



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 3D2C / pdb\_00003d2c  
Title : Structure of 4D3, a thermostable mutant of Bacillus subtilis lipase obtained through directed evolution  
Authors : Sankaranarayanan, R.; Kamal, M.Z.  
Deposited on : 2008-05-08  
Resolution : 2.18 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](mailto: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>.

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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

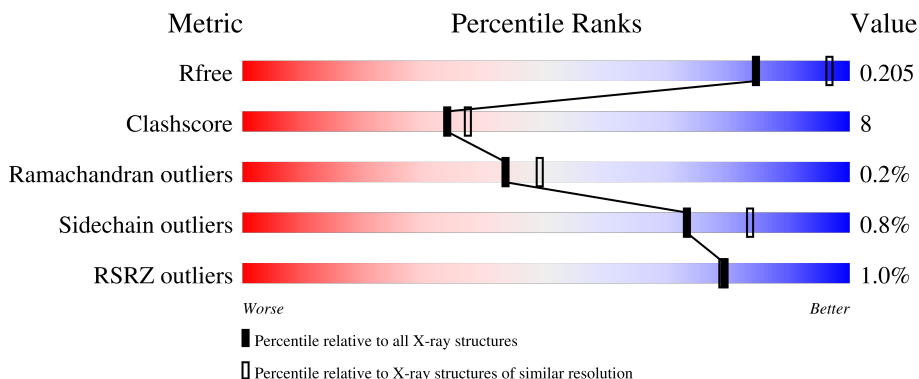
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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  $\geq 3$ , 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	181	 80% 16% ..
1	B	181	 78% 19% ..
1	C	181	 82% 17% ..
1	D	181	 78% 19% ..
1	E	181	 78% 20% ..

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Mol	Chain	Length	Quality of chain
1	F	181	 <p>86% 12% ..</p>
1	G	181	 <p>83% 15% ..</p>
1	H	181	 <p>81% 17% ..</p>
1	I	181	 <p>80% 19% ..</p>
1	J	181	 <p>77% 19% ..</p>
1	K	181	 <p>87% 11% ..</p>
1	L	181	 <p>81% 15% ..</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17510 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 Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	179	1365	857	238	265	5	0	0	0
1	B	179	1365	857	238	265	5	0	0	0
1	C	179	1365	857	238	265	5	0	0	0
1	D	179	1365	857	238	265	5	0	0	0
1	E	179	1365	857	238	265	5	0	0	0
1	F	179	1365	857	238	265	5	0	0	0
1	G	179	1365	857	238	265	5	0	0	0
1	H	179	1365	857	238	265	5	0	0	0
1	I	179	1365	857	238	265	5	0	0	0
1	J	179	1365	857	238	265	5	0	0	0
1	K	179	1365	857	238	265	5	0	0	0
1	L	179	1365	857	238	265	5	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	ALA	engineered mutation	UNP P37957
A	17	SER	PHE	engineered mutation	UNP P37957
A	20	GLU	ALA	engineered mutation	UNP P37957
A	89	TYR	ASN	engineered mutation	UNP P37957
A	111	ASP	GLY	engineered mutation	UNP P37957

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Chain	Residue	Modelled	Actual	Comment	Reference
A	114	PRO	LEU	engineered mutation	UNP P37957
A	132	ASP	ALA	engineered mutation	UNP P37957
A	157	MET	ILE	engineered mutation	UNP P37957
A	166	TYR	ASN	engineered mutation	UNP P37957
B	15	SER	ALA	engineered mutation	UNP P37957
B	17	SER	PHE	engineered mutation	UNP P37957
B	20	GLU	ALA	engineered mutation	UNP P37957
B	89	TYR	ASN	engineered mutation	UNP P37957
B	111	ASP	GLY	engineered mutation	UNP P37957
B	114	PRO	LEU	engineered mutation	UNP P37957
B	132	ASP	ALA	engineered mutation	UNP P37957
B	157	MET	ILE	engineered mutation	UNP P37957
B	166	TYR	ASN	engineered mutation	UNP P37957
C	15	SER	ALA	engineered mutation	UNP P37957
C	17	SER	PHE	engineered mutation	UNP P37957
C	20	GLU	ALA	engineered mutation	UNP P37957
C	89	TYR	ASN	engineered mutation	UNP P37957
C	111	ASP	GLY	engineered mutation	UNP P37957
C	114	PRO	LEU	engineered mutation	UNP P37957
C	132	ASP	ALA	engineered mutation	UNP P37957
C	157	MET	ILE	engineered mutation	UNP P37957
C	166	TYR	ASN	engineered mutation	UNP P37957
D	15	SER	ALA	engineered mutation	UNP P37957
D	17	SER	PHE	engineered mutation	UNP P37957
D	20	GLU	ALA	engineered mutation	UNP P37957
D	89	TYR	ASN	engineered mutation	UNP P37957
D	111	ASP	GLY	engineered mutation	UNP P37957
D	114	PRO	LEU	engineered mutation	UNP P37957
D	132	ASP	ALA	engineered mutation	UNP P37957
D	157	MET	ILE	engineered mutation	UNP P37957
D	166	TYR	ASN	engineered mutation	UNP P37957
E	15	SER	ALA	engineered mutation	UNP P37957
E	17	SER	PHE	engineered mutation	UNP P37957
E	20	GLU	ALA	engineered mutation	UNP P37957
E	89	TYR	ASN	engineered mutation	UNP P37957
E	111	ASP	GLY	engineered mutation	UNP P37957
E	114	PRO	LEU	engineered mutation	UNP P37957
E	132	ASP	ALA	engineered mutation	UNP P37957
E	157	MET	ILE	engineered mutation	UNP P37957
E	166	TYR	ASN	engineered mutation	UNP P37957
F	15	SER	ALA	engineered mutation	UNP P37957
F	17	SER	PHE	engineered mutation	UNP P37957

