



# Full wwPDB X-ray Structure Validation Report

Mar 27, 2014 – 09:47 PM EDT

PDB ID : 3P87  
Title : Structure of human PCNA bound to RNASEH2B PIP box peptide  
Authors : Bubeck, D.; Reijns, M.A.; Graham, S.C.; Astell, K.R.; Jones, E.Y.; Jackson, A.P.  
Deposited on : 2010-10-13  
Resolution : 2.99 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

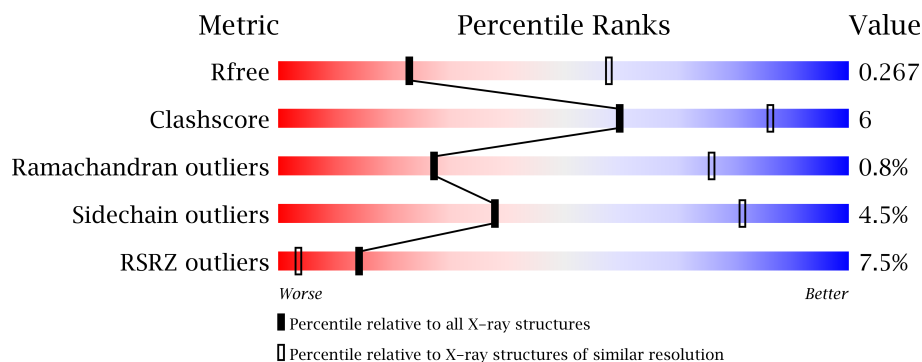
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.99 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	
1	F	261	
2	G	23	
2	H	23	
2	I	23	
2	J	23	
2	K	23	
2	L	23	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11486 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1834	1164	302	352	16			
1	B	245	Total	C	N	O	S	0	0	0
			1827	1161	301	349	16			
1	C	245	Total	C	N	O	S	0	0	0
			1834	1164	301	353	16			
1	D	245	Total	C	N	O	S	0	0	0
			1834	1164	302	352	16			
1	E	245	Total	C	N	O	S	0	0	0
			1842	1168	302	356	16			
1	F	245	Total	C	N	O	S	0	0	0
			1826	1160	301	349	16			

- Molecule 2 is a protein called Ribonuclease H2 subunit B.

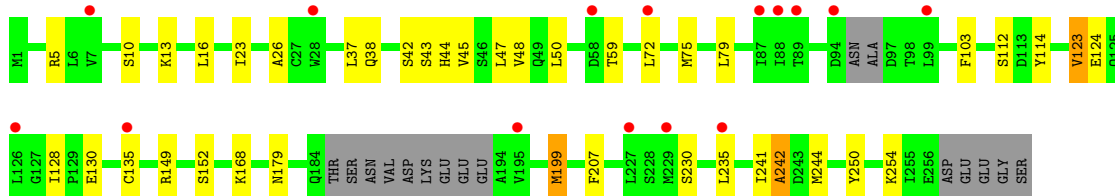
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	11	Total	C	N	O	S	0	0	0
			79	51	11	16	1			
2	H	12	Total	C	N	O	S	0	0	0
			84	54	12	17	1			
2	I	12	Total	C	N	O	S	0	0	0
			84	54	12	17	1			
2	J	11	Total	C	N	O	S	0	0	0
			79	51	11	16	1			
2	K	12	Total	C	N	O	S	0	0	0
			84	54	12	17	1			
2	L	11	Total	C	N	O	S	0	0	0
			79	51	11	16	1			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

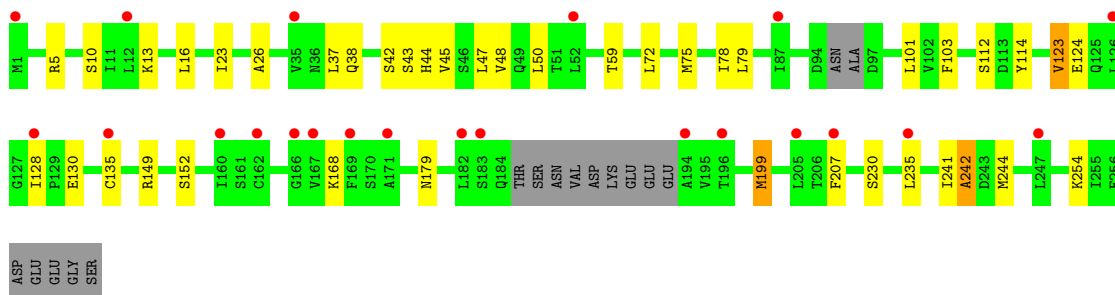
- Molecule 1: Proliferating cell nuclear antigen

