



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:10 PM UTC

PDB ID : 7U1H / pdb_00007u1h
Title : Crystal structure of Lens culinaris vicilin
Authors : Robinson, K.A.; Bakestani, I.D.; Loewen, M.C.
Deposited on : 2022-02-21
Resolution : 2.50 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

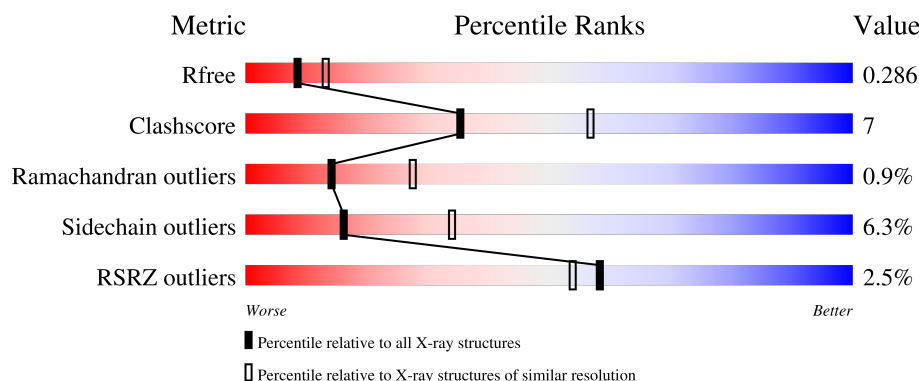
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	2% 67% 16% • 15%
1	B	431	2% 64% 20% • 15%
1	C	431	2% 66% 16% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17579 atoms, of which 8775 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 Allergen Len c 1.0101.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	H	N	O	62	4	0
			5889	1858	2951	518	562			
1	B	365	Total	C	H	N	O	61	4	0
			5857	1848	2930	516	563			
1	C	363	Total	C	H	N	O	61	3	0
			5793	1832	2894	510	557			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q84UI1
A	-16	GLY	-	expression tag	UNP Q84UI1
A	-15	SER	-	expression tag	UNP Q84UI1
A	-14	SER	-	expression tag	UNP Q84UI1
A	-13	HIS	-	expression tag	UNP Q84UI1
A	-12	HIS	-	expression tag	UNP Q84UI1
A	-11	HIS	-	expression tag	UNP Q84UI1
A	-10	HIS	-	expression tag	UNP Q84UI1
A	-9	HIS	-	expression tag	UNP Q84UI1
A	-8	HIS	-	expression tag	UNP Q84UI1
A	-7	LEU	-	expression tag	UNP Q84UI1
A	-6	VAL	-	expression tag	UNP Q84UI1
A	-5	PRO	-	expression tag	UNP Q84UI1
A	-4	ARG	-	expression tag	UNP Q84UI1
A	-3	GLY	-	expression tag	UNP Q84UI1
A	-2	SER	-	expression tag	UNP Q84UI1
A	-1	HIS	-	expression tag	UNP Q84UI1
A	0	MET	-	expression tag	UNP Q84UI1
A	1	MET	-	expression tag	UNP Q84UI1
B	-17	MET	-	expression tag	UNP Q84UI1
B	-16	GLY	-	expression tag	UNP Q84UI1
B	-15	SER	-	expression tag	UNP Q84UI1
B	-14	SER	-	expression tag	UNP Q84UI1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP Q84UI1
B	-12	HIS	-	expression tag	UNP Q84UI1
B	-11	HIS	-	expression tag	UNP Q84UI1
B	-10	HIS	-	expression tag	UNP Q84UI1
B	-9	HIS	-	expression tag	UNP Q84UI1
B	-8	HIS	-	expression tag	UNP Q84UI1
B	-7	LEU	-	expression tag	UNP Q84UI1
B	-6	VAL	-	expression tag	UNP Q84UI1
B	-5	PRO	-	expression tag	UNP Q84UI1
B	-4	ARG	-	expression tag	UNP Q84UI1
B	-3	GLY	-	expression tag	UNP Q84UI1
B	-2	SER	-	expression tag	UNP Q84UI1
B	-1	HIS	-	expression tag	UNP Q84UI1
B	0	MET	-	expression tag	UNP Q84UI1
B	1	MET	-	expression tag	UNP Q84UI1
C	-17	MET	-	expression tag	UNP Q84UI1
C	-16	GLY	-	expression tag	UNP Q84UI1
C	-15	SER	-	expression tag	UNP Q84UI1
C	-14	SER	-	expression tag	UNP Q84UI1
C	-13	HIS	-	expression tag	UNP Q84UI1
C	-12	HIS	-	expression tag	UNP Q84UI1
C	-11	HIS	-	expression tag	UNP Q84UI1
C	-10	HIS	-	expression tag	UNP Q84UI1
C	-9	HIS	-	expression tag	UNP Q84UI1
C	-8	HIS	-	expression tag	UNP Q84UI1
C	-7	LEU	-	expression tag	UNP Q84UI1
C	-6	VAL	-	expression tag	UNP Q84UI1
C	-5	PRO	-	expression tag	UNP Q84UI1
C	-4	ARG	-	expression tag	UNP Q84UI1
C	-3	GLY	-	expression tag	UNP Q84UI1
C	-2	SER	-	expression tag	UNP Q84UI1
C	-1	HIS	-	expression tag	UNP Q84UI1
C	0	MET	-	expression tag	UNP Q84UI1
C	1	MET	-	expression tag	UNP Q84UI1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	17	Total O 17 17	0	0

