Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 10:01 PM JST

PDB ID	:	7BWN
Title	:	Crystal Structure of a Designed Protein Heterocatenane
Authors	:	Liu, Y.J.; Duan, Z.L.; Fang, J.; Zhang, F.; Xiao, J.Y.; Zhang, W.B.
Deposited on	:	2020-04-15
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

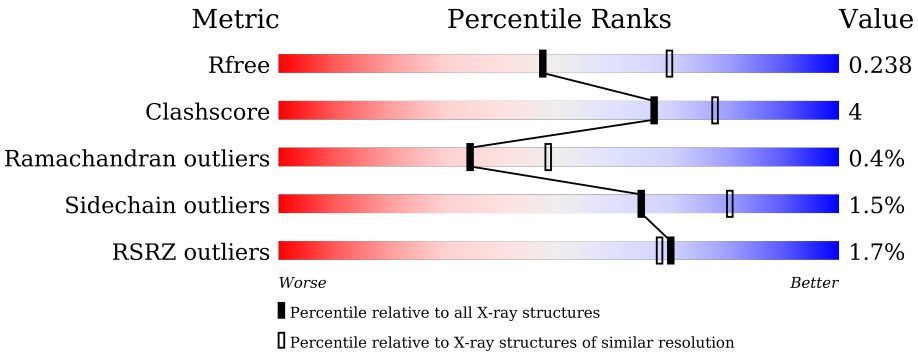
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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.



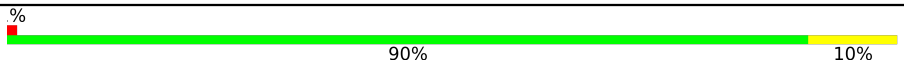
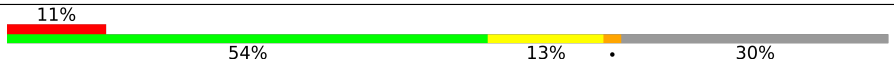
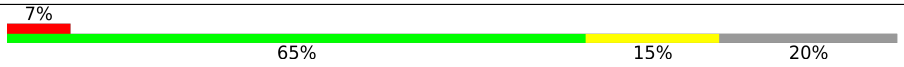
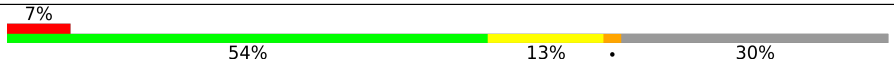
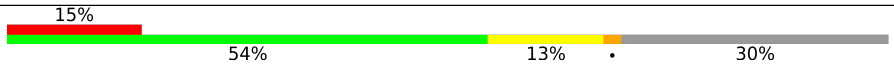
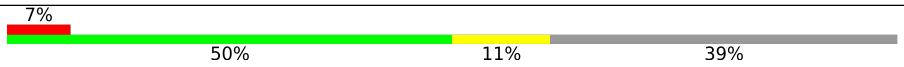
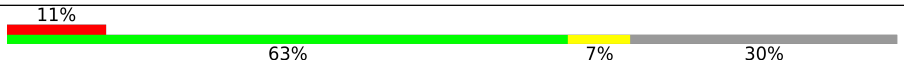
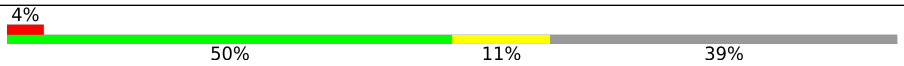
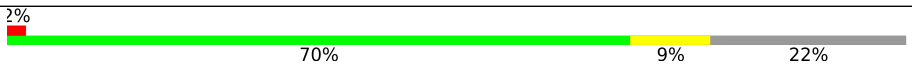
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	280	90% 9%
1	C	280	92% 7%
1	E	280	91% 9%
1	F	280	% 89% 10%
1	H	280	% 87% 12%
1	J	280	88% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	280	
1	O	280	
2	B	46	
2	D	46	
2	G	46	
2	I	46	
2	K	46	
2	L	46	
2	N	46	
2	P	46	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20596 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 Chimera of Green fluorescent protein and p53dim.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	280	Total	C	N	O	S	0	0	0
			2225	1404	384	429	8			
1	A	280	Total	C	N	O	S	0	0	0
			2225	1404	384	429	8			
1	C	280	Total	C	N	O	S	0	0	0
			2225	1404	384	429	8			
1	E	280	Total	C	N	O	S	0	0	0
			2225	1404	384	429	8			
1	H	280	Total	C	N	O	S	0	0	0
			2225	1404	384	429	8			
1	J	280	Total	C	N	O	S	0	0	0
			2225	1404	384	429	8			
1	M	280	Total	C	N	O	S	0	0	0
			2225	1404	384	429	8			
1	O	280	Total	C	N	O	S	0	0	0
			2221	1402	384	427	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	SER	ARG	engineered mutation	UNP A0A059PIQ0
F	30	ARG	SER	engineered mutation	UNP A0A059PIQ0
F	72	SER	ALA	engineered mutation	UNP A0A059PIQ0
F	80	ARG	GLN	engineered mutation	UNP A0A059PIQ0
F	206	VAL	ALA	engineered mutation	UNP A0A059PIQ0
A	2	SER	ARG	engineered mutation	UNP A0A059PIQ0
A	30	ARG	SER	engineered mutation	UNP A0A059PIQ0
A	72	SER	ALA	engineered mutation	UNP A0A059PIQ0
A	80	ARG	GLN	engineered mutation	UNP A0A059PIQ0
A	206	VAL	ALA	engineered mutation	UNP A0A059PIQ0
C	2	SER	ARG	engineered mutation	UNP A0A059PIQ0
C	30	ARG	SER	engineered mutation	UNP A0A059PIQ0
C	72	SER	ALA	engineered mutation	UNP A0A059PIQ0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	80	ARG	GLN	engineered mutation	UNP A0A059PIQ0
C	206	VAL	ALA	engineered mutation	UNP A0A059PIQ0
E	2	SER	ARG	engineered mutation	UNP A0A059PIQ0
E	30	ARG	SER	engineered mutation	UNP A0A059PIQ0
E	72	SER	ALA	engineered mutation	UNP A0A059PIQ0
E	80	ARG	GLN	engineered mutation	UNP A0A059PIQ0
E	206	VAL	ALA	engineered mutation	UNP A0A059PIQ0
H	2	SER	ARG	engineered mutation	UNP A0A059PIQ0
H	30	ARG	SER	engineered mutation	UNP A0A059PIQ0
H	72	SER	ALA	engineered mutation	UNP A0A059PIQ0
H	80	ARG	GLN	engineered mutation	UNP A0A059PIQ0
H	206	VAL	ALA	engineered mutation	UNP A0A059PIQ0
J	2	SER	ARG	engineered mutation	UNP A0A059PIQ0
J	30	ARG	SER	engineered mutation	UNP A0A059PIQ0
J	72	SER	ALA	engineered mutation	UNP A0A059PIQ0
J	80	ARG	GLN	engineered mutation	UNP A0A059PIQ0
J	206	VAL	ALA	engineered mutation	UNP A0A059PIQ0
M	2	SER	ARG	engineered mutation	UNP A0A059PIQ0
M	30	ARG	SER	engineered mutation	UNP A0A059PIQ0
M	72	SER	ALA	engineered mutation	UNP A0A059PIQ0
M	80	ARG	GLN	engineered mutation	UNP A0A059PIQ0
M	206	VAL	ALA	engineered mutation	UNP A0A059PIQ0
O	2	SER	ARG	engineered mutation	UNP A0A059PIQ0
O	30	ARG	SER	engineered mutation	UNP A0A059PIQ0
O	72	SER	ALA	engineered mutation	UNP A0A059PIQ0
O	80	ARG	GLN	engineered mutation	UNP A0A059PIQ0
O	206	VAL	ALA	engineered mutation	UNP A0A059PIQ0