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Chain	Residue	Modelled	Actual	Comment	Reference
F	20	GLU	ALA	engineered mutation	UNP P37957
F	89	TYR	ASN	engineered mutation	UNP P37957
F	111	ASP	GLY	engineered mutation	UNP P37957
F	114	PRO	LEU	engineered mutation	UNP P37957
F	132	ASP	ALA	engineered mutation	UNP P37957
F	157	MET	ILE	engineered mutation	UNP P37957
F	166	TYR	ASN	engineered mutation	UNP P37957
G	15	SER	ALA	engineered mutation	UNP P37957
G	17	SER	PHE	engineered mutation	UNP P37957
G	20	GLU	ALA	engineered mutation	UNP P37957
G	89	TYR	ASN	engineered mutation	UNP P37957
G	111	ASP	GLY	engineered mutation	UNP P37957
G	114	PRO	LEU	engineered mutation	UNP P37957
G	132	ASP	ALA	engineered mutation	UNP P37957
G	157	MET	ILE	engineered mutation	UNP P37957
G	166	TYR	ASN	engineered mutation	UNP P37957
H	15	SER	ALA	engineered mutation	UNP P37957
H	17	SER	PHE	engineered mutation	UNP P37957
H	20	GLU	ALA	engineered mutation	UNP P37957
H	89	TYR	ASN	engineered mutation	UNP P37957
H	111	ASP	GLY	engineered mutation	UNP P37957
H	114	PRO	LEU	engineered mutation	UNP P37957
H	132	ASP	ALA	engineered mutation	UNP P37957
H	157	MET	ILE	engineered mutation	UNP P37957
H	166	TYR	ASN	engineered mutation	UNP P37957
I	15	SER	ALA	engineered mutation	UNP P37957
I	17	SER	PHE	engineered mutation	UNP P37957
I	20	GLU	ALA	engineered mutation	UNP P37957
I	89	TYR	ASN	engineered mutation	UNP P37957
I	111	ASP	GLY	engineered mutation	UNP P37957
I	114	PRO	LEU	engineered mutation	UNP P37957
I	132	ASP	ALA	engineered mutation	UNP P37957
I	157	MET	ILE	engineered mutation	UNP P37957
I	166	TYR	ASN	engineered mutation	UNP P37957
J	15	SER	ALA	engineered mutation	UNP P37957
J	17	SER	PHE	engineered mutation	UNP P37957
J	20	GLU	ALA	engineered mutation	UNP P37957
J	89	TYR	ASN	engineered mutation	UNP P37957
J	111	ASP	GLY	engineered mutation	UNP P37957
J	114	PRO	LEU	engineered mutation	UNP P37957
J	132	ASP	ALA	engineered mutation	UNP P37957
J	157	MET	ILE	engineered mutation	UNP P37957

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Chain	Residue	Modelled	Actual	Comment	Reference
J	166	TYR	ASN	engineered mutation	UNP P37957
K	15	SER	ALA	engineered mutation	UNP P37957
K	17	SER	PHE	engineered mutation	UNP P37957
K	20	GLU	ALA	engineered mutation	UNP P37957
K	89	TYR	ASN	engineered mutation	UNP P37957
K	111	ASP	GLY	engineered mutation	UNP P37957
K	114	PRO	LEU	engineered mutation	UNP P37957
K	132	ASP	ALA	engineered mutation	UNP P37957
K	157	MET	ILE	engineered mutation	UNP P37957
K	166	TYR	ASN	engineered mutation	UNP P37957
L	15	SER	ALA	engineered mutation	UNP P37957
L	17	SER	PHE	engineered mutation	UNP P37957
L	20	GLU	ALA	engineered mutation	UNP P37957
L	89	TYR	ASN	engineered mutation	UNP P37957
L	111	ASP	GLY	engineered mutation	UNP P37957
L	114	PRO	LEU	engineered mutation	UNP P37957
L	132	ASP	ALA	engineered mutation	UNP P37957
L	157	MET	ILE	engineered mutation	UNP P37957
L	166	TYR	ASN	engineered mutation	UNP P37957

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	97	Total O 97 97	0	0
2	B	83	Total O 83 83	0	0
2	C	107	Total O 107 107	0	0
2	D	90	Total O 90 90	0	0
2	E	97	Total O 97 97	0	0
2	F	90	Total O 90 90	0	0
2	G	94	Total O 94 94	0	0
2	H	83	Total O 83 83	0	0
2	I	99	Total O 99 99	0	0
2	J	92	Total O 92 92	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
2	K	93	Total O 93 93	0	0
2	L	105	Total O 105 105	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: Lipase

Chain A:  80% 16% ..




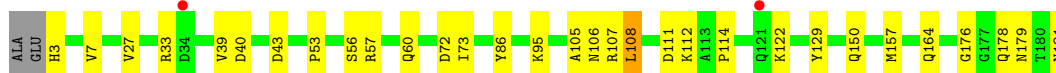
- Molecule 1: Lipase

Chain B:  78% 19% ..




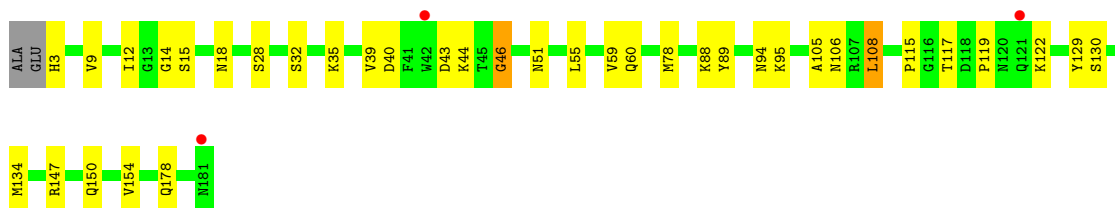
- Molecule 1: Lipase

Chain C:  82% 17% ..

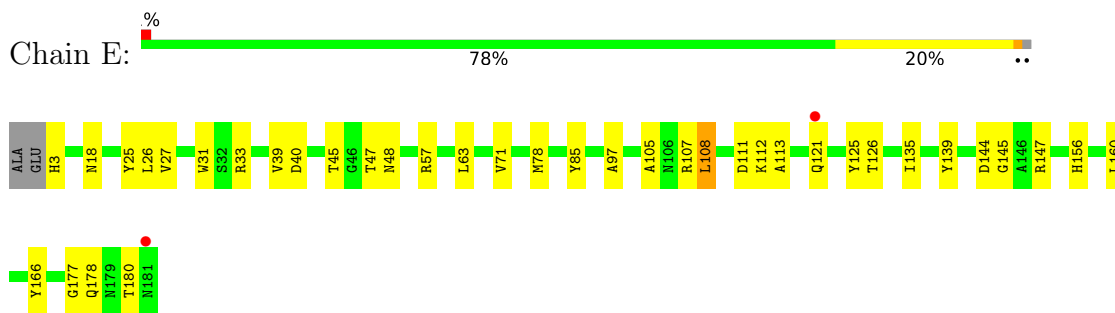


- Molecule 1: Lipase

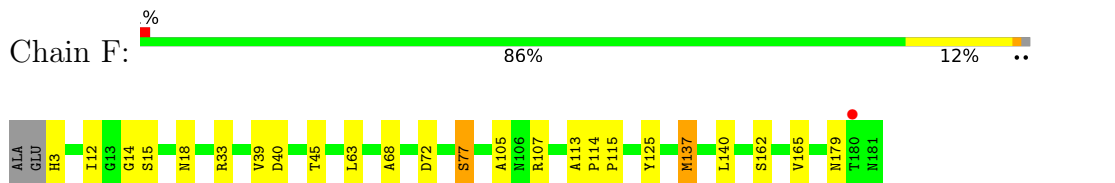
Chain D:  78% 19% ..



