



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:10 AM UTC

PDB ID : 3JYM / pdb_00003jym
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 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

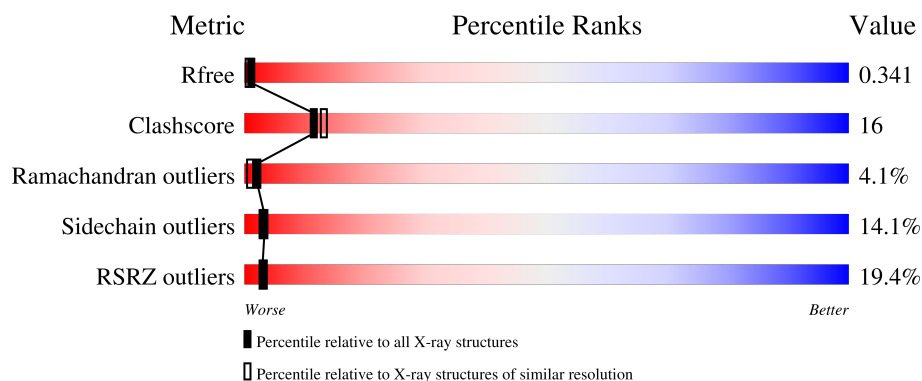
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 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	377	16% 33% 33% 11% • 20%
1	B	377	15% 41% 29% 8% • 18%

2 Entry composition

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.

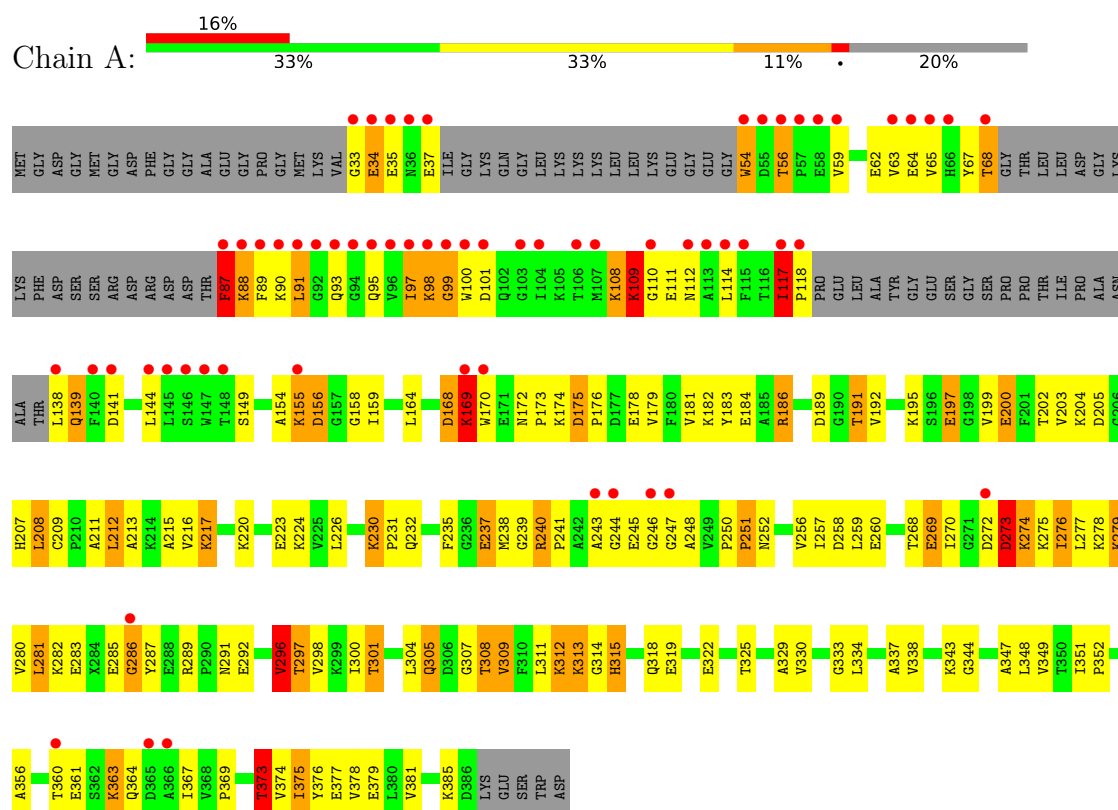
- Molecule 1 is a protein called FK506-binding protein (FKBP) from wheat.