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	L	32	Total C N O 274 172 49 53	0	0	0
2	B	32	Total C N O 285 179 52 54	0	0	0
2	D	37	Total C N O S 312 195 55 61 1	0	0	0
2	G	32	Total C N O 279 175 49 55	0	0	0
2	I	32	Total C N O 285 179 52 54	0	0	0
2	K	28	Total C N O 248 156 44 48	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	N	28	Total C N O 248 156 44 48	0	0	0
2	P	36	Total C N O S 304 191 53 59 1	0	0	0

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	316	GLY	-	expression tag	UNP P04637
L	317	GLY	-	expression tag	UNP P04637
L	318	HIS	-	expression tag	UNP P04637
L	319	HIS	-	expression tag	UNP P04637
L	320	HIS	-	expression tag	UNP P04637
L	321	HIS	-	expression tag	UNP P04637
L	322	HIS	-	expression tag	UNP P04637
L	323	HIS	-	expression tag	UNP P04637
L	324	GLU	-	expression tag	UNP P04637
L	325	LEU	-	expression tag	UNP P04637
L	340	GLU	MET	engineered mutation	UNP P04637
L	344	LYS	LEU	engineered mutation	UNP P04637
L	357	THR	-	expression tag	UNP P04637
L	358	SER	-	expression tag	UNP P04637
L	359	CYS	-	expression tag	UNP P04637
L	360	PHE	-	expression tag	UNP P04637
L	361	ASN	-	expression tag	UNP P04637
B	316	GLY	-	expression tag	UNP P04637
B	317	GLY	-	expression tag	UNP P04637
B	318	HIS	-	expression tag	UNP P04637
B	319	HIS	-	expression tag	UNP P04637
B	320	HIS	-	expression tag	UNP P04637
B	321	HIS	-	expression tag	UNP P04637
B	322	HIS	-	expression tag	UNP P04637
B	323	HIS	-	expression tag	UNP P04637
B	324	GLU	-	expression tag	UNP P04637
B	325	LEU	-	expression tag	UNP P04637
B	340	GLU	MET	engineered mutation	UNP P04637
B	344	LYS	LEU	engineered mutation	UNP P04637
B	357	THR	-	expression tag	UNP P04637
B	358	SER	-	expression tag	UNP P04637
B	359	CYS	-	expression tag	UNP P04637
B	360	PHE	-	expression tag	UNP P04637
B	361	ASN	-	expression tag	UNP P04637

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	316	GLY	-	expression tag	UNP P04637
D	317	GLY	-	expression tag	UNP P04637
D	318	HIS	-	expression tag	UNP P04637
D	319	HIS	-	expression tag	UNP P04637
D	320	HIS	-	expression tag	UNP P04637
D	321	HIS	-	expression tag	UNP P04637
D	322	HIS	-	expression tag	UNP P04637
D	323	HIS	-	expression tag	UNP P04637
D	324	GLU	-	expression tag	UNP P04637
D	325	LEU	-	expression tag	UNP P04637
D	340	GLU	MET	engineered mutation	UNP P04637
D	344	LYS	LEU	engineered mutation	UNP P04637
D	357	THR	-	expression tag	UNP P04637
D	358	SER	-	expression tag	UNP P04637
D	359	CYS	-	expression tag	UNP P04637
D	360	PHE	-	expression tag	UNP P04637
D	361	ASN	-	expression tag	UNP P04637
G	316	GLY	-	expression tag	UNP P04637
G	317	GLY	-	expression tag	UNP P04637
G	318	HIS	-	expression tag	UNP P04637
G	319	HIS	-	expression tag	UNP P04637
G	320	HIS	-	expression tag	UNP P04637
G	321	HIS	-	expression tag	UNP P04637
G	322	HIS	-	expression tag	UNP P04637
G	323	HIS	-	expression tag	UNP P04637
G	324	GLU	-	expression tag	UNP P04637
G	325	LEU	-	expression tag	UNP P04637
G	340	GLU	MET	engineered mutation	UNP P04637
G	344	LYS	LEU	engineered mutation	UNP P04637
G	357	THR	-	expression tag	UNP P04637
G	358	SER	-	expression tag	UNP P04637
G	359	CYS	-	expression tag	UNP P04637
G	360	PHE	-	expression tag	UNP P04637
G	361	ASN	-	expression tag	UNP P04637
I	316	GLY	-	expression tag	UNP P04637
I	317	GLY	-	expression tag	UNP P04637
I	318	HIS	-	expression tag	UNP P04637
I	319	HIS	-	expression tag	UNP P04637
I	320	HIS	-	expression tag	UNP P04637
I	321	HIS	-	expression tag	UNP P04637
I	322	HIS	-	expression tag	UNP P04637
I	323	HIS	-	expression tag	UNP P04637

