Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:21 pm BST

PDB ID	:	3JYM
Title	:	Crystal Structure of the 3 FKBP domains of wheat FKBP73
Authors	:	Dym, O.; Breiman, A.; Israel Structural Proteomics Center (ISPC)
Deposited on	:	2009-09-22
Resolution	:	2.28 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 following versions of software and data (see references ⓘ) were used in the production of this report:

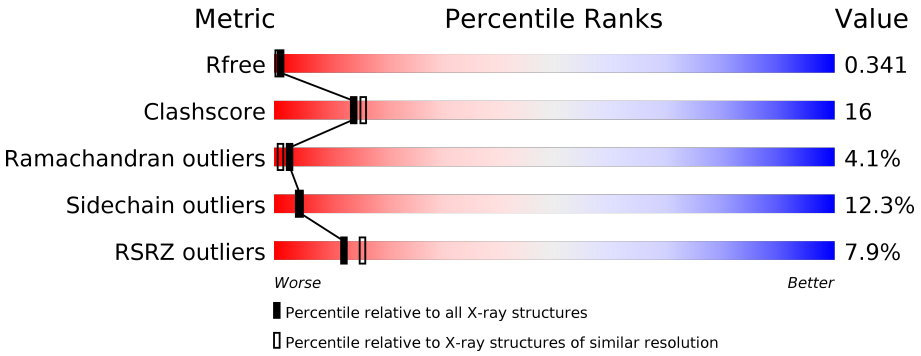
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 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	377	7% 44% 29% 6% • 20%
1	B	377	6% 48% 24% 7% • 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4726 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 FK506-binding protein (FKBP) from wheat.

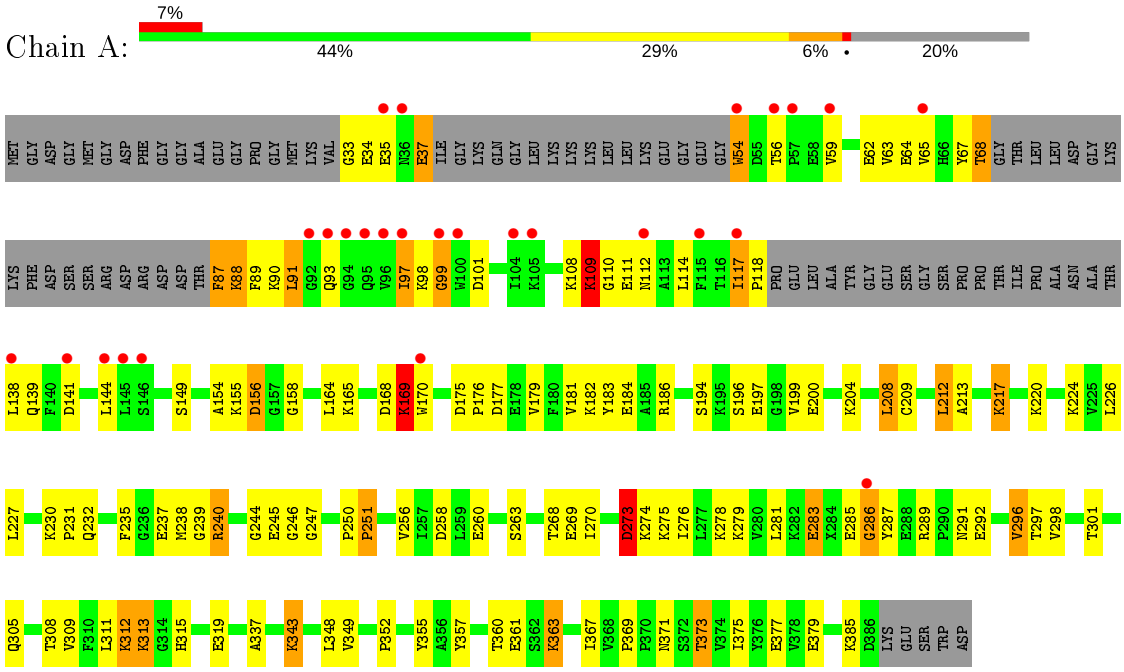
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2344	1501	378	460	5			
1	B	308	Total	C	N	O	S	0	0	0
			2382	1523	385	469	5			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