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			

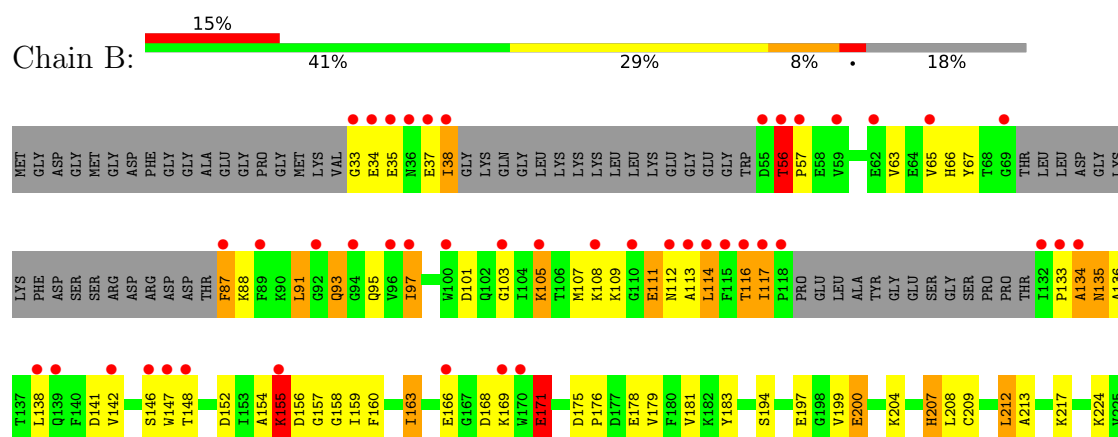
3 Residue-property plots [i](#)

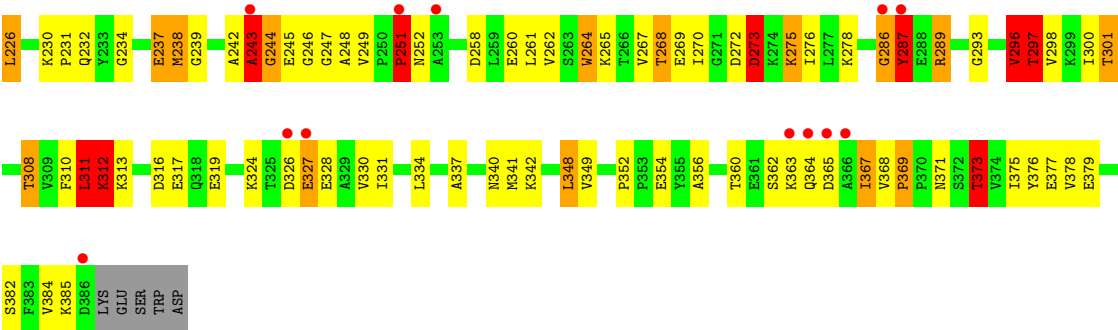
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: FK506-binding protein (FKBP) from wheat



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





4 Data and refinement statistics

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 46.63 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.63-2.28) 98.6 (46.63-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.92%)	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 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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	2.08	83/2382 (3.5%)	1.65	49/3210 (1.5%)
1	B	1.89	52/2419 (2.1%)	1.61	34/3261 (1.0%)
All	All	1.99	135/4801 (2.8%)	1.63	83/6471 (1.3%)

