Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:29 pm BST

PDB ID	:	2WQJ
Title	:	Crystal structure of a truncated variant of the human p73 tetramerization domain
Authors	:	Joerger, A.C.
Deposited on	:	2009-08-21
Resolution	:	2.00 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:

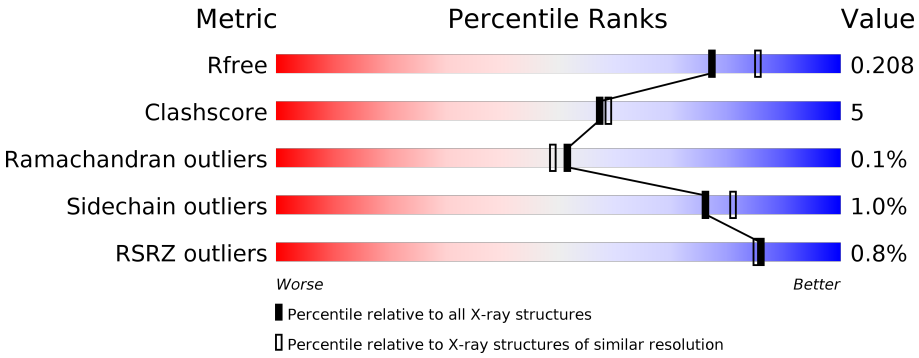
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	1	35	6% 57% 20% 23%
1	2	35	3% 63% 14% • 20%
1	A	35	74% 6% 6% 14%
1	B	35	71% 6% 23%
1	C	35	80% 14% 6%
1	D	35	71% 6% • 20%

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Mol	Chain	Length	Quality of chain
1	E	35	74% 6% 20%
1	F	35	69% 14% 17%
1	G	35	74% 6% 20%
1	H	35	71% 9% 20%
1	I	35	77% 9% 14%
1	J	35	3% 74% 6% 20%
1	K	35	77% 9% 14%
1	L	35	71% 6% 23%
1	M	35	74% 6% 20%
1	N	35	69% 14% 17%
1	O	35	3% 74% 6% 20%
1	P	35	63% 17% 20%
1	Q	35	69% 14% 17%
1	R	35	69% 14% 17%
1	S	35	69% 11% 20%
1	T	35	60% 20% 20%
1	U	35	69% 11% 20%
1	V	35	3% 69% 11% 20%
1	W	35	71% 9% 20%
1	X	35	77% 6% 17%
1	Y	35	63% 11% 26%
1	Z	35	80% 9% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7107 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 TUMOR PROTEIN P73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	30	Total	C	N	O	S	0	0	1
			239	152	37	48	2			
1	B	27	Total	C	N	O	S	0	0	1
			226	145	37	42	2			
1	C	33	Total	C	N	O	S	0	0	1
			266	168	43	53	2			
1	D	28	Total	C	N	O	S	0	0	0
			241	155	38	46	2			
1	E	28	Total	C	N	O	S	0	0	0
			235	152	35	46	2			
1	F	29	Total	C	N	O	S	0	0	1
			243	154	39	48	2			
1	G	28	Total	C	N	O	S	0	0	0
			236	153	35	46	2			
1	H	28	Total	C	N	O	S	0	0	0
			236	153	35	46	2			
1	I	30	Total	C	N	O	S	0	0	1
			245	159	37	47	2			
1	J	28	Total	C	N	O	S	0	1	1
			241	153	41	45	2			
1	K	30	Total	C	N	O	S	0	0	0
			247	159	34	52	2			
1	L	27	Total	C	N	O	S	0	0	1
			221	143	34	42	2			
1	M	28	Total	C	N	O	S	0	0	0
			241	155	38	46	2			
1	N	29	Total	C	N	O	S	0	0	0
			250	160	39	49	2			
1	O	28	Total	C	N	O	S	0	0	1
			228	146	35	45	2			
1	P	28	Total	C	N	O	S	0	0	0
			235	152	35	46	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	29	Total	C	N	O	S	0	0	1
			243	154	39	48	2			
1	R	29	Total	C	N	O	S	0	0	0
			250	160	39	49	2			
1	S	28	Total	C	N	O	S	0	0	0
			241	155	38	46	2			
1	T	28	Total	C	N	O	S	0	0	1
			229	147	35	45	2			
1	U	28	Total	C	N	O	S	0	0	0
			241	155	38	46	2			
1	V	28	Total	C	N	O	S	0	0	0
			235	152	35	46	2			
1	W	28	Total	C	N	O	S	0	0	1
			228	146	35	45	2			
1	X	29	Total	C	N	O	S	0	0	1
			228	149	33	44	2			
1	Y	26	Total	C	N	O	S	0	0	0
			221	142	36	42	1			
1	Z	31	Total	C	N	O	S	0	0	0
			256	166	39	49	2			
1	1	27	Total	C	N	O	S	0	0	1
			226	145	37	42	2			
1	2	28	Total	C	N	O	S	0	0	1
			228	146	35	45	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	O	0	0
			11	11		
2	B	9	Total	O	0	0
			9	9		
2	C	14	Total	O	0	0
			14	14		
2	D	24	Total	O	0	0
			24	24		
2	E	23	Total	O	0	0
			23	23		
2	F	19	Total	O	0	0
			19	19		
2	G	22	Total	O	0	0
			22	22		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	13	Total O 13 13	0	0
2	I	20	Total O 20 20	0	0
2	J	19	Total O 19 19	0	0
2	K	15	Total O 15 15	0	0
2	L	23	Total O 23 23	0	0
2	M	15	Total O 15 15	0	0
2	N	28	Total O 28 28	0	0
2	O	4	Total O 4 4	0	0
2	P	7	Total O 7 7	0	0
2	Q	26	Total O 26 26	0	0
2	R	14	Total O 14 14	0	0
2	S	11	Total O 11 11	0	0
2	T	19	Total O 19 19	0	0
2	U	11	Total O 11 11	0	0
2	V	18	Total O 18 18	0	0
2	W	11	Total O 11 11	0	0
2	X	19	Total O 19 19	0	0
2	Y	10	Total O 10 10	0	0
2	Z	20	Total O 20 20	0	0
2	1	15	Total O 15 15	0	0
2	2	11	Total O 11 11	0	0

