Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 11:43 PM EDT

PDB ID	:	7U1J
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:

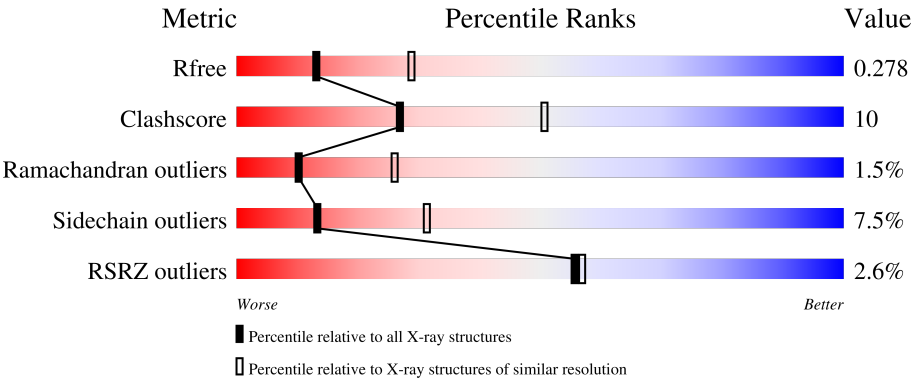
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	65% 17% • 15%
1	B	413	% 58% 23% • 17%
1	C	413	5% 56% 26% • 16%

2 Entry composition (i)

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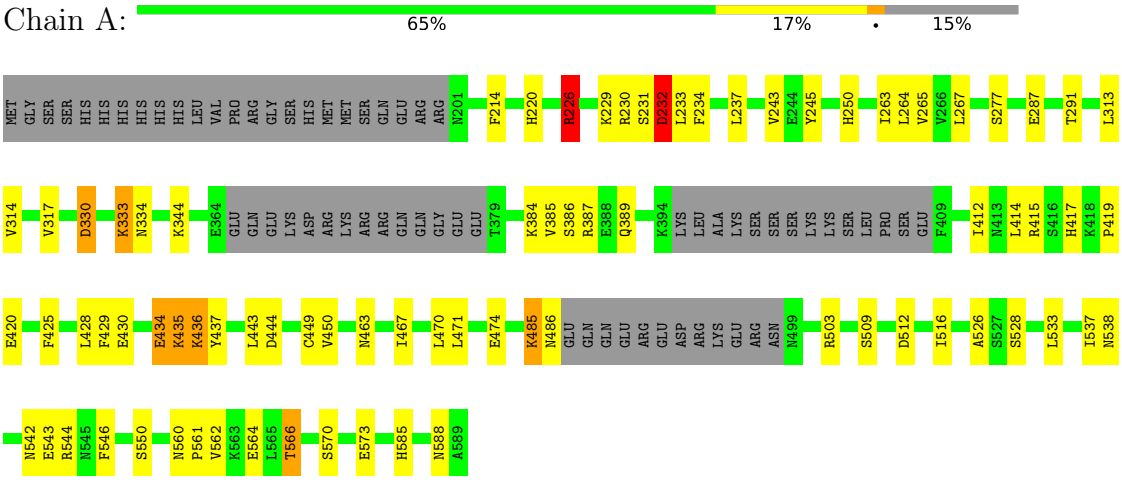
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	14	Total	O	0	0
			14	14		

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.