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 (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	PRO	CA-C	9.56	1.57	1.51
1	A	337	ALA	C-O	-9.48	1.13	1.24
1	A	312	LYS	C-O	-9.48	1.13	1.24
1	A	374	VAL	C-O	-9.24	1.14	1.24
1	A	174	LYS	CA-C	-8.72	1.41	1.52
1	B	159	ILE	CA-CB	8.49	1.66	1.54
1	B	313	LYS	C-O	-8.29	1.14	1.23
1	B	213	ALA	CA-CB	-8.21	1.40	1.53
1	A	244	GLY	N-CA	8.17	1.57	1.45
1	A	269	GLU	CA-C	-8.11	1.42	1.52
1	A	377	GLU	C-O	-8.03	1.14	1.24
1	A	213	ALA	CA-CB	-7.98	1.40	1.53
1	A	319	GLU	C-O	-7.93	1.13	1.23
1	A	159	ILE	CA-CB	7.80	1.65	1.54
1	B	377	GLU	C-O	-7.77	1.14	1.24
1	B	268	THR	CA-C	7.57	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	GLN	C-O	-7.52	1.14	1.24
1	B	312	LYS	C-O	-7.47	1.15	1.24
1	B	207	HIS	C-O	-7.41	1.14	1.23
1	A	164	LEU	N-CA	-7.40	1.36	1.46
1	A	309	VAL	CA-CB	7.37	1.64	1.53
1	A	268	THR	CA-C	7.24	1.61	1.52
1	A	375	ILE	C-O	-7.18	1.16	1.24
1	A	176	PRO	CA-C	7.13	1.63	1.52
1	A	215	ALA	CA-CB	-7.07	1.42	1.53
1	A	209	CYS	C-O	-7.06	1.17	1.24
1	A	117	ILE	CA-CB	7.04	1.63	1.54
1	B	311	LEU	C-O	-7.04	1.16	1.23
1	A	308	THR	CA-CB	7.00	1.62	1.53
1	A	211	ALA	CA-CB	-7.00	1.42	1.53
1	A	172	ASN	C-O	-6.95	1.15	1.24
1	A	351	ILE	N-CA	6.92	1.55	1.46
1	A	313	LYS	C-O	-6.89	1.15	1.23
1	A	330	VAL	CA-CB	6.88	1.65	1.54
1	B	163	ILE	CA-C	-6.87	1.45	1.52
1	A	318	GLN	C-O	-6.75	1.15	1.23
1	A	296	VAL	C-O	-6.66	1.17	1.24
1	B	337	ALA	C-O	-6.64	1.16	1.24
1	B	371	ASN	CA-C	6.59	1.62	1.52
1	A	216	VAL	C-O	-6.58	1.16	1.24
1	A	279	LYS	C-O	-6.57	1.16	1.24
1	B	376	TYR	C-O	-6.56	1.16	1.24
1	B	301	THR	CA-CB	6.54	1.65	1.53
1	A	207	HIS	C-O	-6.42	1.15	1.23
1	A	56	THR	CA-C	6.38	1.58	1.52
1	B	243	ALA	CA-C	6.33	1.61	1.52
1	A	281	LEU	N-CA	6.24	1.54	1.46
1	A	378	VAL	C-O	-6.23	1.17	1.24
1	B	289	ARG	CA-C	-6.22	1.46	1.52
1	B	316	ASP	N-CA	6.22	1.53	1.46
1	A	192	VAL	C-O	-6.18	1.18	1.24
1	B	375	ILE	C-O	-6.16	1.17	1.24
1	A	197	GLU	C-O	-6.15	1.15	1.24
1	A	181	VAL	CA-CB	6.13	1.65	1.55
1	B	349	VAL	C-O	-6.05	1.17	1.24
1	A	376	TYR	C-O	-6.05	1.17	1.24
1	A	191	THR	CA-CB	6.03	1.61	1.53
1	A	268	THR	CB-CG2	-6.01	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	ILE	CA-CB	5.97	1.61	1.54
1	B	209	CYS	CB-SG	-5.95	1.61	1.81
1	A	181	VAL	N-CA	-5.91	1.39	1.46
1	A	315	HIS	N-CA	5.90	1.53	1.45
1	B	269	GLU	CA-C	-5.90	1.45	1.52
1	A	375	ILE	CG1-CD1	-5.88	1.28	1.51
1	A	273	ASP	C-O	-5.88	1.16	1.24
