



• Molecule 1: BIEst2



• Molecule 1: BIEst2



ALA	ILE	LYS	ASN	PRO	ALA	GLY	THR	TRP	LYS	ILE	ALA	SER	SER	LYS	GLN	LYS	GLU	ALA	ALA	PHE	PHE	PHE	THR	ASP	SER	PRO	LEU	ASN	GLN	ILE	LYS	ASN	ALA	ALA	VAL	VAL	THR	ARG	GLU	GLY	SER	SER	ASN	LEU	ALA	ASN	VAL	LYS	ALA	ALA	SER	SER	VAL	ARG	SER	ILE	ARG	TYR	THR	ILE
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ASN	GLY	LYS	GLN	ALA	GLU	LYS	LYS	LYS	LEU	SER	LYS	PRO	ALA	ALA	SER	ILE	ASN	ASN	ALA	ALA	LEU	GLN	ASN	ASN	SER	SER	SER	PHE	LYS	LYS	LYS	GLY	GLY	MET	TYR	SER	VAL	THR	THR	ILE	ILE	ASP	LEU	SER	SER	GLY	LYS	LYS	THR	ALA	ASP	ASN	ASN	SER	SER	PRO	PHE	PHE	ASN	ARG	ASN	ILE	THR	ILE	ILE	ILE	ARG	SER	SER	ILE	TYR	VAL	ASN	ASN	ASP	ASN	LYS	TYR
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GLU
LYS
PHE
GLU
ASN
SER
PRO
LEU
SER
ASP

- Molecule 1: BlEst2

Chain F: 41% 7% 50%

Label	Value	Color
MET	100	Grey
LYS	98	Grey
LYS	95	Grey
LEU	92	Grey
VAL	90	Grey
LEU	88	Grey
LEU	85	Grey
MET	82	Grey
LEU	80	Grey
VAL	78	Grey
LEU	75	Grey
LEU	72	Grey
VAL	70	Grey
TYR	68	Grey
PRO	65	Grey
HIS	62	Grey
VAL	60	Grey
SER	58	Grey
LYS	55	Grey
ALA	52	Grey
GLY	50	Grey
PHE	48	Grey
LYS	45	Grey
GLY	42	Grey
GLY	40	Grey
GLY	38	Grey
G29	35	Red
D38	32	Yellow
V51	30	Yellow
F52	28	Green
V53	25	Orange
H54	22	Green
G55	20	Yellow
W63	18	Yellow
N67	15	Yellow
D79	12	Yellow
K89	10	Yellow
R103	8	Yellow
Y106	5	Yellow
L115	3	Yellow
V116	2	Green
S117	1	White
Y118	0	Green
S119	-2	White
K120	-5	Orange
D124	-8	Yellow
L132	-10	Yellow

[illegible]

ASN	LEU	SER	TYR	PRO	PHE	ILE	GLY	GLY	GLU	ASN	HIS	GLY	LEU	ARG	GLY	GLU	GLU	GLU	PHE	VAL	ALA	ALA	GLU	THR	VAL	HIS	TRP	LYS	LEU	SER	ASN	HIS	SER	SER	GLY	ILE	LYS	LEU	THR	ASP	PRO	ARG	GLY	LYS	PRO	PHE	LYS	ASP	PHE	SER	ILE	ALA	LYS	THR
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ALA	ASP	VAL	PHE	GLU	GLY	PHE	GLY	VAL	VAL	HIS	SER	ALA	ALA	ALA	LYS	ASN	PRO	ALA	ALA	GLY	THR	TRP	LYS	ILE	ALA	ALA	SER	SER	VAL	LYS	GLN	LYS	GLU	PHE	ALA	LEU	PHE	ILE	VAL	THR	THR	ASP	SER	PRO	LEU	ASN	GLN	GLN	ILE	LYS	ALA	ALA	VAL	THR	ARG	GLU	SER	SER	ASN	LEU	ALA
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ASN	VAL	LYS	ALA	SER	VAL	ARG	SER	ILE	ARG	TYR	GLU	ASN	GLY	LYS	GLN	ALA	ALA	GLU	LYS	LYS	SER	SER	LEU	LYS	PRO	ALA	ALA	ILE	SER	ASN	ASN	LEU	GLN	LEU	GLN	ASN	ASN	LEU	LEU	SER	PER	PER	LYS	LYS	ALA	ALA	GLY	MET	TYR	SER	VAL	THR	ILE	ASP	LEU	SER	GLY	LYS	THR	ALA	ASP	ASN	SER	SER	PRO	PER	ASN	ASN	ARG
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THR ILE ILE ARG SER ILE TYR VAL ASN ASP LYS GLY GLU LYS PHE GLU ASN SER PRO LEU SER ASP

