



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 03:17 AM UTC

PDB ID : 7U1J / pdb_00007u1j
Title : Crystal structure of Pisum sativum convicilin
Authors : Bakestani, I.D.; Robinson, K.A.; Loewen, M.C.
Deposited on : 2022-02-21
Resolution : 2.70 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

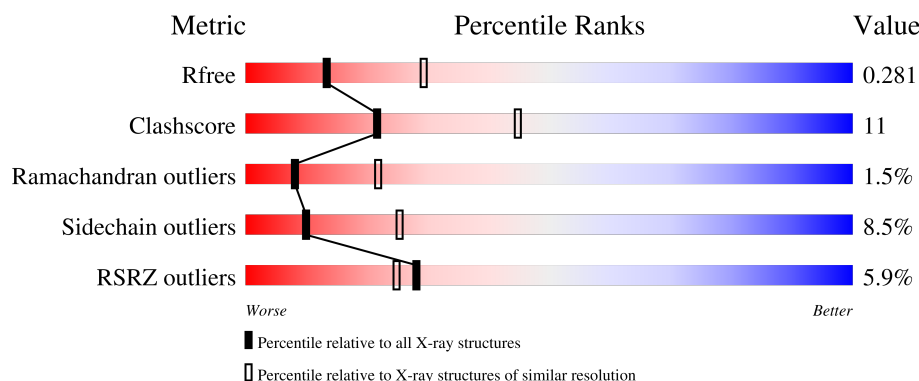
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	413	 2% 62% 20% 15%
1	B	413	 5% 55% 25% 17%
1	C	413	 8% 54% 27% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16811 atoms, of which 8362 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 Convicilin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	349	Total	C	H	N	O	S	59	0	0
			5622	1782	2820	484	534	2			
1	B	344	Total	C	H	N	O	S	59	0	0
			5521	1754	2763	476	526	2			
1	C	346	Total	C	H	N	O	S	59	0	0
			5548	1762	2779	478	527	2			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	MET	-	expression tag	UNP Q9M3X6
A	178	GLY	-	expression tag	UNP Q9M3X6
A	179	SER	-	expression tag	UNP Q9M3X6
A	180	SER	-	expression tag	UNP Q9M3X6
A	181	HIS	-	expression tag	UNP Q9M3X6
A	182	HIS	-	expression tag	UNP Q9M3X6
A	183	HIS	-	expression tag	UNP Q9M3X6
A	184	HIS	-	expression tag	UNP Q9M3X6
A	185	HIS	-	expression tag	UNP Q9M3X6
A	186	HIS	-	expression tag	UNP Q9M3X6
A	187	LEU	-	expression tag	UNP Q9M3X6
A	188	VAL	-	expression tag	UNP Q9M3X6
A	189	PRO	-	expression tag	UNP Q9M3X6
A	190	ARG	-	expression tag	UNP Q9M3X6
A	191	GLY	-	expression tag	UNP Q9M3X6
A	192	SER	-	expression tag	UNP Q9M3X6
A	193	HIS	-	expression tag	UNP Q9M3X6
A	194	MET	-	expression tag	UNP Q9M3X6
A	195	MET	-	expression tag	UNP Q9M3X6
B	177	MET	-	expression tag	UNP Q9M3X6
B	178	GLY	-	expression tag	UNP Q9M3X6
B	179	SER	-	expression tag	UNP Q9M3X6
B	180	SER	-	expression tag	UNP Q9M3X6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	181	HIS	-	expression tag	UNP Q9M3X6
B	182	HIS	-	expression tag	UNP Q9M3X6
B	183	HIS	-	expression tag	UNP Q9M3X6
B	184	HIS	-	expression tag	UNP Q9M3X6
B	185	HIS	-	expression tag	UNP Q9M3X6
B	186	HIS	-	expression tag	UNP Q9M3X6
B	187	LEU	-	expression tag	UNP Q9M3X6
B	188	VAL	-	expression tag	UNP Q9M3X6
B	189	PRO	-	expression tag	UNP Q9M3X6
B	190	ARG	-	expression tag	UNP Q9M3X6
B	191	GLY	-	expression tag	UNP Q9M3X6
B	192	SER	-	expression tag	UNP Q9M3X6
B	193	HIS	-	expression tag	UNP Q9M3X6
B	194	MET	-	expression tag	UNP Q9M3X6
B	195	MET	-	expression tag	UNP Q9M3X6
C	177	MET	-	expression tag	UNP Q9M3X6
C	178	GLY	-	expression tag	UNP Q9M3X6
C	179	SER	-	expression tag	UNP Q9M3X6
C	180	SER	-	expression tag	UNP Q9M3X6
C	181	HIS	-	expression tag	UNP Q9M3X6
C	182	HIS	-	expression tag	UNP Q9M3X6
C	183	HIS	-	expression tag	UNP Q9M3X6
C	184	HIS	-	expression tag	UNP Q9M3X6
C	185	HIS	-	expression tag	UNP Q9M3X6
C	186	HIS	-	expression tag	UNP Q9M3X6
C	187	LEU	-	expression tag	UNP Q9M3X6
C	188	VAL	-	expression tag	UNP Q9M3X6
C	189	PRO	-	expression tag	UNP Q9M3X6
C	190	ARG	-	expression tag	UNP Q9M3X6
C	191	GLY	-	expression tag	UNP Q9M3X6
C	192	SER	-	expression tag	UNP Q9M3X6
C	193	HIS	-	expression tag	UNP Q9M3X6
C	194	MET	-	expression tag	UNP Q9M3X6
C	195	MET	-	expression tag	UNP Q9M3X6