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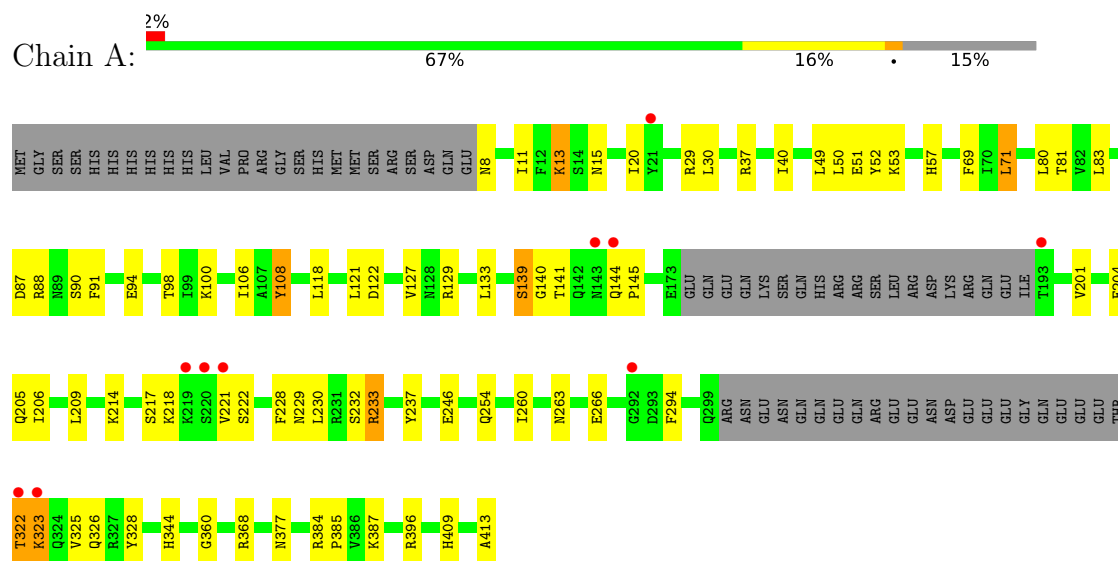
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	11	Total	O	0	0
			11	11		