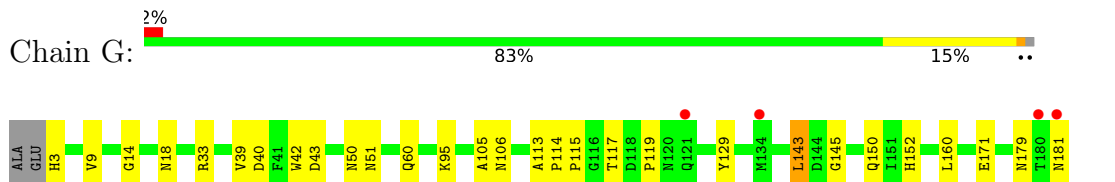
- Molecule 1: Lipase



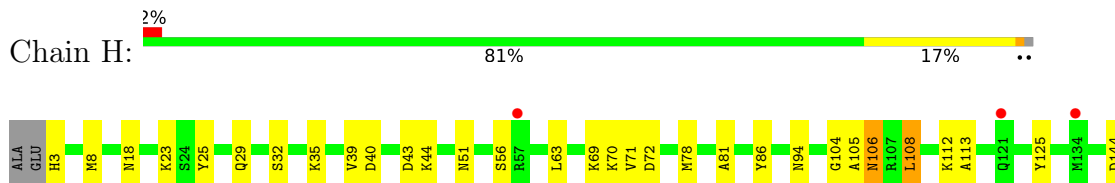
- Molecule 1: Lipase



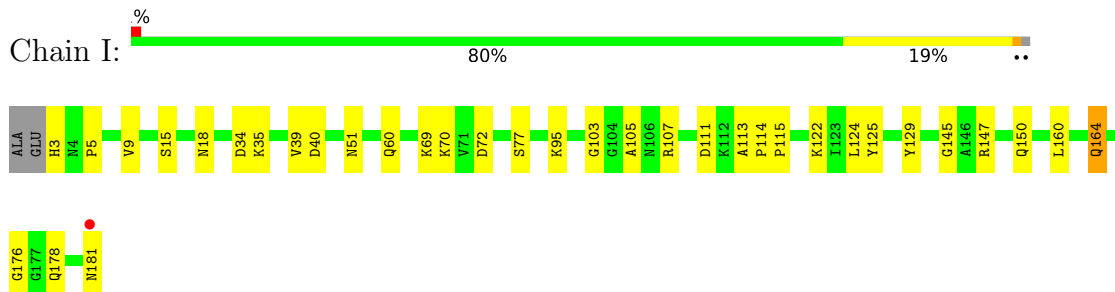
- Molecule 1: Lipase



- Molecule 1: Lipase



- Molecule 1: Lipase

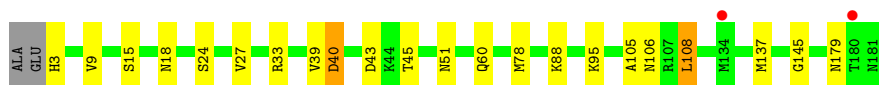
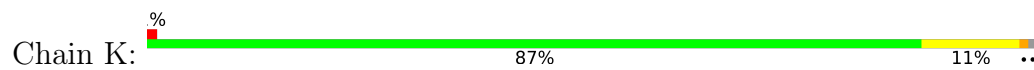


- Molecule 1: Lipase

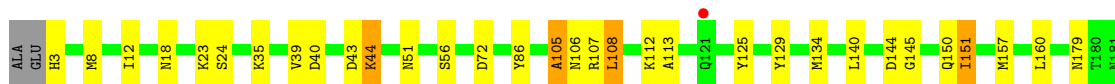
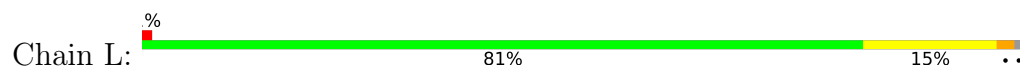