1	B	199	VAL	C-O	-5.86	1.17	1.23
1	A	200	GLU	N-CA	-5.84	1.38	1.46
1	A	322	GLU	N-CA	-5.80	1.38	1.45
1	A	209	CYS	CB-SG	-5.79	1.62	1.81
1	B	181	VAL	CA-CB	5.77	1.64	1.55
1	B	200	GLU	C-O	-5.71	1.17	1.23
1	A	314	GLY	C-O	-5.69	1.16	1.23
1	A	178	GLU	CA-C	5.67	1.60	1.52
1	A	200	GLU	C-O	-5.67	1.17	1.23
1	A	347	ALA	C-O	-5.65	1.16	1.23
1	B	297	THR	N-CA	5.65	1.53	1.46
1	B	356	ALA	CA-CB	5.64	1.63	1.53
1	B	296	VAL	C-O	-5.63	1.18	1.24
1	A	280	VAL	C-O	5.61	1.29	1.24
1	A	364	GLN	N-CA	-5.60	1.42	1.46
1	A	257	ILE	CA-CB	5.60	1.61	1.54
1	A	381	VAL	CA-CB	5.59	1.60	1.54
1	A	373	THR	CA-CB	5.55	1.61	1.53
1	A	159	ILE	C-O	-5.54	1.17	1.24
1	A	209	CYS	N-CA	-5.53	1.41	1.46
1	B	378	VAL	C-O	-5.53	1.18	1.24
1	B	301	THR	C-N	-5.52	1.29	1.33
1	B	209	CYS	C-O	-5.51	1.18	1.24
1	A	277	LEU	N-CA	5.49	1.52	1.46
1	A	274	LYS	C-O	-5.48	1.16	1.23
1	B	155	LYS	N-CA	5.45	1.53	1.46
1	A	205	ASP	C-O	-5.44	1.16	1.24
1	B	97	ILE	CA-CB	5.41	1.59	1.54
1	A	300	ILE	CA-CB	5.39	1.62	1.54
1	B	348	LEU	C-O	-5.38	1.17	1.24
1	A	176	PRO	C-O	-5.36	1.17	1.24
1	A	322	GLU	C-O	-5.34	1.17	1.23
1	A	186	ARG	N-CA	-5.33	1.39	1.45
1	B	276	ILE	CA-C	5.33	1.59	1.52
1	B	247	GLY	N-CA	5.30	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	301	THR	CB-CG2	-5.29	1.35	1.52
1	A	175	ASP	CA-C	-5.29	1.47	1.52
1	B	349	VAL	CA-CB	5.29	1.60	1.53
1	A	273	ASP	CB-CG	-5.28	1.38	1.52
1	A	379	GLU	C-O	-5.26	1.17	1.24
1	B	181	VAL	C-O	-5.26	1.18	1.23
1	B	300	ILE	CG1-CD1	5.26	1.72	1.51
1	B	384	VAL	CA-CB	5.25	1.61	1.54
1	B	231	PRO	C-O	-5.21	1.17	1.24
1	A	297	THR	N-CA	5.21	1.52	1.46
1	B	249	VAL	N-CA	5.21	1.51	1.46
1	B	341	MET	CA-C	-5.20	1.46	1.52
1	A	203	VAL	CA-CB	-5.20	1.48	1.54
1	A	337	ALA	C-N	-5.20	1.27	1.33
1	B	319	GLU	C-O	-5.20	1.17	1.23
1	A	159	ILE	CA-C	-5.17	1.46	1.52
1	A	282	LYS	C-O	-5.17	1.18	1.24
1	A	199	VAL	CA-C	-5.16	1.46	1.52
1	B	316	ASP	CG-OD2	5.15	1.35	1.25
1	A	329	ALA	N-CA	5.14	1.52	1.46
1	A	334	LEU	CA-C	5.12	1.59	1.52
1	A	243	ALA	CA-C	5.11	1.59	1.52
1	A	289	ARG	C-O	-5.11	1.18	1.24
1	B	297	THR	CB-CG2	-5.10	1.35	1.52
1	B	242	ALA	CA-CB	-5.09	1.46	1.53
1	A	259	LEU	C-O	-5.09	1.17	1.23
1	A	274	LYS	CA-C	-5.05	1.46	1.53
1	B	275	LYS	CG-CD	5.03	1.67	1.52
1	A	272	ASP	C-O	-5.03	1.18	1.24
1	B	197	GLU	C-O	-5.03	1.17	1.24
1	B	342	LYS	C-O	5.02	1.30	1.23
1	A	356	ALA	C-O	5.01	1.30	1.24
1	B	178	GLU	CA-C	5.01	1.59	1.52
1	B	379	GLU	C-O	-5.01	1.18	1.24
1	A	173	PRO	C-O	-5.00	1.17	1.23