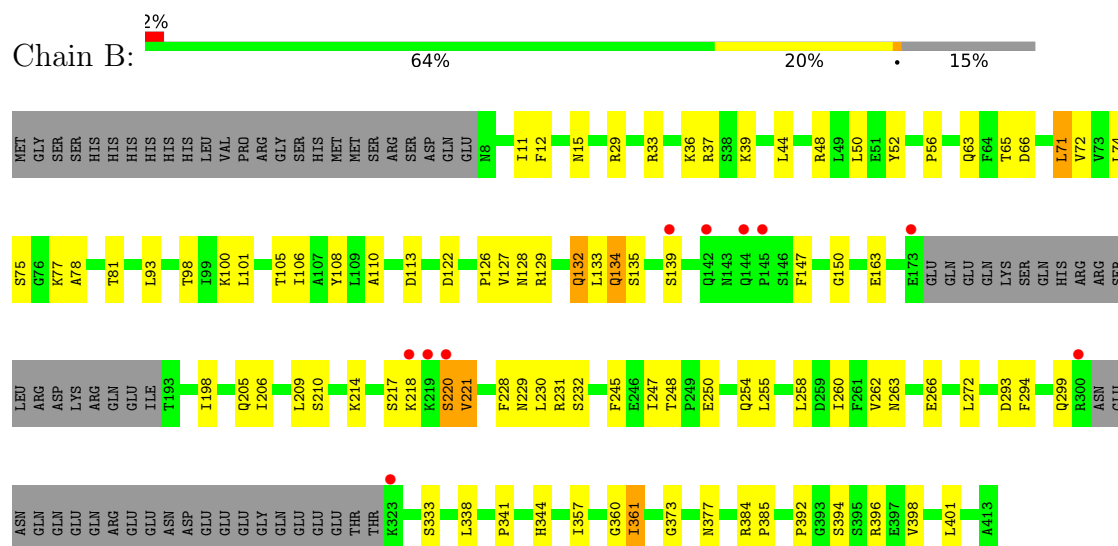
3 Residue-property plots [i](#)