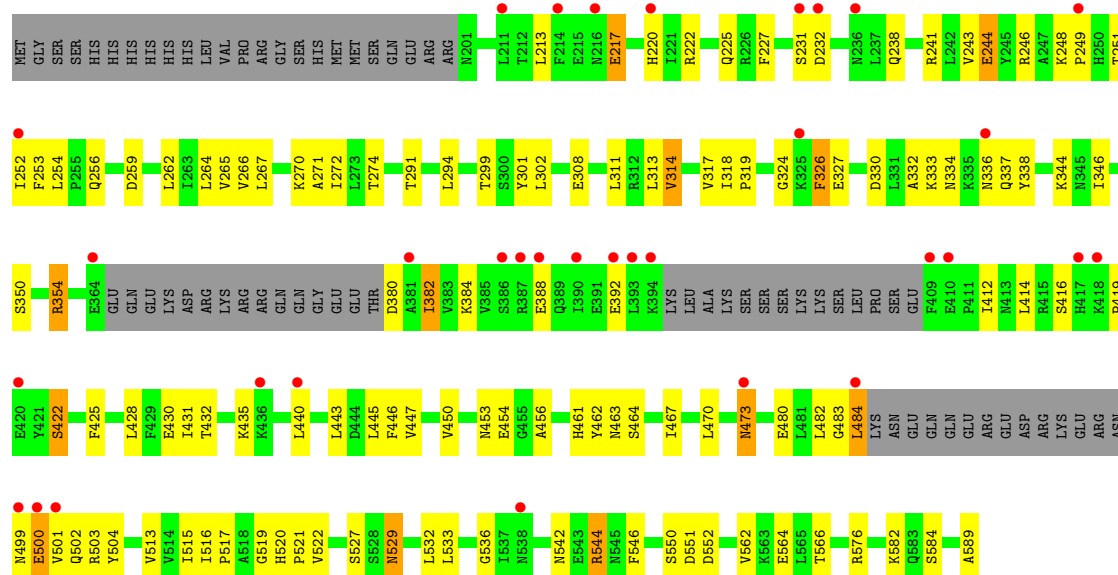
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	72	Total O 72 72	0	0
2	B	34	Total O 34 34	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	14	Total	O	0	0
			14	14		



