



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2022 – 12:03 PM EST

PDB ID : 7U1I  
Title : Crystal structure of Pisum sativum vicilin  
Authors : Beavington, B.A.G.; Bakestani, I.D.; Robinson, K.A.; Loewen, M.C.  
Deposited on : 2022-02-21  
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](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.

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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	:	2.27
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)	:	2.27

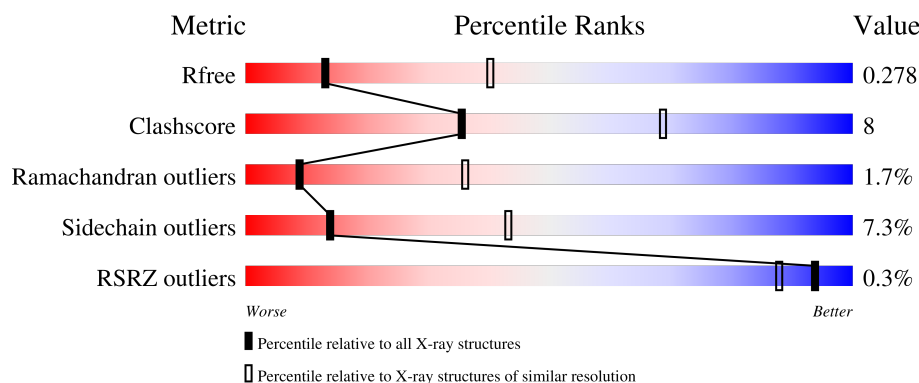
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 3.10 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 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	428	
1	B	428	
1	C	428	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16934 atoms, of which 8426 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 Vicilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	H	N	O	61	0	0
			5708	1812	2850	490	556			
1	B	360	Total	C	H	N	O	60	0	0
			5666	1801	2824	488	553			
1	C	359	Total	C	H	N	O	59	0	0
			5540	1770	2752	475	543			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q702P1
A	-16	GLY	-	expression tag	UNP Q702P1
A	-15	SER	-	expression tag	UNP Q702P1
A	-14	SER	-	expression tag	UNP Q702P1
A	-13	HIS	-	expression tag	UNP Q702P1
A	-12	HIS	-	expression tag	UNP Q702P1
A	-11	HIS	-	expression tag	UNP Q702P1
A	-10	HIS	-	expression tag	UNP Q702P1
A	-9	HIS	-	expression tag	UNP Q702P1
A	-8	HIS	-	expression tag	UNP Q702P1
A	-7	LEU	-	expression tag	UNP Q702P1
A	-6	VAL	-	expression tag	UNP Q702P1
A	-5	PRO	-	expression tag	UNP Q702P1
A	-4	ARG	-	expression tag	UNP Q702P1
A	-3	GLY	-	expression tag	UNP Q702P1
A	-2	SER	-	expression tag	UNP Q702P1
A	-1	HIS	-	expression tag	UNP Q702P1
A	0	MET	-	expression tag	UNP Q702P1
A	1	MET	-	expression tag	UNP Q702P1
B	-17	MET	-	expression tag	UNP Q702P1
B	-16	GLY	-	expression tag	UNP Q702P1
B	-15	SER	-	expression tag	UNP Q702P1
B	-14	SER	-	expression tag	UNP Q702P1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP Q702P1
B	-12	HIS	-	expression tag	UNP Q702P1
B	-11	HIS	-	expression tag	UNP Q702P1
B	-10	HIS	-	expression tag	UNP Q702P1
B	-9	HIS	-	expression tag	UNP Q702P1
B	-8	HIS	-	expression tag	UNP Q702P1
B	-7	LEU	-	expression tag	UNP Q702P1
B	-6	VAL	-	expression tag	UNP Q702P1
B	-5	PRO	-	expression tag	UNP Q702P1
B	-4	ARG	-	expression tag	UNP Q702P1
B	-3	GLY	-	expression tag	UNP Q702P1
B	-2	SER	-	expression tag	UNP Q702P1
B	-1	HIS	-	expression tag	UNP Q702P1
B	0	MET	-	expression tag	UNP Q702P1
B	1	MET	-	expression tag	UNP Q702P1
C	-17	MET	-	expression tag	UNP Q702P1
C	-16	GLY	-	expression tag	UNP Q702P1
C	-15	SER	-	expression tag	UNP Q702P1
C	-14	SER	-	expression tag	UNP Q702P1
C	-13	HIS	-	expression tag	UNP Q702P1
C	-12	HIS	-	expression tag	UNP Q702P1
C	-11	HIS	-	expression tag	UNP Q702P1
C	-10	HIS	-	expression tag	UNP Q702P1
C	-9	HIS	-	expression tag	UNP Q702P1
C	-8	HIS	-	expression tag	UNP Q702P1
C	-7	LEU	-	expression tag	UNP Q702P1
C	-6	VAL	-	expression tag	UNP Q702P1
C	-5	PRO	-	expression tag	UNP Q702P1
C	-4	ARG	-	expression tag	UNP Q702P1
C	-3	GLY	-	expression tag	UNP Q702P1
C	-2	SER	-	expression tag	UNP Q702P1
C	-1	HIS	-	expression tag	UNP Q702P1
C	0	MET	-	expression tag	UNP Q702P1
C	1	MET	-	expression tag	UNP Q702P1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	9	Total O 9 9	0	0

