



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:52 AM UTC

PDB ID : 1PXY / pdb_00001pxy
Title : Crystal structure of the actin-crosslinking core of Arabidopsis fimbrin
Authors : Klein, M.G.; Shi, W.; Tseng, Y.; Wirtz, D.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2003-07-07
Resolution : 2.40 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

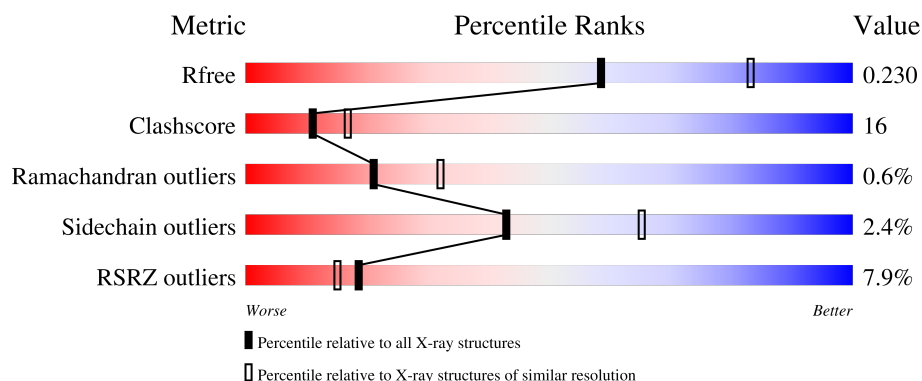
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	506	6% 66% 24% • 8%
1	B	506	8% 59% 34% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7708 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called fimbrin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3725	2386	653	668	18			
1	B	477	Total	C	N	O	S	0	0	0
			3793	2428	663	684	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	GLY	-	cloning artifact	UNP Q7G188
A	119	SER	-	cloning artifact	UNP Q7G188
A	120	PRO	-	cloning artifact	UNP Q7G188
A	121	GLY	-	cloning artifact	UNP Q7G188
A	122	ILE	-	cloning artifact	UNP Q7G188
A	240	LEU	VAL	engineered mutation	UNP Q7G188
B	118	GLY	-	cloning artifact	UNP Q7G188
B	119	SER	-	cloning artifact	UNP Q7G188
B	120	PRO	-	cloning artifact	UNP Q7G188
B	121	GLY	-	cloning artifact	UNP Q7G188
B	122	ILE	-	cloning artifact	UNP Q7G188
B	240	LEU	VAL	engineered mutation	UNP Q7G188

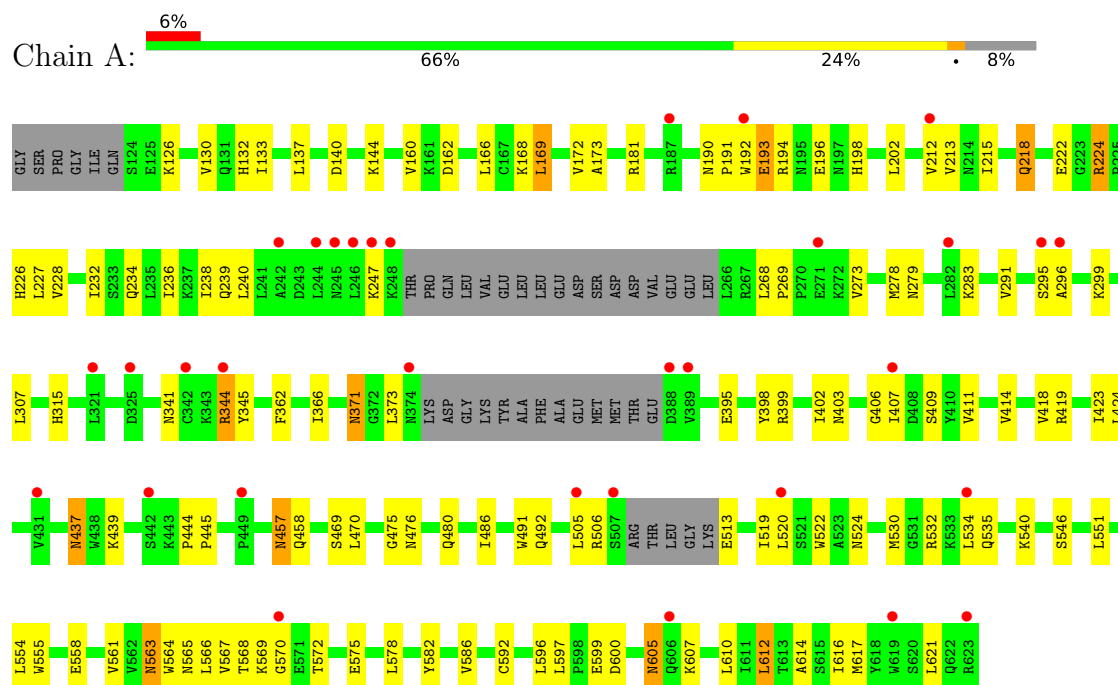
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	112	Total	O	0	0
			112	112		
2	B	78	Total	O	0	0
			78	78		

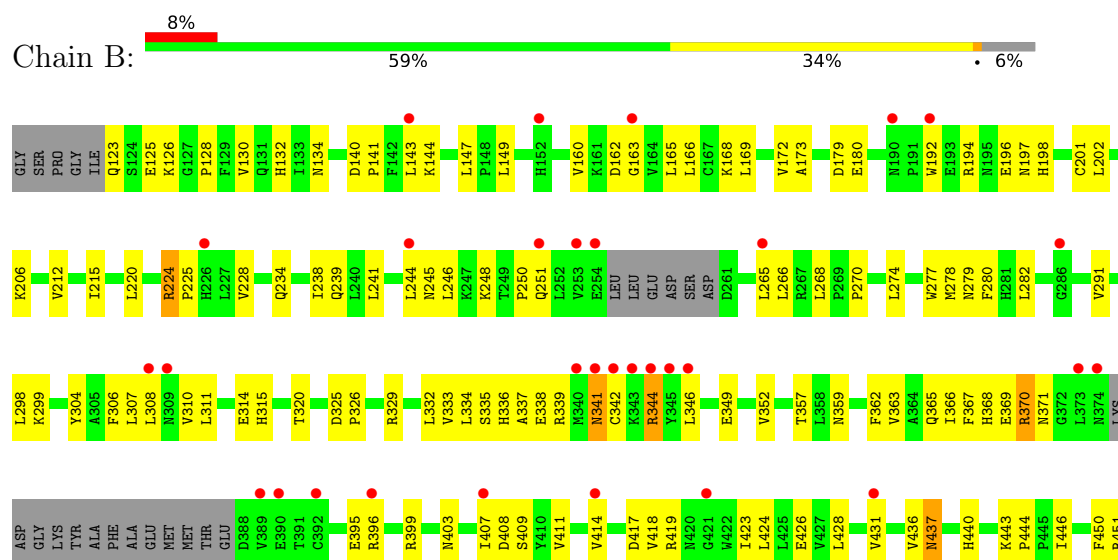
3 Residue-property plots