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	269.15Å 269.15Å 269.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.94 – 2.70 134.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (134.94-2.70) 91.5 (134.94-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.215 , 0.281 0.213 , 0.281	Depositor DCC
R_{free} test set	2246 reflections (0.56%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16811	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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	1.06	0/2851	1.43	9/3855 (0.2%)
1	B	1.15	2/2807 (0.1%)	1.46	6/3797 (0.2%)
1	C	1.19	1/2817 (0.0%)	1.49	6/3811 (0.2%)
All	All	1.13	3/8475 (0.0%)	1.46	21/11463 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	432	THR	N-CA	5.83	1.50	1.46
1	B	224	LEU	C-O	5.04	1.29	1.23
1	B	216	ASN	N-CA	5.02	1.49	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	ASN	CA-CB-CG	-7.31	105.29	112.60
1	A	549	GLY	CA-C-O	-7.17	115.17	122.56
1	A	432	THR	CA-CB-OG1	-6.83	99.35	109.60
1	B	551	ASP	CB-CA-C	6.46	120.45	109.53
1	A	475	GLY	CA-C-O	-6.46	117.42	122.52
1	A	507	ARG	N-CA-C	-6.23	101.88	110.35
1	C	326	PHE	CB-CA-C	-6.15	102.23	109.80
1	C	551	ASP	CB-CA-C	5.58	119.20	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	446	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	552	ASP	N-CA-C	-5.43	105.95	112.58
1	C	589	ALA	CA-C-O	-5.43	111.57	120.80
1	C	576	ARG	CA-C-N	5.38	127.93	120.29
1	C	576	ARG	C-N-CA	5.38	127.93	120.29
1	A	353	THR	CA-CB-OG1	-5.37	101.55	109.60
1	A	486	ASN	CA-CB-CG	-5.37	107.23	112.60
1	B	291	THR	CA-CB-OG1	-5.16	101.85	109.60
1	A	244	GLU	CB-CG-CD	5.13	121.33	112.60
1	B	357	THR	CA-CB-OG1	-5.11	101.93	109.60
1	B	510	PRO	N-CA-C	5.11	119.22	111.15
1	C	354	ARG	CB-CA-C	5.02	118.24	109.65

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	ASP	Peptide
1	C	464	SER	Peptide

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	2802	2820	2809	45	1
1	B	2758	2763	2747	63	1
1	C	2769	2779	2760	71	0
2	A	72	0	0	1	0
2	B	34	0	0	1	0
2	C	14	0	0	1	0
All	All	8449	8362	8316	179	1

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 11.