- Molecule 1: Lipase



- Molecule 1: Lipase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.28Å 198.04Å 197.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.18 25.00 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-2.18) 98.8 (25.00-2.18)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.17Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.202 , 0.245 0.204 , 0.205	Depositor DCC
$R_{free}$ test set	6671 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17510	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.38	0/1392	0.92	6/1884 (0.3%)
1	B	0.39	0/1392	0.92	6/1884 (0.3%)
1	C	0.39	0/1392	0.94	4/1884 (0.2%)
1	D	0.38	0/1392	0.93	5/1884 (0.3%)
1	E	0.38	0/1392	0.90	2/1884 (0.1%)
1	F	0.38	0/1392	0.95	2/1884 (0.1%)
1	G	0.38	0/1392	0.92	3/1884 (0.2%)
1	H	0.39	0/1392	0.93	4/1884 (0.2%)
1	I	0.38	0/1392	0.95	5/1884 (0.3%)
1	J	0.36	0/1392	0.92	6/1884 (0.3%)
1	K	0.38	0/1392	0.91	5/1884 (0.3%)
1	L	0.39	0/1392	0.92	3/1884 (0.2%)
All	All	0.38	0/16704	0.93	51/22608 (0.2%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ASN	N-CA-C	7.60	119.20	111.07
1	J	106	ASN	N-CA-C	7.33	119.27	111.28
1	L	106	ASN	N-CA-C	7.13	119.06	111.28
1	D	106	ASN	N-CA-C	7.13	119.05	111.28
1	J	121	GLN	N-CA-C	7.00	119.83	108.34
1	F	105	ALA	N-CA-C	-6.90	102.10	111.55
1	H	105	ALA	N-CA-C	-6.68	102.19	111.81
1	B	105	ALA	N-CA-C	-6.64	102.25	111.81
1	A	105	ALA	N-CA-C	-6.46	102.50	111.81
1	C	105	ALA	N-CA-C	-6.24	102.82	111.81
1	D	105	ALA	N-CA-C	-6.18	102.91	111.81
1	K	105	ALA	N-CA-C	-6.14	102.97	111.81
1	D	108	LEU	N-CA-C	-6.00	105.81	113.01
1	C	106	ASN	N-CA-C	5.99	118.58	111.33
1	K	88	LYS	N-CA-C	5.98	117.60	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	72	ASP	N-CA-C	-5.96	100.48	109.95
1	E	108	LEU	N-CA-C	-5.93	106.00	113.18
1	H	108	LEU	N-CA-C	-5.89	106.05	113.18
1	E	105	ALA	N-CA-C	-5.89	102.49	110.68
1	K	108	LEU	N-CA-C	-5.89	106.05	113.18
1	D	46	GLY	N-CA-C	5.83	121.99	113.48
1	I	72	ASP	N-CA-C	-5.72	100.56	109.72
1	B	106	ASN	N-CA-C	5.69	117.48	111.28
1	G	105	ALA	N-CA-C	-5.68	103.62	111.81
1	L	105	ALA	N-CA-C	-5.68	102.78	110.68
1	B	108	LEU	N-CA-C	-5.67	106.37	113.28
1	C	108	LEU	N-CA-C	-5.64	106.35	113.18
1	J	135	ILE	N-CA-C	5.57	116.96	111.67
1	H	106	ASN	N-CA-C	5.51	118.00	111.33
1	I	105	ALA	N-CA-C	-5.51	103.88	111.81
1	I	9	VAL	N-CA-C	5.45	115.44	107.37
1	H	72	ASP	N-CA-C	-5.45	101.29	109.95
1	J	105	ALA	N-CA-C	-5.44	103.98	111.81
1	B	72	ASP	N-CA-C	-5.38	101.11	109.72
1	A	9	VAL	N-CA-C	5.33	115.26	107.37
1	G	9	VAL	N-CA-C	5.31	115.23	107.37
1	G	106	ASN	N-CA-C	5.31	117.48	111.11
1	F	72	ASP	N-CA-C	-5.30	101.53	109.95
1	I	51	ASN	N-CA-C	5.30	117.13	111.36
1	D	9	VAL	N-CA-C	5.29	115.19	107.37
1	K	106	ASN	N-CA-C	5.27	117.71	111.33
1	A	108	LEU	N-CA-C	-5.25	106.13	112.54
1	B	114	PRO	CA-C-N	5.25	124.75	119.19
1	B	114	PRO	C-N-CA	5.25	124.75	119.19
1	A	19	PHE	N-CA-C	5.21	118.67	112.72
1	J	125	TYR	N-CA-C	5.21	117.94	109.24
1	C	72	ASP	N-CA-C	-5.13	101.79	109.95
1	J	72	ASP	N-CA-C	-5.13	102.19	110.14
1	I	5	PRO	N-CA-C	-5.10	103.10	111.21
1	K	9	VAL	N-CA-C	5.05	115.31	107.28
1	A	125	TYR	N-CA-C	5.01	117.56	109.40

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	1365	0	1339	27	0
1	B	1365	0	1339	24	0
1	C	1365	0	1339	20	0
1	D	1365	0	1339	28	0
1	E	1365	0	1339	25	0
1	F	1365	0	1339	17	0
1	G	1365	0	1339	17	0
1	H	1365	0	1339	19	0
1	I	1365	0	1339	23	0
1	J	1365	0	1339	29	0
1	K	1365	0	1339	13	0
1	L	1365	0	1339	21	0
2	A	97	0	0	3	0
2	B	83	0	0	5	0
2	C	107	0	0	3	0
2	D	90	0	0	4	0
2	E	97	0	0	4	0
2	F	90	0	0	4	0
2	G	94	0	0	2	0
2	H	83	0	0	6	0
2	I	99	0	0	3	0
2	J	92	0	0	2	0
2	K	93	0	0	3	0
2	L	105	0	0	2	0
All	All	17510	0	16068	250	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 8.