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: Allergen Len c 1.0101

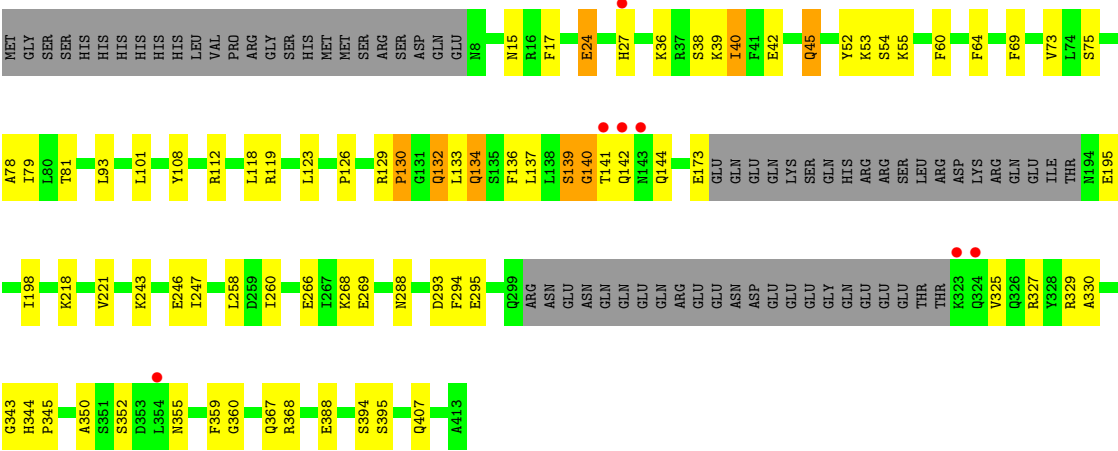


• Molecule 1: Allergen Len c 1.0101



• Molecule 1: Allergen Len c 1.0101





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.44Å 92.50Å 143.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.91 – 2.50 77.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (77.91-2.50) 97.9 (77.79-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.199 , 0.284 0.198 , 0.286	Depositor DCC
R_{free} test set	2075 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.980	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17579	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	1.05	0/3000	1.42	4/4052 (0.1%)
1	B	1.07	1/2988 (0.0%)	1.41	3/4037 (0.1%)
1	C	1.05	0/2955	1.44	3/3994 (0.1%)
All	All	1.05	1/8943 (0.0%)	1.42	10/12083 (0.1%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	PRO	C-O	-5.27	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	44	LEU	CA-C-N	5.81	128.34	120.38
1	B	44	LEU	C-N-CA	5.81	128.34	120.38
1	A	387	LYS	CA-C-N	5.39	127.45	120.44
1	A	387	LYS	C-N-CA	5.39	127.45	120.44
1	A	413	ALA	CA-C-O	-5.38	111.65	120.80
1	C	388	GLU	CA-C-N	5.37	127.75	120.44
1	C	388	GLU	C-N-CA	5.37	127.75	120.44
1	A	108	TYR	CB-CA-C	5.24	119.73	109.35
1	C	17	PHE	CA-CB-CG	5.13	118.93	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	218	LYS	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	2938	2951	2944	43	2
1	B	2927	2930	2919	51	0
1	C	2899	2894	2875	38	2
2	A	12	0	0	1	0
2	B	17	0	0	0	0
2	C	11	0	0	0	0
All	All	8804	8775	8738	129	2

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 7.