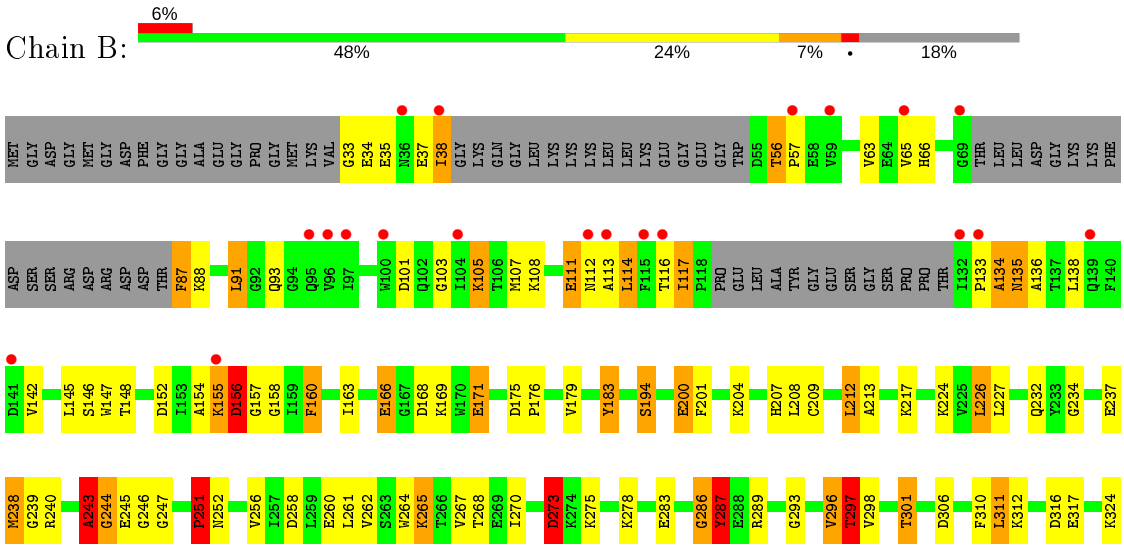
- Molecule 1: FK506-binding protein (FKBP) from wheat

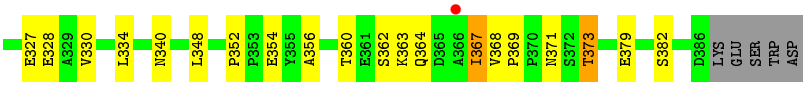
Chain A:



- Molecule 1: FK506-binding protein (FKBP) from wheat

Chain B:




E327
E328
A329
V330
L334
N340
L348
P352
P353
E354
Y355
A356
T360
E361
S362
K363
Q364
D365
A366
I367
V368
P369
P370
N371
S372
T373
E379
S382
D386
LYS
GLU
SER
TRP
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	186.96Å 31.01Å 68.98Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	46.63 – 2.28 46.65 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.63-2.28) 98.6 (46.65-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.97 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.270 , 0.343 0.271 , 0.341	Depositor DCC
R_{free} test set	1834 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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	1.68	32/2382 (1.3%)	1.29	10/3210 (0.3%)
1	B	1.54	19/2419 (0.8%)	1.25	11/3261 (0.3%)
All	All	1.61	51/4801 (1.1%)	1.27	21/6471 (0.3%)