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.08Å 122.52Å 157.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.49 – 3.60 40.49 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.49-3.60) 99.8 (40.49-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.214 , 0.258 0.229 , 0.279	Depositor DCC
R_{free} test set	1203 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11889	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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	0.82	1/1998 (0.1%)	1.22	7/2714 (0.3%)
1	B	0.82	0/1998	1.22	1/2714 (0.0%)
1	C	0.83	1/1998 (0.1%)	1.27	3/2714 (0.1%)
1	D	0.80	1/1998 (0.1%)	1.26	3/2714 (0.1%)
1	E	0.80	0/1998	1.28	3/2714 (0.1%)
1	F	0.79	1/1998 (0.1%)	1.31	5/2714 (0.2%)
All	All	0.81	4/11988 (0.0%)	1.26	22/16284 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	226	MET	SD-CE	-6.99	1.62	1.79
1	A	159	SER	CA-C	5.87	1.59	1.52
1	C	47	LYS	C-N	5.52	1.38	1.33
1	D	159	SER	CA-C	5.20	1.59	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	SER	CA-C-N	7.41	133.19	122.44
1	A	159	SER	C-N-CA	7.41	133.19	122.44
1	D	231	ASP	CA-CB-CG	7.26	119.86	112.60
1	C	231	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	119	SER	CA-CB-OG	6.45	123.99	111.10
1	B	119	SER	CA-CB-OG	5.99	123.07	111.10
1	F	253	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	44	ASP	CA-CB-CG	5.72	118.32	112.60
1	E	253	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	253	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	218	PHE	N-CA-C	-5.58	105.11	111.14
1	F	167	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	253	ASP	CA-CB-CG	5.55	118.15	112.60
1	F	267	PHE	CA-CB-CG	5.48	119.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	44	ASP	CA-CB-CG	5.29	117.89	112.60
1	E	163	GLY	CA-C-N	5.28	128.09	120.38
1	E	163	GLY	C-N-CA	5.28	128.09	120.38
1	A	218	PHE	N-CA-C	-5.13	105.60	111.14
1	A	90	ASP	CA-CB-CG	5.10	117.70	112.60
1	F	158	TYR	CA-C-N	5.02	131.13	121.54
1	F	158	TYR	C-N-CA	5.02	131.13	121.54

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	1935	0	1837	23	0
1	B	1935	0	1837	14	0
1	C	1935	0	1837	22	0
1	D	1935	0	1837	23	0
1	E	1935	0	1837	20	0
1	F	1935	0	1837	20	0
2	A	59	0	0	0	0
2	B	54	0	0	2	0
2	C	44	0	0	0	0
2	D	45	0	0	0	0
2	E	40	0	0	0	0
2	F	37	0	0	2	0
All	All	11889	0	11022	116	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 5.