All (129) 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:288:ASN:HD22	1:C:355[B]:ASN:HD22	1.24	0.85
1:B:71:LEU:HD12	1:B:122:ASP:OD1	1.79	0.83
1:C:129:ARG:HB2	1:C:132:GLN:HG3	1.61	0.82
1:A:20:ILE:HD11	1:A:30:LEU:HB2	1.61	0.82
1:B:258:LEU:HB3	1:B:260:ILE:HD12	1.69	0.74
1:B:71:LEU:O	1:B:98:THR:HA	1.89	0.72
1:B:29:ARG:O	1:B:50:LEU:HA	1.93	0.68
1:B:71:LEU:CD1	1:B:122:ASP:OD1	2.43	0.66
1:A:246:GLU:CD	1:A:368:ARG:HH22	2.04	0.65
1:C:343:GLY:O	1:C:345:PRO:HD3	1.97	0.65
1:B:48:ARG:HG3	1:B:133:LEU:CD2	2.28	0.64
1:B:394:SER:O	1:B:398:VAL:HG23	1.99	0.63
1:C:38:SER:OG	1:C:40:ILE:HB	1.99	0.62
1:C:246:GLU:CD	1:C:368:ARG:HH22	2.08	0.61
1:C:78:ALA:HB3	1:C:93:LEU:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLY:HA2	1:A:145:PRO:HA	1.84	0.60
1:C:288:ASN:HD22	1:C:355[B]:ASN:ND2	1.96	0.59
1:B:78:ALA:HA	1:B:110:ALA:O	2.02	0.59
1:B:11:ILE:O	1:B:37:ARG:NH2	2.36	0.58
1:A:322:THR:O	1:A:323:LYS:HB2	2.03	0.58
1:B:205:GLN:O	1:B:209:LEU:HG	2.04	0.58
1:B:81:THR:HB	1:B:108:TYR:CE2	2.39	0.58
1:A:29:ARG:O	1:A:50:LEU:HA	2.03	0.57
1:B:129[A]:ARG:NH1	1:B:132:GLN:HG2	2.19	0.57
1:C:39:LYS:O	1:C:42[B]:GLU:HG3	2.04	0.57
1:B:134:GLN:OE1	1:C:344:HIS:NE2	2.37	0.57
1:B:228:PHE:CE2	1:B:247:ILE:HG21	2.40	0.57
1:B:48:ARG:HG3	1:B:133:LEU:HD21	1.85	0.57
1:C:79:ILE:HD11	1:C:112:ARG:HD3	1.87	0.57
1:A:83:LEU:HD12	1:A:106:ILE:CG2	2.36	0.56
1:B:260:ILE:HA	1:B:360:GLY:O	2.07	0.55
1:C:129:ARG:CB	1:C:132:GLN:HG3	2.36	0.53
1:A:384[B]:ARG:HB3	1:A:385:PRO:CD	2.38	0.53
1:A:326:GLN:HG2	1:A:328:TYR:CZ	2.44	0.52
1:C:73:VAL:HG21	1:C:93:LEU:HB3	1.92	0.51
1:A:57:HIS:HA	1:A:206:ILE:HD11	1.93	0.51
1:B:98:THR:HG21	1:B:230:LEU:HD21	1.93	0.51
1:B:220:SER:OG	1:B:221:VAL:N	2.44	0.51
1:A:13:LYS:HA	1:A:13:LYS:HE2	1.93	0.50
1:A:260:ILE:HA	1:A:360:GLY:O	2.12	0.50
1:C:295:GLU:HG2	1:C:329:ARG:HG2	1.92	0.50
1:A:377:ASN:OD1	1:A:377:ASN:C	2.54	0.50
1:A:221:VAL:HG11	1:A:233:ARG:HD2	1.93	0.49
1:A:229:ASN:HB3	1:A:232:SER:HB3	1.94	0.49
1:B:384:ARG:HB3	1:B:385:PRO:HD3	1.94	0.49
1:A:57:HIS:HA	1:A:206:ILE:CD1	2.42	0.49
1:C:81:THR:HB	1:C:108:TYR:CE2	2.46	0.49
1:C:294:PHE:CE2	1:C:330:ALA:HB3	2.47	0.49
1:A:69:PHE:CD1	1:A:122[B]:ASP:OD2	2.66	0.49
1:B:361:ILE:HD12	1:B:361:ILE:N	2.28	0.49
1:C:126:PRO:HB3	1:C:132:GLN:O	2.13	0.48
1:C:139:SER:O	1:C:140:GLY:O	2.30	0.48
1:B:220:SER:O	1:B:221:VAL:HB	2.13	0.48
1:B:401:LEU:C	1:B:401:LEU:HD23	2.39	0.48
1:B:74:LEU:CD2	1:B:357:ILE:HG13	2.43	0.47
1:B:71:LEU:HD13	1:B:101:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD22	1:A:122[A]:ASP:CG	2.39	0.47
1:B:100:LYS:HE2	1:B:254:GLN:O	2.15	0.47
1:A:8:ASN:N	2:A:502:HOH:O	2.47	0.47
1:B:294:PHE:CE2	1:B:338:LEU:HD13	2.50	0.47
1:B:229:ASN:HB3	1:B:232:SER:OG	2.14	0.46
1:B:12:PHE:CZ	1:B:37:ARG:HG2	2.50	0.46