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	1	1
1	B	0	4
All	All	1	5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	CYS	CB-SG	-12.13	1.61	1.82
1	A	209	CYS	CB-SG	-11.82	1.62	1.82
1	A	355	TYR	CD2-CE2	-7.48	1.28	1.39
1	A	244	GLY	N-CA	7.44	1.57	1.46
1	A	283	GLU	CB-CG	-7.09	1.38	1.52
1	A	355	TYR	CD1-CE1	-6.50	1.29	1.39
1	B	379	GLU	CD-OE1	-6.50	1.18	1.25
1	A	273	ASP	CB-CG	-6.15	1.38	1.51
1	A	377	GLU	CD-OE1	-6.14	1.18	1.25
1	B	201	PHE	CE1-CZ	6.00	1.48	1.37
1	B	166	GLU	CG-CD	5.99	1.60	1.51
1	A	268	THR	CB-CG2	-5.95	1.32	1.52
1	A	199	VAL	CB-CG2	5.93	1.65	1.52
1	A	377	GLU	CD-OE2	-5.91	1.19	1.25
1	B	200	GLU	CD-OE2	-5.86	1.19	1.25
1	B	194	SER	CB-OG	-5.85	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	ALA	CA-CB	-5.70	1.40	1.52
1	A	313	LYS	CE-NZ	-5.59	1.35	1.49
1	A	213	ALA	CA-CB	-5.56	1.40	1.52
1	A	343	LYS	CE-NZ	5.54	1.62	1.49
1	B	371	ASN	CB-CG	5.50	1.63	1.51
1	A	263	SER	CB-OG	-5.47	1.35	1.42
1	A	357	TYR	CB-CG	-5.46	1.43	1.51
1	B	247	GLY	N-CA	5.46	1.54	1.46
1	A	296	VAL	CB-CG1	-5.42	1.41	1.52
1	B	265	LYS	CB-CG	5.41	1.67	1.52
1	B	183	TYR	CD2-CE2	5.39	1.47	1.39
1	A	312	LYS	C-O	-5.36	1.13	1.23
1	A	165	LYS	CE-NZ	5.36	1.62	1.49
1	A	337	ALA	C-O	-5.35	1.13	1.23
1	B	262	VAL	CB-CG2	-5.33	1.41	1.52
1	A	371	ASN	CB-CG	5.27	1.63	1.51
1	A	312	LYS	CB-CG	-5.26	1.38	1.52
1	A	283	GLU	CG-CD	-5.26	1.44	1.51
1	B	301	THR	CB-CG2	-5.23	1.35	1.52
1	A	37	GLU	C-O	5.22	1.33	1.23
1	A	196	SER	CB-OG	-5.22	1.35	1.42
1	A	292	GLU	CG-CD	5.20	1.59	1.51
1	B	379	GLU	CD-OE2	-5.17	1.20	1.25
1	A	176	PRO	CA-C	5.13	1.63	1.52
1	B	283	GLU	CD-OE2	5.13	1.31	1.25
1	A	379	GLU	CD-OE1	-5.09	1.20	1.25
1	B	160	PHE	CD1-CE1	5.09	1.49	1.39
1	A	181	VAL	CA-CB	5.08	1.65	1.54
1	A	194	SER	CB-OG	-5.06	1.35	1.42
1	A	379	GLU	CD-OE2	-5.04	1.20	1.25
1	B	297	THR	CB-CG2	-5.04	1.35	1.52
1	A	319	GLU	C-O	-5.04	1.13	1.23
1	A	164	LEU	N-CA	-5.04	1.36	1.46
1	B	356	ALA	CA-CB	5.03	1.63	1.52
1	B	256	VAL	CB-CG2	5.01	1.63	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	GLY	N-CA-C	-8.12	92.80	113.10
1	A	240	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	B	316	ASP	CB-CG-OD1	-7.08	111.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	244	GLY	N-CA-C	-6.96	95.69	113.10
1	B	88	LYS	N-CA-C	-6.31	93.97	111.00
1	B	306	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	240	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	B	156	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	B	227	LEU	CB-CG-CD1	-5.84	101.06	111.00
1	A	286	GLY	N-CA-C	5.84	127.71	113.10
1	A	227	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	B	273	ASP	CB-CA-C	-5.69	99.02	110.40
1	B	287	TYR	CB-CA-C	5.61	121.62	110.40
1	A	177	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	234	GLY	N-CA-C	-5.19	100.12	113.10
1	A	273	ASP	N-CA-C	5.18	124.99	111.00
1	A	268	THR	OG1-CB-CG2	5.17	121.90	110.00
1	A	244	GLY	N-CA-C	-5.16	100.19	113.10
1	A	289	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	240	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	B	145	LEU	CA-CB-CG	5.04	126.88	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	268	THR	CB