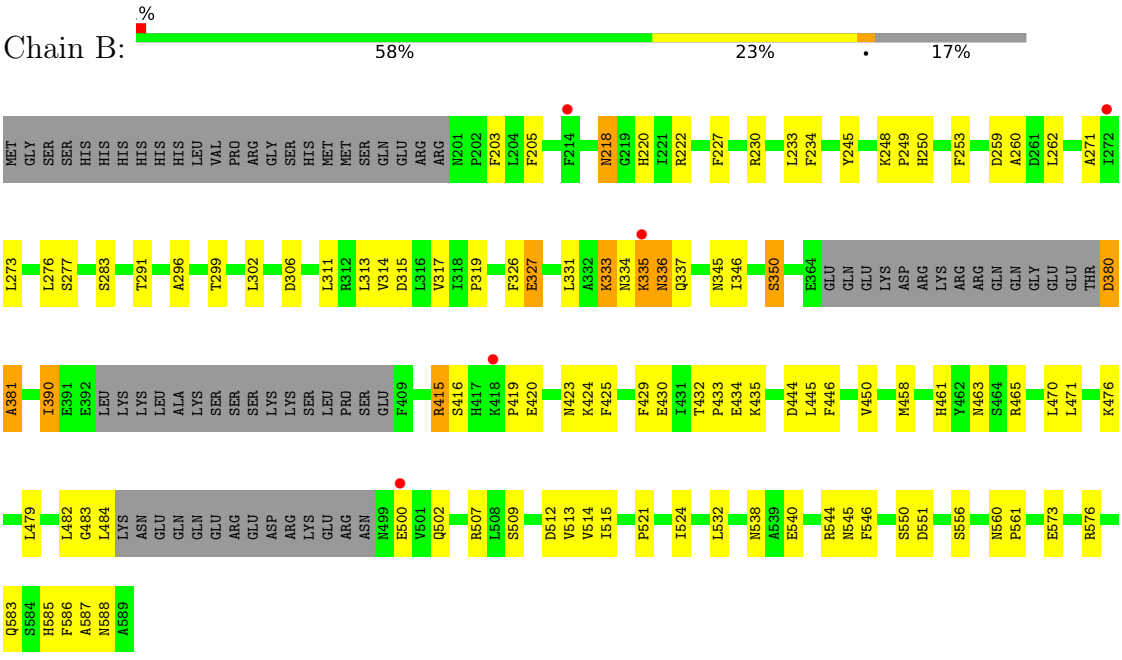
- Molecule 1: Convicilin

Chain A:



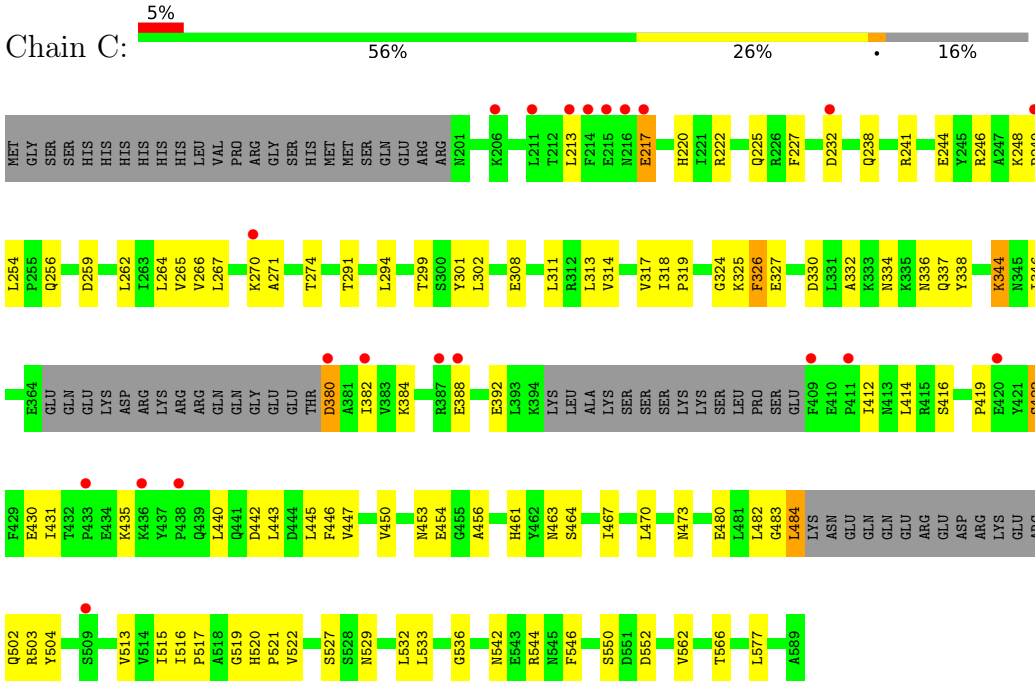
- Molecule 1: Convicilin

Chain B:



