



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:24 pm GMT

PDB ID : 1PXY
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

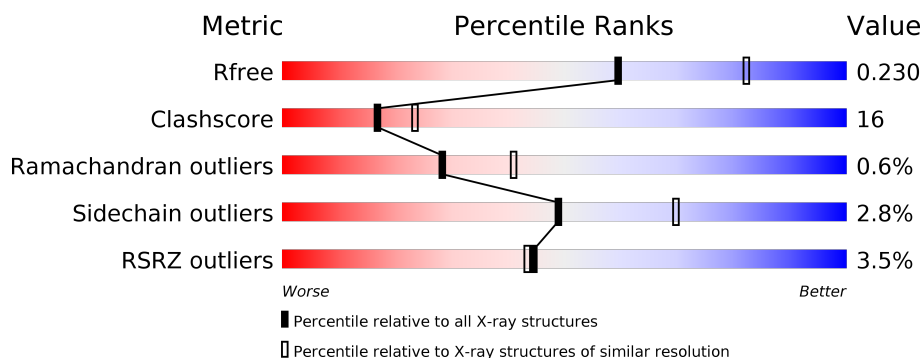
1 Overall quality at a glance

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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>• 8%</div> </div> </div>
1	B	506	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>• 6%</div> </div> </div>

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.

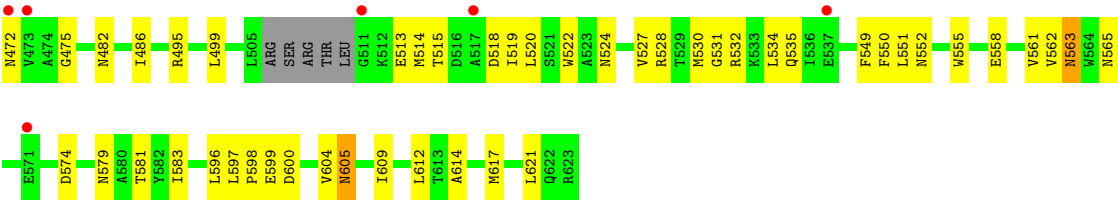
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3725	2386	653	668	18			
1	B	477	Total	C	N	O	S	0	0	0
			3793	2428	663	684	18			

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	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	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		



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 29.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.40) 93.8 (29.22-2.40)	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	No test flags present.	DCC
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 , 57.2	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

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	0.28	0/3794	0.50	0/5129
1	B	0.27	0/3863	0.48	0/5226
All	All	0.28	0/7657	0.49	0/10355

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3725	0	3834	106	0
1	B	3793	0	3877	135	0
2	A	112	0	0	4	0
2	B	78	0	0	4	0
All	All	7708	0	7711	239	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 (239) 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:HG23	1:A:617:MET:HE3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:SER:H	1:A:492:GLN:HE22	1.20	0.89
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:B:403:ASN:HD21	1:B:411:VAL:H	1.31	0.76
1:A:519:ILE:HA	1:A:617:MET:HE1	1.68	0.75
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:278:MET:HE2	1:B:291:VAL:HG21	1.76	0.67
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: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
1:B:179:ASP:HB2	1:B:581:THR:HG22	1.78	0.64
1:A:437:ASN:C	1:A:437:ASN:HD22	2.01	0.64
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:202:LEU:HG	1:B:212:VAL:HG21	1.81	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ILE:HG21	1:B:452:LYS:HG3	1.83	0.60
1:A:224:ARG:O	1:A:228:VAL:HG23	2.02	0.60
1:B:519:ILE:HG23	1:B:617:MET:HE3	1.82	0.60
1:A:212:VAL:O	1:A:212:VAL:HG22	2.01	0.59
1:A:522:TRP:HB3	1:A:617:MET:HE1	1.83	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:A:522:TRP:CE3	1:A:617:MET:HE2	2.39	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: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:H	1:A:534:LEU:HD23	1.69	0.57
1:B:519:ILE:HD13	1:B:614:ALA:HB2	1.87	0.57
1:A:519:ILE:HA	1:A:617:MET:CE	2.33	0.56
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
1:B:299:LYS:HG2	2:B:2129:HOH:O	2.06	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: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:A:563:ASN:HD22	1:A:563:ASN:C	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:162:ASP:CG	1:A:194:ARG:HH12	2.11	0.52
1:A:592:CYS:SG	1:A:616:ILE:HD13	2.49	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:522:TRP:CE3	1:B:617:MET:HE2	2.44	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:A:437:ASN:HD22	1:A:439:LYS:H	1.57	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:469:SER:C	1:A:470:LEU:HD22	2.31	0.51
1:A:519:ILE:HD13	1:A:614:ALA:HB2	1.92	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: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:B:599:GLU:H	1:B:599:GLU:CD	2.14	0.50
1:B:519:ILE:HA	1:B:617:MET:CE	2.41	0.50
1:A:226:HIS:CE1	1:A:227:LEU:HG	2.46	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:A:181:ARG:HB3	1:A:566:LEU:HD13	1.94	0.50
1:B:437:ASN:C	1:B:437:ASN:HD22	2.15	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: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:A:522:TRP:HB3	1:A:617:MET:CE	2.42	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:HH11	1:B:344:ARG:HG3	1.76	0.49
1:A:563:ASN:HD22	1:A:565:ASN:H	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:522:TRP:HB3	1:B:617:MET:HE1	1.95	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: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:N	1:B:344:ARG:HD3	2.28	0.47
1:A:133:ILE:HG23	1:A:137:LEU:HD12	1.95	0.47
1:A:444:PRO:HA	1:A:445:PRO:C	2.34	0.47
1:A:457:ASN:HD21	1:A:475:GLY:H	1.61	0.47
1:B:165:LEU:C	1:B:165:LEU:HD13	2.35	0.47
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:B:173:ALA:HA	1:B:239:GLN:HB2	1.96	0.47
1:A:445:PRO:HD2	1:B:349:GLU:HG3	1.97	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:A:605:ASN:C	1:A:605:ASN:HD22	2.18	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:A:540:LYS:O	1:A:540:LYS:HG2	2.15	0.46
1:B:522:TRP:HB3	1:B:617:MET:CE	2.45	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:CD2	1:B:534:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD12	1:B:266:LEU:HD23	1.98	0.45
1:A:344:ARG:HE	1:A:344:ARG:C	2.19	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:530:MET:CE	1:B:532:ARG:HG2	2.47	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:A:437:ASN:ND2	1:A:437:ASN:C	2.66	0.44
1:B:514:MET:SD	1:B:518:ASP:HB3	2.58	0.44
1:B:519:ILE:HA	1:B:617:MET:HE1	1.99	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: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
1:B:532:ARG:HB3	1:B:534:LEU:HD23	2.00	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:367:PHE:C	1:B:369:GLU:H	2.22	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:B:194:ARG:HG3	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: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:B:325:ASP:OD1	1:B:326:PRO:HD2	2.21	0.41
1:B:522:TRP:CH2	1:B:617:MET:HA	2.56	0.41
1:A:520:LEU:HD13	1:A:524:ASN:ND2	2.36	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: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:N	1:B:534:LEU:HD23	2.29	0.40
1:B:563:ASN:HD21	1:B:565:ASN:HD22	1.69	0.40
1:A:506:ARG:HH22	1:A:513:GLU:CG	2.35	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%)	51	67
1	B	469/506 (93%)	438 (93%)	26 (6%)	5 (1%)	17	23
All	All	926/1012 (92%)	877 (95%)	43 (5%)	6 (1%)	28	41