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLY	N-CA-C	-10.67	92.80	111.46
1	B	230	LYS	CA-C-N	9.38	130.01	119.32
1	B	230	LYS	C-N-CA	9.38	130.01	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LYS	CA-C-N	8.60	130.59	119.84
1	A	230	LYS	C-N-CA	8.60	130.59	119.84
1	B	234	GLY	CA-C-N	-8.54	109.27	122.60
1	B	234	GLY	C-N-CA	-8.54	109.27	122.60
1	A	289	ARG	CA-C-N	-8.47	111.65	120.03
1	A	289	ARG	C-N-CA	-8.47	111.65	120.03
1	A	292	GLU	N-CA-C	-7.84	99.45	110.50
1	A	34	GLU	N-CA-C	7.62	118.02	108.19
1	A	95	GLN	N-CA-C	7.58	121.78	112.23
1	A	100	TRP	N-CA-C	7.57	122.10	113.01
1	B	248	ALA	CA-C-N	-7.49	115.23	123.02
1	B	248	ALA	C-N-CA	-7.49	115.23	123.02
1	B	56	THR	CA-C-N	7.20	127.19	119.78
1	B	56	THR	C-N-CA	7.20	127.19	119.78
1	A	296	VAL	N-CA-CB	-6.72	102.13	111.41
1	A	273	ASP	N-CA-C	6.66	124.99	110.80
1	A	301	THR	CB-CA-C	6.62	120.73	110.14
1	A	223	GLU	CB-CA-C	6.43	119.93	109.90
1	B	327	GLU	N-CA-C	-6.40	104.69	114.16
1	B	373	THR	CB-CA-C	6.37	120.23	109.84
1	A	297	THR	CB-CA-C	6.36	120.49	110.19
1	A	268	THR	OG1-CB-CG2	6.30	121.90	109.30
1	A	272	ASP	CA-C-N	6.30	133.57	121.54
1	A	272	ASP	C-N-CA	6.30	133.57	121.54
1	A	344	GLY	N-CA-C	-6.20	106.76	115.32
1	A	286	GLY	N-CA-C	6.13	127.71	113.18
1	B	88	LYS	N-CA-C	-6.08	93.97	111.00
1	B	244	GLY	N-CA-C	-6.07	95.69	113.30
1	B	287	TYR	CB-CA-C	6.06	121.62	110.10
1	A	268	THR	CA-CB-OG1	6.03	118.64	109.60
1	B	365	ASP	N-CA-C	-6.03	104.40	110.97
1	B	247	GLY	N-CA-C	5.94	120.69	112.37
1	A	304	LEU	N-CA-C	-5.91	102.91	110.53
1	B	331	ILE	CB-CG1-CD1	-5.89	101.44	113.80
1	B	296	VAL	N-CA-CB	-5.87	102.07	111.58
1	B	262	VAL	N-CA-C	-5.83	106.03	111.45
1	A	202	THR	N-CA-C	-5.77	100.59	109.76
1	B	273	ASP	CB-CA-C	-5.73	99.02	110.42