- Molecule 1: Convicilin

Chain C:


5%
56%
26%
16%
MET GLY SER SER HIS HIS HIS HIS HIS HIS LEU VAL PRO ARG GLY SER HIS MET MET SER GLN GLU ARG ARG N201 K206 L211 T212 L213 F214 E215 N216 E217 H220 I221 R222 Q225 R226 F227 D232 Q238 R241 E244 Y245 R246 A247 K248 P249 H250 T251 I252 F253
L254 P255 Q256 D259 L262 I263 L264 V265 V266 L267 K270 A271 T274 T291 L294 T299 S300 Y301 L302 E308 L311 R312 L313 V314 V317 I318 P319 G324 K325 F326 E327 D330 L331 A332 K333 N334 K335 N336 Q337 Y338 K344 N345 I346 S350 R354
E364 GLU GLN GLU LYS ASP ARG LYS ARG ARG GLN GLN GLY GLU GLU THR D380 A381 I382 V383 K384 R387 E388 E392 L393 K394 LYS LEU ALA LYS SER SER SER LYS LYS SER LEU PRO SER GLU F409 E410 P411 I412 N413 L414 R415 S416 P419 E420 Y421 S422 F425 L428
F429 E430 I431 T432 P433 E434 K435 K436 Y437 P438 Q439 L440 Q441 D442 L443 D444 L445 F446 V447 V450 N453 E454 G455 A456 H461 Y462 N463 S464 I467 L470 N473 E480 L481 L482 G483 L484 LYS ASN GLU GLN GLN GLU ARG GLU ASP ARG LYS GLU ARG ASN N499 E500 V501
Q502 R503 Y504 S509 V513 V514 I515 I516 P517 A518 G519 H520 P521 V522 S527 S528 N529 L532 L533 G536 N542 E543 R544 N545 F546 S550 D551 D552 V562 T566 L577 A589

4 Data and refinement statistics (i)

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 – 2.70 134.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (134.94-2.70) 91.5 (134.58-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.215 , 0.281 0.215 , 0.278	Depositor DCC
R_{free} test set	2069 reflections (5.11%)	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)	0.37 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.74	0/2851	0.99	2/3855 (0.1%)
1	B	0.77	0/2807	0.99	2/3797 (0.1%)
1	C	0.79	0/2817	0.96	0/3811
All	All	0.77	0/8475	0.98	4/11463 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	415	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	226	ARG	CG-CD-NE	5.09	122.49	111.80
1	A	226	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	551	ASP	CB-CA-C	5.03	120.45	110.40

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 (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	2802	2820	2809	41	1
1	B	2758	2763	2747	59	1
1	C	2769	2779	2760	69	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	169	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 10.