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	GLU	Peptide
1	B	155	LYS	Peptide
1	B	243	ALA	Peptide
1	B	286	GLY	Peptide
1	B	87	PHE	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	2344	0	2347	63	0
1	B	2382	0	2392	85	0
All	All	4726	0	4739	148	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 (148) 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:273:ASP:OD1	1:A:275:LYS:HD2	1.27	1.33
1:B:273:ASP:OD1	1:B:275:LYS:CD	1.90	1.18
1:B:273:ASP:OD1	1:B:275:LYS:HD2	0.93	1.10
1:B:243:ALA:HB1	1:B:244:GLY:HA3	1.11	1.06
1:A:65:VAL:O	1:A:87:PHE:N	2.00	0.94
1:B:35:GLU:OE1	1:B:113:ALA:HB1	1.67	0.94
1:B:243:ALA:CB	1:B:244:GLY:HA3	1.98	0.94
1:B:243:ALA:HB1	1:B:244:GLY:CA	1.99	0.91
1:B:324:LYS:HD3	1:B:327:GLU:OE2	1.74	0.87
1:A:175:ASP:OD1	1:A:217:LYS:HE3	1.77	0.84
1:B:65:VAL:H	1:B:87:PHE:N	1.77	0.82
1:A:269:GLU:HB3	1:A:274:LYS:HB3	1.64	0.79
1:B:183:TYR:OH	1:B:207:HIS:HE1	1.67	0.78
1:A:273:ASP:OD1	1:A:275:LYS:CD	2.23	0.73
1:B:311:LEU:HD12	1:B:312:LYS:N	2.05	0.72
1:A:89:PHE:HE1	1:A:101:ASP:OD1	1.74	0.69
1:A:87:PHE:HA	1:A:88:LYS:HB2	1.75	0.69
1:B:134:ALA:O	1:B:136:ALA:N	2.25	0.69
1:B:108:LYS:O	1:B:111:GLU:HB3	1.93	0.69
1:B:65:VAL:O	1:B:87:PHE:HB2	1.93	0.68
1:A:184:GLU:OE2	1:A:186:ARG:NH1	2.27	0.68
1:A:63:VAL:CG1	1:A:91:LEU:HD12	2.25	0.66
1:B:107:MET:HE3	1:B:111:GLU:HG2	1.78	0.64
1:A:34:GLU:HG2	1:A:35:GLU:H	1.62	0.64
1:B:226:LEU:C	1:B:226:LEU:HD23	2.18	0.64
1:B:152:ASP:HB2	1:B:160:PHE:CE1	2.33	0.64
1:A:90:LYS:HB3	1:A:93:GLN:HG3	1.80	0.63
1:A:226:LEU:HD21	1:A:256:VAL:HG13	1.80	0.63
1:B:107:MET:HE1	1:B:142:VAL:O	1.99	0.62
1:B:117:ILE:O	1:B:117:ILE:CG2	2.48	0.61
1:A:367:ILE:O	1:A:369:PRO:HD3	2.02	0.60
1:A:237:GLU:O	1:A:251:PRO:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PRO:HA	1:B:373:THR:HB	1.84	0.59
1:B:293:GLY:HA2	1:B:324:LYS:HE3	1.84	0.58
1:A:63:VAL:HG11	1:A:91:LEU:HD12	1.85	0.58
1:B:237:GLU:HA	1:B:252:ASN:OD1	2.03	0.58
1:B:38:ILE:O	1:B:112:ASN:HB2	2.03	0.58
1:A:183:TYR:HA	1:A:258:ASP:O	2.03	0.57
1:B:34:GLU:CG	1:B:35:GLU:H	2.17	0.57
1:B:154:ALA:C	1:B:156:ASP:HB2	2.25	0.57
1:B:367:ILE:O	1:B:369:PRO:HD3	2.05	0.57
1:A:97:ILE:O	1:A:99:GLY:N	2.37	0.57
1:A:179:VAL:O	1:A:200:GLU:HA	2.06	0.56
1:B:91:LEU:HD21	1:B:105:LYS:HB2	1.86	0.56
1:B:243:ALA:CB	1:B:244:GLY:CA	2.70	0.56
1:B:38:ILE:HB	1:B:112:ASN:HB3	1.86	0.56
1:A:311:LEU:HD12	1:A:312:LYS:N	2.20	0.56
1:B:200:GLU:OE2	1:B:265:LYS:NZ	2.35	0.55