All (116) 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:49:PRO:HG2	1:C:113:VAL:HG12	1.53	0.91
1:E:165:LEU:H	1:E:165:LEU:HD23	1.44	0.82
1:B:71:GLU:HG3	1:E:133:ASN:CG	2.11	0.76
1:D:157:ALA:HB1	1:D:161:TRP:HE3	1.55	0.71
1:B:162:ALA:H	1:B:165:LEU:HD12	1.57	0.69
1:D:157:ALA:HB1	1:D:161:TRP:CE3	2.28	0.68
1:D:156:LEU:O	1:D:156:LEU:HG	1.92	0.68
1:C:236:GLU:HG3	1:C:249:THR:CG2	2.23	0.68
1:B:273:ILE:HG21	2:B:507:HOH:O	1.95	0.65
1:D:161:TRP:CG	1:D:162:ALA:H	2.15	0.65
1:A:103:ARG:NH1	1:A:107:GLN:HB2	2.13	0.63
1:D:106:TYR:HB2	1:D:137:TYR:HB3	1.83	0.60
1:A:103:ARG:NE	1:B:47:LYS:HZ2	1.99	0.60
1:F:63:TRP:HA	1:F:67:ASN:HD22	1.67	0.59
1:C:236:GLU:HG3	1:C:249:THR:HG23	1.85	0.58
1:A:201:LYS:HZ1	1:A:273:ILE:HG21	1.67	0.58
1:D:55:GLY:HA2	1:D:121:GLY:H	1.69	0.56
1:C:53:VAL:HB	1:C:117:SER:HB3	1.89	0.55
1:F:106:TYR:HB2	1:F:137:TYR:HB3	1.89	0.55
1:A:162:ALA:HB3	1:A:165:LEU:HB2	1.89	0.55
1:C:106:TYR:HB2	1:C:137:TYR:HB3	1.87	0.54
1:E:106:TYR:HB2	1:E:137:TYR:HB3	1.88	0.54
1:A:201:LYS:NZ	1:A:273:ILE:HG21	2.23	0.53
1:B:56:LEU:HD21	1:B:176:VAL:HG22	1.90	0.53
2:B:536:HOH:O	1:E:103:ARG:HG2	2.09	0.52
1:C:211:GLY:HA3	1:C:217:LEU:HB2	1.91	0.52
1:A:103:ARG:HD3	1:A:137:TYR:CZ	2.44	0.52
1:F:177:TYR:HE2	2:F:513:HOH:O	1.91	0.52
1:E:53:VAL:HB	1:E:117:SER:HB3	1.92	0.52
1:C:78:TYR:HE1	1:C:268:MET:HE3	1.74	0.52
1:E:165:LEU:HD23	1:E:165:LEU:N	2.20	0.52
1:A:103:ARG:HH12	1:A:107:GLN:HB2	1.75	0.52
1:A:103:ARG:HD3	1:A:137:TYR:CE1	2.46	0.51
1:D:53:VAL:HB	1:D:117:SER:HB3	1.93	0.51
1:E:78:TYR:HE2	1:E:268:MET:HE3	1.77	0.50
1:F:120:LYS:HE2	1:F:124:ASP:OD1	2.12	0.50
1:B:136:HIS:HB2	1:B:137:TYR:CE2	2.46	0.50
1:D:78:TYR:HE2	1:D:268:MET:HE3	1.77	0.50
1:A:146:THR:O	1:A:239:ALA:HA	2.12	0.50
1:C:201:LYS:HZ1	1:C:273:ILE:HG21	1.77	0.50
1:C:210:ILE:HB	1:C:221:GLY:HA3	1.94	0.49
1:C:120:LYS:HE2	1:C:124:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LYS:NZ	1:F:273:ILE:HG21	2.27	0.49
1:F:63:TRP:HA	1:F:67:ASN:ND2	2.27	0.49
1:E:120:LYS:HE2	1:E:124:ASP:OD1	2.12	0.49
1:A:161:TRP:CZ3	1:A:172:LYS:HG3	2.49	0.48
1:F:264:PHE:CD2	1:F:264:PHE:C	2.91	0.48
1:A:56:LEU:HD21	1:A:176:VAL:HG22	1.96	0.48
1:C:201:LYS:NZ	1:C:273:ILE:HG21	2.28	0.48
1:D:146:THR:O	1:D:239:ALA:HA	2.14	0.47
1:B:146:THR:O	1:B:239:ALA:HA	2.13	0.47
1:D:55:GLY:HA3	1:D:119:SER:HB3	1.97	0.47
1:E:153:LEU:HG	1:E:224:LEU:HD21	1.97	0.47
1:E:236:GLU:HG3	1:E:249:THR:CG2	2.45	0.46
1:C:146:THR:O	1:C:239:ALA:HA	2.16	0.46
1:D:56:LEU:HD21	1:D:176:VAL:HG22	1.96	0.46
1:F:53:VAL:HB	1:F:117:SER:HB3	1.97	0.46
1:B:135:TYR:CE2	1:B:199:LYS:HD3	2.51	0.46
1:E:146:THR:O	1:E:239:ALA:HA	2.15	0.46
1:F:146:THR:O	1:F:239:ALA:HA	2.16	0.46
1:E:102:LEU:HD21	1:E:115:LEU:HD21	1.99	0.45
1:C:51:VAL:HB	1:C:115:LEU:HD23	1.99	0.45
1:B:53:VAL:HB	1:B:117:SER:HB3	1.99	0.45