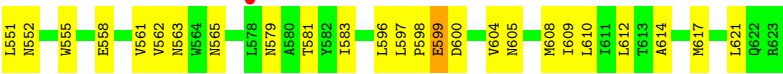
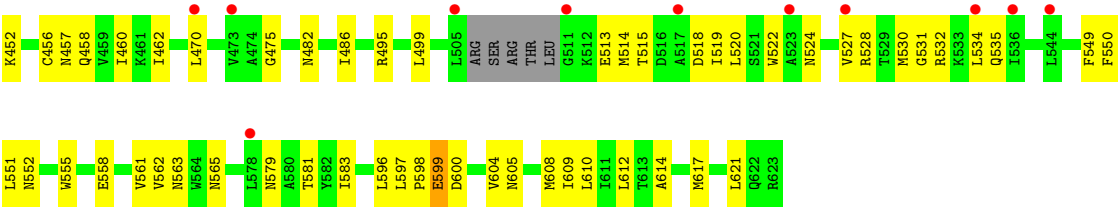
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: fimbrin-like protein



• Molecule 1: fimbrin-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.69Å 104.98Å 104.41Å 90.00° 103.93° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.40) 93.6 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.42Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.270 0.199 , 0.230	Depositor DCC
R_{free} test set	1137 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7708	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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 [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	0.32	0/3794	0.83	5/5129 (0.1%)
1	B	0.31	0/3863	0.82	5/5226 (0.1%)
All	All	0.32	0/7657	0.83	10/10355 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ARG	N-CA-C	6.08	119.80	112.38
1	A	224	ARG	CA-C-N	5.81	125.28	119.24
1	A	224	ARG	C-N-CA	5.81	125.28	119.24
1	B	341	ASN	N-CA-C	5.71	120.06	113.38
1	B	224	ARG	CA-C-N	5.61	126.85	119.84
1	B	224	ARG	C-N-CA	5.61	126.85	119.84
1	B	419	ARG	N-CA-C	5.54	118.25	111.82
1	A	341	ASN	N-CA-C	5.17	118.72	111.74
1	A	193	GLU	N-CA-C	-5.05	105.90	111.71
1	B	436	VAL	N-CA-C	5.03	115.54	108.89

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	3725	0	3834	112	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3793	0	3877	139	0
2	A	112	0	0	4	0
2	B	78	0	0	4	0
All	All	7708	0	7711	249	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 16.