All (179) 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:562:VAL:O	1:C:566:THR:HG22	1.69	0.92
1:B:271:ALA:HB2	1:B:311:LEU:HD22	1.61	0.82
1:B:250:HIS:ND1	1:B:390:ILE:HD13	1.96	0.80
1:A:562:VAL:O	1:A:566:THR:HG22	1.82	0.78
1:B:334:ASN:C	1:B:336:ASN:H	1.98	0.71
1:B:423:ASN:HB3	1:B:425:PHE:H	1.55	0.69
1:C:430:GLU:CD	1:C:544:ARG:HH22	2.03	0.66
1:B:483:GLY:C	1:B:484:LEU:HD23	2.20	0.65
1:B:271:ALA:HB2	1:B:311:LEU:CD2	2.27	0.64
1:C:265:VAL:HG11	1:C:533:LEU:HD11	1.81	0.63
1:A:232:ASP:O	1:A:234:PHE:N	2.31	0.62
1:A:263:ILE:HD11	1:A:443:LEU:HD13	1.81	0.62
1:A:435:LYS:O	1:A:436:LYS:CB	2.46	0.62
1:A:264:LEU:O	1:A:291:THR:HA	2.01	0.61
1:C:227:PHE:CD1	1:C:515:ILE:HD11	2.36	0.61
1:C:318:ILE:HD13	1:C:443:LEU:HD22	1.82	0.60
1:B:479:LEU:HD12	1:B:524:ILE:HG12	1.83	0.60
1:A:485:LYS:O	1:A:486:ASN:CG	2.43	0.60
1:B:276:LEU:HD12	1:B:299:THR:HG22	1.83	0.60
1:C:259:ASP:OD2	1:C:327:GLU:OE1	2.19	0.60
1:B:276:LEU:HD12	1:B:299:THR:CG2	2.31	0.60
1:B:259:ASP:OD2	1:B:327:GLU:HG2	2.01	0.60
1:A:267:LEU:HD11	1:A:314:VAL:HG23	1.84	0.59
1:A:385:VAL:HG22	1:A:389:GLN:HB2	1.84	0.59
1:B:461:HIS:O	1:B:521:PRO:HA	2.04	0.58
1:B:250:HIS:HA	1:B:390:ILE:HD11	1.84	0.58
1:B:423:ASN:ND2	1:B:586:PHE:O	2.36	0.58
1:A:562:VAL:O	1:A:566:THR:CG2	2.52	0.58
1:B:250:HIS:HA	1:B:390:ILE:CD1	2.34	0.57
1:C:252:ILE:HA	1:C:302:LEU:O	2.04	0.57
1:B:249:PRO:HB3	1:B:306:ASP:O	2.05	0.56
1:A:420:GLU:HB2	2:A:666:HOH:O	2.06	0.56
1:B:334:ASN:C	1:B:336:ASN:N	2.64	0.56
1:C:414:LEU:HD21	1:C:447:VAL:HG12	1.88	0.56
1:B:346:ILE:O	1:B:350:SER:OG	2.24	0.55
1:C:334:ASN:HD21	1:C:380:ASP:N	2.04	0.55
1:A:435:LYS:O	1:A:436:LYS:HB3	2.06	0.55
1:C:252:ILE:O	1:C:382:ILE:HA	2.06	0.55
1:C:430:GLU:OE2	1:C:544:ARG:NH2	2.34	0.55
1:C:267:LEU:HD11	1:C:314:VAL:HG22	1.89	0.54
1:A:430:GLU:CD	1:A:544:ARG:HH22	2.15	0.54
1:C:412:ILE:HG22	1:C:431:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASN:N	1:B:218:ASN:OD1	2.40	0.53
1:A:430:GLU:OE2	1:A:544:ARG:NH2	2.36	0.53
1:C:482:LEU:HD12	1:C:521:PRO:HG2	1.92	0.52
1:C:546:PHE:HB2	1:C:552:ASP:O	2.10	0.52
1:A:226:ARG:HG2	1:A:226:ARG:HH11	1.74	0.52
1:C:453:ASN:O	1:C:456:ALA:HB3	2.10	0.51
1:A:570:SER:OG	1:A:573:GLU:HG3	2.11	0.51
1:C:461:HIS:HB3	1:C:546:PHE:CD1	2.46	0.51
1:C:502:GLN:HG2	1:C:504:TYR:CZ	2.44	0.51
1:B:262:LEU:HD11	1:B:317:VAL:HG22	1.93	0.51
1:C:256:GLN:O	1:C:299:THR:HA	2.11	0.51
1:C:271:ALA:HB2	1:C:311:LEU:CD2	2.40	0.51
1:C:483:GLY:C	1:C:484:LEU:HD23	2.35	0.51
1:A:330:ASP:CG	1:A:334:ASN:OD1	2.54	0.51
1:B:203:PHE:O	1:B:514:VAL:HA	2.10	0.51
1:C:354:ARG:NH1	2:C:601:HOH:O	2.29	0.50
1:B:458:MET:CE	1:B:524:ILE:HD12	2.41	0.50
1:A:245:TYR:HB3	1:A:313:LEU:HB2	1.93	0.50