1	A	319	GLU	CA-C-N	-5.72	114.72	120.21
1	A	319	GLU	C-N-CA	-5.72	114.72	120.21
1	B	268	THR	N-CA-CB	-5.71	101.32	110.63
1	B	67	TYR	N-CA-C	5.69	118.06	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	THR	CB-CA-C	5.59	119.45	110.16
1	B	272	ASP	CA-C-N	5.55	132.13	121.54
1	B	272	ASP	C-N-CA	5.55	132.13	121.54
1	B	234	GLY	N-CA-C	-5.51	100.12	113.18
1	A	308	THR	N-CA-CB	5.49	118.83	109.87
1	A	373	THR	N-CA-CB	5.49	118.35	110.06
1	A	244	GLY	N-CA-C	-5.48	100.19	113.18
1	A	325	THR	CB-CA-C	-5.47	100.16	109.51
1	B	297	THR	CB-CA-C	5.45	119.12	110.19
1	A	195	LYS	CA-C-N	-5.45	112.21	121.85
1	A	195	LYS	C-N-CA	-5.45	112.21	121.85
1	A	381	VAL	N-CA-C	5.43	115.52	110.42
1	B	242	ALA	CA-C-N	5.41	131.88	121.54
1	B	242	ALA	C-N-CA	5.41	131.88	121.54
1	B	171	GLU	N-CA-C	5.41	118.53	110.52
1	B	141	ASP	N-CA-C	-5.34	99.07	108.20
1	A	333	GLY	N-CA-C	5.32	120.21	113.24
1	A	252	ASN	N-CA-C	5.32	119.35	112.86
1	A	87	PHE	CA-C-N	5.30	131.24	121.70
1	A	87	PHE	C-N-CA	5.30	131.24	121.70
1	A	211	ALA	N-CA-C	5.28	117.72	111.33
1	B	308	THR	N-CA-CB	5.25	118.08	109.95
1	A	248	ALA	CA-C-N	-5.17	117.64	123.02
1	A	248	ALA	C-N-CA	-5.17	117.64	123.02
1	A	241	PRO	CA-C-N	5.17	128.69	121.24
1	A	241	PRO	C-N-CA	5.17	128.69	121.24
1	A	307	GLY	CA-C-N	-5.15	114.26	121.72
1	A	307	GLY	C-N-CA	-5.15	114.26	121.72
1	B	264	TRP	N-CA-C	5.14	116.10	108.60
1	A	237	GLU	CA-C-N	5.13	129.29	120.72
1	A	237	GLU	C-N-CA	5.13	129.29	120.72
1	A	373	THR	CB-CA-C	5.12	118.19	109.53
1	A	168	ASP	N-CA-C	5.10	118.12	109.76
1	A	155	LYS	N-CA-C	-5.10	104.27	111.56
1	B	237	GLU	CA-C-N	5.07	131.22	121.54
1	B	237	GLU	C-N-CA	5.07	131.22	121.54
1	A	240	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	A	308	THR	CB-CA-C	5.03	118.53	110.29