All (249) 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:A:519:ILE:HA	1:A:617:MET:HE1	1.39	1.02
1:A:469:SER:H	1:A:492:GLN:HE22	1.20	0.89
1:B:519:ILE:HA	1:B:617:MET:HE1	1.54	0.87
1:A:437:ASN:H	1:A:458:GLN:HE22	1.24	0.86
1:A:403:ASN:HD21	1:A:411:VAL:H	1.23	0.85
1:A:522:TRP:HB3	1:A:617:MET:HE2	1.64	0.79
1:B:522:TRP:HB3	1:B:617:MET:HE2	1.67	0.77
1:B:403:ASN:HD21	1:B:411:VAL:H	1.31	0.76
1:A:546:SER:HB2	1:A:570:GLY:HA3	1.69	0.75
1:B:395:GLU:HG2	1:B:414:VAL:HG22	1.69	0.74
1:B:534:LEU:HD23	1:B:534:LEU:H	1.53	0.74
1:A:371:ASN:HD22	1:A:373:LEU:H	1.37	0.71
1:B:407:ILE:HG22	2:B:2150:HOH:O	1.90	0.70
1:B:141:PRO:HA	1:B:144:LYS:HE3	1.72	0.70
1:B:245:ASN:HB3	1:B:248:LYS:HG2	1.73	0.69
1:B:304:TYR:HB3	1:B:333:VAL:HG11	1.76	0.68
1:A:476:ASN:O	1:A:480:GLN:HG3	1.93	0.68
1:A:212:VAL:HG23	1:A:215:ILE:HB	1.75	0.68
1:B:212:VAL:HG23	1:B:215:ILE:HD12	1.76	0.67
1:A:279:ASN:O	1:A:283:LYS:HG3	1.94	0.67
1:A:457:ASN:ND2	1:A:475:GLY:H	1.92	0.67
1:A:418:VAL:CG2	1:A:424:LEU:HG	2.26	0.66
1:A:437:ASN:C	1:A:437:ASN:HD22	2.01	0.66
1:B:407:ILE:HG13	1:B:426:GLU:HB3	1.77	0.66
1:A:212:VAL:CG2	1:A:215:ILE:HB	2.26	0.65
1:A:558:GLU:O	1:A:561:VAL:HG22	1.97	0.65
1:B:140:ASP:O	1:B:144:LYS:HG3	1.96	0.65
1:A:371:ASN:ND2	1:A:373:LEU:H	1.95	0.65
1:B:524:ASN:HB3	1:B:535:GLN:OE1	1.97	0.65
1:A:296:ALA:HA	1:A:299:LYS:HG3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ASP:HB2	1:B:581:THR:HG22	1.78	0.64
1:B:278:MET:HE2	1:B:282:LEU:HD11	1.78	0.63
1:A:140:ASP:O	1:A:144:LYS:HB2	1.99	0.62
1:A:279:ASN:HD21	1:A:291:VAL:H	1.44	0.62
1:A:173:ALA:HA	1:A:239:GLN:HB2	1.82	0.62
1:B:457:ASN:HD22	1:B:475:GLY:HA3	1.64	0.62
1:A:132:HIS:HE1	1:A:239:GLN:HE22	1.48	0.62
1:B:134:ASN:HD21	1:B:149:LEU:H	1.48	0.62
1:A:407:ILE:HG12	1:A:409:SER:H	1.65	0.61
1:B:125:GLU:OE1	1:B:357:THR:HG22	2.01	0.61
1:A:395:GLU:HG2	1:A:414:VAL:HG22	1.83	0.61
1:B:530:MET:HE2	1:B:532:ARG:HG2	1.81	0.61
1:B:202:LEU:HG	1:B:212:VAL:HG21	1.81	0.61
1:A:278:MET:HE3	1:A:307:LEU:HD22	1.83	0.60
1:B:265:LEU:HD23	1:B:268:LEU:HD12	1.82	0.60
1:B:399:ARG:HG3	1:B:411:VAL:HG12	1.83	0.60
1:B:522:TRP:CB	1:B:617:MET:HE2	2.30	0.60
1:B:446:ILE:HG21	1:B:452:LYS:HG3	1.83	0.60
1:A:563:ASN:C	1:A:563:ASN:HD22	2.10	0.60
1:A:224:ARG:O	1:A:228:VAL:HG23	2.02	0.60
1:A:212:VAL:HG22	1:A:212:VAL:O	2.01	0.59
1:B:192:TRP:O	1:B:196:GLU:HG3	2.02	0.59