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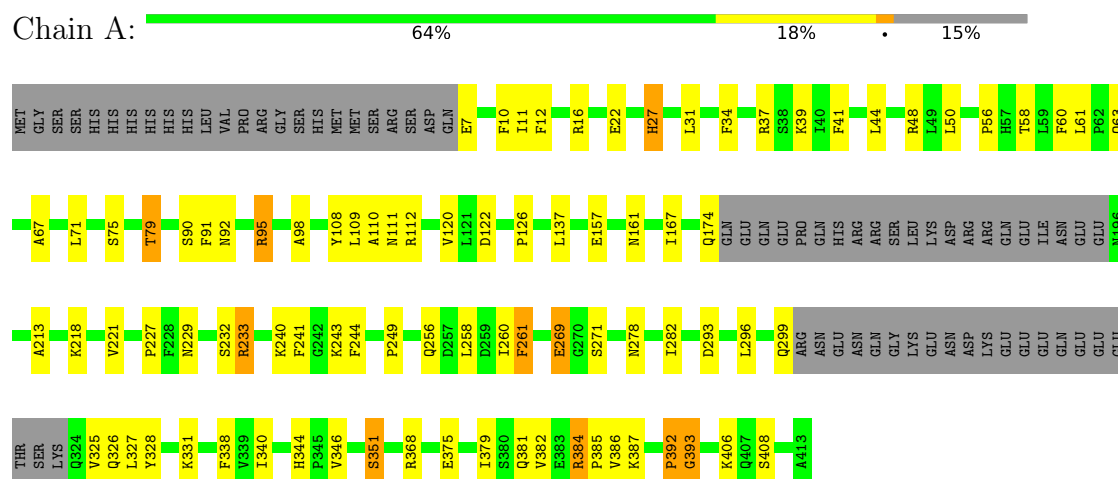
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	O	0	0
			2	2		