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: TUMOR PROTEIN P73

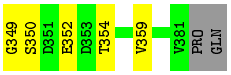
Chain A:

- Molecule 1: TUMOR PROTEIN P73

Chain B:

- Molecule 1: TUMOR PROTEIN P73

Chain C:



- Molecule 1: TUMOR PROTEIN P73

Chain D:

- Molecule 1: TUMOR PROTEIN P73

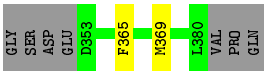
Chain E:

- Molecule 1: TUMOR PROTEIN P73

Chain F:

• Molecule 1: TUMOR PROTEIN P73

Chain G:

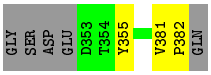


• Molecule 1: TUMOR PROTEIN P73

Chain H:

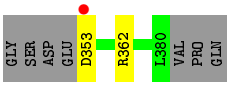
• Molecule 1: TUMOR PROTEIN P73

Chain I:



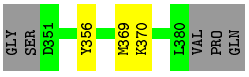
• Molecule 1: TUMOR PROTEIN P73

Chain J:



• Molecule 1: TUMOR PROTEIN P73

Chain K:



• Molecule 1: TUMOR PROTEIN P73

Chain L:

• Molecule 1: TUMOR PROTEIN P73

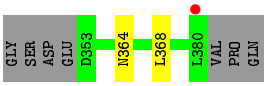
Chain M:

• Molecule 1: TUMOR PROTEIN P73

Chain N:

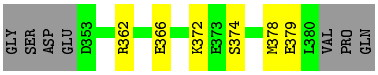
• Molecule 1: TUMOR PROTEIN P73

Chain O:



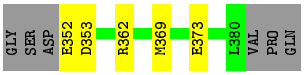
• Molecule 1: TUMOR PROTEIN P73

Chain P:



• Molecule 1: TUMOR PROTEIN P73

Chain Q:



• Molecule 1: TUMOR PROTEIN P73

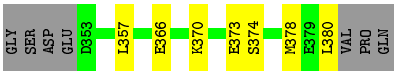
Chain R:

• Molecule 1: TUMOR PROTEIN P73

Chain S:

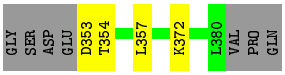
• Molecule 1: TUMOR PROTEIN P73

Chain T:



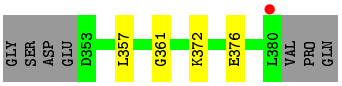
• Molecule 1: TUMOR PROTEIN P73

Chain U:



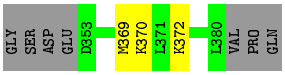
• Molecule 1: TUMOR PROTEIN P73

Chain V:



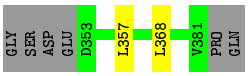
• Molecule 1: TUMOR PROTEIN P73

Chain W:



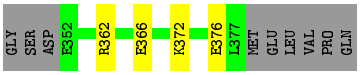
• Molecule 1: TUMOR PROTEIN P73

Chain X:



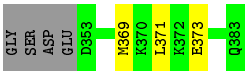
• Molecule 1: TUMOR PROTEIN P73

Chain Y:



• Molecule 1: TUMOR PROTEIN P73

Chain Z:

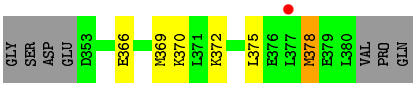


• Molecule 1: TUMOR PROTEIN P73

Chain 1:

- Molecule 1: TUMOR PROTEIN P73

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.85Å 98.93Å 120.12Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	24.96 – 2.00 60.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (24.96-2.00) 99.6 (60.03-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.248 0.208 , 0.208	Depositor DCC
R_{free} test set	4578 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7107	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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	1	0.43	0/228	0.50	0/303
1	2	0.42	0/230	0.46	0/307
1	A	0.47	0/240	0.54	0/318
1	B	0.49	0/228	0.48	0/303
1	C	0.46	0/268	0.55	0/357
1	D	0.38	0/243	0.54	0/323
1	E	0.39	0/237	0.49	0/316
1	F	0.44	0/245	0.49	0/326
1	G	0.31	0/238	0.46	0/317
1	H	0.32	0/238	0.48	0/317
1	I	0.55	1/247 (0.4%)	0.49	0/330
1	J	0.48	0/247	0.51	0/328
1	K	0.37	0/249	0.51	0/333
1	L	0.51	0/223	0.59	0/297
1	M	0.37	0/243	0.54	0/323
1	N	0.44	0/252	0.50	0/335
1	O	0.41	0/230	0.48	0/307
1	P	0.29	0/237	0.42	0/316
1	Q	0.48	0/245	0.53	0/326
1	R	0.33	0/252	0.43	0/335
1	S	0.32	0/243	0.48	0/323
1	T	0.43	0/231	0.49	0/308
1	U	0.33	0/242	0.46	0/320
1	V	0.32	0/237	0.46	0/316
1	W	0.44	0/230	0.52	0/307
1	X	0.43	0/230	0.45	0/308
1	Y	0.31	0/223	0.43	0/297
1	Z	0.33	0/259	0.45	0/346
All	All	0.41	1/6715 (0.0%)	0.49	0/8942

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	381	VAL	C-N	-5.44	1.24	1.34

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	1	226	0	230	5	0
1	2	228	0	223	4	0
1	A	239	0	232	4	0
1	B	226	0	230	2	0
1	C	266	0	261	5	0
1	D	241	0	245	4	0
1	E	235	0	234	2	0
1	F	243	0	240	4	0
1	G	236	0	236	1	0
1	H	236	0	236	2	0
1	I	245	0	247	3	0
1	J	241	0	243	1	0
1	K	247	0	235	3	0
1	L	221	0	221	1	0
1	M	241	0	245	2	0
1	N	250	0	251	4	0
1	O	228	0	223	2	0
1	P	235	0	234	5	0
1	Q	243	0	240	6	0
1	R	250	0	251	3	0
1	S	241	0	245	3	0
1	T	229	0	225	6	0
1	U	241	0	244	5	0
1	V	235	0	234	3	0
1	W	228	0	223	3	0
1	X	228	0	223	2	0
1	Y	221	0	221	3	0
1	Z	256	0	256	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	15	0	0	0	0
2	2	11	0	0	0	0
2	A	11	0	0	0	0
2	B	9	0	0	0	0
2	C	14	0	0	0	0
2	D	24	0	0	1	0
2	E	23	0	0	0	0
2	F	19	0	0	2	0
2	G	22	0	0	0	0
2	H	13	0	0	0	0
2	I	20	0	0	2	0
2	J	19	0	0	0	0
2	K	15	0	0	1	0
2	L	23	0	0	0	0
2	M	15	0	0	0	0
2	N	28	0	0	0	0
2	O	4	0	0	0	0
2	P	7	0	0	0	0
2	Q	26	0	0	0	0
2	R	14	0	0	0	0
2	S	11	0	0	0	0
2	T	19	0	0	2	0
2	U	11	0	0	0	0
2	V	18	0	0	0	0
2	W	11	0	0	0	0
2	X	19	0	0	0	0
2	Y	10	0	0	0	0
2	Z	20	0	0	0	0
All	All	7107	0	6628	65	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 5.