All (250) 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:I:69:LYS:HG2	1:I:70:LYS:HG3	1.48	0.92
1:I:147:ARG:HB2	1:I:178:GLN:HG2	1.60	0.84
1:E:156:HIS:HB3	1:F:137:MET:HE1	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:HB2	1:D:178:GLN:HG2	1.66	0.77
1:H:112:LYS:HG2	1:H:144:ASP:HB2	1.67	0.76
1:L:112:LYS:HG2	1:L:144:ASP:HB2	1.67	0.74
1:D:15:SER:H	1:D:18:ASN:ND2	1.84	0.74
1:A:134:MET:HE3	1:D:134:MET:SD	2.27	0.73
1:L:44:LYS:HE3	1:L:44:LYS:HA	1.72	0.71
1:L:107:ARG:HG3	1:L:140:LEU:HA	1.73	0.70
1:J:18:ASN:HB3	1:J:160:LEU:HD13	1.73	0.70
1:A:107:ARG:NH1	1:A:111:ASP:HB2	2.09	0.68
1:B:107:ARG:HG3	1:B:140:LEU:HA	1.74	0.68
1:F:33:ARG:HD2	2:F:269:HOH:O	1.93	0.67
1:L:129:TYR:O	1:L:151:ILE:HD13	1.96	0.66
1:B:18:ASN:HB3	1:B:160:LEU:HD13	1.76	0.66
1:J:145:GLY:O	1:J:179:ASN:HA	1.97	0.65
1:D:12:ILE:HD11	1:D:78:MET:HG3	1.79	0.65
1:C:107:ARG:NH1	1:C:111:ASP:HB2	2.12	0.65
1:L:18:ASN:HB3	1:L:160:LEU:HD13	1.79	0.64
1:B:3:HIS:HE1	2:B:183:HOH:O	1.80	0.64
1:A:60:GLN:NE2	1:A:95:LYS:NZ	2.47	0.63
1:F:3:HIS:HD2	2:F:188:HOH:O	1.81	0.63
1:A:88:LYS:HD3	1:A:89:TYR:CE1	2.34	0.62
1:D:78:MET:SD	1:D:108:LEU:HD12	2.40	0.62
1:E:107:ARG:HD3	1:E:111:ASP:OD1	2.00	0.61
1:K:3:HIS:HD2	2:K:249:HOH:O	1.82	0.61
1:D:115:PRO:HB3	1:D:122:LYS:HD2	1.81	0.61
1:I:3:HIS:HE1	2:I:192:HOH:O	1.83	0.61
1:I:176:GLY:O	1:K:24:SER:HB3	2.00	0.60
1:J:60:GLN:NE2	1:J:95:LYS:HZ3	1.99	0.60
1:C:164:GLN:HG2	2:C:239:HOH:O	2.02	0.59
1:D:12:ILE:HG12	2:D:271:HOH:O	2.02	0.59
1:H:78:MET:SD	1:H:108:LEU:HD12	2.42	0.59
1:K:60:GLN:NE2	1:K:95:LYS:NZ	2.51	0.59
1:J:107:ARG:NH1	1:J:111:ASP:HB2	2.17	0.59
1:H:8:MET:HE1	1:H:23:LYS:HG2	1.85	0.59
1:K:60:GLN:NE2	1:K:95:LYS:HZ3	2.01	0.59
1:J:15:SER:H	1:J:18:ASN:ND2	2.01	0.58
1:H:3:HIS:HD2	2:H:212:HOH:O	1.85	0.58
1:B:3:HIS:HD2	2:B:187:HOH:O	1.85	0.58
1:D:44:LYS:HB2	2:K:230:HOH:O	2.02	0.58
1:C:53:PRO:O	1:C:57:ARG:HD3	2.03	0.58
1:I:3:HIS:HD2	2:I:203:HOH:O	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:HIS:HD2	2:L:285:HOH:O	1.87	0.58
1:J:45:THR:OG1	1:J:47:THR:HG23	2.03	0.58
1:E:178:GLN:NE2	2:E:217:HOH:O	2.37	0.58
1:F:39:VAL:HG22	1:F:40:ASP:N	2.18	0.58
1:J:122:LYS:HD2	1:J:179:ASN:HB3	1.87	0.57
1:H:78:MET:HE3	1:H:81:ALA:HB3	1.86	0.57
1:B:12:ILE:HG23	1:B:44:LYS:O	2.03	0.57
1:I:122:LYS:NZ	1:I:181:ASN:O	2.34	0.57
1:C:60:GLN:NE2	1:C:95:LYS:NZ	2.54	0.56
1:I:15:SER:H	1:I:18:ASN:ND2	2.03	0.56
1:F:3:HIS:HE1	2:F:185:HOH:O	1.89	0.56
1:C:3:HIS:HD2	2:C:222:HOH:O	1.89	0.56
1:J:63:LEU:HD21	1:J:71:VAL:HG13	1.86	0.56
1:A:60:GLN:HE21	1:A:95:LYS:NZ	2.04	0.55
1:D:3:HIS:HE1	2:D:182:HOH:O	1.88	0.55
1:J:134:MET:HE2	1:J:134:MET:HA	1.88	0.55
1:F:107:ARG:HG3	1:F:140:LEU:HA	1.89	0.55
1:B:39:VAL:HG22	1:B:40:ASP:N	2.22	0.55
1:E:3:HIS:HE1	2:E:189:HOH:O	1.90	0.55
1:K:27:VAL:HG21	1:K:33:ARG:HD2	1.87	0.55
1:A:3:HIS:HD2	2:A:209:HOH:O	1.89	0.54
1:G:33:ARG:HD2	2:G:217:HOH:O	2.06	0.54
1:B:23:LYS:HE3	2:B:214:HOH:O	2.08	0.54
1:D:3:HIS:HD2	2:D:183:HOH:O	1.89	0.54
1:D:60:GLN:NE2	1:D:95:LYS:NZ	2.55	0.54
1:D:117:THR:O	1:D:119:PRO:HD3	2.08	0.54
1:E:45:THR:OG1	1:E:47:THR:HG23	2.08	0.53
1:A:88:LYS:HD3	1:A:89:TYR:HE1	1.74	0.53
1:K:78:MET:SD	1:K:108:LEU:HD12	2.48	0.53
1:I:60:GLN:NE2	1:I:95:LYS:NZ	2.57	0.53
1:L:3:HIS:HE1	2:L:302:HOH:O	1.91	0.53
1:A:39:VAL:HG22	1:A:40:ASP:N	2.23	0.52
1:J:60:GLN:NE2	1:J:95:LYS:NZ	2.57	0.52
1:E:3:HIS:HD2	2:E:191:HOH:O	1.91	0.52
1:I:34:ASP:OD1	1:I:35:LYS:HG2	2.10	0.52
1:I:39:VAL:HG22	1:I:40:ASP:N	2.25	0.52
1:G:3:HIS:HE1	2:G:212:HOH:O	1.92	0.52
1:A:112:LYS:HG2	1:A:144:ASP:HB2	1.91	0.52
1:A:179:ASN:C	1:A:181:ASN:H	2.18	0.52
1:L:145:GLY:O	1:L:179:ASN:HA	2.10	0.52
1:E:112:LYS:HD3	1:E:144:ASP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:ASN:HB3	1:I:160:LEU:HD13	1.92	0.52
1:E:63:LEU:HD21	1:E:71:VAL:HG13	1.90	0.52
1:B:78:MET:SD	1:B:108:LEU:HD12	2.50	0.52