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
1	B	250	PRO
1	B	604	VAL

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	416/452 (92%)	407 (98%)	9 (2%)	57	76
1	B	420/452 (93%)	406 (97%)	14 (3%)	43	64
All	All	836/904 (92%)	813 (97%)	23 (3%)	49	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	169	LEU
1	A	344	ARG
1	A	371	ASN
1	A	437	ASN
1	A	563	ASN
1	A	577	ARG
1	A	605	ASN
1	A	612	LEU
1	B	169	LEU
1	B	187	ARG
1	B	245	ASN
1	B	341	ASN
1	B	344	ARG
1	B	370	ARG
1	B	374	ASN
1	B	437	ASN
1	B	472	ASN
1	B	513	GLU
1	B	563	ASN
1	B	574	ASP
1	B	605	ASN
1	B	612	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	132	HIS
1	A	134	ASN
1	A	190	ASN
1	A	226	HIS
1	A	239	GLN
1	A	279	ASN
1	A	315	HIS
1	A	359	ASN
1	A	371	ASN
1	A	374	ASN
1	A	403	ASN
1	A	437	ASN
1	A	440	HIS
1	A	457	ASN
1	A	458	GLN

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Mol	Chain	Res	Type
1	A	465	GLN
1	A	492	GLN
1	A	563	ASN
1	A	605	ASN
1	B	132	HIS
1	B	134	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	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 carbohydrates 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%)	-0.08	11 (2%) 59 56	15, 33, 64, 81	0
1	B	477/506 (94%)	0.16	22 (4%) 33 31	21, 44, 70, 80	0
All	All	942/1012 (93%)	0.04	33 (3%) 44 43	15, 39, 68, 81	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	TRP	6.7
1	A	187	ARG	5.0
1	B	389	VAL	4.9
1	A	192	TRP	4.5
1	A	623	ARG	3.9
1	B	246	LEU	3.9
1	A	213	VAL	3.7
1	A	267	ARG	3.6
1	A	507	SER	3.5
1	B	390	GLU	3.4
1	B	517	ALA	3.4
1	A	246	LEU	3.2
1	A	374	ASN	3.2
1	B	341	ASN	3.0
1	B	471	VAL	2.7
1	A	245	ASN	2.7
1	B	374	ASN	2.7
1	B	267	ARG	2.7
1	B	345	TYR	2.6
1	B	250	PRO	2.6
1	B	511	GLY	2.5
1	B	373	LEU	2.4
1	B	288	LYS	2.4
1	B	388	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	265	LEU	2.3
1	B	473	VAL	2.3
1	B	472	ASN	2.2
1	B	324	LYS	2.2
1	A	268	LEU	2.2
1	B	537	GLU	2.2
1	B	190	ASN	2.1
1	B	571	GLU	2.1
1	A	152	HIS	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 carbohydrates 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.