1:C:319:PRO:HG2	1:C:324:GLY:CA	2.41	0.50
1:C:467:ILE:HG23	1:C:517:PRO:HA	1.94	0.49
1:C:317:VAL:HG11	1:C:326:PHE:CD1	2.46	0.49
1:C:302:LEU:HD11	1:C:313:LEU:CD1	2.42	0.49
1:B:430:GLU:OE2	1:B:544:ARG:NH2	2.45	0.49
1:B:333:LYS:O	1:B:334:ASN:CG	2.55	0.49
1:C:319:PRO:HG2	1:C:324:GLY:HA2	1.95	0.49
1:C:428:LEU:HD23	1:C:450:VAL:HG22	1.94	0.49
1:A:509:SER:HB2	1:A:512:ASP:OD2	2.13	0.49
1:B:482:LEU:HB2	1:B:521:PRO:HG2	1.94	0.49
1:A:537:ILE:N	1:A:537:ILE:HD12	2.28	0.49
1:A:435:LYS:HA	1:A:435:LYS:HD3	1.59	0.48
1:C:470:LEU:HD22	1:C:516:ILE:HD11	1.94	0.48
1:B:470:LEU:O	1:B:513:VAL:HA	2.13	0.48
1:B:319:PRO:HG3	1:B:326:PHE:HB3	1.93	0.48
1:C:431:ILE:HG22	1:C:440:LEU:HD22	1.95	0.48
1:C:271:ALA:HB2	1:C:311:LEU:HD22	1.95	0.48
1:A:434:GLU:OE1	1:A:436:LYS:HD3	2.14	0.48
1:C:262:LEU:HD22	1:C:294:LEU:HD23	1.95	0.48
1:A:526:ALA:HB1	1:A:528:SER:O	2.14	0.48
1:A:415:ARG:C	1:A:417:HIS:H	2.23	0.47
1:B:434:GLU:CD	1:B:435:LYS:H	2.23	0.47
1:A:237:LEU:HD21	1:A:467:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ARG:HA	1:C:311:LEU:O	2.15	0.47
1:A:463:ASN:HB3	1:A:542:ASN:OD1	2.15	0.47
1:B:484:LEU:HD23	1:B:484:LEU:N	2.30	0.47
1:A:428:LEU:HD12	1:A:450:VAL:HG22	1.97	0.47
1:B:262:LEU:CD1	1:B:317:VAL:HG22	2.45	0.46
1:B:509:SER:O	1:B:512:ASP:HB2	2.15	0.46
1:C:241:ARG:HB2	1:C:317:VAL:HB	1.97	0.46
1:C:274:THR:HB	1:C:301:TYR:CE1	2.50	0.46
1:B:314:VAL:HG21	1:B:471:LEU:HD13	1.96	0.46
1:B:273:LEU:HD23	1:B:302:LEU:HD13	1.96	0.46
1:B:430:GLU:HG2	1:B:432:THR:HG23	1.97	0.46
1:A:265:VAL:HG11	1:A:533:LEU:HD11	1.97	0.46
1:A:546:PHE:CE2	1:A:585:HIS:HA	2.50	0.46
1:C:431:ILE:O	1:C:446:PHE:HB2	2.16	0.46
1:C:445:LEU:HD23	1:C:536:GLY:O	2.16	0.46
1:C:450:VAL:HB	1:C:532:LEU:HD11	1.97	0.46
1:B:380:ASP:O	1:B:381:ALA:HB3	2.16	0.46
1:B:425:PHE:CE1	1:B:588:ASN:HB2	2.51	0.46
1:C:248:LYS:HB3	1:C:249:PRO:HD2	1.97	0.45
1:A:419:PRO:HB3	1:A:429:PHE:CE2	2.51	0.45
1:A:560:ASN:N	1:A:561:PRO:HD2	2.32	0.45
1:B:334:ASN:O	1:B:336:ASN:N	2.45	0.45
1:B:463:ASN:HB2	2:B:602:HOH:O	2.17	0.45
1:C:425:PHE:HB3	1:C:456:ALA:HB1	1.99	0.45
1:A:333:LYS:H	1:A:333:LYS:HG3	1.61	0.45
1:B:205:PHE:CE2	1:B:230:ARG:HG3	2.51	0.45
1:B:218:ASN:HA	1:B:248:LYS:HD2	2.00	0.44
1:B:227:PHE:CD1	1:B:515:ILE:HD11	2.52	0.44
1:A:214:PHE:O	1:A:220:HIS:HA	2.17	0.44
1:C:248:LYS:HB3	1:C:249:PRO:CD	2.47	0.44
1:B:444:ASP:OD2	1:B:538:ASN:HA	2.18	0.44
1:B:220:HIS:NE2	1:B:222:ARG:HD3	2.33	0.44
1:A:453:ASN:O	1:A:454:GLU:C	2.61	0.44
1:C:419:PRO:HG2	1:C:422:SER:OG	2.18	0.44
1:B:583:GLN:HB2	1:B:587:ALA:HB2	2.00	0.44
1:A:412:ILE:HD13	1:A:437:TYR:CD1	2.53	0.44
1:C:428:LEU:CD2	1:C:450:VAL:HG22	2.48	0.44