1:E:39:VAL:HG22	1:E:40:ASP:N	2.25	0.51
1:F:15:SER:H	1:F:18:ASN:ND2	2.08	0.51
1:H:113:ALA:HB1	1:H:125:TYR:CD1	2.46	0.51
1:C:129:TYR:CE1	1:C:150:GLN:HB2	2.45	0.51
1:E:48:ASN:HB3	1:E:85:TYR:CG	2.47	0.50
1:E:145:GLY:HA2	1:E:180:THR:OG1	2.10	0.50
1:A:60:GLN:NE2	1:A:95:LYS:HZ1	2.09	0.50
1:D:43:ASP:HB3	1:D:51:ASN:HD21	1.75	0.50
1:J:12:ILE:HG23	1:J:44:LYS:O	2.12	0.50
1:G:179:ASN:C	1:G:181:ASN:H	2.20	0.50
1:I:145:GLY:HA3	1:I:181:ASN:ND2	2.27	0.50
1:J:108:LEU:HD21	1:L:12:ILE:CG2	2.41	0.50
1:H:44:LYS:HE2	1:H:44:LYS:HA	1.92	0.50
1:F:162:SER:HB3	1:F:165:VAL:HG23	1.94	0.49
1:J:157:MET:HE3	1:J:160:LEU:HD12	1.94	0.49
1:B:91:ASP:OD2	1:B:95:LYS:NZ	2.44	0.49
1:C:39:VAL:HG22	1:C:40:ASP:N	2.27	0.49
1:H:178:GLN:HG2	1:H:179:ASN:N	2.27	0.49
1:A:60:GLN:NE2	1:A:95:LYS:HZ3	2.09	0.49
1:A:3:HIS:HE1	2:A:185:HOH:O	1.95	0.49
1:B:50:ASN:O	1:B:54:VAL:HG23	2.12	0.49
1:L:56:SER:HA	1:L:86:TYR:CE1	2.48	0.49
1:B:86:TYR:O	1:B:90:LEU:HB2	2.12	0.49
1:G:43:ASP:HB3	1:G:51:ASN:HD21	1.77	0.49
1:K:39:VAL:HG22	1:K:40:ASP:N	2.28	0.49
1:A:162:SER:HB3	1:A:165:VAL:HG23	1.95	0.49
1:D:60:GLN:NE2	1:D:95:LYS:HZ3	2.11	0.49
1:E:27:VAL:HG21	1:E:33:ARG:NH1	2.27	0.49
1:A:18:ASN:HB3	1:A:160:LEU:HD13	1.94	0.48
1:D:35:LYS:HE3	2:D:188:HOH:O	2.13	0.48
1:E:18:ASN:HB3	1:E:160:LEU:HD13	1.93	0.48
1:E:113:ALA:HB1	1:E:125:TYR:CD1	2.48	0.48
1:B:113:ALA:HB1	1:B:125:TYR:CD1	2.48	0.48
1:G:60:GLN:NE2	1:G:95:LYS:HE2	2.28	0.48
1:J:39:VAL:HG22	1:J:40:ASP:N	2.28	0.48
1:J:3:HIS:HE1	2:J:269:HOH:O	1.96	0.48
1:C:176:GLY:O	1:L:24:SER:HB3	2.14	0.48
1:G:145:GLY:HA3	1:G:181:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:SER:HB3	2:F:199:HOH:O	2.13	0.48
1:C:60:GLN:NE2	1:C:95:LYS:HZ1	2.11	0.48
1:C:157:MET:HE2	1:E:139:TYR:CD1	2.48	0.48
1:L:105:ALA:O	1:L:108:LEU:HB2	2.13	0.48
1:B:137:MET:HE2	2:B:213:HOH:O	2.13	0.47
1:C:33:ARG:NH2	2:C:218:HOH:O	2.47	0.47
1:E:25:TYR:CD2	1:E:166:TYR:HB3	2.49	0.47
1:A:15:SER:H	1:A:18:ASN:ND2	2.11	0.47
1:J:157:MET:HE3	1:J:160:LEU:CD1	2.44	0.47
1:D:129:TYR:CE1	1:D:150:GLN:HB2	2.50	0.47
1:J:5:PRO:HG3	1:J:35:LYS:HE3	1.96	0.47
1:A:105:ALA:O	1:A:108:LEU:HB2	2.15	0.47
1:E:78:MET:SD	1:E:108:LEU:HD12	2.55	0.47
1:G:18:ASN:HB3	1:G:160:LEU:HD13	1.97	0.47
1:D:32:SER:HB3	1:D:35:LYS:HE2	1.97	0.47
1:G:114:PRO:HA	1:G:115:PRO:HD3	1.77	0.46
1:J:147:ARG:HB2	1:J:178:GLN:HB3	1.97	0.46
1:K:137:MET:HG3	2:K:306:HOH:O	2.15	0.46
1:I:77:SER:HA	1:I:103:GLY:O	2.15	0.46
1:J:113:ALA:HB1	1:J:125:TYR:CD1	2.50	0.46
1:F:113:ALA:HB1	1:F:125:TYR:CD1	2.50	0.46
1:A:61:LYS:NZ	1:A:61:LYS:HB3	2.31	0.46
1:D:55:LEU:O	1:D:59:VAL:HG23	2.16	0.46
1:K:43:ASP:HB3	1:K:51:ASN:HD21	1.80	0.46
1:B:88:LYS:HD3	1:B:89:TYR:CZ	2.50	0.46
1:B:145:GLY:O	1:B:179:ASN:HA	2.15	0.46
1:B:89:TYR:O	1:B:90:LEU:HD23	2.15	0.46
1:L:113:ALA:HB1	1:L:125:TYR:CD1	2.51	0.46
1:G:14:GLY:CA	1:G:18:ASN:HD21	2.29	0.46
1:H:39:VAL:HG22	1:H:40:ASP:N	2.31	0.46
1:E:97:ALA:CB	1:E:121:GLN:HE22	2.28	0.46
1:L:12:ILE:HG23	1:L:44:LYS:O	2.15	0.46
1:C:7:VAL:HB	1:C:73:ILE:HD13	1.98	0.45
1:G:39:VAL:HG22	1:G:40:ASP:N	2.31	0.45
1:B:88:LYS:HD3	1:B:89:TYR:CE1	2.51	0.45
1:D:130:SER:HB2	1:D:154:VAL:HG13	1.98	0.45
1:I:114:PRO:HA	1:I:115:PRO:HD3	1.86	0.45
1:L:151:ILE:HD13	1:L:151:ILE:H	1.81	0.45
1:A:108:LEU:HD12	1:K:45:THR:HG22	1.98	0.45
1:H:63:LEU:HD21	1:H:71:VAL:HG13	1.99	0.45
1:K:145:GLY:O	1:K:179:ASN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:VAL:HG22	1:L:40:ASP:N	2.32	0.45
1:J:20:GLU:HA	1:J:20:GLU:OE1	2.16	0.45
1:C:27:VAL:HG21	1:C:33:ARG:HD2	1.98	0.45
1:F:162:SER:HB3	1:F:165:VAL:CG2	2.46	0.45
1:I:60:GLN:NE2	1:I:95:LYS:HZ3	2.14	0.45
1:B:170:LYS:HE2	2:H:240:HOH:O	2.16	0.44
1:J:59:VAL:O	1:J:63:LEU:HG	2.17	0.44
1:C:56:SER:HA	1:C:86:TYR:CE1	2.52	0.44
1:C:60:GLN:HE21	1:C:95:LYS:NZ	2.14	0.44
1:D:39:VAL:HG22	1:D:40:ASP:N	2.32	0.44
1:F:14:GLY:CA	1:F:18:ASN:HD21	2.30	0.44