1:F:201:LYS:HZ1	1:F:273:ILE:HG21	1.81	0.45
1:F:248:ASP:HA	2:F:505:HOH:O	2.16	0.45
1:C:208:ASN:HD22	1:C:249:THR:HG22	1.81	0.45
1:C:236:GLU:HG3	1:C:249:THR:HG21	1.97	0.45
1:D:51:VAL:HB	1:D:115:LEU:HD23	1.99	0.45
1:C:35:PHE:CE1	1:C:82:PHE:HB2	2.52	0.45
1:A:78:TYR:HE2	1:A:268:MET:HE3	1.81	0.45
1:F:51:VAL:HB	1:F:115:LEU:HD23	1.98	0.45
1:A:162:ALA:HB1	1:A:164:TRP:NE1	2.32	0.44
1:D:54:HIS:O	1:D:121:GLY:HA3	2.17	0.44
1:D:129:LEU:HD11	1:D:138:VAL:HG21	2.00	0.44
1:A:103:ARG:CZ	1:B:47:LYS:HZ2	2.31	0.44
1:E:129:LEU:HD11	1:E:138:VAL:HG21	2.00	0.44
1:E:162:ALA:H	1:E:165:LEU:HD21	1.82	0.44
1:D:268:MET:N	1:D:269:PRO:HD2	2.33	0.43
1:A:211:GLY:HA3	1:A:217:LEU:HB2	2.00	0.43
1:B:156:LEU:HD23	1:B:165:LEU:HD21	1.99	0.43
1:D:102:LEU:HD21	1:D:115:LEU:HD21	1.98	0.43
1:A:268:MET:N	1:A:269:PRO:HD2	2.33	0.43
1:E:51:VAL:HB	1:E:115:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:MET:N	1:E:269:PRO:HD2	2.33	0.43
1:C:268:MET:N	1:C:269:PRO:HD2	2.34	0.43
1:D:135:TYR:CE2	1:D:199:LYS:HD3	2.53	0.43
1:A:103:ARG:HH21	1:B:47:LYS:HD2	1.82	0.43
1:A:210:ILE:HB	1:A:221:GLY:HA3	1.99	0.43
1:E:161:TRP:CZ2	1:E:166:ALA:HB2	2.54	0.43
1:E:231:ASP:OD1	1:E:254:HIS:HB2	2.19	0.42
1:B:51:VAL:HB	1:B:115:LEU:HD23	2.00	0.42
1:C:213:PHE:CE1	1:D:219:PHE:HD1	2.38	0.42
1:D:161:TRP:CD1	1:D:162:ALA:H	2.38	0.42
1:B:268:MET:N	1:B:269:PRO:HD2	2.33	0.42
1:F:203:PHE:CD2	1:F:245:THR:HB	2.54	0.42
1:F:223:TYR:O	1:F:226:MET:HG2	2.20	0.42
1:A:161:TRP:HZ2	1:A:166:ALA:HB2	1.85	0.42
1:E:161:TRP:HZ2	1:E:166:ALA:HB2	1.85	0.42
1:F:55:GLY:HA3	1:F:119:SER:HB3	2.02	0.42
1:F:129:LEU:HD11	1:F:138:VAL:HG21	2.02	0.42
1:A:103:ARG:HA	1:A:103:ARG:HD2	1.81	0.42
1:A:51:VAL:HB	1:A:115:LEU:HD23	2.02	0.41
1:D:56:LEU:HD12	1:D:175:ALA:HB1	2.01	0.41
1:D:203:PHE:CD2	1:D:245:THR:HB	2.55	0.41
1:A:103:ARG:HH22	1:A:107:GLN:CD	2.28	0.41
1:F:268:MET:HA	1:F:271:LEU:HD12	2.02	0.41
1:A:53:VAL:HB	1:A:117:SER:HB3	2.01	0.41
1:C:135:TYR:CE2	1:C:199:LYS:HD3	2.56	0.41
1:C:214:GLY:HA3	1:D:164:TRP:CD1	2.56	0.41
1:C:161:TRP:CZ2	1:C:166:ALA:HB2	2.56	0.41
1:C:162:ALA:H	1:C:165:LEU:HD12	1.85	0.41
1:E:135:TYR:CE2	1:E:199:LYS:HD3	2.56	0.41
1:F:264:PHE:CE2	1:F:268:MET:HB2	2.56	0.41
1:D:161:TRP:CG	1:D:162:ALA:N	2.87	0.40
1:F:161:TRP:HB2	1:F:172:LYS:HE3	2.03	0.40
1:F:268:MET:N	1:F:269:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	244/487 (50%)	240 (98%)	4 (2%)	0	100	100
1	B	244/487 (50%)	241 (99%)	3 (1%)	0	100	100
1	C	244/487 (50%)	236 (97%)	7 (3%)	1 (0%)	30	61
1	D	244/487 (50%)	232 (95%)	10 (4%)	2 (1%)	16	49
1	E	244/487 (50%)	235 (96%)	9 (4%)	0	100	100
1	F	244/487 (50%)	230 (94%)	13 (5%)	1 (0%)	30	61
All	All	1464/2922 (50%)	1414 (97%)	46 (3%)	4 (0%)	36	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	249	THR
1	D	161	TRP
1	D	162	ALA
1	F	159	SER