1:A:71:LEU:HD22	1:A:122[A]:ASP:OD1	2.16	0.46
1:A:57:HIS:HB3	1:A:201:VAL:O	2.15	0.46
1:B:48:ARG:CG	1:B:133:LEU:HD21	2.46	0.46
1:A:218:LYS:O	1:A:221:VAL:HG12	2.15	0.46
1:A:53:LYS:HA	1:A:118:LEU:O	2.16	0.45
1:B:66:ASP:HB2	1:B:128:ASN:ND2	2.32	0.45
1:A:15:ASN:OD1	1:A:15:ASN:C	2.60	0.45
1:B:98:THR:OG1	1:B:228:PHE:CE2	2.70	0.45
1:A:87:ASP:CG	1:A:88:ARG:H	2.25	0.45
1:C:60:PHE:CD1	1:C:198:ILE:HG12	2.52	0.44
1:C:266:GLU:HG2	1:C:355[A]:ASN:ND2	2.32	0.44
1:A:29:ARG:NH1	1:A:51:GLU:OE1	2.49	0.44
1:A:217:SER:OG	1:A:218:LYS:N	2.49	0.44
1:C:350:ALA:HB1	1:C:352:SER:O	2.18	0.44
1:C:260:ILE:HA	1:C:360:GLY:O	2.18	0.44
1:B:255:LEU:HB3	1:B:260:ILE:O	2.18	0.43
1:A:52:TYR:CE2	1:A:122[A]:ASP:OD2	2.72	0.43
1:B:230:LEU:HD21	1:B:262:VAL:HG12	2.00	0.43
1:A:81:THR:HB	1:A:108:TYR:CE2	2.53	0.43
1:A:91:PHE:HA	1:A:214:LYS:O	2.19	0.43
1:A:221:VAL:HG11	1:A:233:ARG:CD	2.48	0.43
1:B:245:PHE:O	1:B:263:ASN:HB2	2.18	0.43
1:C:54:SER:HB3	1:C:60:PHE:CZ	2.53	0.43
1:A:11:ILE:O	1:A:37:ARG:NH2	2.36	0.43
1:B:341:PRO:O	1:B:344:HIS:HB2	2.19	0.43
1:B:78:ALA:HB3	1:B:93:LEU:HB2	2.00	0.43
1:A:83:LEU:HD12	1:A:106:ILE:HG21	2.00	0.42
1:B:150:GLY:O	1:C:327:ARG:NE	2.50	0.42
1:B:373:GLY:O	1:B:377:ASN:HB2	2.19	0.42
1:C:129:ARG:HB2	1:C:132:GLN:CG	2.42	0.42
1:B:56:PRO:HB3	1:B:113:ASP:O	2.19	0.42
1:C:258:LEU:HB3	1:C:260:ILE:HD12	2.01	0.42
1:C:141:THR:N	1:C:144:GLN:O	2.53	0.42
1:C:394:SER:O	1:C:395:SER:C	2.62	0.42
1:C:24:GLU:OE2	1:C:195:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HE2	1:A:254:GLN:O	2.19	0.42
1:B:248:THR:OG1	1:B:250[B]:GLU:HG2	2.19	0.42
1:B:250[B]:GLU:CD	1:B:250[B]:GLU:H	2.27	0.42
1:A:71:LEU:O	1:A:98:THR:HA	2.20	0.42
1:A:71:LEU:HD23	1:A:71:LEU:N	2.34	0.42
1:C:221:VAL:HG21	1:C:247:ILE:HD12	2.02	0.42
1:C:53:LYS:HA	1:C:118:LEU:O	2.20	0.41
1:B:48:ARG:HG3	1:B:133:LEU:HD23	2.03	0.41
1:B:384:ARG:N	1:B:385:PRO:HD2	2.35	0.41
1:C:52:TYR:O	1:C:119:ARG:HA	2.21	0.41
1:B:33:ARG:HB2	1:B:36:LYS:HG2	2.03	0.41
1:B:384:ARG:HB3	1:B:385:PRO:CD	2.51	0.41
1:C:123:LEU:HD22	1:C:359:PHE:HB3	2.02	0.41
1:B:66:ASP:CB	1:B:128:ASN:HD22	2.34	0.41
1:B:72:VAL:HG22	1:B:98:THR:HG22	2.03	0.41
1:A:246:GLU:HG3	1:A:263:ASN:HB3	2.02	0.41
1:B:231:ARG:NH2	1:B:266:GLU:OE2	2.54	0.41
1:C:268:LYS:O	1:C:269:GLU:C	2.64	0.41
1:A:80:LEU:O	1:A:90:SER:HA	2.21	0.41
1:A:205:GLN:O	1:A:209:LEU:HG	2.20	0.41
1:B:65:THR:HG21	1:B:133:LEU:HD12	2.03	0.41
1:C:64:PHE:CE1	1:C:136:PHE:HB2	2.56	0.41
1:C:69:PHE:HB2	1:C:101:LEU:HB3	2.03	0.41
1:B:147:PHE:HA	1:C:325:VAL:HG11	2.03	0.41
1:B:231:ARG:HH21	1:B:266:GLU:CD	2.29	0.41
1:A:98:THR:OG1	1:A:230:LEU:HD21	2.22	0.40
1:A:294:PHE:CD1	1:A:294:PHE:C	2.98	0.40
1:A:221:VAL:HA	1:A:228:PHE:HB2	2.03	0.40
1:A:237:TYR:HB3	1:A:409:HIS:CG	2.57	0.40