All (169) 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:423:ASN:HB3	1:B:425:PHE:H	1.55	0.69
1:B:334:ASN:C	1:B:336:ASN:H	1.98	0.66
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:430:GLU:CD	1:C:544:ARG:HH22	2.03	0.61
1:B:483:GLY:C	1:B:484:LEU:HD23	2.20	0.60
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:414:LEU:HD21	1:C:447:VAL:HG12	1.88	0.56
1:A:485:LYS:O	1:A:486:ASN:CG	2.43	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:C:412:ILE:HG22	1:C:431:ILE:HD11	1.90	0.54
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:B:334:ASN:C	1:B:336:ASN:N	2.64	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:A:430:GLU:CD	1:A:544:ARG:HH22	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:LEU:HD21	1:A:467:ILE:HG21	1.96	0.47
1:C:246:ARG:HA	1:C:311:LEU:O	2.15	0.47
1:B:346:ILE:O	1:B:350:SER:OG	2.24	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:C:483:GLY:C	1:C:484:LEU:HD23	2.35	0.46
1:B:273:LEU:HD23	1:B:302:LEU:HD13	1.96	0.46
1:A:330:ASP:CG	1:A:334:ASN:OD1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:333:LYS:O	1:B:334:ASN:CG	2.55	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: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: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: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:A:415:ARG:C	1:A:417:HIS:H	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:434:GLU:CD	1:B:435:LYS:H	2.23	0.41
1:C:217:GLU:H	1:C:217:GLU:HG3	1.62	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
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: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%)	17 40
1	B	336/413 (81%)	307 (91%)	22 (6%)	7 (2%)	7 18
1	C	338/413 (82%)	304 (90%)	29 (9%)	5 (2%)	10 26
All	All	1015/1239 (82%)	934 (92%)	66 (6%)	15 (2%)	10 26

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 (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	314/374 (84%)	293 (93%)	21 (7%)	16 37
1	B	307/374 (82%)	283 (92%)	24 (8%)	12 29
1	C	308/374 (82%)	283 (92%)	25 (8%)	11 27
All	All	929/1122 (83%)	859 (92%)	70 (8%)	13 31

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	ARG
1	A	229	LYS
1	A	230	ARG
1	A	231	SER
1	A	232	ASP
1	A	250	HIS
1	A	277	SER
1	A	287	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	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	336	ASN
1	B	345	ASN
1	B	350	SER
1	B	380	ASP
1	B	390	ILE
1	B	416	SER
1	B	420	GLU
1	B	424	LYS
1	B	446	PHE
1	B	476	LYS
1	B	502	GLN
1	B	507	ARG

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Mol	Chain	Res	Type
1	B	550	SER
1	B	556	SER
1	B	576	ARG
1	C	217	GLU
1	C	220	HIS
1	C	232	ASP
1	C	238	GLN
1	C	270	LYS
1	C	308	GLU
1	C	325	LYS
1	C	326	PHE
1	C	330	ASP
1	C	336	ASN
1	C	344	LYS
1	C	354	ARG
1	C	380	ASP
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	442	ASP
1	C	473	ASN
1	C	484	LEU
1	C	503	ARG
1	C	550	SER
1	C	577	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	ASN
1	A	588	ASN
1	B	238	GLN
1	B	538	ASN
1	B	585	HIS
1	C	583	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.06	0 100 100	16, 30, 56, 86	0
1	B	344/413 (83%)	0.06	5 (1%) 73 76	24, 41, 77, 111	0
1	C	346/413 (83%)	0.40	22 (6%) 19 18	31, 55, 96, 128	0
All	All	1039/1239 (83%)	0.18	27 (2%) 56 57	16, 42, 83, 128	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	214	PHE	4.1
1	C	388	GLU	4.1
1	C	409	PHE	3.4
1	C	216	ASN	3.4
1	B	335	LYS	3.2
1	C	211	LEU	3.1
1	C	213	LEU	3.1
1	C	215	GLU	2.9
1	C	420	GLU	2.7
1	B	418	LYS	2.7
1	C	217	GLU	2.7
1	B	214	PHE	2.6
1	C	206	LYS	2.5
1	C	387	ARG	2.4
1	C	232	ASP	2.4
1	C	433	PRO	2.4
1	C	438	PRO	2.4
1	C	270	LYS	2.4
1	C	249	PRO	2.3
1	C	252	ILE	2.3
1	B	500	GLU	2.3
1	C	411	PRO	2.2
1	C	509	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	380	ASP	2.1
1	B	272	ILE	2.1
1	C	382	ILE	2.1
1	C	436	LYS	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 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.