1:A:362:PHE:O	1:A:366:ILE:HG12	2.03	0.59
1:A:572:THR:OG1	1:A:575:GLU:HG3	2.03	0.58
1:B:482:ASN:O	1:B:486:ILE:HG12	2.03	0.58
1:A:437:ASN:ND2	1:A:439:LYS:H	2.01	0.58
1:A:437:ASN:H	1:A:458:GLN:NE2	1.98	0.58
1:B:346:LEU:H	1:B:346:LEU:HD23	1.67	0.58
1:B:336:HIS:HA	1:B:339:ARG:NH1	2.19	0.58
1:A:234:GLN:O	1:A:238:ILE:HG12	2.03	0.58
1:A:522:TRP:CB	1:A:617:MET:HE2	2.32	0.58
1:B:224:ARG:O	1:B:228:VAL:HG23	2.04	0.58
1:B:579:ASN:O	1:B:583:ILE:HG12	2.03	0.58
1:B:437:ASN:H	1:B:458:GLN:HE22	1.52	0.57
1:B:558:GLU:O	1:B:561:VAL:HG22	2.05	0.57
1:A:534:LEU:HD23	1:A:534:LEU:H	1.69	0.57
1:A:162:ASP:CG	1:A:194:ARG:HH12	2.11	0.57
1:B:519:ILE:HD13	1:B:614:ALA:HB2	1.87	0.57
1:A:232:ILE:O	1:A:236:ILE:HG12	2.05	0.56
1:B:362:PHE:O	1:B:366:ILE:HG12	2.05	0.56
1:A:524:ASN:HB3	1:A:535:GLN:OE1	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LYS:HG2	2:B:2129:HOH:O	2.06	0.56
1:B:599:GLU:H	1:B:599:GLU:CD	2.14	0.56
1:A:469:SER:C	1:A:470:LEU:HD22	2.31	0.56
1:B:551:LEU:HG	1:B:583:ILE:HD11	1.86	0.56
1:B:418:VAL:CG2	1:B:424:LEU:HG	2.36	0.56
1:A:519:ILE:HG23	1:A:617:MET:HE3	1.87	0.55
1:B:437:ASN:H	1:B:458:GLN:NE2	2.05	0.55
1:A:437:ASN:HD21	1:A:439:LYS:HB3	1.71	0.55
1:B:437:ASN:C	1:B:437:ASN:HD22	2.15	0.55
1:A:190:ASN:HB3	1:A:191:PRO:HD2	1.89	0.54
1:B:551:LEU:HG	1:B:583:ILE:CD1	2.37	0.54
1:A:399:ARG:HG3	1:A:411:VAL:HG12	1.87	0.54
1:B:605:ASN:O	1:B:609:ILE:HG12	2.08	0.54
1:A:371:ASN:HD22	1:A:373:LEU:N	2.04	0.54
1:B:520:LEU:HD13	1:B:520:LEU:O	2.08	0.54
1:A:437:ASN:C	1:A:437:ASN:ND2	2.66	0.54
1:B:132:HIS:HE1	1:B:239:GLN:HE22	1.56	0.53
1:B:311:LEU:HB3	1:B:370:ARG:HG2	1.90	0.53
1:B:450:PHE:CZ	1:B:451:ARG:NH1	2.76	0.53
1:B:495:ARG:CZ	1:B:499:LEU:HD11	2.38	0.53
1:A:554:LEU:HD21	1:A:616:ILE:HD12	1.90	0.53
1:B:234:GLN:O	1:B:238:ILE:HG12	2.09	0.53
1:B:306:PHE:O	1:B:310:VAL:HG23	2.09	0.53
1:A:592:CYS:SG	1:A:616:ILE:HD13	2.49	0.52
1:B:278:MET:HE1	1:B:298:LEU:CD2	2.38	0.52
1:B:279:ASN:HD21	1:B:291:VAL:H	1.56	0.52
1:B:524:ASN:O	1:B:528:ARG:HD3	2.09	0.52
1:B:212:VAL:CG2	1:B:215:ILE:HB	2.39	0.52
1:B:550:PHE:HZ	1:B:609:ILE:HG23	1.73	0.52
1:B:277:TRP:O	1:B:280:PHE:HB3	2.10	0.52
1:B:314:GLU:HG2	1:B:315:HIS:CD2	2.45	0.52
1:B:165:LEU:HD13	1:B:165:LEU:C	2.35	0.52
1:A:437:ASN:HD22	1:A:439:LYS:H	1.57	0.51
1:A:444:PRO:HA	1:A:445:PRO:C	2.34	0.51
1:B:555:TRP:HD1	1:B:562:VAL:HB	1.75	0.51