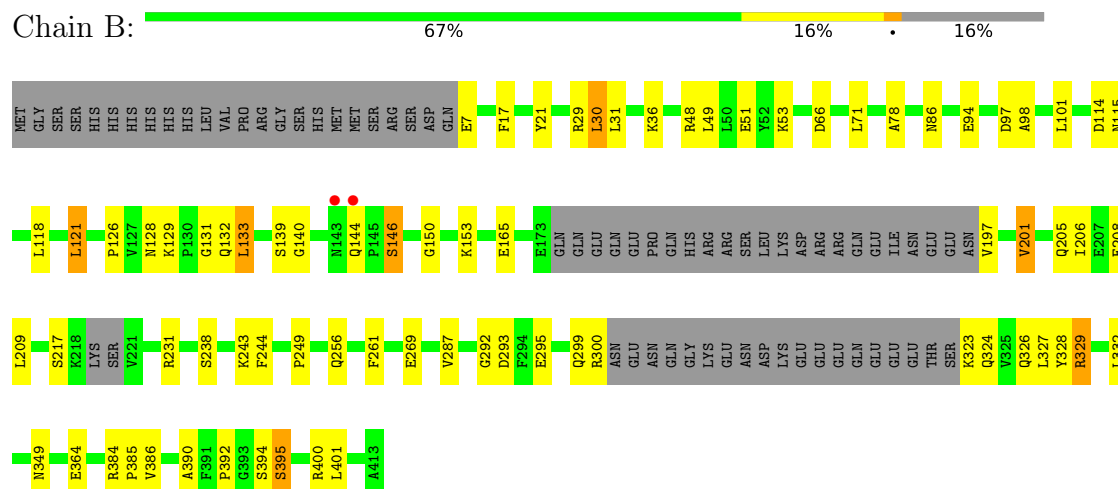
### 3 Residue-property plots

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: Vicilin

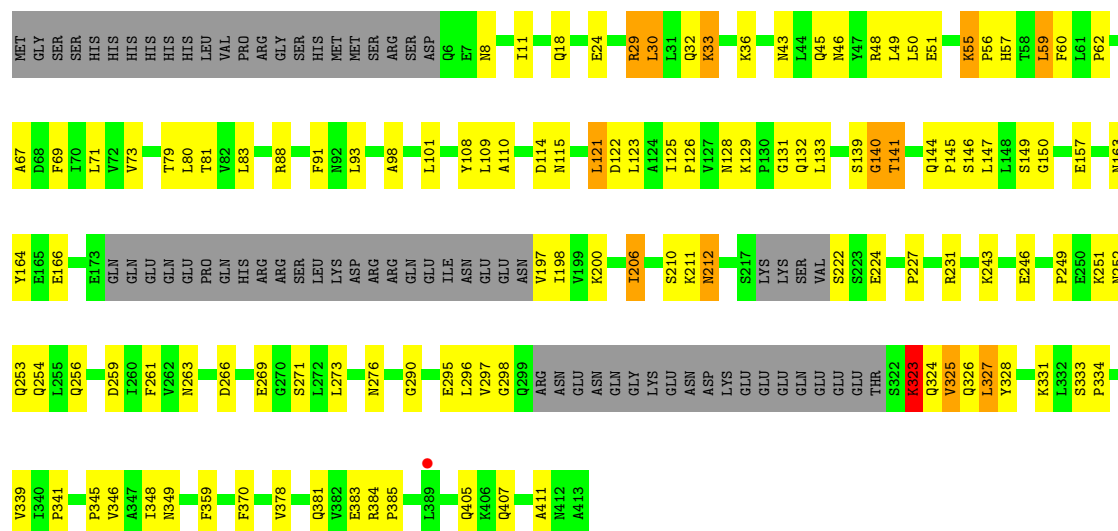


#### • Molecule 1: Vicilin



#### • Molecule 1: Vicilin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.32Å 52.69Å 127.84Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	98.10 – 3.10 97.91 – 3.10	Depositor EDS
% Data completeness (in resolution range)	84.4 (98.10-3.10) 68.3 (97.91-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.185 , 0.285 0.184 , 0.278	Depositor DCC
$R_{free}$ test set	822 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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	0.68	1/2907 (0.0%)	0.86	0/3930
1	B	0.68	0/2890	0.84	0/3908
1	C	0.69	0/2836	0.83	0/3844
All	All	0.69	1/8633 (0.0%)	0.85	0/11682

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	GLU	CD-OE2	6.53	1.32	1.25

There are no bond angle outliers.