1:H:43:ASP:HB3	1:H:51:ASN:HD21	1.82	0.44
1:E:135:ILE:HG13	1:F:137:MET:CE	2.48	0.44
1:A:162:SER:HB3	1:A:165:VAL:CG2	2.47	0.44
1:A:115:PRO:HB3	1:A:122:LYS:HG3	2.00	0.44
1:G:150:GLN:HE21	1:G:152:HIS:CE1	2.36	0.44
1:J:134:MET:HE1	1:L:134:MET:HG3	2.00	0.44
1:G:117:THR:O	1:G:119:PRO:HD3	2.18	0.44
1:L:43:ASP:HB3	1:L:51:ASN:HD21	1.83	0.44
1:A:115:PRO:HG2	2:A:222:HOH:O	2.17	0.43
1:B:77:SER:HA	1:B:103:GLY:O	2.18	0.43
1:H:25:TYR:O	1:H:29:GLN:HG2	2.18	0.43
1:H:94:ASN:HA	2:H:189:HOH:O	2.17	0.43
1:I:124:LEU:HD22	1:I:178:GLN:HA	1.99	0.43
1:E:26:LEU:O	1:E:31:TRP:HB2	2.17	0.43
1:E:135:ILE:HG13	1:F:137:MET:HE3	2.00	0.43
1:I:34:ASP:OD1	1:I:35:LYS:HE3	2.18	0.43
1:J:44:LYS:HA	2:J:282:HOH:O	2.17	0.43
1:D:46:GLY:HA2	1:D:51:ASN:OD1	2.19	0.43
1:G:113:ALA:N	1:G:143:LEU:HD22	2.34	0.43
1:J:5:PRO:HG3	1:J:35:LYS:CE	2.48	0.43
1:L:129:TYR:CE1	1:L:150:GLN:HB2	2.54	0.43
1:G:129:TYR:CE1	1:G:150:GLN:HB2	2.54	0.43
1:B:107:ARG:NH1	1:B:111:ASP:HB3	2.33	0.43
1:D:14:GLY:O	1:D:44:LYS:HE3	2.18	0.43
1:D:43:ASP:C	1:D:43:ASP:OD1	2.61	0.43
1:A:107:ARG:HA	1:A:110:THR:O	2.19	0.43
1:H:3:HIS:HE1	2:H:213:HOH:O	2.01	0.43
1:A:43:ASP:OD1	1:A:43:ASP:C	2.61	0.42
1:I:60:GLN:HE22	1:I:95:LYS:HZ3	1.66	0.42
1:D:88:LYS:HD3	1:D:89:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:GLY:C	1:H:106:ASN:H	2.28	0.42
1:C:157:MET:HE2	1:E:139:TYR:CG	2.54	0.42
1:J:126:THR:OG1	1:J:177:GLY:HA2	2.19	0.42
1:K:15:SER:H	1:K:18:ASN:ND2	2.17	0.42
1:J:105:ALA:HB1	1:J:108:LEU:HD12	2.00	0.42
1:J:177:GLY:O	1:J:178:GLN:HB2	2.20	0.42
1:B:14:GLY:CA	1:B:18:ASN:HD21	2.33	0.42
1:D:94:ASN:HB3	1:D:117:THR:OG1	2.20	0.42
1:F:12:ILE:HG12	1:F:45:THR:O	2.19	0.42
1:F:114:PRO:HA	1:F:115:PRO:HD3	1.80	0.42
1:J:139:TYR:CD2	1:L:157:MET:HE2	2.55	0.42
1:B:137:MET:HG3	2:B:242:HOH:O	2.18	0.41
1:G:42:TRP:CH2	1:G:50:ASN:HB3	2.55	0.41
1:A:60:GLN:HE21	1:A:95:LYS:HZ3	1.67	0.41
1:H:32:SER:HB2	1:H:35:LYS:CG	2.51	0.41
1:I:113:ALA:HB1	1:I:125:TYR:CD1	2.56	0.41
1:C:112:LYS:O	1:C:114:PRO:HD3	2.20	0.41
1:H:56:SER:HA	1:H:86:TYR:CE1	2.55	0.41
1:I:164:GLN:HG2	2:I:240:HOH:O	2.19	0.41
1:A:104:GLY:C	1:A:106:ASN:H	2.29	0.41
1:B:56:SER:HA	1:B:86:TYR:CE1	2.56	0.41
1:B:118:ASP:HB3	1:B:121:GLN:O	2.21	0.41
1:D:28:SER:HB2	1:G:171:GLU:HA	2.02	0.41
1:D:60:GLN:HE21	1:D:95:LYS:NZ	2.18	0.41
1:I:107:ARG:HG2	1:I:111:ASP:OD1	2.20	0.41
1:I:60:GLN:HE22	1:I:95:LYS:NZ	2.19	0.41
1:I:129:TYR:CE1	1:I:150:GLN:HB2	2.56	0.41
1:J:122:LYS:CD	1:J:179:ASN:HB3	2.51	0.41
1:D:60:GLN:HE21	1:D:95:LYS:HZ3	1.69	0.41
1:G:150:GLN:HE21	1:G:152:HIS:HE1	1.69	0.41
1:H:18:ASN:ND2	2:H:192:HOH:O	2.54	0.41
1:E:126:THR:OG1	1:E:177:GLY:HA2	2.21	0.41
1:L:8:MET:HE1	1:L:23:LYS:HG2	2.03	0.40
1:C:122:LYS:HE2	1:C:181:ASN:O	2.22	0.40
1:F:63:LEU:HD22	1:F:68:ALA:O	2.21	0.40
1:A:12:ILE:HG23	1:A:44:LYS:O	2.22	0.40
1:H:70:LYS:HE3	2:H:189:HOH:O	2.21	0.40
1:C:43:ASP:OD1	1:C:43:ASP:C	2.65	0.40
1:C:178:GLN:HG2	1:C:179:ASN:N	2.36	0.40
1:E:57:ARG:HG3	1:E:57:ARG:HH11	1.87	0.40
1:E:147:ARG:NH2	2:E:223:HOH:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:MET:HE1	1:K:108:LEU:CD1	2.52	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	177/181 (98%)	170 (96%)	5 (3%)	2 (1%)	11	9
1	B	177/181 (98%)	171 (97%)	6 (3%)	0	100	100
1	C	177/181 (98%)	172 (97%)	5 (3%)	0	100	100
1	D	177/181 (98%)	173 (98%)	4 (2%)	0	100	100
1	E	177/181 (98%)	172 (97%)	5 (3%)	0	100	100
1	F	177/181 (98%)	171 (97%)	5 (3%)	1 (1%)	21	20
1	G	177/181 (98%)	171 (97%)	6 (3%)	0	100	100
1	H	177/181 (98%)	171 (97%)	6 (3%)	0	100	100
1	I	177/181 (98%)	170 (96%)	7 (4%)	0	100	100
1	J	177/181 (98%)	167 (94%)	8 (4%)	2 (1%)	11	9
1	K	177/181 (98%)	172 (97%)	5 (3%)	0	100	100
1	L	177/181 (98%)	173 (98%)	4 (2%)	0	100	100
All	All	2124/2172 (98%)	2053 (97%)	66 (3%)	5 (0%)	43	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	180	THR
1	J	177	GLY