All (65) 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)
1:2:366:GLU:O	1:2:370:LYS:HG2	1.76	0.85
1:1:358:GLN:O	1:2:372:LYS:HE2	1.93	0.68
1:Z:369:MET:O	1:Z:373:GLU:HG2	1.93	0.67
1:T:366:GLU:O	1:T:370:LYS:HG2	1.95	0.66
1:Y:362:ARG:O	1:Y:366:GLU:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:352:GLU:HG2	1:Q:353:ASP:H	1.64	0.63
1:U:353:ASP:N	1:V:361:GLY:H	1.98	0.62
1:K:370:LYS:HE3	2:K:2011:HOH:O	1.99	0.62
1:1:362:ARG:O	1:1:366:GLU:HG3	2.00	0.61
1:I:382:PRO:N	2:I:2020:HOH:O	2.35	0.60
1:S:375:LEU:O	1:S:379:GLU:HG2	2.02	0.59
1:U:353:ASP:N	1:U:354:THR:N	2.49	0.59
1:1:374:SER:HB3	1:1:378:MET:HE1	1.85	0.58
1:N:362:ARG:O	1:N:366:GLU:HG3	2.05	0.56
1:T:373:GLU:OE2	1:W:370:LYS:HE2	2.07	0.54
1:2:375:LEU:HD23	1:2:378:MET:HE1	1.90	0.54
1:H:366:GLU:O	1:H:370:LYS:HG2	2.08	0.53
1:W:372:LYS:HG3	1:X:368:LEU:HD11	1.91	0.53
1:Y:372:LYS:O	1:Y:376:GLU:HG2	2.10	0.52
1:M:372:LYS:HD3	1:N:357:LEU:HD21	1.93	0.51
1:F:358:GLN:OE1	1:Q:362:ARG:HD2	2.11	0.51
1:S:369:MET:HG2	1:T:357:LEU:HD11	1.95	0.49
1:B:369:MET:SD	1:N:366:GLU:HG2	2.53	0.49
1:O:368:LEU:HD11	1:P:372:LYS:HG3	1.94	0.48
1:U:372:LYS:HD3	1:V:357:LEU:HD21	1.95	0.48
1:F:356:TYR:O	1:Q:362:ARG:HD3	2.14	0.48
1:1:357:LEU:HD21	1:2:369:MET:HG2	1.97	0.47
1:H:362:ARG:HH21	1:H:362:ARG:HG2	1.80	0.47
1:W:369:MET:HG2	1:X:357:LEU:CD1	2.45	0.47
1:K:369:MET:HG2	1:L:357:LEU:HD13	1.96	0.46
1:Y:376:GLU:HA	1:Y:376:GLU:OE2	2.15	0.46
1:C:349:GLY:N	1:C:354:THR:HG1	2.13	0.46
1:A:362:ARG:HG2	1:A:363:GLU:OE2	2.16	0.46
1:R:373:GLU:O	1:R:377:LEU:HG	2.16	0.46
1:U:357:LEU:HD21	1:V:372:LYS:HD3	1.98	0.46
1:I:355:TYR:OH	1:J:362:ARG:NE	2.41	0.45
1:E:366:GLU:HG2	1:Q:369:MET:SD	2.56	0.45
1:F:380:LEU:N	2:F:2019:HOH:O	2.48	0.45
1:A:362:ARG:HG2	1:A:363:GLU:N	2.31	0.45
1:I:382:PRO:N	2:I:2018:HOH:O	2.49	0.44
1:P:374:SER:O	1:P:378:MET:HG3	2.18	0.44
1:M:367:ILE:HD13	1:P:378:MET:HG2	1.98	0.44
1:Q:369:MET:HG2	1:Q:373:GLU:OE1	2.18	0.44
1:Z:371:LEU:HD23	1:1:371:LEU:HD21	1.98	0.44
1:C:359:VAL:HA	1:D:372:LYS:HZ3	1.83	0.43
1:T:380:LEU:N	2:T:2018:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:SER:HB2	1:K:356:TYR:HD1	1.84	0.43
1:R:362:ARG:O	1:R:366:GLU:HG2	2.19	0.43
1:C:359:VAL:HA	1:D:372:LYS:NZ	2.33	0.43
1:U:353:ASP:HB3	1:U:354:THR:N	2.32	0.43
1:E:371:LEU:HD23	1:E:371:LEU:HA	1.87	0.42
1:A:355:TYR:N	1:A:355:TYR:CD1	2.88	0.42
1:C:352:GLU:O	1:C:354:THR:HG23	2.20	0.42
1:T:374:SER:O	1:T:378:MET:HG3	2.20	0.42
1:D:362:ARG:NH2	2:D:2012:HOH:O	2.53	0.41
2:F:2004:HOH:O	1:R:352:GLU:HG2	2.18	0.41
1:O:364:ASN:OD1	1:P:379:GLU:OE1	2.39	0.41
1:B:366:GLU:HG2	1:N:369:MET:HE1	2.02	0.41
1:T:357:LEU:HD12	2:T:2005:HOH:O	2.21	0.41
1:A:367:ILE:HD13	1:D:378:MET:HG2	2.02	0.41
1:G:365:PHE:CE2	1:G:369:MET:HE2	2.56	0.40
1:P:362:ARG:O	1:P:366:GLU:HG2	2.21	0.40
1:F:366:GLU:O	1:F:370:LYS:HG2	2.21	0.40
1:S:380:LEU:HD12	1:S:380:LEU:C	2.42	0.40
1:Q:352:GLU:CG	1:Q:353:ASP:H	2.33	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	1	25/35 (71%)	23 (92%)	2 (8%)	0	100 100
1	2	26/35 (74%)	23 (88%)	2 (8%)	1 (4%)	3 1
1	A	26/35 (74%)	26 (100%)	0	0	100 100
1	B	25/35 (71%)	25 (100%)	0	0	100 100
1	C	31/35 (89%)	31 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	26/35 (74%)	26 (100%)	0	0	100	100
1	E	26/35 (74%)	26 (100%)	0	0	100	100
1	F	27/35 (77%)	27 (100%)	0	0	100	100
1	G	26/35 (74%)	26 (100%)	0	0	100	100
1	H	26/35 (74%)	26 (100%)	0	0	100	100
1	I	28/35 (80%)	28 (100%)	0	0	100	100
1	J	27/35 (77%)	27 (100%)	0	0	100	100
1	K	28/35 (80%)	28 (100%)	0	0	100	100
1	L	25/35 (71%)	25 (100%)	0	0	100	100
1	M	26/35 (74%)	26 (100%)	0	0	100	100
1	N	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
1	O	26/35 (74%)	26 (100%)	0	0	100	100
1	P	26/35 (74%)	26 (100%)	0	0	100	100
1	Q	27/35 (77%)	27 (100%)	0	0	100	100
1	R	27/35 (77%)	27 (100%)	0	0	100	100
1	S	26/35 (74%)	26 (100%)	0	0	100	100
1	T	26/35 (74%)	26 (100%)	0	0	100	100
1	U	25/35 (71%)	25 (100%)	0	0	100	100
1	V	26/35 (74%)	26 (100%)	0	0	100	100
1	W	26/35 (74%)	26 (100%)	0	0	100	100
1	X	27/35 (77%)	27 (100%)	0	0	100	100
1	Y	24/35 (69%)	24 (100%)	0	0	100	100
1	Z	29/35 (83%)	29 (100%)	0	0	100	100
All	All	740/980 (76%)	734 (99%)	5 (1%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	378	MET