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	2858	2850	2832	46	0
1	B	2842	2824	2804	39	0
1	C	2788	2752	2710	61	0
2	A	9	0	0	0	0
2	B	9	0	0	1	0
2	C	2	0	0	0	0
All	All	8508	8426	8346	136	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 (136) 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:24:GLU:OE1	1:C:200:LYS:NZ	2.20	0.74
1:B:71:LEU:HD13	1:B:101:LEU:HD13	1.71	0.72
1:B:29:ARG:NH1	1:B:51:GLU:OE1	2.26	0.69
1:A:392:PRO:O	1:A:393:GLY:O	2.16	0.63
1:B:150:GLY:O	1:C:327:LEU:HB2	2.00	0.61
1:B:205:GLN:O	1:B:208:GLU:HB3	2.01	0.61
1:A:327:LEU:HB2	1:C:150:GLY:O	2.01	0.60
1:A:379:ILE:O	1:A:382:VAL:HG23	2.01	0.60
1:B:7:GLU:N	2:B:503:HOH:O	2.36	0.59
1:C:8:ASN:HD21	1:C:328:TYR:HB3	1.69	0.58
1:A:10:PHE:O	1:A:338:PHE:HA	2.06	0.56
1:B:323:LYS:O	1:B:324:GLN:HG2	2.05	0.56
1:C:83:LEU:HD23	1:C:88:ARG:HG3	1.88	0.56
1:B:327:LEU:CD1	1:B:329:ARG:HG3	2.36	0.55
1:C:141:THR:HG21	1:C:197:VAL:HG21	1.87	0.55
1:C:253:GLN:HA	1:C:256:GLN:HG3	1.88	0.55
1:C:405:GLN:OE1	1:C:407:GLN:HB2	2.06	0.55
1:C:59:LEU:CD2	1:C:110:ALA:HB2	2.37	0.54
1:A:44:LEU:HD21	1:A:282:ILE:HG21	1.90	0.54
1:C:81:THR:HB	1:C:108:TYR:CE2	2.42	0.54
1:C:276:ASN:HB3	1:C:370:PHE:CD1	2.43	0.53
1:A:120:VAL:HG12	1:A:122:ASP:OD1	2.08	0.53
1:C:73:VAL:HG21	1:C:93:LEU:HB3	1.89	0.53
1:B:384:ARG:HG3	1:B:395:SER:HB2	1.91	0.53
1:A:11:ILE:O	1:A:37:ARG:NH2	2.42	0.53
1:C:249:PRO:HB3	1:C:256:GLN:HA	1.90	0.53
1:C:157:GLU:OE1	1:C:163:ASN:HA	2.09	0.52
1:C:91:PHE:CD2	1:C:227:PRO:HD3	2.44	0.52
1:C:8:ASN:ND2	1:C:328:TYR:HB3	2.24	0.52
1:C:384:ARG:N	1:C:385:PRO:HD2	2.26	0.51
1:B:71:LEU:O	1:B:98:ALA:HA	2.10	0.51
1:C:246:GLU:HG3	1:C:263:ASN:HB3	1.92	0.51
1:C:57:HIS:HA	1:C:206:ILE:CD1	2.41	0.51
1:B:53:LYS:HA	1:B:118:LEU:O	2.10	0.51
1:A:56:PRO:HA	1:A:111:ASN:OD1	2.10	0.51
1:B:209:LEU:N	1:B:209:LEU:HD23	2.25	0.51
1:A:71:LEU:O	1:A:98:ALA:HA	2.11	0.50
1:A:229:ASN:HB3	1:A:232:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:C	1:B:392:PRO:HB2	2.32	0.50
1:B:209:LEU:HD22	1:C:383:GLU:OE1	2.11	0.50
1:B:249:PRO:HB3	1:B:256:GLN:HA	1.94	0.50
1:A:61:LEU:HD22	1:B:390:ALA:HA	1.94	0.50
1:B:48:ARG:NH1	1:B:131:GLY:O	2.37	0.50