1:A:398:TYR:O	1:A:402:ILE:HG13	2.10	0.51
1:A:519:ILE:HD13	1:A:614:ALA:HB2	1.92	0.51
1:A:605:ASN:C	1:A:605:ASN:HD22	2.18	0.51
1:A:582:TYR:O	1:A:586:VAL:HG23	2.10	0.51
1:B:212:VAL:HG22	1:B:215:ILE:HB	1.92	0.51
1:B:278:MET:HE1	1:B:298:LEU:HD21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:THR:H	1:B:518:ASP:HB2	1.74	0.51
1:A:469:SER:N	1:A:492:GLN:HE22	2.00	0.50
1:A:198:HIS:O	1:A:202:LEU:HD13	2.12	0.50
1:A:226:HIS:CE1	1:A:227:LEU:HG	2.46	0.50
1:A:181:ARG:HB3	1:A:566:LEU:HD13	1.94	0.50
1:A:212:VAL:HG23	1:A:215:ILE:HD12	1.92	0.50
1:A:268:LEU:HB2	2:A:2018:HOH:O	2.11	0.50
1:B:598:PRO:HD2	1:B:599:GLU:OE2	2.11	0.50
1:A:546:SER:CB	1:A:570:GLY:HA3	2.40	0.50
1:A:612:LEU:O	1:A:616:ILE:HG12	2.11	0.50
1:B:329:ARG:O	1:B:333:VAL:HG23	2.12	0.50
1:A:597:LEU:O	1:A:600:ASP:HB2	2.12	0.50
1:A:344:ARG:HE	1:A:344:ARG:C	2.19	0.50
1:B:437:ASN:OD1	1:B:440:HIS:HD2	1.95	0.50
1:B:336:HIS:HA	1:B:339:ARG:HH11	1.76	0.49
1:B:359:ASN:O	1:B:363:VAL:HG23	2.12	0.49
1:A:418:VAL:HG22	1:A:424:LEU:HG	1.93	0.49
1:B:344:ARG:HG3	1:B:344:ARG:HH11	1.76	0.49
1:A:563:ASN:HD22	1:A:565:ASN:H	1.61	0.49
1:B:168:LYS:O	1:B:172:VAL:HG23	2.13	0.49
1:B:244:LEU:HB2	1:B:270:PRO:HB3	1.95	0.49
1:B:278:MET:HG3	1:B:307:LEU:HD22	1.94	0.49
1:A:269:PRO:O	1:A:273:VAL:HG23	2.13	0.48
1:A:126:LYS:O	1:A:130:VAL:HG23	2.13	0.48
1:B:320:THR:HA	1:B:332:LEU:HD13	1.94	0.48
1:A:218:GLN:O	1:A:222:GLU:HG3	2.13	0.48
1:B:334:LEU:HB3	1:B:344:ARG:NH1	2.28	0.48
1:B:163:GLY:O	1:B:197:ASN:HB3	2.14	0.48
1:B:212:VAL:HG22	1:B:212:VAL:O	2.14	0.48
1:A:168:LYS:O	1:A:172:VAL:HG23	2.14	0.48
1:A:519:ILE:HG23	1:A:617:MET:CE	2.44	0.48
1:B:335:SER:O	1:B:338:GLU:HB3	2.14	0.48
1:B:428:LEU:HA	1:B:431:VAL:HG12	1.95	0.48
1:A:522:TRP:CD2	1:A:617:MET:HG3	2.49	0.48
1:B:617:MET:O	1:B:621:LEU:HG	2.14	0.48
1:A:399:ARG:NH2	2:A:2050:HOH:O	2.44	0.47
1:B:344:ARG:HD3	1:B:344:ARG:N	2.28	0.47
1:B:522:TRP:CG	1:B:617:MET:HE2	2.48	0.47
1:A:133:ILE:HG23	1:A:137:LEU:HD12	1.95	0.47
1:A:555:TRP:CD1	1:A:564:TRP:HE1	2.31	0.47
1:A:457:ASN:HD21	1:A:475:GLY:H	1.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:HIS:O	1:B:201:CYS:HB3	2.14	0.47
1:B:320:THR:HG22	1:B:332:LEU:HB3	1.97	0.47
1:A:563:ASN:ND2	1:A:565:ASN:H	2.13	0.47
1:B:337:ALA:HB1	1:B:342:CYS:SG	2.55	0.47
1:A:445:PRO:HD2	1:B:349:GLU:HG3	1.97	0.47
1:B:173:ALA:HA	1:B:239:GLN:HB2	1.96	0.47