1:A:208:LEU:HB3	1:A:212:LEU:HD22	1.88	0.55
1:B:293:GLY:O	1:B:324:LYS:HE3	2.07	0.55
1:B:111:GLU:HG3	1:B:112:ASN:O	2.07	0.55
1:A:273:ASP:HB3	1:A:275:LYS:H	1.71	0.54
1:B:293:GLY:O	1:B:324:LYS:HG3	2.08	0.54
1:A:111:GLU:HG2	1:A:112:ASN:H	1.72	0.54
1:A:34:GLU:CG	1:A:35:GLU:H	2.19	0.54
1:A:305:GLN:HG2	1:A:375:ILE:HD11	1.90	0.54
1:A:312:LYS:HG2	1:A:315:HIS:CE1	2.43	0.54
1:B:117:ILE:HG22	1:B:117:ILE:O	2.07	0.53
1:B:34:GLU:HG2	1:B:35:GLU:H	1.74	0.53
1:B:183:TYR:HA	1:B:258:ASP:O	2.09	0.52
1:A:111:GLU:HG2	1:A:112:ASN:N	2.24	0.52
1:A:291:ASN:HB3	1:A:385:LYS:HE3	1.91	0.52
1:B:156:ASP:HB3	1:B:158:GLY:H	1.74	0.52
1:A:33:GLY:HA3	1:A:118:PRO:HD3	1.91	0.52
1:A:235:PHE:CE1	1:A:240:ARG:HD3	2.45	0.51
1:A:67:TYR:HA	1:A:141:ASP:O	2.10	0.51
1:A:230:LYS:HB3	1:A:231:PRO:HD2	1.93	0.51
1:B:63:VAL:HG11	1:B:91:LEU:HD12	1.93	0.51
1:B:330:VAL:HB	1:B:334:LEU:HD23	1.91	0.51
1:B:208:LEU:HB3	1:B:212:LEU:HD22	1.91	0.51
1:B:157:GLY:HA2	1:B:160:PHE:CZ	2.45	0.50
1:B:33:GLY:HA3	1:B:116:THR:O	2.12	0.50
1:B:35:GLU:HA	1:B:114:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PRO:O	1:B:134:ALA:O	2.29	0.50
1:B:152:ASP:HB2	1:B:160:PHE:HE1	1.76	0.50
1:B:224:LYS:HG2	1:B:260:GLU:HG3	1.93	0.50
1:B:297:THR:HG23	1:B:382:SER:OG	2.11	0.49
1:B:57:PRO:HG3	1:B:147:TRP:CD2	2.48	0.49
1:A:109:LYS:O	1:A:144:LEU:O	2.31	0.49
1:B:101:ASP:O	1:B:105:LYS:HB3	2.13	0.48
1:B:35:GLU:OE1	1:B:113:ALA:CB	2.51	0.48
1:B:175:ASP:OD1	1:B:217:LYS:HE3	2.14	0.48
1:A:62:GLU:HG3	1:A:90:LYS:HG3	1.95	0.48
1:B:293:GLY:CA	1:B:324:LYS:HE3	2.43	0.48
1:B:354:GLU:N	1:B:354:GLU:OE2	2.40	0.48
1:B:65:VAL:N	1:B:87:PHE:N	2.57	0.47
1:A:312:LYS:HG2	1:A:315:HIS:NE2	2.29	0.47
1:A:278:LYS:HG3	1:A:349:VAL:HG22	1.95	0.47
1:B:330:VAL:CB	1:B:334:LEU:HD23	2.44	0.47
1:B:293:GLY:O	1:B:324:LYS:CG	2.62	0.47
1:A:63:VAL:HG13	1:A:91:LEU:HD12	1.93	0.47
1:B:57:PRO:HG3	1:B:147:TRP:CE3	2.49	0.47
1:A:54:TRP:HA	1:A:54:TRP:CE3	2.50	0.47
1:A:168:ASP:C	1:A:169:LYS:HG3	2.36	0.46
1:A:278:LYS:HB3	1:A:278:LYS:HE3	1.75	0.46
1:A:285:GLU:OE2	1:A:343:LYS:HD3	2.14	0.46
1:A:352:PRO:HA	1:A:373:THR:HB	1.97	0.46
1:A:54:TRP:HE3	1:A:108:LYS:HZ1	1.62	0.46
1:B:362:SER:HB3	1:B:368:VAL:HB	1.98	0.46
1:A:64:GLU:HG3	1:A:88:LYS:HD2	1.98	0.46
1:A:361:GLU:OE2	1:A:363:LYS:NZ	2.44	0.45
1:A:270:ILE:HG21	1:A:270:ILE:HD13	1.75	0.45
1:A:281:LEU:HD11	1:A:348:LEU:HG	1.97	0.45
1:A:270:ILE:N	1:A:276:ILE:O	2.32	0.45
1:A:54:TRP:HA	1:A:54:TRP:HE3	1.81	0.45