1:C:71:LEU:O	1:C:98:ALA:HA	2.13	0.49
1:A:167:ILE:HA	1:B:401:LEU:HD11	1.95	0.49
1:B:126:PRO:HG3	1:B:133:LEU:HD13	1.95	0.49
1:C:290:GLY:O	1:C:334:PRO:HD3	2.13	0.49
1:A:91:PHE:CD1	1:A:227:PRO:HD3	2.48	0.49
1:B:49:LEU:HD22	1:B:121:LEU:CD2	2.43	0.48
1:C:140:GLY:HA3	1:C:146:SER:HB2	1.96	0.48
1:A:31:LEU:O	1:A:48:ARG:NH2	2.36	0.47
1:A:58:THR:O	1:A:110:ALA:HA	2.14	0.47
1:B:384:ARG:N	1:B:385:PRO:HD2	2.29	0.47
1:A:34:PHE:HB3	1:A:41:PHE:HB3	1.97	0.47
1:A:90:SER:HB3	1:A:213:ALA:HB2	1.97	0.47
1:A:293:ASP:HB3	1:A:331:LYS:HA	1.96	0.47
1:C:67:ALA:HA	1:C:125:ILE:O	2.15	0.47
1:C:126:PRO:HB3	1:C:132:GLN:O	2.15	0.47
1:B:201:VAL:CG1	1:B:206:ILE:HG12	2.45	0.47
1:C:222:SER:HA	1:C:252:ASN:HD22	1.79	0.47
1:C:49:LEU:HD22	1:C:121:LEU:CD2	2.45	0.46
1:C:249:PRO:C	1:C:251:LYS:H	2.18	0.46
1:C:297:VAL:HB	1:C:345:PRO:HD2	1.97	0.46
1:A:326:GLN:HB3	1:A:328:TYR:CE1	2.50	0.46
1:B:384:ARG:HG3	1:B:395:SER:CB	2.46	0.46
1:C:60:PHE:CD1	1:C:198:ILE:HG12	2.51	0.45
1:C:30:LEU:HD22	1:C:48:ARG:NH2	2.31	0.45
1:C:327:LEU:HD12	1:C:328:TYR:N	2.31	0.45
1:B:150:GLY:O	1:C:327:LEU:CB	2.65	0.45
1:A:241:PHE:HB3	1:A:271:SER:HB3	1.98	0.45
1:A:249:PRO:HB3	1:A:256:GLN:HA	1.99	0.45
1:B:30:LEU:O	1:B:31:LEU:C	2.53	0.45
1:C:33:LYS:HB3	1:C:36:LYS:HG2	1.98	0.45
1:C:147:LEU:HD12	1:C:147:LEU:C	2.38	0.45
1:C:296:LEU:HB3	1:C:328:TYR:HB2	1.98	0.45
1:A:381:GLN:O	1:C:83:LEU:HD21	2.17	0.45
1:B:17:PHE:HA	1:B:31:LEU:HA	1.99	0.45
1:C:378:VAL:O	1:C:381:GLN:HB2	2.17	0.45
1:B:287:VAL:HG21	1:B:332:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:PHE:HB2	1:C:101:LEU:HB2	2.00	0.44
1:A:12:PHE:HA	1:A:16:ARG:HD2	2.00	0.44
1:A:67:ALA:HB2	1:A:126:PRO:HA	2.00	0.44
1:C:144:GLN:HG2	1:C:144:GLN:O	2.18	0.44
1:B:326:GLN:HB3	1:B:328:TYR:CE1	2.53	0.43
1:C:49:LEU:HD22	1:C:121:LEU:HD22	1.99	0.43
1:C:55:LYS:HB3	1:C:56:PRO:CD	2.49	0.43
1:C:29:ARG:NH1	1:C:51:GLU:OE1	2.51	0.43
1:B:128:ASN:O	1:C:43:ASN:ND2	2.52	0.43
1:A:375:GLU:HB2	1:A:408:SER:HB3	2.01	0.43
1:A:261:PHE:C	1:A:261:PHE:CD2	2.92	0.43
1:A:108:TYR:CE1	1:B:386:VAL:HG21	2.54	0.42
1:A:384:ARG:HB3	1:A:385:PRO:HD3	2.01	0.42