1:B:123:GLN:N	2:B:2114:HOH:O	2.48	0.46
1:B:530:MET:HG3	1:B:531:GLY:N	2.31	0.46
1:A:532:ARG:HB3	1:A:534:LEU:CD2	2.46	0.46
1:B:458:GLN:HE21	1:B:462:ILE:HD11	1.80	0.46
1:B:456:CYS:O	1:B:460:ILE:HD13	2.15	0.46
1:B:367:PHE:C	1:B:369:GLU:H	2.22	0.46
1:A:540:LYS:HG2	1:A:540:LYS:O	2.15	0.46
1:A:522:TRP:CG	1:A:617:MET:HE2	2.51	0.46
1:B:520:LEU:HD13	1:B:524:ASN:ND2	2.31	0.46
1:B:407:ILE:HG23	1:B:409:SER:O	2.16	0.46
1:B:534:LEU:H	1:B:534:LEU:CD2	2.26	0.46
1:A:411:VAL:HG22	1:A:423:ILE:HD13	1.98	0.45
1:B:140:ASP:HB3	1:B:143:LEU:HB2	1.98	0.45
1:B:246:LEU:HD12	1:B:266:LEU:HD23	1.98	0.45
1:B:160:VAL:HG23	1:B:166:LEU:HG	1.98	0.45
1:A:491:TRP:NE1	1:A:607:LYS:HE3	2.32	0.45
1:A:596:LEU:H	1:A:596:LEU:HD23	1.82	0.45
1:B:147:LEU:HD23	1:B:149:LEU:HG	1.99	0.45
1:A:569:LYS:O	1:A:575:GLU:HB3	2.17	0.45
1:B:241:LEU:HB3	1:B:244:LEU:HD12	1.99	0.45
1:B:362:PHE:CZ	1:B:366:ILE:HD11	2.51	0.45
1:B:396:ARG:NH1	1:B:597:LEU:HD21	2.32	0.45
1:B:344:ARG:HD3	1:B:344:ARG:H	1.81	0.45
1:B:202:LEU:O	1:B:206:LYS:HG3	2.16	0.44
1:B:320:THR:HG22	1:B:332:LEU:HD13	1.99	0.44
1:A:160:VAL:HG23	1:A:166:LEU:HG	1.99	0.44
1:B:514:MET:SD	1:B:518:ASP:HB3	2.58	0.44
1:A:418:VAL:HG11	1:A:486:ILE:HD13	2.00	0.44
1:A:470:LEU:HD22	1:A:470:LEU:N	2.33	0.44
1:B:514:MET:CE	1:B:518:ASP:HB3	2.48	0.44
1:B:555:TRP:CD1	1:B:562:VAL:HB	2.52	0.44
1:B:534:LEU:HD11	1:B:552:ASN:HD22	1.83	0.43
1:A:522:TRP:HB3	1:A:617:MET:CE	2.42	0.43
1:A:315:HIS:HD2	2:A:2039:HOH:O	2.00	0.43
1:B:162:ASP:OD1	1:B:194:ARG:NH1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ARG:HB3	1:B:534:LEU:HD23	2.00	0.43
1:A:520:LEU:HD13	1:A:520:LEU:C	2.44	0.43
1:B:443:LYS:HA	1:B:444:PRO:HD3	1.89	0.43
1:A:551:LEU:HD13	1:A:567:VAL:CG1	2.49	0.43
1:A:568:THR:HG21	1:A:578:LEU:HD23	2.01	0.43
1:B:460:ILE:N	1:B:460:ILE:HD12	2.34	0.43
1:A:192:TRP:O	1:A:196:GLU:HG3	2.18	0.43
1:A:169:LEU:O	1:A:172:VAL:HB	2.19	0.43
1:B:597:LEU:O	1:B:600:ASP:HB2	2.18	0.42
1:A:403:ASN:ND2	1:A:411:VAL:H	2.04	0.42
1:B:125:GLU:C	1:B:128:PRO:HD2	2.44	0.42
1:B:534:LEU:HD11	1:B:552:ASN:ND2	2.34	0.42
1:B:245:ASN:HD22	1:B:246:LEU:N	2.17	0.42
1:B:530:MET:CE	1:B:532:ARG:HG2	2.47	0.42
1:A:215:ILE:HG12	1:A:227:LEU:HD22	1.99	0.42
1:B:308:LEU:HD13	1:B:336:HIS:HB3	2.02	0.42
1:B:342:CYS:HB2	1:B:365:GLN:HE21	1.84	0.42
1:B:457:ASN:ND2	1:B:475:GLY:HA3	2.34	0.42
1:A:437:ASN:HD21	1:A:439:LYS:CB	2.32	0.42