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	199/400 (50%)	192 (96%)	7 (4%)	32	57
1	B	199/400 (50%)	191 (96%)	8 (4%)	28	54
1	C	199/400 (50%)	191 (96%)	8 (4%)	28	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	199/400 (50%)	189 (95%)	10 (5%)	22	49
1	E	199/400 (50%)	186 (94%)	13 (6%)	15	43
1	F	199/400 (50%)	183 (92%)	16 (8%)	11	37
All	All	1194/2400 (50%)	1132 (95%)	62 (5%)	21	48

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	79	ASP
1	A	103	ARG
1	A	117	SER
1	A	190	GLN
1	A	200	THR
1	A	273	ILE
1	B	38	ASP
1	B	79	ASP
1	B	103	ARG
1	B	117	SER
1	B	171	GLN
1	B	190	GLN
1	B	200	THR
1	B	273	ILE
1	C	38	ASP
1	C	79	ASP
1	C	103	ARG
1	C	117	SER
1	C	120	LYS
1	C	137	TYR
1	C	200	THR
1	C	273	ILE
1	D	38	ASP
1	D	79	ASP
1	D	85	LEU
1	D	103	ARG
1	D	120	LYS
1	D	137	TYR
1	D	156	LEU
1	D	158	TYR
1	D	200	THR
1	D	273	ILE

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Mol	Chain	Res	Type
1	E	38	ASP
1	E	79	ASP
1	E	103	ARG
1	E	117	SER
1	E	119	SER
1	E	120	LYS
1	E	137	TYR
1	E	165	LEU
1	E	167	ASP
1	E	200	THR
1	E	249	THR
1	E	256	SER
1	E	273	ILE
1	F	38	ASP
1	F	53	VAL
1	F	79	ASP
1	F	89	LYS
1	F	103	ARG
1	F	117	SER
1	F	120	LYS
1	F	137	TYR
1	F	167	ASP
1	F	172	LYS
1	F	200	THR
1	F	259	LYS
1	F	261	ASN
1	F	262	LEU
1	F	268	MET
1	F	273	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	86	HIS
1	A	160	ASN
1	A	208	ASN
1	B	57	ASN
1	B	86	HIS
1	B	132	HIS
1	B	171	GLN
1	C	57	ASN

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Mol	Chain	Res	Type
1	C	92	GLN
1	C	208	ASN
1	D	57	ASN
1	D	86	HIS
1	D	160	ASN
1	D	171	GLN
1	D	208	ASN
1	E	57	ASN
1	E	76	ASN
1	E	86	HIS
1	F	57	ASN
1	F	86	HIS
1	F	208	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [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	245/487 (50%)	-0.31	1 (0%) 88 70	3, 28, 54, 122	1 (0%)
1	B	245/487 (50%)	-0.20	1 (0%) 88 70	3, 27, 53, 121	1 (0%)
1	C	245/487 (50%)	-0.28	0 100 100	3, 31, 58, 126	1 (0%)
1	D	245/487 (50%)	-0.13	1 (0%) 88 70	6, 38, 64, 132	1 (0%)
1	E	245/487 (50%)	-0.14	1 (0%) 88 70	8, 40, 66, 134	1 (0%)
1	F	245/487 (50%)	0.04	2 (0%) 82 58	22, 54, 80, 148	1 (0%)
All	All	1470/2922 (50%)	-0.17	6 (0%) 88 70	3, 36, 66, 148	6 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	29	GLY	2.8
1	F	273	ILE	2.8
1	D	273	ILE	2.6
1	B	273	ILE	2.3
1	E	273	ILE	2.1
1	A	273	ILE	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 oligosaccharides 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.