1:C:266:VAL:HA	1:C:313:LEU:HD23	1.99	0.43
1:B:248:LYS:HB3	1:B:249:PRO:CD	2.49	0.43
1:C:253:PHE:CZ	1:C:256:GLN:OE1	2.71	0.43
1:B:423:ASN:C	1:B:425:PHE:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ILE:O	1:C:350:SER:HB3	2.19	0.43
1:A:425:PHE:CE1	1:A:588:ASN:HB2	2.53	0.43
1:B:253:PHE:HB3	1:B:302:LEU:HB3	2.00	0.43
1:C:463:ASN:HB3	1:C:542:ASN:OD1	2.17	0.43
1:C:267:LEU:HD22	1:C:473:ASN:CG	2.43	0.43
1:C:264:LEU:O	1:C:291:THR:HA	2.18	0.43
1:C:222:ARG:NH1	1:C:244:GLU:OE1	2.50	0.43
1:C:344:LYS:HD2	1:C:344:LYS:H	1.84	0.43
1:A:470:LEU:HD22	1:A:516:ILE:HD11	2.00	0.43
1:A:485:LYS:O	1:A:486:ASN:OD1	2.36	0.43
1:B:445:LEU:HA	1:B:445:LEU:HD23	1.80	0.43
1:B:465:ARG:HD3	1:B:540:GLU:O	2.19	0.43
1:C:251:THR:HB	1:C:382:ILE:HG22	2.01	0.43
1:C:482:LEU:HB2	1:C:521:PRO:HG2	2.00	0.43
1:A:414:LEU:HD13	1:A:449:CYS:HB2	2.01	0.42
1:C:266:VAL:HG22	1:C:313:LEU:CD2	2.49	0.42
1:C:450:VAL:HB	1:C:532:LEU:CD1	2.49	0.42
1:C:499:ASN:O	1:C:500:GLU:O	2.37	0.42
1:C:517:PRO:HB2	1:C:520:HIS:ND1	2.34	0.42
1:C:454:GLU:HG3	1:C:527:SER:O	2.19	0.42
1:C:254:LEU:HD12	1:C:380:ASP:O	2.19	0.42
1:B:415:ARG:HG2	1:B:429:PHE:CZ	2.55	0.42
1:B:528:SER:O	1:B:529:ASN:C	2.63	0.42
1:C:462:TYR:CD1	1:C:462:TYR:C	2.97	0.42
1:A:386:SER:OG	1:A:389:GLN:HG3	2.20	0.42
1:B:245:TYR:CE1	1:B:302:LEU:HD23	2.54	0.42
1:B:333:LYS:O	1:B:334:ASN:OD1	2.37	0.42
1:A:243:VAL:HG23	1:A:317:VAL:HG21	2.01	0.42
1:B:461:HIS:HA	1:B:545:ASN:O	2.19	0.42
1:C:213:LEU:HD23	1:C:213:LEU:HA	1.92	0.42
1:B:262:LEU:HG	1:B:315:ASP:HB3	2.01	0.42
1:C:262:LEU:HB2	1:C:294:LEU:HB3	2.02	0.42
1:B:331:LEU:O	1:B:337:GLN:HG3	2.20	0.41
1:C:217:GLU:H	1:C:217:GLU:HG3	1.62	0.41
1:A:577:LEU:C	1:A:577:LEU:HD23	2.46	0.41
1:B:428:LEU:C	1:B:428:LEU:HD13	2.46	0.41
1:A:444:ASP:OD2	1:A:538:ASN:HA	2.20	0.41
1:B:450:VAL:HB	1:B:532:LEU:HB2	2.02	0.41
1:C:332:ALA:O	1:C:337:GLN:HG3	2.20	0.41
1:C:470:LEU:O	1:C:513:VAL:HA	2.20	0.41
1:B:419:PRO:HB3	1:B:429:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:VAL:O	1:C:501:VAL:HG23	2.21	0.41
1:B:560:ASN:N	1:B:561:PRO:CD	2.84	0.41
1:C:445:LEU:HD23	1:C:445:LEU:HA	1.85	0.41
1:A:314:VAL:HG21	1:A:471:LEU:HD22	2.03	0.40
1:B:560:ASN:HB2	1:B:561:PRO:HD3	2.03	0.40
1:B:577:LEU:C	1:B:577:LEU:HD23	2.46	0.40
1:A:428:LEU:HD23	1:A:428:LEU:C	2.46	0.40
1:A:541:ASN:C	1:A:542:ASN:O	2.64	0.40
1:C:482:LEU:HA	1:C:502:GLN:O	2.21	0.40
1:B:331:LEU:HD23	1:B:331:LEU:HA	1.94	0.40
1:C:265:VAL:HG11	1:C:533:LEU:CD1	2.50	0.40
1:C:480:GLU:O	1:C:522:VAL:HA	2.21	0.40
1:B:546:PHE:CE2	1:B:585:HIS:HA	2.57	0.40
1:C:461:HIS:HB3	1:C:546:PHE:CE1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:HH21	1:B:573:GLU:OE1[48_445]	1.58	0.02