1:B:270:ILE:HD13	1:B:270:ILE:HG21	1.60	0.44
1:B:286:GLY:HA2	1:B:287:TYR:HB3	1.99	0.44
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.84	0.44
1:B:176:PRO:HA	1:B:204:LYS:HE2	1.99	0.44
1:B:179:VAL:O	1:B:200:GLU:HA	2.18	0.44
1:A:87:PHE:CA	1:A:88:LYS:HB2	2.46	0.44
1:A:170:TRP:HA	1:A:220:LYS:HE3	1.98	0.44
1:B:171:GLU:HG3	1:B:264:TRP:CZ2	2.52	0.44
1:B:57:PRO:HB2	1:B:91:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:VAL:HG13	1:A:298:VAL:HG13	2.00	0.44
1:A:114:LEU:HD11	1:A:139:GLN:HG2	1.99	0.43
1:B:168:ASP:HB3	1:B:169:LYS:HE2	2.00	0.43
1:B:237:GLU:O	1:B:251:PRO:HB3	2.19	0.43
1:B:286:GLY:CA	1:B:287:TYR:HB3	2.48	0.43
1:B:103:GLY:O	1:B:107:MET:HG3	2.18	0.43
1:A:224:LYS:HG2	1:A:260:GLU:HG3	2.00	0.43
1:B:56:THR:HA	1:B:57:PRO:HD3	1.91	0.43
1:A:117:ILE:O	1:A:138:LEU:N	2.52	0.43
1:B:324:LYS:CD	1:B:327:GLU:OE2	2.58	0.43
1:B:330:VAL:HG21	1:B:334:LEU:HD23	2.00	0.43
1:B:297:THR:CG2	1:B:382:SER:OG	2.67	0.43
1:B:163:ILE:HD13	1:B:163:ILE:HG21	1.62	0.42
1:A:154:ALA:O	1:A:155:LYS:HB2	2.20	0.42
1:A:67:TYR:CD1	1:A:68:THR:N	2.88	0.42
1:A:291:ASN:CB	1:A:385:LYS:HE3	2.49	0.42
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.82	0.42
1:A:250:PRO:O	1:A:251:PRO:C	2.58	0.42
1:A:309:VAL:HG11	1:A:312:LYS:HE2	2.01	0.42
1:B:183:TYR:OH	1:B:207:HIS:CE1	2.59	0.41
1:B:310:PHE:O	1:B:364:GLN:CB	2.68	0.41
1:B:317:GLU:O	1:B:317:GLU:HG2	2.18	0.41
1:B:296:VAL:HG13	1:B:298:VAL:HG13	2.02	0.41
1:A:156:ASP:HB3	1:A:158:GLY:H	1.85	0.41
1:B:267:VAL:HA	1:B:278:LYS:O	2.20	0.41
1:B:37:GLU:HG3	1:B:38:ILE:N	2.35	0.41
1:B:261:LEU:HD12	1:B:261:LEU:HA	1.80	0.41
1:B:107:MET:CE	1:B:111:GLU:HG2	2.47	0.41
1:B:330:VAL:CG2	1:B:334:LEU:HD23	2.51	0.41
1:B:289:ARG:NH1	1:B:340:ASN:O	2.53	0.41
1:B:273:ASP:HB3	1:B:275:LYS:H	1.86	0.41
1:B:208:LEU:HA	1:B:208:LEU:HD12	1.86	0.40
1:A:117:ILE:HA	1:A:118:PRO:HD3	1.95	0.40
1:B:134:ALA:C	1:B:136:ALA:N	2.75	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	292/377 (78%)	261 (89%)	17 (6%)	14 (5%)	2	1
1	B	299/377 (79%)	266 (89%)	23 (8%)	10 (3%)	4	2
All	All	591/754 (78%)	527 (89%)	40 (7%)	24 (4%)	3	1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
1	A	246	GLY
1	B	134	ALA
1	B	135	ASN
1	B	287	TYR
1	A	59	VAL
1	A	88	LYS
1	A	98	LYS
1	A	99	GLY
1	A	251	PRO
1	A	286	GLY
1	B	146	SER
1	B	238	MET
1	A	110	GLY
1	B	155	LYS
1	B	251	PRO
1	A	97	ILE
1	A	208	LEU
1	B	243	ALA
1	A	169	LYS
1	A	239	GLY
1	A	273	ASP
1	B	239	GLY
1	B	246	GLY