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	1	25/33 (76%)	25 (100%)	0	100 100
1	2	25/33 (76%)	25 (100%)	0	100 100
1	A	26/33 (79%)	24 (92%)	2 (8%)	13 8
1	B	25/33 (76%)	25 (100%)	0	100 100
1	C	29/33 (88%)	29 (100%)	0	100 100
1	D	27/33 (82%)	26 (96%)	1 (4%)	34 32
1	E	26/33 (79%)	26 (100%)	0	100 100
1	F	27/33 (82%)	27 (100%)	0	100 100
1	G	26/33 (79%)	26 (100%)	0	100 100
1	H	26/33 (79%)	26 (100%)	0	100 100
1	I	27/33 (82%)	27 (100%)	0	100 100
1	J	27/33 (82%)	26 (96%)	1 (4%)	34 32
1	K	27/33 (82%)	27 (100%)	0	100 100
1	L	24/33 (73%)	23 (96%)	1 (4%)	30 27
1	M	27/33 (82%)	27 (100%)	0	100 100
1	N	28/33 (85%)	27 (96%)	1 (4%)	35 34
1	O	25/33 (76%)	25 (100%)	0	100 100
1	P	26/33 (79%)	26 (100%)	0	100 100
1	Q	27/33 (82%)	27 (100%)	0	100 100
1	R	28/33 (85%)	28 (100%)	0	100 100
1	S	27/33 (82%)	27 (100%)	0	100 100
1	T	25/33 (76%)	25 (100%)	0	100 100
1	U	27/33 (82%)	27 (100%)	0	100 100
1	V	26/33 (79%)	25 (96%)	1 (4%)	33 31
1	W	25/33 (76%)	25 (100%)	0	100 100
1	X	24/33 (73%)	24 (100%)	0	100 100
1	Y	24/33 (73%)	24 (100%)	0	100 100
1	Z	28/33 (85%)	28 (100%)	0	100 100
All	All	734/924 (79%)	727 (99%)	7 (1%)	76 81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	ARG
1	A	363	GLU
1	D	362	ARG
1	J	353	ASP
1	L	362	ARG
1	N	352	GLU
1	V	376	GLU