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	324	GLU	-	expression tag	UNP P04637
I	325	LEU	-	expression tag	UNP P04637
I	340	GLU	MET	engineered mutation	UNP P04637
I	344	LYS	LEU	engineered mutation	UNP P04637
I	357	THR	-	expression tag	UNP P04637
I	358	SER	-	expression tag	UNP P04637
I	359	CYS	-	expression tag	UNP P04637
I	360	PHE	-	expression tag	UNP P04637
I	361	ASN	-	expression tag	UNP P04637
K	316	GLY	-	expression tag	UNP P04637
K	317	GLY	-	expression tag	UNP P04637
K	318	HIS	-	expression tag	UNP P04637
K	319	HIS	-	expression tag	UNP P04637
K	320	HIS	-	expression tag	UNP P04637
K	321	HIS	-	expression tag	UNP P04637
K	322	HIS	-	expression tag	UNP P04637
K	323	HIS	-	expression tag	UNP P04637
K	324	GLU	-	expression tag	UNP P04637
K	325	LEU	-	expression tag	UNP P04637
K	340	GLU	MET	engineered mutation	UNP P04637
K	344	LYS	LEU	engineered mutation	UNP P04637
K	357	THR	-	expression tag	UNP P04637
K	358	SER	-	expression tag	UNP P04637
K	359	CYS	-	expression tag	UNP P04637
K	360	PHE	-	expression tag	UNP P04637
K	361	ASN	-	expression tag	UNP P04637
N	316	GLY	-	expression tag	UNP P04637
N	317	GLY	-	expression tag	UNP P04637
N	318	HIS	-	expression tag	UNP P04637
N	319	HIS	-	expression tag	UNP P04637
N	320	HIS	-	expression tag	UNP P04637
N	321	HIS	-	expression tag	UNP P04637
N	322	HIS	-	expression tag	UNP P04637
N	323	HIS	-	expression tag	UNP P04637
N	324	GLU	-	expression tag	UNP P04637
N	325	LEU	-	expression tag	UNP P04637
N	340	GLU	MET	engineered mutation	UNP P04637
N	344	LYS	LEU	engineered mutation	UNP P04637
N	357	THR	-	expression tag	UNP P04637
N	358	SER	-	expression tag	UNP P04637
N	359	CYS	-	expression tag	UNP P04637
N	360	PHE	-	expression tag	UNP P04637

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	361	ASN	-	expression tag	UNP P04637
P	316	GLY	-	expression tag	UNP P04637
P	317	GLY	-	expression tag	UNP P04637
P	318	HIS	-	expression tag	UNP P04637
P	319	HIS	-	expression tag	UNP P04637
P	320	HIS	-	expression tag	UNP P04637
P	321	HIS	-	expression tag	UNP P04637
P	322	HIS	-	expression tag	UNP P04637
P	323	HIS	-	expression tag	UNP P04637
P	324	GLU	-	expression tag	UNP P04637
P	325	LEU	-	expression tag	UNP P04637
P	340	GLU	MET	engineered mutation	UNP P04637
P	344	LYS	LEU	engineered mutation	UNP P04637
P	357	THR	-	expression tag	UNP P04637
P	358	SER	-	expression tag	UNP P04637
P	359	CYS	-	expression tag	UNP P04637
P	360	PHE	-	expression tag	UNP P04637
P	361	ASN	-	expression tag	UNP P04637

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	73	Total O 73 73	0	0
3	L	8	Total O 8 8	0	0
3	A	62	Total O 62 62	0	0
3	B	9	Total O 9 9	0	0
3	C	56	Total O 56 56	0	0
3	D	8	Total O 8 8	0	0
3	E	71	Total O 71 71	0	0
3	G	8	Total O 8 8	0	0
3	H	60	Total O 60 60	0	0
3	I	8	Total O 8 8	0	0

Continued on next page...

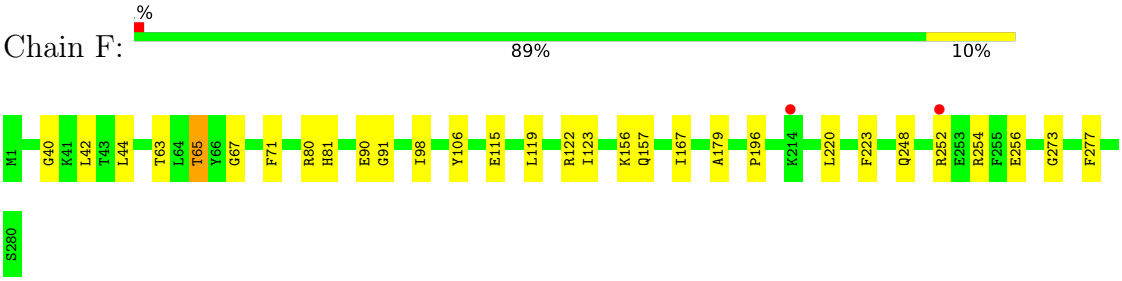
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	60	Total O 60 60	0	0
3	K	6	Total O 6 6	0	0
3	M	71	Total O 71 71	0	0
3	N	5	Total O 5 5	0	0
3	O	56	Total O 56 56	0	0
3	P	4	Total O 4 4	0	0

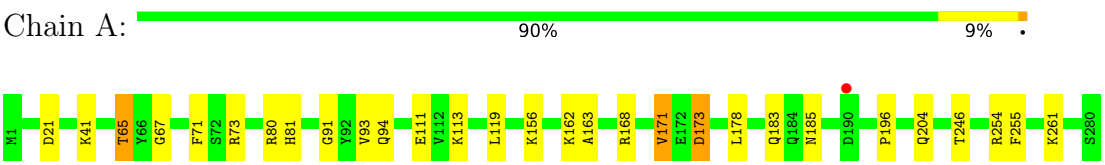
3 Residue-property plots (i)

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.