Chain A: 



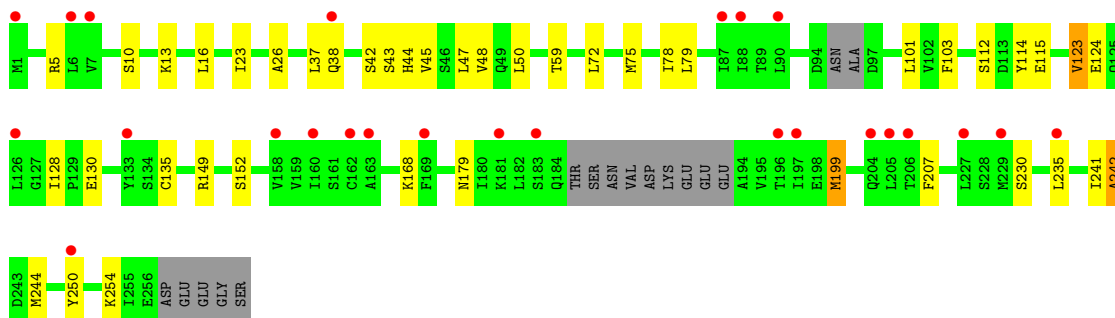
- Molecule 1: Proliferating cell nuclear antigen

Chain B: 



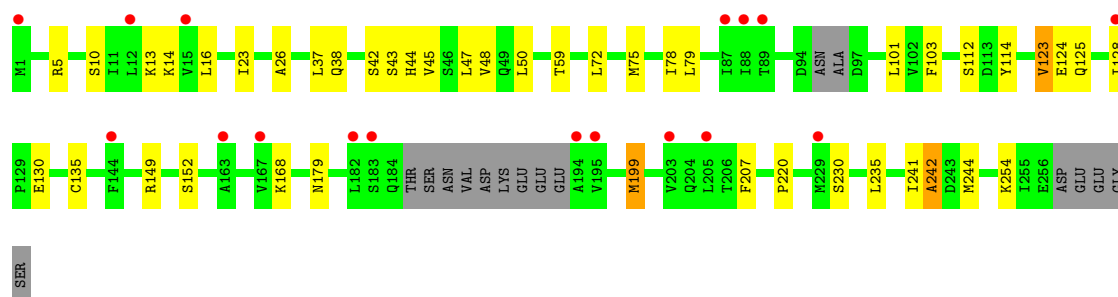
- Molecule 1: Proliferating cell nuclear antigen

Chain C: 



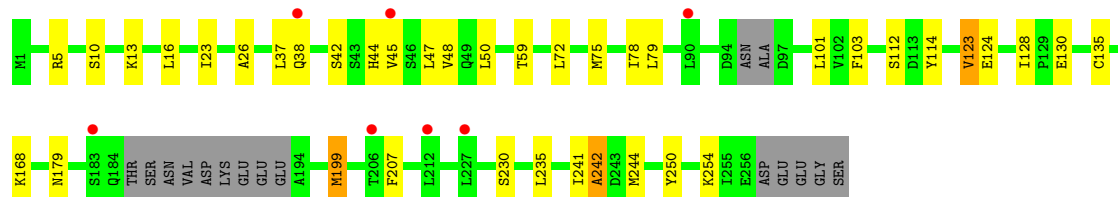
- Molecule 1: Proliferating cell nuclear antigen

Chain D: 



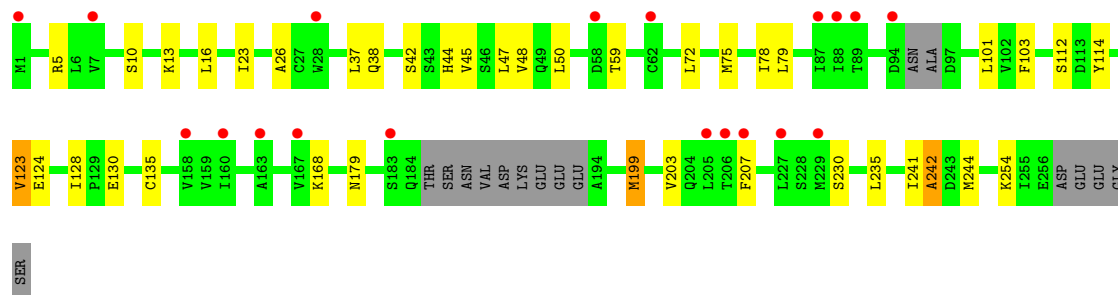
- Molecule 1: Proliferating cell nuclear antigen