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	341/413 (83%)	323 (95%)	15 (4%)	3 (1%)	14	35
1	B	336/413 (81%)	307 (91%)	22 (6%)	7 (2%)	5	15
1	C	338/413 (82%)	304 (90%)	29 (9%)	5 (2%)	8	22
All	All	1015/1239 (82%)	934 (92%)	66 (6%)	15 (2%)	8	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	LYS
1	B	335	LYS
1	C	500	GLU
1	A	232	ASP
1	B	296	ALA
1	B	500	GLU
1	C	519	GLY
1	A	233	LEU
1	B	233	LEU
1	B	381	ALA
1	B	260	ALA
1	C	225	GLN
1	C	338	TYR
1	C	529	ASN
1	B	433	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	314/374 (84%)	292 (93%)	22 (7%)	14	34
1	B	307/374 (82%)	280 (91%)	27 (9%)	9	23
1	C	308/374 (82%)	278 (90%)	30 (10%)	8	20
All	All	929/1122 (83%)	850 (92%)	79 (8%)	10	25

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	LYS
1	A	226	ARG
1	A	229	LYS
1	A	230	ARG
1	A	231	SER
1	A	232	ASP
1	A	277	SER
1	A	287	GLU

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Mol	Chain	Res	Type
1	A	308	GLU
1	A	330	ASP
1	A	333	LYS
1	A	344	LYS
1	A	384	LYS
1	A	434	GLU
1	A	435	LYS
1	A	474	GLU
1	A	485	LYS
1	A	503	ARG
1	A	543	GLU
1	A	550	SER
1	A	564	GLU
1	A	566	THR
1	B	218	ASN
1	B	234	PHE
1	B	244	GLU
1	B	262	LEU
1	B	275	VAL
1	B	277	SER
1	B	283	SER
1	B	291	THR
1	B	313	LEU
1	B	327	GLU
1	B	333	LYS
1	B	335	LYS
1	B	350	SER
1	B	380	ASP
1	B	385	VAL
1	B	390	ILE
1	B	416	SER
1	B	420	GLU
1	B	424	LYS
1	B	440	LEU
1	B	464	SER
1	B	476	LYS
1	B	484	LEU
1	B	507	ARG
1	B	550	SER
1	B	556	SER
1	B	576	ARG
1	C	217	GLU