1:A:140:ASP:O	1:A:144:LYS:N	2.53	0.42
1:A:418:VAL:CG1	1:A:486:ILE:HD13	2.50	0.42
1:B:220:LEU:N	1:B:220:LEU:HD22	2.34	0.42
1:B:194:ARG:HG3	1:B:194:ARG:HH11	1.84	0.42
1:A:578:LEU:HG	2:A:2015:HOH:O	2.19	0.42
1:B:368:HIS:HB3	2:B:2182:HOH:O	2.19	0.42
1:B:407:ILE:HG12	1:B:408:ASP:N	2.35	0.42
1:B:563:ASN:ND2	1:B:565:ASN:H	2.18	0.41
1:A:162:ASP:HA	1:A:194:ARG:HH11	1.85	0.41
1:B:244:LEU:HD13	1:B:274:LEU:HB2	2.02	0.41
1:B:417:ASP:O	1:B:423:ILE:HD12	2.19	0.41
1:B:304:TYR:HB3	1:B:333:VAL:CG1	2.47	0.41
1:A:191:PRO:HG2	1:A:192:TRP:CD1	2.56	0.41
1:B:126:LYS:O	1:B:130:VAL:HG23	2.20	0.41
1:B:527:VAL:HG21	1:B:549:PHE:CE1	2.56	0.41
1:A:295:SER:O	1:A:299:LYS:HG3	2.20	0.41
1:A:445:PRO:HG3	1:B:352:VAL:HG21	2.03	0.41
1:B:437:ASN:C	1:B:437:ASN:ND2	2.78	0.41
1:A:213:VAL:HG11	1:A:406:GLY:HA2	2.02	0.41
1:A:132:HIS:HE1	1:A:239:GLN:NE2	2.14	0.41
1:A:520:LEU:HD13	1:A:524:ASN:ND2	2.36	0.41
1:B:325:ASP:OD1	1:B:326:PRO:HD2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:TRP:CH2	1:B:617:MET:HA	2.56	0.41
1:A:132:HIS:HD2	1:A:345:TYR:OH	2.03	0.40
1:A:190:ASN:ND2	1:A:193:GLU:OE1	2.54	0.40
1:B:335:SER:O	1:B:339:ARG:HG3	2.21	0.40
1:A:505:LEU:HD23	1:A:621:LEU:HB2	2.03	0.40
1:A:610:LEU:HD23	1:A:610:LEU:C	2.46	0.40
1:B:224:ARG:HA	1:B:225:PRO:HD2	1.76	0.40
1:B:470:LEU:HD22	1:B:470:LEU:N	2.37	0.40
1:B:534:LEU:HD23	1:B:534:LEU:N	2.29	0.40
1:B:563:ASN:HD21	1:B:565:ASN:HD22	1.69	0.40
1:B:608:MET:HE2	1:B:608:MET:HA	2.03	0.40
1:A:506:ARG:HH22	1:A:513:GLU:CG	2.35	0.40
1:A:530:MET:HE3	1:A:555:TRP:CH2	2.57	0.40
1:B:596:LEU:H	1:B:596:LEU:HD23	1.86	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	457/506 (90%)	439 (96%)	17 (4%)	1 (0%)	43	58
1	B	469/506 (93%)	438 (93%)	26 (6%)	5 (1%)	11	18
All	All	926/1012 (92%)	877 (95%)	43 (5%)	6 (1%)	21	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	GLU
1	B	251	GLN
1	A	247	LYS
1	B	371	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	250	PRO
1	B	604	VAL

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	416/452 (92%)	405 (97%)	11 (3%)	40	63
1	B	420/452 (93%)	411 (98%)	9 (2%)	47	69
All	All	836/904 (92%)	816 (98%)	20 (2%)	43	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	218	GLN
1	A	240	LEU
1	A	344	ARG
1	A	371	ASN
1	A	437	ASN
1	A	457	ASN
1	A	563	ASN
1	A	599	GLU
1	A	605	ASN
1	A	612	LEU
1	B	169	LEU