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Mol	Chain	Res	Type
1	F	179	ASN
1	J	93	GLY

### 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	148/149 (99%)	147 (99%)	1 (1%)	76	86
1	B	148/149 (99%)	147 (99%)	1 (1%)	76	86
1	C	148/149 (99%)	147 (99%)	1 (1%)	76	86
1	D	148/149 (99%)	148 (100%)	0	100	100
1	E	148/149 (99%)	148 (100%)	0	100	100
1	F	148/149 (99%)	146 (99%)	2 (1%)	59	72
1	G	148/149 (99%)	147 (99%)	1 (1%)	76	86
1	H	148/149 (99%)	147 (99%)	1 (1%)	76	86
1	I	148/149 (99%)	147 (99%)	1 (1%)	76	86
1	J	148/149 (99%)	147 (99%)	1 (1%)	76	86
1	K	148/149 (99%)	147 (99%)	1 (1%)	76	86
1	L	148/149 (99%)	144 (97%)	4 (3%)	39	50
All	All	1776/1788 (99%)	1762 (99%)	14 (1%)	73	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	B	121	GLN
1	C	108	LEU
1	F	77	SER
1	F	137	MET
1	G	143	LEU
1	H	69	LYS
1	I	164	GLN

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Mol	Chain	Res	Type
1	J	157	MET
1	K	40	ASP
1	L	35	LYS
1	L	44	LYS
1	L	108	LEU
1	L	151	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	18	ASN
1	A	60	GLN
1	A	106	ASN
1	A	150	GLN
1	A	164	GLN
1	A	178	GLN
1	B	3	HIS
1	B	18	ASN
1	B	60	GLN
1	B	150	GLN
1	C	3	HIS
1	C	18	ASN
1	C	60	GLN
1	C	106	ASN
1	C	164	GLN
1	C	178	GLN
1	D	3	HIS
1	D	18	ASN
1	D	51	ASN
1	D	60	GLN
1	D	82	ASN
1	D	150	GLN
1	D	164	GLN
1	D	174	ASN
1	D	181	ASN
1	E	3	HIS
1	E	18	ASN
1	E	51	ASN
1	E	60	GLN
1	E	82	ASN
1	E	106	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	121	GLN
1	E	150	GLN
1	E	164	GLN
1	E	178	GLN
1	F	3	HIS
1	F	18	ASN
1	F	51	ASN
1	F	60	GLN
1	F	106	ASN
1	F	178	GLN
1	G	3	HIS
1	G	18	ASN
1	G	51	ASN
1	G	60	GLN
1	G	82	ASN
1	G	150	GLN
1	G	164	GLN
1	H	3	HIS
1	H	51	ASN
1	H	60	GLN
1	H	82	ASN
1	H	106	ASN
1	H	150	GLN
1	I	3	HIS
1	I	18	ASN
1	I	60	GLN
1	I	98	ASN
1	I	106	ASN
1	I	164	GLN
1	I	178	GLN
1	J	3	HIS
1	J	18	ASN
1	J	51	ASN
1	J	60	GLN
1	J	82	ASN
1	J	106	ASN
1	J	120	ASN
1	J	150	GLN
1	J	178	GLN
1	K	3	HIS
1	K	18	ASN
1	K	51	ASN

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Mol	Chain	Res	Type
1	K	60	GLN
1	K	82	ASN
1	K	106	ASN
1	K	138	ASN
1	K	150	GLN
1	L	3	HIS
1	L	18	ASN
1	L	51	ASN
1	L	60	GLN
1	L	82	ASN
1	L	106	ASN
1	L	121	GLN
1	L	150	GLN
1	L	164	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	179/181 (98%)	-0.11	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	19, 30, 46, 59	0
1	B	179/181 (98%)	0.02	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">85</span> <span style="border: 1px solid black; padding: 0 2px;">84</span>	21, 32, 49, 66	0
1	C	179/181 (98%)	-0.31	2 (1%) <span style="border: 1px solid black; padding: 0 2px;">78</span> <span style="border: 1px solid black; padding: 0 2px;">77</span>	17, 26, 39, 51	0
1	D	179/181 (98%)	-0.10	3 (1%) <span style="border: 1px solid black; padding: 0 2px;">69</span> <span style="border: 1px solid black; padding: 0 2px;">68</span>	19, 30, 43, 55	0
1	E	179/181 (98%)	-0.17	2 (1%) <span style="border: 1px solid black; padding: 0 2px;">78</span> <span style="border: 1px solid black; padding: 0 2px;">77</span>	20, 29, 42, 51	0
1	F	179/181 (98%)	-0.19	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">85</span> <span style="border: 1px solid black; padding: 0 2px;">84</span>	20, 30, 40, 57	0
1	G	179/181 (98%)	-0.14	4 (2%) <span style="border: 1px solid black; padding: 0 2px;">62</span> <span style="border: 1px solid black; padding: 0 2px;">61</span>	21, 29, 43, 61	0
1	H	179/181 (98%)	-0.13	3 (1%) <span style="border: 1px solid black; padding: 0 2px;">69</span> <span style="border: 1px solid black; padding: 0 2px;">68</span>	20, 30, 42, 53	0
1	I	179/181 (98%)	-0.20	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">85</span> <span style="border: 1px solid black; padding: 0 2px;">84</span>	21, 29, 42, 54	0
1	J	179/181 (98%)	-0.03	2 (1%) <span style="border: 1px solid black; padding: 0 2px;">78</span> <span style="border: 1px solid black; padding: 0 2px;">77</span>	21, 31, 48, 59	0
1	K	179/181 (98%)	-0.21	2 (1%) <span style="border: 1px solid black; padding: 0 2px;">78</span> <span style="border: 1px solid black; padding: 0 2px;">77</span>	19, 28, 42, 56	0
1	L	179/181 (98%)	-0.23	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">85</span> <span style="border: 1px solid black; padding: 0 2px;">84</span>	19, 27, 41, 52	0
All	All	2148/2172 (98%)	-0.15	22 (1%) <span style="border: 1px solid black; padding: 0 2px;">79</span> <span style="border: 1px solid black; padding: 0 2px;">79</span>	17, 29, 43, 66	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	121	GLN	3.4
1	G	121	GLN	3.4
1	D	42	TRP	3.4
1	H	121	GLN	2.9
1	H	57	ARG	2.7
1	J	49	TYR	2.7
1	L	121	GLN	2.6
1	H	134	MET	2.6
1	G	181	ASN	2.5
1	D	121	GLN	2.5
1	E	181	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	134	MET	2.4
1	K	180	THR	2.4
1	D	181	ASN	2.3
1	J	181	ASN	2.3
1	F	180	THR	2.3
1	I	181	ASN	2.3
1	C	34	ASP	2.1
1	G	180	THR	2.1
1	K	134	MET	2.1
1	B	134	MET	2.1
1	C	121	GLN	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.