All (2) 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:344:HIS:HE2	1:C:134:GLN:OE1[2_555]	1.58	0.02
1:A:344:HIS:NE2	1:C:134:GLN:OE1[2_555]	2.19	0.01

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	363/431 (84%)	324 (89%)	36 (10%)	3 (1%)	16	31
1	B	363/431 (84%)	333 (92%)	27 (7%)	3 (1%)	16	31
1	C	360/431 (84%)	332 (92%)	24 (7%)	4 (1%)	11	22
All	All	1086/1293 (84%)	989 (91%)	87 (8%)	10 (1%)	14	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	LYS
1	B	15	ASN
1	B	220	SER
1	B	221	VAL
1	C	15	ASN
1	C	140	GLY
1	A	139	SER
1	C	142	GLN
1	A	144	GLN
1	C	130	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	330/391 (84%)	312 (94%)	18 (6%)	19	40
1	B	328/391 (84%)	302 (92%)	26 (8%)	11	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	323/391 (83%)	303 (94%)	20 (6%)	16	34
All	All	981/1173 (84%)	917 (94%)	64 (6%)	16	32

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	40	ILE
1	A	71	LEU
1	A	94	GLU
1	A	121	LEU
1	A	127	VAL
1	A	129	ARG
1	A	133	LEU
1	A	139	SER
1	A	141	THR
1	A	204	GLU
1	A	222	SER
1	A	233	ARG
1	A	266	GLU
1	A	322	THR
1	A	325	VAL
1	A	396[A]	ARG
1	A	396[B]	ARG
1	B	39	LYS
1	B	52	TYR
1	B	63	GLN
1	B	71	LEU
1	B	75	SER
1	B	77	LYS
1	B	105	THR
1	B	106	ILE
1	B	126	PRO
1	B	127	VAL
1	B	132	GLN
1	B	134	GLN
1	B	135	SER
1	B	139[A]	SER
1	B	139[B]	SER
1	B	163	GLU
1	B	198	ILE
1	B	206	ILE

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Mol	Chain	Res	Type
1	B	210	SER
1	B	214	LYS
1	B	217	SER
1	B	272	LEU
1	B	299	GLN
1	B	333	SER
1	B	361	ILE
1	B	396	ARG
1	C	24	GLU
1	C	27[A]	HIS
1	C	27[B]	HIS
1	C	36	LYS
1	C	40	ILE
1	C	45	GLN
1	C	55	LYS
1	C	75	SER
1	C	130	PRO
1	C	132	GLN
1	C	133	LEU
1	C	134	GLN
1	C	137	LEU
1	C	139	SER
1	C	173	GLU
1	C	218	LYS
1	C	243	LYS
1	C	293	ASP
1	C	367	GLN
1	C	407	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	27	HIS
1	A	142	GLN
1	B	18	GLN
1	B	365	ASN
1	C	45	GLN
1	C	63	GLN
1	C	132	GLN
1	C	212	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	365/431 (84%)	-0.01	10 (2%) 56 51	16, 35, 66, 118	4 (1%)
1	B	365/431 (84%)	-0.07	10 (2%) 56 51	16, 33, 59, 93	4 (1%)
1	C	363/431 (84%)	-0.05	7 (1%) 66 62	13, 35, 60, 96	3 (0%)
All	All	1093/1293 (84%)	-0.04	27 (2%) 58 54	13, 34, 63, 118	11 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	GLN	4.8
1	A	220	SER	4.3
1	A	221	VAL	4.0
1	B	323	LYS	3.8
1	A	322	THR	3.7
1	B	218	LYS	3.3
1	C	323	LYS	3.3
1	C	141	THR	3.1
1	B	145	PRO	2.9
1	C	27[A]	HIS	2.8
1	A	144	GLN	2.8
1	C	324	GLN	2.7
1	C	142	GLN	2.6
1	B	300	ARG	2.5
1	A	292	GLY	2.5
1	B	219	LYS	2.5
1	B	139[A]	SER	2.5
1	A	219	LYS	2.5
1	B	173	GLU	2.4
1	B	142	GLN	2.4
1	A	323	LYS	2.2
1	C	143	ASN	2.1
1	A	193	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	354	LEU	2.1
1	B	220	SER	2.1
1	A	143	ASN	2.1
1	A	21[A]	TYR	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 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.