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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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	64	0
1	B	2382	0	2392	88	0
All	All	4726	0	4739	152	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 (152) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:226:LEU:C	1:B:226:LEU:HD23	2.18	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:A:34:GLU:HG2	1:A:35:GLU:H	1.62	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:154:ALA:C	1:B:156:ASP:HB2	2.25	0.62
1:B:117:ILE:CG2	1:B:117:ILE:O	2.48	0.61
1:B:107:MET:HE3	1:B:113:ALA:HB3	1.83	0.60
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
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: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:38:ILE:HB	1:B:112:ASN:HB3	1.86	0.56
1:B:243:ALA:CB	1:B:244:GLY:CA	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:GLU:CG	1:A:35:GLU:H	2.19	0.54
1:A:111:GLU:HG2	1:A:112:ASN:H	1.72	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:O	1:B:117:ILE:HG22	2.07	0.53
1:B:34:GLU:HG2	1:B:35:GLU:H	1.74	0.53
1:B:107:MET:HE2	1:B:111:GLU:HG2	1.91	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:B:107:MET:HE1	1:B:142:VAL:O	2.09	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:A:168:ASP:C	1:A:169:LYS:HG3	2.36	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
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:A:54:TRP:HE3	1:A:108:LYS:HZ1	1.59	0.48
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:OE2	1:B:354:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:250:PRO:O	1:A:251:PRO:C	2.58	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: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:B:93:GLN:C	1:B:95:GLN:H	2.24	0.45
1:A:361:GLU:OE2	1:A:363:LYS:NZ	2.44	0.45
1:A:270:ILE:HD13	1:A:270:ILE:HG21	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:B:134:ALA:C	1:B:136:ALA:N	2.75	0.45
1:A:54:TRP:HE3	1:A:54:TRP:HA	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:HB3	1:A:279:LYS:HE2	1.84	0.44
1:B:107:MET:CE	1:B:111:GLU:HG2	2.47	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
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:326:ASP:O	1:B:326:ASP:CG	2.60	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:A:189:ASP:OD1	1:A:191:THR:OG1	2.25	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:297:THR:CG2	1:B:382:SER:OG	2.67	0.43
1:B:324:LYS:CD	1:B:327:GLU:OE2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:HG21	1:B:334:LEU:HD23	2.00	0.43
1:B:163:ILE:HD13	1:B:163:ILE:HG21	1.62	0.42
1:A:67:TYR:CD1	1:A:68:THR:N	2.88	0.42
1:A:154:ALA:O	1:A:155:LYS:HB2	2.20	0.42
1:A:291:ASN:CB	1:A:385:LYS:HE3	2.49	0.42
1:A:212:LEU:HA	1:A:212:LEU:HD12	1.82	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:261:LEU:HA	1:B:261:LEU:HD12	1.80	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:37:GLU:HG3	1:B:38:ILE:N	2.35	0.41
1:B:208:LEU:HD12	1:B:208:LEU:HA	1.86	0.40
1:A:117:ILE:HA	1:A:118:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	3	1
All	All	591/754 (78%)	527 (89%)	40 (7%)	24 (4%)	2	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%)	221 (87%)	33 (13%)	4	4
1	B	258/311 (83%)	219 (85%)	39 (15%)	3	2
All	All	512/622 (82%)	440 (86%)	72 (14%)	3	3