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	254/311 (82%)	226 (89%)	28 (11%)	6	6
1	B	258/311 (83%)	223 (86%)	35 (14%)	3	3
All	All	512/622 (82%)	449 (88%)	63 (12%)	4	4

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	54	TRP
1	A	56	THR
1	A	68	THR
1	A	87	PHE
1	A	91	LEU
1	A	109	LYS
1	A	117	ILE
1	A	149	SER
1	A	156	ASP
1	A	169	LYS
1	A	182	LYS
1	A	197	GLU
1	A	204	LYS
1	A	212	LEU
1	A	217	LYS
1	A	232	GLN
1	A	238	MET
1	A	273	ASP
1	A	283	GLU
1	A	287	TYR
1	A	297	THR
1	A	301	THR
1	A	308	THR
1	A	313	LYS
1	A	360	THR
1	A	363	LYS

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Mol	Chain	Res	Type
1	A	373	THR
1	B	38	ILE
1	B	56	THR
1	B	66	HIS
1	B	91	LEU
1	B	93	GLN
1	B	105	LYS
1	B	111	GLU
1	B	114	LEU
1	B	117	ILE
1	B	135	ASN
1	B	138	LEU
1	B	148	THR
1	B	156	ASP
1	B	166	GLU
1	B	171	GLU
1	B	194	SER
1	B	212	LEU
1	B	226	LEU
1	B	232	GLN
1	B	238	MET
1	B	245	GLU
1	B	251	PRO
1	B	268	THR
1	B	273	ASP
1	B	287	TYR
1	B	296	VAL
1	B	297	THR
1	B	301	THR
1	B	311	LEU
1	B	328	GLU
1	B	348	LEU
1	B	360	THR
1	B	363	LYS
1	B	367	ILE
1	B	373	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	232	GLN

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Mol	Chain	Res	Type
1	B	207	HIS
1	B	232	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 carbohydrates 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	300/377 (79%)	0.52	27 (9%)	9	12	8, 26, 67, 81	0
1	B	307/377 (81%)	0.41	21 (6%)	17	21	11, 30, 61, 80	0
All	All	607/754 (80%)	0.46	48 (7%)	12	16	8, 28, 63, 81	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	TRP	7.3
1	A	59	VAL	6.4
1	A	54	TRP	6.3
1	B	59	VAL	5.9
1	B	96	VAL	4.7
1	A	56	THR	4.4
1	B	115	PHE	4.3
1	B	97	ILE	4.2
1	B	100	TRP	4.0
1	A	35	GLU	4.0
1	A	104	ILE	3.4
1	A	144	LEU	3.3
1	A	145	LEU	3.3
1	A	94	GLY	3.2
1	A	112	ASN	3.2
1	A	96	VAL	3.2
1	A	95	GLN	3.2
1	A	115	PHE	3.0
1	A	93	GLN	2.9
1	A	36	ASN	2.9
1	A	170	TRP	2.9
1	B	95	GLN	2.8
1	A	146	SER	2.7
1	B	65	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	133	PRO	2.6
1	B	38	ILE	2.6
1	B	113	ALA	2.6
1	B	57	PRO	2.5
1	A	65	VAL	2.5
1	B	112	ASN	2.4
1	B	132	ILE	2.4
1	B	69	GLY	2.4
1	B	116	THR	2.3
1	A	57	PRO	2.3
1	B	104	ILE	2.3
1	A	99	GLY	2.3
1	B	366	ALA	2.3
1	A	105	LYS	2.1
1	B	139	GLN	2.1
1	A	286	GLY	2.1
1	B	36	ASN	2.1
1	A	117	ILE	2.1
1	A	138	LEU	2.1
1	B	155	LYS	2.1
1	A	141	ASP	2.0
1	A	92	GLY	2.0
1	B	141	ASP	2.0
1	A	97	ILE	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.