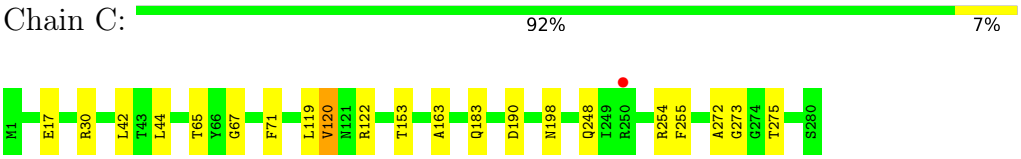
• Molecule 1: Chimera of Green fluorescent protein and p53dim



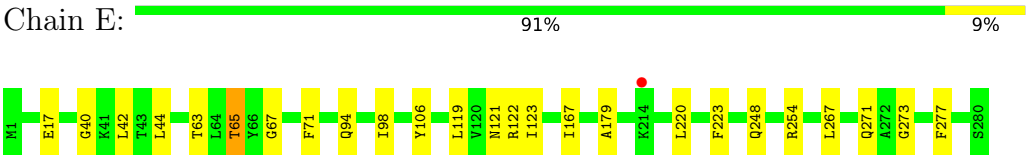
• Molecule 1: Chimera of Green fluorescent protein and p53dim



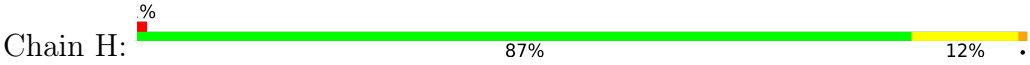
• Molecule 1: Chimera of Green fluorescent protein and p53dim

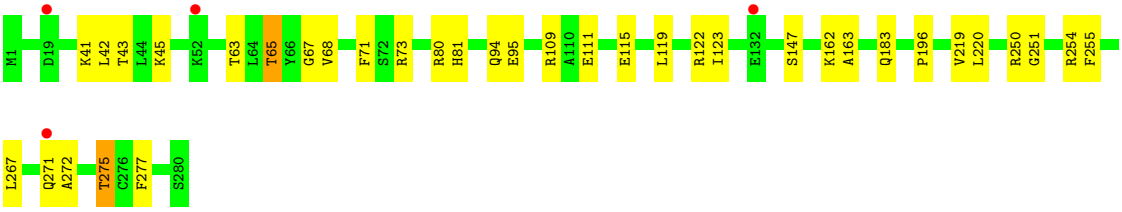


• Molecule 1: Chimera of Green fluorescent protein and p53dim

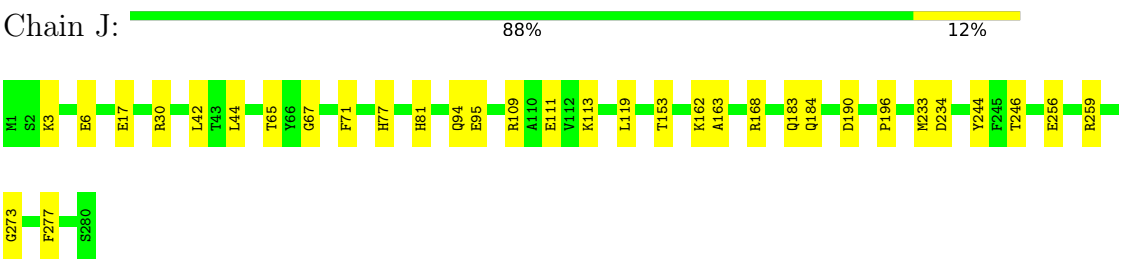


• Molecule 1: Chimera of Green fluorescent protein and p53dim

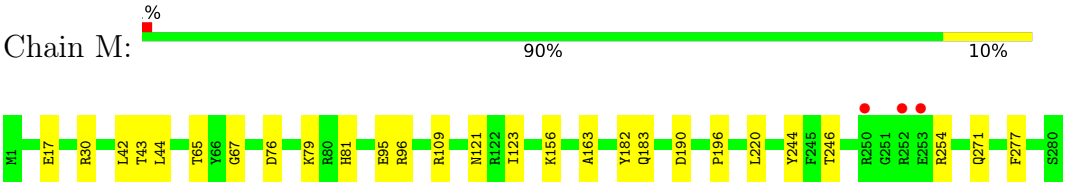




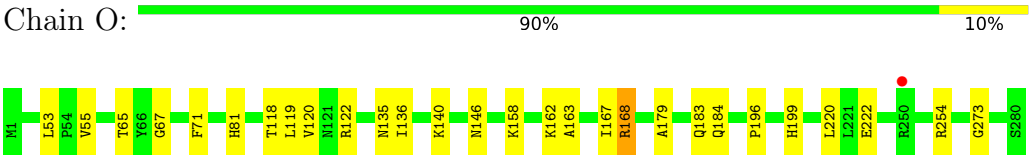
• Molecule 1: Chimera of Green fluorescent protein and p53dim



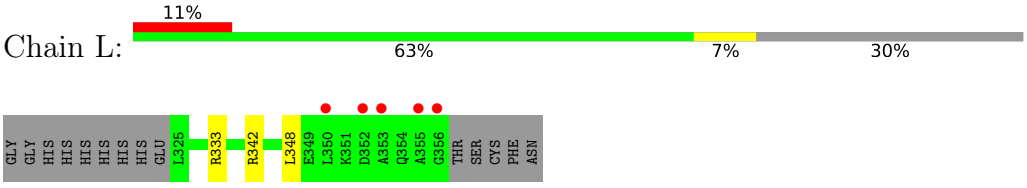
• Molecule 1: Chimera of Green fluorescent protein and p53dim



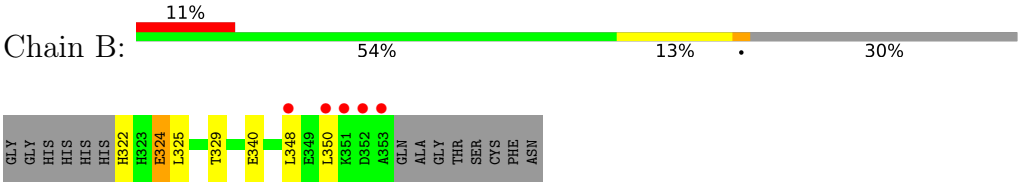
• Molecule 1: Chimera of Green fluorescent protein and p53dim