1:C:157:GLU:OE1	1:C:164:TYR:N	2.51	0.42
1:A:157:GLU:O	1:A:161:ASN:N	2.51	0.42
1:A:382:VAL:O	1:A:387:LYS:HE3	2.18	0.42
1:C:339:VAL:O	1:C:341:PRO:HD3	2.19	0.42
1:A:218:LYS:O	1:A:221:VAL:HG12	2.19	0.42
1:B:78:ALA:HB2	1:B:118:LEU:HD22	2.00	0.42
1:C:50:LEU:HB2	1:C:122:ASP:HB2	2.00	0.42
1:B:129:LYS:HD3	1:B:132:GLN:HG3	2.01	0.42
1:C:295:GLU:O	1:C:346:VAL:HA	2.20	0.42
1:A:269:GLU:HG3	1:A:351:SER:O	2.20	0.42
1:A:50:LEU:N	1:A:50:LEU:HD12	2.35	0.42
1:B:94:GLU:O	1:B:97:ASP:HB2	2.20	0.42
1:B:292:GLY:O	1:B:332:LEU:N	2.46	0.42
1:C:259:ASP:O	1:C:259:ASP:CG	2.57	0.42
1:A:221:VAL:HG21	1:A:233:ARG:HB2	2.00	0.42
1:A:278:ASN:OD1	1:A:368:ARG:NH1	2.52	0.42
1:A:382:VAL:HG12	1:A:386:VAL:HB	2.02	0.42
1:B:66:ASP:OD1	1:B:128:ASN:HB2	2.20	0.42
1:A:137:LEU:HD22	1:A:137:LEU:N	2.34	0.42
1:C:123:LEU:HD22	1:C:359:PHE:CG	2.55	0.42
1:A:92:ASN:HD22	1:A:112:ARG:CZ	2.32	0.41
1:C:273:LEU:HB3	1:C:348:ILE:HB	2.01	0.41
1:A:22:GLU:OE2	1:A:27:HIS:CD2	2.73	0.41
1:A:296:LEU:HD11	1:A:344:HIS:HB3	2.03	0.41
1:C:224:GLU:N	1:C:224:GLU:OE2	2.54	0.41
1:C:271:SER:HB3	1:C:411:ALA:O	2.20	0.41
1:A:340:ILE:HD13	1:A:346:VAL:HG11	2.03	0.41
1:B:140:GLY:HA2	1:B:146:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ARG:HH22	1:C:266:ASP:CG	2.23	0.41
1:C:126:PRO:HG2	1:C:131:GLY:CA	2.51	0.41
1:A:79:THR:HG23	1:A:92:ASN:OD1	2.21	0.41
1:C:83:LEU:CD2	1:C:88:ARG:HG3	2.51	0.41
1:C:139:SER:O	1:C:139:SER:OG	2.29	0.41
1:A:75:SER:HA	1:A:95:ARG:HG3	2.02	0.41
1:B:49:LEU:HD23	1:B:49:LEU:HA	1.83	0.41
1:C:252:ASN:OD1	1:C:254:GLN:HB2	2.20	0.41
1:C:145:PRO:HB2	1:C:149:SER:CB	2.50	0.40
1:B:295:GLU:HB3	1:B:327:LEU:HD21	2.01	0.40
1:A:60:PHE:HD2	1:A:109:LEU:O	2.04	0.40
1:A:258:LEU:HB2	1:A:260:ILE:HD12	2.04	0.40
1:B:21:TYR:HH	1:B:197:VAL:N	2.19	0.40
1:B:86:ASN:CG	1:B:86:ASN:O	2.60	0.40
1:C:323:LYS:HD3	1:C:323:LYS:O	2.22	0.40
1:C:298:GLY:O	1:C:325:VAL:HA	2.21	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	356/428 (83%)	310 (87%)	42 (12%)	4 (1%)	14	46
1	B	352/428 (82%)	303 (86%)	45 (13%)	4 (1%)	14	46
1	C	351/428 (82%)	301 (86%)	40 (11%)	10 (3%)	5	25
All	All	1059/1284 (82%)	914 (86%)	127 (12%)	18 (2%)	9	36