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Mol	Chain	Res	Type
1	C	220	HIS
1	C	231	SER
1	C	232	ASP
1	C	238	GLN
1	C	243	VAL
1	C	244	GLU
1	C	270	LYS
1	C	272	ILE
1	C	308	GLU
1	C	314	VAL
1	C	330	ASP
1	C	333	LYS
1	C	336	ASN
1	C	382	ILE
1	C	384	LYS
1	C	388	GLU
1	C	392	GLU
1	C	416	SER
1	C	422	SER
1	C	435	LYS
1	C	473	ASN
1	C	484	LEU
1	C	503	ARG
1	C	529	ASN
1	C	544	ARG
1	C	550	SER
1	C	564	GLU
1	C	582	LYS
1	C	584	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
1	A	486	ASN
1	A	541	ASN
1	B	588	ASN
1	C	334	ASN
1	C	502	GLN
1	C	545	ASN
1	C	581	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

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	349/413 (84%)	-0.25	8 (2%) 61 58	16, 30, 57, 87	0
1	B	344/413 (83%)	0.26	20 (5%) 29 25	23, 41, 77, 114	0
1	C	346/413 (83%)	0.77	33 (9%) 14 11	29, 55, 93, 130	0
All	All	1039/1239 (83%)	0.26	61 (5%) 28 25	16, 42, 83, 130	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	409	PHE	7.1
1	B	409	PHE	5.9
1	B	214	PHE	5.5
1	B	392	GLU	5.0
1	C	394	LYS	4.8
1	A	409	PHE	4.6
1	A	394	LYS	4.3
1	B	380	ASP	4.3
1	C	231	SER	4.2
1	B	335	LYS	4.2
1	C	501	VAL	4.0
1	C	211	LEU	3.8
1	C	388	GLU	3.4
1	C	387	ARG	3.4
1	C	417	HIS	3.4
1	B	272	ILE	3.1
1	A	379	THR	3.0
1	C	392	GLU	3.0
1	C	214	PHE	3.0
1	C	216	ASN	2.9
1	B	387	ARG	2.9
1	C	499	ASN	2.9
1	C	436	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	417	HIS	2.8
1	B	500	GLU	2.8
1	C	325	LYS	2.8
1	A	486	ASN	2.7
1	B	220	HIS	2.7
1	C	220	HIS	2.7
1	C	364	GLU	2.7
1	C	473	ASN	2.6
1	C	484	LEU	2.6
1	C	500	GLU	2.5
1	C	249	PRO	2.5
1	B	388	GLU	2.5
1	C	420	GLU	2.4
1	C	440	LEU	2.4
1	C	386	SER	2.3
1	C	390	ILE	2.3
1	B	417	HIS	2.3
1	C	538	ASN	2.3
1	B	285	ASN	2.3
1	C	336	ASN	2.3
1	C	381	ALA	2.3
1	C	236	ASN	2.3
1	B	385	VAL	2.3
1	B	499	ASN	2.2
1	A	435	LYS	2.2
1	B	327	GLU	2.2
1	C	232	ASP	2.2
1	C	418	LYS	2.2
1	C	410	GLU	2.2
1	B	386	SER	2.2
1	C	252	ILE	2.2
1	A	424	LYS	2.2
1	C	393	LEU	2.2
1	A	335	LYS	2.1
1	B	434	GLU	2.1
1	B	390	ILE	2.0
1	B	305	GLN	2.0
1	B	439	GLN	2.0

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 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.