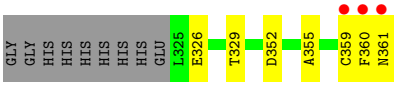
• Molecule 2: Cellular tumor antigen p53



• Molecule 2: Cellular tumor antigen p53



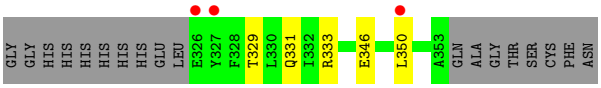
• Molecule 2: Cellular tumor antigen p53



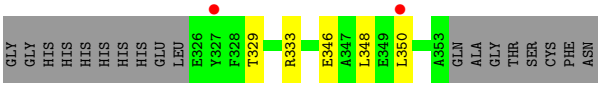
• Molecule 2: Cellular tumor antigen p53

• Molecule 2: Cellular tumor antigen p53

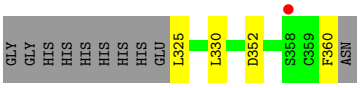
• Molecule 2: Cellular tumor antigen p53



• Molecule 2: Cellular tumor antigen p53



• Molecule 2: Cellular tumor antigen p53



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	108.90Å 108.90Å 684.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.15 – 2.40 49.15 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.15-2.40) 96.3 (49.15-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14_3247	Depositor
R, R_{free}	0.187 , 0.239 0.187 , 0.238	Depositor DCC
R_{free} test set	2007 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 22.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.480 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20596	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 4.88% 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	0.45	1/2272 (0.0%)	0.59	1/3062 (0.0%)
1	C	0.30	0/2272	0.56	0/3062
1	E	0.38	0/2272	0.58	1/3062 (0.0%)
1	F	0.42	1/2272 (0.0%)	0.58	1/3062 (0.0%)
1	H	0.34	0/2272	0.57	1/3062 (0.0%)
1	J	0.43	0/2272	0.58	0/3062
1	M	0.47	1/2272 (0.0%)	0.57	0/3062
1	O	0.37	0/2268	0.56	0/3057
2	B	0.37	0/290	0.57	0/385
2	D	0.49	0/316	0.58	0/420
2	G	0.65	0/282	0.72	1/374 (0.3%)
2	I	0.32	0/290	0.51	0/385
2	K	0.44	0/251	0.55	0/332
2	L	0.32	0/277	0.54	0/367
2	N	0.34	0/251	0.51	0/332
2	P	0.31	0/308	0.48	0/409
All	All	0.40	3/20437 (0.0%)	0.57	5/27495 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	244	TYR	CE1-CZ	-5.59	1.31	1.38
1	F	91	GLY	C-O	-5.12	1.15	1.23
1	A	91	GLY	C-O	-5.07	1.15	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	65	THR	C-N-CA	-5.64	107.61	121.70
1	F	65	THR	C-N-CA	-5.51	107.92	121.70
2	G	352	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	65	THR	C-N-CA	-5.18	108.75	121.70
1	H	65	THR	C-N-CA	-5.09	108.97	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2225	0	2169	22	0
1	C	2225	0	2169	11	0
1	E	2225	0	2168	16	0
1	F	2225	0	2169	20	0
1	H	2225	0	2169	25	0
1	J	2225	0	2169	21	0
1	M	2225	0	2169	18	0
1	O	2221	0	2165	17	0
2	B	285	0	268	5	0
2	D	312	0	296	3	0
2	G	279	0	267	3	0
2	I	285	0	268	4	0
2	K	248	0	237	6	0
2	L	274	0	264	3	0
2	N	248	0	237	4	0
2	P	304	0	290	2	0
3	A	62	0	0	1	0
3	B	9	0	0	0	0
3	C	56	0	0	0	0
3	D	8	0	0	0	0
3	E	71	0	0	0	0
3	F	73	0	0	1	0
3	G	8	0	0	0	0
3	H	60	0	0	3	0
3	I	8	0	0	0	0
3	J	60	0	0	0	0
3	K	6	0	0	0	0
3	L	8	0	0	0	0
3	M	71	0	0	1	0
3	N	5	0	0	0	0
3	O	56	0	0	0	0
3	P	4	0	0	0	0
All	All	20596	0	19474	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 4.