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	364	ASN
1	E	364	ASN
1	F	364	ASN
1	O	358	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	353:ASP	C	354:THR	N	3.08

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	1	27/35 (77%)	0.47	2 (7%) 14 13	26, 39, 71, 77	0
1	2	28/35 (80%)	0.25	1 (3%) 42 42	33, 46, 67, 84	0
1	A	30/35 (85%)	0.16	0 100 100	25, 39, 51, 53	0
1	B	27/35 (77%)	0.20	0 100 100	25, 38, 51, 55	0
1	C	33/35 (94%)	0.03	0 100 100	25, 35, 55, 62	0
1	D	28/35 (80%)	0.06	0 100 100	23, 30, 45, 51	0
1	E	28/35 (80%)	-0.03	0 100 100	25, 32, 42, 51	0
1	F	29/35 (82%)	0.07	0 100 100	28, 35, 51, 61	0
1	G	28/35 (80%)	-0.02	0 100 100	25, 37, 54, 67	0
1	H	28/35 (80%)	0.07	0 100 100	31, 44, 56, 63	0
1	I	30/35 (85%)	0.03	0 100 100	21, 32, 48, 53	0
1	J	28/35 (80%)	0.14	1 (3%) 42 42	23, 31, 49, 58	0
1	K	30/35 (85%)	-0.01	0 100 100	28, 40, 47, 55	0
1	L	27/35 (77%)	-0.04	0 100 100	23, 32, 44, 49	0
1	M	28/35 (80%)	0.00	0 100 100	26, 34, 47, 57	0
1	N	29/35 (82%)	-0.16	0 100 100	22, 32, 48, 61	0
1	O	28/35 (80%)	0.27	1 (3%) 42 42	37, 47, 55, 63	0
1	P	28/35 (80%)	0.18	0 100 100	37, 45, 62, 68	0
1	Q	29/35 (82%)	-0.12	0 100 100	26, 34, 54, 56	0
1	R	29/35 (82%)	-0.07	0 100 100	30, 38, 49, 62	0
1	S	28/35 (80%)	-0.16	0 100 100	32, 41, 61, 63	0
1	T	28/35 (80%)	-0.19	0 100 100	32, 40, 50, 60	0
1	U	28/35 (80%)	0.04	0 100 100	32, 40, 57, 68	0
1	V	28/35 (80%)	-0.00	1 (3%) 42 42	33, 40, 53, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	W	28/35 (80%)	0.04	0	100	100	30, 38, 49, 55	0
1	X	29/35 (82%)	-0.26	0	100	100	30, 38, 51, 64	0
1	Y	26/35 (74%)	0.02	0	100	100	27, 44, 57, 67	0
1	Z	31/35 (88%)	-0.14	0	100	100	25, 32, 43, 49	0
All	All	798/980 (81%)	0.03	6 (0%)	86	85	21, 38, 57, 84	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	380	LEU	3.5
1	2	377	LEU	3.3
1	O	380	LEU	3.1
1	1	378	MET	2.7
1	J	353	ASP	2.2
1	V	380	LEU	2.2

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.