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	GLY

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Mol	Chain	Res	Type
1	C	212	ASN
1	C	323	LYS
1	C	140	GLY
1	C	210	SER
1	C	211	LYS
1	B	269	GLU
1	B	146	SER
1	B	217	SER
1	C	141	THR
1	C	324	GLN
1	A	269	GLU
1	B	153	LYS
1	C	269	GLU
1	C	325	VAL
1	A	384	ARG
1	A	392	PRO
1	C	62	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	318/386 (82%)	304 (96%)	14 (4%)	28	61
1	B	315/386 (82%)	291 (92%)	24 (8%)	13	41
1	C	303/386 (78%)	273 (90%)	30 (10%)	8	29
All	All	936/1158 (81%)	868 (93%)	68 (7%)	14	43

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	39	LYS
1	A	63	GLN
1	A	79	THR
1	A	95	ARG

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Mol	Chain	Res	Type
1	A	233	ARG
1	A	240	LYS
1	A	243	LYS
1	A	244	PHE
1	A	261	PHE
1	A	299	GLN
1	A	325	VAL
1	A	351	SER
1	A	406	LYS
1	B	30	LEU
1	B	36	LYS
1	B	114	ASP
1	B	115	ASN
1	B	121	LEU
1	B	133	LEU
1	B	139	SER
1	B	144	GLN
1	B	165	GLU
1	B	201	VAL
1	B	231	ARG
1	B	238	SER
1	B	243	LYS
1	B	244	PHE
1	B	261	PHE
1	B	293	ASP
1	B	299	GLN
1	B	300	ARG
1	B	329	ARG
1	B	349	ASN
1	B	364	GLU
1	B	394	SER
1	B	395	SER
1	B	400	ARG
1	C	11	ILE
1	C	18	GLN
1	C	29	ARG
1	C	30	LEU
1	C	32	GLN
1	C	33	LYS
1	C	45	GLN
1	C	46	ASN
1	C	55	LYS

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Mol	Chain	Res	Type
1	C	59	LEU
1	C	79	THR
1	C	80	LEU
1	C	109	LEU
1	C	114	ASP
1	C	115	ASN
1	C	121	LEU
1	C	128	ASN
1	C	129	LYS
1	C	133	LEU
1	C	166	GLU
1	C	206	ILE
1	C	212	ASN
1	C	243	LYS
1	C	261	PHE
1	C	323	LYS
1	C	326	GLN
1	C	327	LEU
1	C	331	LYS
1	C	333	SER
1	C	349	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	GLN
1	C	45	GLN

### 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 ⓘ

There are no monosaccharides 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	362/428 (84%)	-0.13	0 100 100	20, 40, 63, 101	0
1	B	360/428 (84%)	-0.06	2 (0%) 89 78	20, 42, 86, 141	0
1	C	359/428 (83%)	0.10	1 (0%) 94 88	34, 58, 80, 101	0
All	All	1081/1284 (84%)	-0.03	3 (0%) 94 88	20, 47, 79, 141	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	389	LEU	2.9
1	B	143	ASN	2.3
1	B	144	GLN	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.