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:J:233:MET:HE1	1:O:199:HIS:HA	1.68	0.76
1:J:256:GLU:OE2	1:J:259:ARG:NH2	2.21	0.74
1:J:17:GLU:OE2	1:J:30:ARG:NH1	2.23	0.71
1:O:146:ASN:HB3	1:O:168:ARG:NH2	2.07	0.70
2:B:324:GLU:HG2	2:B:325:LEU:HG	1.75	0.69
1:H:115:GLU:OE2	1:H:122:ARG:NH2	2.28	0.67
1:H:254:ARG:HD2	2:I:348:LEU:HD13	1.77	0.67
1:E:17:GLU:OE2	1:E:122:ARG:NH1	2.27	0.67
1:A:254:ARG:HD2	2:B:348:LEU:HD13	1.78	0.66
1:M:76:ASP:OD1	1:M:79:LYS:NZ	2.30	0.64
1:E:42:LEU:HD13	1:E:44:LEU:HD23	1.78	0.64
1:J:233:MET:CE	1:O:199:HIS:HA	2.27	0.64
1:E:65:THR:C	1:E:67:GLY:H	2.01	0.63
1:M:65:THR:C	1:M:67:GLY:H	2.01	0.63
1:F:65:THR:C	1:F:67:GLY:H	2.02	0.62
1:C:17:GLU:OE1	1:C:30:ARG:NH1	2.32	0.61
1:F:42:LEU:HD13	1:F:44:LEU:HD23	1.82	0.61
1:J:65:THR:C	1:J:67:GLY:H	2.02	0.60
1:H:65:THR:C	1:H:67:GLY:H	2.04	0.60
1:C:65:THR:C	1:C:67:GLY:H	2.03	0.60
1:O:65:THR:C	1:O:67:GLY:H	2.04	0.60
1:A:65:THR:C	1:A:67:GLY:H	2.03	0.60
1:H:65:THR:HG21	1:H:220:LEU:HD23	1.83	0.60
1:E:65:THR:HG21	1:E:220:LEU:HD23	1.85	0.59
1:A:246:THR:HG23	2:B:329:THR:HG23	1.84	0.58
1:J:65:THR:C	1:J:67:GLY:N	2.57	0.58
1:H:272:ALA:O	1:H:275:THR:OG1	2.21	0.57
1:F:65:THR:C	1:F:67:GLY:N	2.57	0.57
1:A:171:VAL:HG22	1:A:173:ASP:H	1.69	0.57
1:E:254:ARG:HD2	2:G:348:LEU:HD13	1.85	0.57
1:J:246:THR:HG23	2:K:329:THR:HG23	1.86	0.57
1:E:65:THR:C	1:E:67:GLY:N	2.57	0.56
1:O:158:LYS:HD2	1:O:184:GLN:NE2	2.19	0.56
1:M:65:THR:C	1:M:67:GLY:N	2.57	0.55
1:F:65:THR:HG21	1:F:220:LEU:HD23	1.89	0.55
1:H:65:THR:C	1:H:67:GLY:N	2.60	0.55
1:O:65:THR:C	1:O:67:GLY:N	2.60	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:C	1:A:67:GLY:N	2.59	0.53
1:C:65:THR:C	1:C:67:GLY:N	2.60	0.53
1:H:250:ARG:NH1	2:I:327:TYR:OH	2.25	0.53
1:A:111:GLU:OE1	1:M:190:ASP:HB3	2.08	0.53
1:H:73:ARG:NH1	3:H:304:HOH:O	2.42	0.53
1:J:3:LYS:O	1:J:6:GLU:HG2	2.08	0.53
1:M:65:THR:HG21	1:M:220:LEU:HD23	1.92	0.52
1:M:42:LEU:HD13	1:M:44:LEU:HD23	1.92	0.52
1:A:168:ARG:HG2	1:A:178:LEU:CD2	2.39	0.51
1:H:71:PHE:CE2	1:H:119:LEU:HD22	2.46	0.51
2:G:346:GLU:OE2	1:H:162:LYS:NZ	2.44	0.51
1:E:71:PHE:CE2	1:E:119:LEU:HD22	2.46	0.51
1:M:271:GLN:NE2	3:M:301:HOH:O	2.36	0.51
1:F:71:PHE:CE2	1:F:119:LEU:HD22	2.46	0.51
1:F:254:ARG:HD2	2:L:348:LEU:HD13	1.92	0.50
1:A:71:PHE:CE2	1:A:119:LEU:HD22	2.46	0.50
1:J:162:LYS:NZ	1:J:184:GLN:OE1	2.43	0.50
1:J:246:THR:OG1	2:K:331:GLN:NE2	2.45	0.50
1:H:111:GLU:OE2	1:J:190:ASP:HB3	2.12	0.49
1:H:267:LEU:O	1:H:271:GLN:HG3	2.11	0.49
2:D:360:PHE:O	2:D:361:ASN:C	2.50	0.49
1:J:42:LEU:HD13	1:J:44:LEU:HD23	1.94	0.49
1:A:168:ARG:HG2	1:A:178:LEU:HD21	1.94	0.49
2:D:355:ALA:HB1	2:D:359:CYS:HB2	1.94	0.49
1:F:90:GLU:H	1:F:90:GLU:CD	2.16	0.49
1:M:156:LYS:O	1:M:156:LYS:HD3	2.13	0.48
1:O:220:LEU:HD21	1:O:222:GLU:HB2	1.95	0.48
1:H:45:LYS:HD3	1:H:219:VAL:HG22	1.95	0.48
1:A:21:ASP:OD2	1:M:109:ARG:HD3	2.14	0.48
1:C:42:LEU:HD13	1:C:44:LEU:HD12	1.95	0.48
1:C:71:PHE:HE2	1:C:119:LEU:HD22	1.79	0.47
1:J:111:GLU:OE2	1:J:113:LYS:NZ	2.47	0.47
1:F:80:ARG:NH2	3:F:303:HOH:O	2.48	0.47
1:C:71:PHE:CE2	1:C:119:LEU:HD22	2.49	0.47
1:M:163:ALA:HB3	1:M:183:GLN:HB3	1.95	0.47
1:F:167:ILE:HB	1:F:179:ALA:HB3	1.97	0.47
1:A:156:LYS:HD3	2:B:340:GLU:OE2	2.15	0.47
1:A:67:GLY:HA2	1:A:94:GLN:NE2	2.29	0.47
1:A:71:PHE:HE2	1:A:119:LEU:HD22	1.80	0.47
1:E:98:ILE:HB	1:E:106:TYR:HB2	1.97	0.46
1:H:71:PHE:HE2	1:H:119:LEU:HD22	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:17:GLU:OE1	1:M:30:ARG:NH1	2.48	0.46
1:H:67:GLY:HA2	1:H:94:GLN:NE2	2.29	0.46
2:N:346:GLU:O	2:N:350:LEU:HG	2.16	0.46
1:O:71:PHE:CE2	1:O:119:LEU:HD22	2.51	0.45
1:H:277:PHE:CZ	2:I:333:ARG:HG2	2.51	0.45
1:J:71:PHE:CE2	1:J:119:LEU:HD22	2.51	0.45
1:H:163:ALA:HB3	1:H:183:GLN:HB3	1.98	0.45
1:F:115:GLU:OE1	1:F:122:ARG:NH1	2.34	0.45
1:A:163:ALA:HB3	1:A:183:GLN:HB3	1.98	0.45
1:F:252:ARG:NH2	1:F:256:GLU:OE1	2.50	0.45
1:E:71:PHE:HE2	1:E:119:LEU:HD22	1.82	0.45
1:H:95:GLU:HG2	1:H:109:ARG:HG3	1.98	0.45
1:J:244:TYR:OH	2:K:333:ARG:HD3	2.17	0.45
1:O:158:LYS:HD2	1:O:184:GLN:HE22	1.80	0.44
1:O:135:ASN:HA	1:O:140:LYS:HB2	1.99	0.44
1:F:98:ILE:HB	1:F:106:TYR:HB2	2.00	0.44
1:O:167:ILE:HB	1:O:179:ALA:HB3	2.00	0.44
1:A:41:LYS:HB2	1:A:41:LYS:HE3	1.86	0.44
1:F:71:PHE:HE2	1:F:119:LEU:HD22	1.82	0.44
1:A:67:GLY:HA2	1:A:94:GLN:HE22	1.82	0.43
1:C:272:ALA:O	1:C:275:THR:HG23	2.18	0.43
1:F:40:GLY:O	1:F:223:PHE:HA	2.18	0.43
1:E:40:GLY:O	1:E:223:PHE:HA	2.18	0.43
2:K:346:GLU:OE2	1:O:162:LYS:NZ	2.52	0.43
1:C:120:VAL:HG13	1:C:122:ARG:HG3	2.01	0.43
1:H:41:LYS:HE3	1:H:41:LYS:HB2	1.81	0.43
1:E:277:PHE:CZ	2:G:333:ARG:HG2	2.53	0.43
1:J:77:HIS:ND1	1:J:234:ASP:OD2	2.37	0.43
1:J:163:ALA:HB3	1:J:183:GLN:HB3	2.01	0.43
1:M:277:PHE:CZ	2:N:333:ARG:HG2	2.54	0.43
1:C:254:ARG:NH2	2:D:352:ASP:OD2	2.50	0.43
1:H:42:LEU:HD21	1:H:68:VAL:HG23	2.01	0.43
1:M:95:GLU:HG2	1:M:109:ARG:HG3	2.01	0.42
2:L:342:ARG:HD2	1:A:162:LYS:HE2	2.02	0.42
1:O:120:VAL:HG12	1:O:122:ARG:HG3	2.00	0.42
1:H:63:THR:CG2	1:H:123:ILE:HG21	2.49	0.42
1:J:95:GLU:HG2	1:J:109:ARG:HG3	2.01	0.42
1:E:167:ILE:HB	1:E:179:ALA:HB3	2.01	0.42
1:E:267:LEU:O	1:E:271:GLN:HG3	2.19	0.42
1:M:254:ARG:HD2	2:N:348:LEU:HD13	2.02	0.42
1:H:251:GLY:HA3	3:H:354:HOH:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:PHE:CZ	2:L:333:ARG:HG2	2.55	0.42
1:J:277:PHE:CZ	2:K:333:ARG:HG2	2.55	0.41
1:M:246:THR:HG23	2:N:329:THR:HG23	2.02	0.41
1:C:163:ALA:HB3	1:C:183:GLN:HB3	2.01	0.41
2:K:346:GLU:O	2:K:350:LEU:HG	2.20	0.41
1:O:55:VAL:HG22	1:O:136:ILE:CG2	2.50	0.41
1:F:115:GLU:CD	1:F:122:ARG:HH12	2.21	0.41
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.86	0.41
1:O:81:HIS:O	1:O:196:PRO:HB3	2.20	0.41
1:F:63:THR:CG2	1:F:123:ILE:HG21	2.51	0.41
1:A:171:VAL:HG22	1:A:173:ASP:HB3	2.01	0.41
1:M:81:HIS:O	1:M:196:PRO:HB3	2.20	0.41
1:E:63:THR:CG2	1:E:123:ILE:HG21	2.51	0.41
1:O:163:ALA:HB3	1:O:183:GLN:HB3	2.03	0.41
1:A:113:LYS:HE2	3:A:359:HOH:O	2.20	0.41
1:M:96:ARG:HA	1:M:182:TYR:O	2.20	0.41
1:C:153:THR:HG22	1:C:198:ASN:OD1	2.20	0.41
1:H:67:GLY:HA2	1:H:94:GLN:HE22	1.84	0.41
1:H:81:HIS:O	1:H:196:PRO:HB3	2.21	0.41
1:H:277:PHE:O	3:H:301:HOH:O	2.22	0.41
1:J:67:GLY:HA2	1:J:94:GLN:NE2	2.35	0.41
1:J:81:HIS:O	1:J:196:PRO:HB3	2.21	0.41
1:F:81:HIS:O	1:F:196:PRO:HB3	2.20	0.41
1:A:93:VAL:O	1:A:185:ASN:HA	2.21	0.41
1:F:156:LYS:H	1:F:156:LYS:HG2	1.73	0.40
1:M:121:ASN:ND2	1:M:123:ILE:HD11	2.37	0.40
1:E:67:GLY:HA2	1:E:94:GLN:NE2	2.36	0.40
1:E:121:ASN:ND2	1:E:123:ILE:HD11	2.36	0.40
1:O:254:ARG:NH2	2:P:352:ASP:OD2	2.50	0.40
1:A:81:HIS:O	1:A:196:PRO:HB3	2.22	0.40
1:F:157:GLN:HE21	2:B:350:LEU:HD12	1.87	0.40
2:I:322:HIS:CG	2:I:323:HIS:N	2.89	0.40
2:P:330:LEU:HD12	2:P:330:LEU:HA	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	278/280 (99%)	268 (96%)	9 (3%)	1 (0%)	34 48
1	C	278/280 (99%)	268 (96%)	8 (3%)	2 (1%)	22 32
1	E	278/280 (99%)	266 (96%)	11 (4%)	1 (0%)	34 48
1	F	278/280 (99%)	270 (97%)	7 (2%)	1 (0%)	34 48
1	H	278/280 (99%)	266 (96%)	11 (4%)	1 (0%)	34 48
1	J	278/280 (99%)	270 (97%)	7 (2%)	1 (0%)	34 48
1	M	278/280 (99%)	268 (96%)	10 (4%)	0	100 100
1	O	278/280 (99%)	269 (97%)	8 (3%)	1 (0%)	34 48
2	B	30/46 (65%)	29 (97%)	1 (3%)	0	100 100
2	D	35/46 (76%)	33 (94%)	2 (6%)	0	100 100
2	G	30/46 (65%)	29 (97%)	0	1 (3%)	4 3
2	I	30/46 (65%)	28 (93%)	2 (7%)	0	100 100
2	K	26/46 (56%)	25 (96%)	1 (4%)	0	100 100
2	L	30/46 (65%)	27 (90%)	3 (10%)	0	100 100
2	N	26/46 (56%)	26 (100%)	0	0	100 100
2	P	34/46 (74%)	34 (100%)	0	0	100 100
All	All	2465/2608 (94%)	2376 (96%)	80 (3%)	9 (0%)	34 48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	273	GLY
2	G	353	ALA
1	J	273	GLY
1	O	273	GLY
1	F	273	GLY
1	A	255	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	273	GLY
1	H	255	PHE
1	C	255	PHE