All (72) 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	98	LYS
1	A	108	LYS
1	A	109	LYS
1	A	117	ILE
1	A	139	GLN
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	296	VAL
1	A	297	THR
1	A	301	THR
1	A	308	THR
1	A	313	LYS
1	A	338	VAL
1	A	360	THR
1	A	363	LYS
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	97	ILE
1	B	105	LYS
1	B	109	LYS
1	B	111	GLU
1	B	114	LEU

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Mol	Chain	Res	Type
1	B	117	ILE
1	B	135	ASN
1	B	138	LEU
1	B	148	THR
1	B	155	LYS
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	296	VAL
1	B	297	THR
1	B	301	THR
1	B	308	THR
1	B	311	LEU
1	B	312	LYS
1	B	328	GLU
1	B	348	LEU
1	B	360	THR
1	B	363	LYS
1	B	367	ILE
1	B	373	THR
1	B	385	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	112	ASN
1	A	172	ASN
1	A	232	GLN
1	A	315	HIS
1	B	172	ASN
1	B	207	HIS
1	B	232	GLN

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	300/377 (79%)	0.88	62 (20%)  	8, 26, 67, 81	0
1	B	307/377 (81%)	0.91	56 (18%)  	11, 30, 61, 80	0
All	All	607/754 (80%)	0.89	118 (19%)  	8, 28, 63, 81	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	TRP	9.3
1	A	54	TRP	7.2
1	A	59	VAL	6.9
1	B	38	ILE	6.5
1	B	33	GLY	6.4
1	A	97	ILE	6.0
1	A	56	THR	5.9
1	A	33	GLY	5.8
1	A	87	PHE	5.8
1	B	56	THR	5.0
1	A	244	GLY	4.8
1	B	87	PHE	4.7
1	B	366	ALA	4.6
1	A	35	GLU	4.6
1	A	99	GLY	4.5
1	B	36	ASN	4.5
1	B	97	ILE	4.5
1	B	134	ALA	4.4
1	B	365	ASP	4.4
1	B	96	VAL	4.3
1	A	104	ILE	4.3
1	A	246	GLY	4.2
1	B	35	GLU	4.2
1	A	96	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLY	4.0
1	B	243	ALA	4.0
1	B	59	VAL	3.9
1	B	113	ALA	3.8
1	B	118	PRO	3.7
1	A	98	LYS	3.6
1	A	68	THR	3.6
1	A	95	GLN	3.6
1	A	147	TRP	3.6
1	A	138	LEU	3.5
1	A	170	TRP	3.5
1	A	94	GLY	3.5
1	A	91	LEU	3.5
1	B	132	ILE	3.4
1	A	55	ASP	3.4
1	B	115	PHE	3.4
1	A	65	VAL	3.4
1	B	363	LYS	3.4
1	A	57	PRO	3.4
1	B	142	VAL	3.4
1	B	146	SER	3.4
1	B	170	TRP	3.4
1	A	148	THR	3.3
1	A	146	SER	3.3
1	A	36	ASN	3.3
1	A	92	GLY	3.2
1	B	138	LEU	3.2
1	B	37	GLU	3.1
1	A	37	GLU	3.1
1	B	166	GLU	3.1
1	B	69	GLY	3.1
1	B	155	LYS	3.1
1	A	115	PHE	3.1
1	A	145	LEU	3.0
1	B	386	ASP	3.0
1	A	93	GLN	3.0
1	A	90	LYS	3.0
1	B	65	VAL	3.0
1	B	57	PRO	2.9
1	B	117	ILE	2.9
1	A	89	PHE	2.9
1	B	139	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	364	GLN	2.9
1	A	286	GLY	2.8
1	B	108	LYS	2.8
1	A	101	ASP	2.8
1	A	66	HIS	2.7
1	A	114	LEU	2.7
1	B	89	PHE	2.7
1	A	118	PRO	2.7
1	A	155	LYS	2.6
1	B	114	LEU	2.6
1	B	169	LYS	2.6
1	A	360	THR	2.5
1	A	144	LEU	2.5
1	A	113	ALA	2.5
1	A	141	ASP	2.5
1	B	110	GLY	2.5
1	A	117	ILE	2.5
1	A	366	ALA	2.5
1	B	55	ASP	2.5
1	B	253	ALA	2.5
1	B	92	GLY	2.5
1	B	133	PRO	2.5
1	B	148	THR	2.5
1	B	94	GLY	2.5
1	B	116	THR	2.4
1	B	147	TRP	2.4
1	A	107	MET	2.4
1	B	100	TRP	2.4
1	A	58	GLU	2.4
1	B	251	PRO	2.4
1	A	34	GLU	2.3
1	B	34	GLU	2.3
1	B	287	TYR	2.3
1	A	169	LYS	2.3
1	A	365	ASP	2.2
1	B	112	ASN	2.2
1	A	88	LYS	2.2
1	B	62	GLU	2.2
1	A	243	ALA	2.2
1	B	326	ASP	2.1
1	B	327	GLU	2.1
1	A	103	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	286	GLY	2.1
1	A	112	ASN	2.1
1	A	272	ASP	2.1
1	B	103	GLY	2.1
1	A	140	PHE	2.1
1	A	64	GLU	2.1
1	A	63	VAL	2.1
1	B	105	LYS	2.0
1	A	106	THR	2.0
1	A	247	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.