1	B	341	ASN
1	B	344	ARG
1	B	370	ARG
1	B	437	ASN
1	B	513	GLU
1	B	599	GLU
1	B	610	LEU
1	B	612	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	132	HIS
1	A	134	ASN
1	A	154	ASN
1	A	190	ASN
1	A	226	HIS
1	A	239	GLN
1	A	279	ASN
1	A	315	HIS
1	A	371	ASN
1	A	374	ASN
1	A	403	ASN
1	A	412	ASN
1	A	437	ASN
1	A	440	HIS
1	A	457	ASN
1	A	458	GLN
1	A	465	GLN
1	A	480	GLN
1	A	492	GLN
1	A	563	ASN
1	A	605	ASN
1	A	622	GLN
1	B	132	HIS
1	B	134	ASN
1	B	154	ASN
1	B	239	GLN
1	B	245	ASN
1	B	279	ASN
1	B	315	HIS
1	B	341	ASN
1	B	365	GLN
1	B	374	ASN
1	B	403	ASN
1	B	437	ASN
1	B	440	HIS
1	B	457	ASN
1	B	458	GLN
1	B	472	ASN
1	B	480	GLN
1	B	552	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	563	ASN
1	B	605	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	465/506 (91%)	0.87	32 (6%)	23 19	15, 33, 64, 81	0
1	B	477/506 (94%)	1.00	42 (8%)	15 12	21, 44, 70, 80	0
All	All	942/1012 (93%)	0.94	74 (7%)	18 15	15, 39, 68, 81	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	CYS	5.0
1	A	192	TRP	4.2
1	A	407	ILE	4.1
1	A	246	LEU	4.1
1	B	253	VAL	3.8
1	B	192	TRP	3.6
1	B	517	ALA	3.5
1	B	374	ASN	3.4
1	B	341	ASN	3.4
1	B	373	LEU	3.3
1	A	248	LYS	3.3
1	A	247	LYS	3.1
1	B	407	ILE	3.1
1	B	251	GLN	3.0
1	A	271	GLU	3.0
1	A	321	LEU	3.0
1	B	396	ARG	2.9
1	B	265	LEU	2.9
1	A	245	ASN	2.9
1	A	505	LEU	2.9
1	A	242	ALA	2.8
1	B	511	GLY	2.8
1	B	346	LEU	2.8
1	B	414	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	623	ARG	2.7
1	B	343	LYS	2.7
1	B	226	HIS	2.7
1	A	296	ALA	2.6
1	B	392	CYS	2.6
1	A	507	SER	2.6
1	A	342	CYS	2.6
1	A	534	LEU	2.6
1	B	389	VAL	2.6
1	B	470	LEU	2.6
1	B	344	ARG	2.5
1	A	570	GLY	2.5
1	A	374	ASN	2.5
1	B	536	ILE	2.5
1	B	244	LEU	2.5
1	B	534	LEU	2.4
1	B	152	HIS	2.4
1	A	212	VAL	2.4
1	A	431	VAL	2.4
1	B	143	LEU	2.4
1	A	520	LEU	2.4
1	B	308	LEU	2.4
1	B	473	VAL	2.3
1	B	527	VAL	2.3
1	A	295	SER	2.3
1	B	286	GLY	2.2
1	A	187	ARG	2.2
1	B	309	ASN	2.2
1	A	389	VAL	2.2
1	B	431	VAL	2.2
1	B	544	LEU	2.2
1	A	388	ASP	2.2
1	B	254	GLU	2.2
1	B	345	TYR	2.2
1	A	442	SER	2.2
1	B	390	GLU	2.1
1	A	606	GLN	2.1
1	A	244	LEU	2.1
1	A	282	LEU	2.1
1	B	505	LEU	2.1
1	B	578	LEU	2.1
1	A	344	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	190	ASN	2.0
1	A	619	TRP	2.0
1	B	421	GLY	2.0
1	A	325	ASP	2.0
1	A	449	PRO	2.0
1	B	340	MET	2.0
1	B	523	ALA	2.0
1	B	163	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.