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	241/241 (100%)	236 (98%)	5 (2%)	53 72
1	C	241/241 (100%)	238 (99%)	3 (1%)	71 85
1	E	241/241 (100%)	240 (100%)	1 (0%)	91 96
1	F	241/241 (100%)	240 (100%)	1 (0%)	91 96
1	H	241/241 (100%)	237 (98%)	4 (2%)	60 78
1	J	241/241 (100%)	239 (99%)	2 (1%)	81 91
1	M	241/241 (100%)	240 (100%)	1 (0%)	91 96
1	O	240/241 (100%)	237 (99%)	3 (1%)	69 84
2	B	29/39 (74%)	27 (93%)	2 (7%)	15 25
2	D	32/39 (82%)	30 (94%)	2 (6%)	18 28
2	G	28/39 (72%)	25 (89%)	3 (11%)	6 9
2	I	29/39 (74%)	26 (90%)	3 (10%)	7 10
2	K	25/39 (64%)	25 (100%)	0	100 100
2	L	27/39 (69%)	27 (100%)	0	100 100
2	N	25/39 (64%)	25 (100%)	0	100 100
2	P	31/39 (80%)	29 (94%)	2 (6%)	17 27
All	All	2153/2240 (96%)	2121 (98%)	32 (2%)	65 80

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	248	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	ARG
1	A	80	ARG
1	A	171	VAL
1	A	173	ASP
1	A	204	GLN
2	B	322	HIS
2	B	324	GLU
1	C	120	VAL
1	C	190	ASP
1	C	248	GLN
2	D	326	GLU
2	D	329	THR
1	E	248	GLN
2	G	324	GLU
2	G	352	ASP
2	G	354	GLN
1	H	43	THR
1	H	80	ARG
1	H	147	SER
1	H	275	THR
2	I	323	HIS
2	I	329	THR
2	I	344	LYS
1	J	153	THR
1	J	168	ARG
1	M	43	THR
1	O	53	LEU
1	O	118	THR
1	O	168	ARG
2	P	325	LEU
2	P	360	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	139	HIS
1	F	157	GLN
1	A	139	HIS
2	K	331	GLN
1	O	184	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 monosaccharides 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	280/280 (100%)	0.08	1 (0%) 92 91	25, 37, 56, 67	0
1	C	280/280 (100%)	0.09	1 (0%) 92 91	27, 36, 54, 68	0
1	E	280/280 (100%)	-0.10	1 (0%) 92 91	22, 34, 51, 61	0
1	F	280/280 (100%)	0.00	2 (0%) 87 86	23, 34, 52, 65	0
1	H	280/280 (100%)	-0.01	4 (1%) 75 73	25, 38, 58, 72	0
1	J	280/280 (100%)	-0.13	0 100 100	26, 36, 52, 65	0
1	M	280/280 (100%)	0.07	3 (1%) 80 79	26, 35, 52, 70	0
1	O	280/280 (100%)	-0.01	1 (0%) 92 91	28, 36, 56, 66	0
2	B	32/46 (69%)	0.57	5 (15%) 2 1	30, 54, 75, 81	0
2	D	37/46 (80%)	0.53	3 (8%) 12 11	31, 46, 74, 79	0
2	G	32/46 (69%)	0.63	3 (9%) 8 7	30, 46, 78, 83	0
2	I	32/46 (69%)	0.83	7 (21%) 0 0	32, 52, 80, 92	0
2	K	28/46 (60%)	0.54	3 (10%) 6 5	30, 46, 73, 77	0
2	L	32/46 (69%)	0.65	5 (15%) 2 1	29, 48, 81, 84	0
2	N	28/46 (60%)	0.54	2 (7%) 16 14	31, 45, 74, 75	0
2	P	36/46 (78%)	0.34	1 (2%) 53 51	32, 47, 68, 75	0
All	All	2497/2608 (95%)	0.06	42 (1%) 70 68	22, 36, 58, 92	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	327	TYR	5.9
2	G	355	ALA	5.3
2	I	322	HIS	5.2
1	C	250	ARG	4.6
1	H	271	GLN	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	353	ALA	4.3
2	L	356	GLY	4.0
2	D	361	ASN	3.9
2	G	353	ALA	3.7
1	O	250	ARG	3.6
1	F	252	ARG	3.4
2	I	352	ASP	3.4
2	N	327	TYR	3.4
2	N	350	LEU	3.3
2	L	352	ASP	3.1
2	B	352	ASP	3.0
1	F	214	LYS	3.0
2	B	353	ALA	3.0
2	P	358	SER	3.0
2	I	351	LYS	2.9
2	K	350	LEU	2.9
2	L	355	ALA	2.8
2	B	350	LEU	2.6
2	I	325	LEU	2.6
2	I	348	LEU	2.6
2	I	350	LEU	2.6
2	D	359	CYS	2.6
1	A	190	ASP	2.6
1	H	52	LYS	2.6
2	B	351	LYS	2.5
1	H	19	ASP	2.5
2	K	326	GLU	2.4
1	M	253	GLU	2.4
2	L	350	LEU	2.3
2	D	360	PHE	2.3
1	M	252	ARG	2.2
1	E	214	LYS	2.2
2	G	351	LYS	2.1
1	M	250	ARG	2.1
2	B	348	LEU	2.0
1	H	132	GLU	2.0
2	L	353	ALA	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 monosaccharides 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.