Chain E:



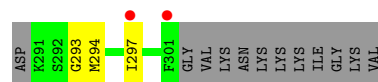
- Molecule 1: Proliferating cell nuclear antigen

Chain F:



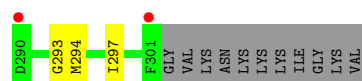
- Molecule 2: Ribonuclease H2 subunit B

Chain G:



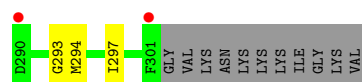
- Molecule 2: Ribonuclease H2 subunit B

Chain H:



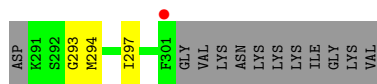
- Molecule 2: Ribonuclease H2 subunit B

Chain I:



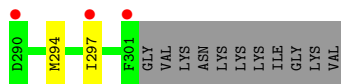
- Molecule 2: Ribonuclease H2 subunit B

Chain J: 



- Molecule 2: Ribonuclease H2 subunit B

Chain K: 



- Molecule 2: Ribonuclease H2 subunit B

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.11Å 81.79Å 116.56Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	47.45 – 2.99 47.45 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.45-2.99) 99.7 (47.45-2.99)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.223 , 0.248 0.250 , 0.267	Depositor DCC
$R_{free}$ test set	1601 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.2	EDS
Estimated twinning fraction	0.000 for k,h,-l 0.011 for -k,-h,-l 0.017 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31867 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11486	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.23 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.8786e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.42	0/1858	0.62	0/2513
1	B	0.42	0/1851	0.63	0/2504
1	C	0.41	0/1858	0.63	0/2513
1	D	0.42	0/1858	0.63	0/2513
1	E	0.42	0/1866	0.63	0/2523
1	F	0.42	0/1850	0.63	0/2503
2	G	0.59	0/80	0.75	0/106
2	H	0.54	0/85	0.72	0/113
2	I	0.56	0/85	0.73	0/113
2	J	0.56	0/80	0.72	0/106
2	K	0.59	0/85	0.73	0/113
2	L	0.54	0/80	0.73	0/106
All	All	0.43	0/11636	0.63	0/15726

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1834	0	1833	23	0
1	B	1827	0	1825	23	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1834	0	1831	25	0
1	D	1834	0	1833	24	0
1	E	1842	0	1841	22	0
1	F	1826	0	1823	22	0
2	G	79	0	65	2	0
2	H	84	0	67	2	0
2	I	84	0	67	2	0
2	J	79	0	65	2	0
2	K	84	0	67	1	0
2	L	79	0	65	1	0
All	All	11486	0	11382	137	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:CYS:SG	1:A:199:MET:HG3	2.34	0.68
1:D:135:CYS:SG	1:D:199:MET:HG3	2.35	0.67
1:C:135:CYS:SG	1:C:199:MET:HG3	2.35	0.67
1:B:135:CYS:SG	1:B:199:MET:HG3	2.35	0.67
1:E:135:CYS:SG	1:E:199:MET:HG3	2.35	0.66
1:F:135:CYS:SG	1:F:199:MET:HG3	2.36	0.65
1:A:5:ARG:HB3	1:A:59:THR:HB	1.83	0.61
1:A:44:HIS:HE1	2:J:294:MET:O	1.86	0.59
1:B:123:VAL:HG13	2:I:293:GLY:HA3	1.84	0.59
1:E:5:ARG:HB3	1:E:59:THR:HB	1.85	0.58
1:F:5:ARG:HB3	1:F:59:THR:HB	1.86	0.58
1:A:16:LEU:HD23	1:A:79:LEU:HD12	1.86	0.58
1:B:5:ARG:HB3	1:B:59:THR:HB	1.85	0.58
1:C:5:ARG:HB3	1:C:59:THR:HB	1.85	0.58
1:D:5:ARG:HB3	1:D:59:THR:HB	1.85	0.57
1:F:16:LEU:HD23	1:F:79:LEU:HD12	1.87	0.57
1:C:47:LEU:HD22	1:C:128:ILE:HD11	1.87	0.57
1:E:47:LEU:HD22	1:E:128:ILE:HD11	1.86	0.56
1:B:47:LEU:HD22	1:B:128:ILE:HD11	1.88	0.56
1:F:47:LEU:HD22	1:F:128:ILE:HD11	1.87	0.56
1:A:47:LEU:HD22	1:A:128:ILE:HD11	1.88	0.56
1:D:47:LEU:HD22	1:D:128:ILE:HD11	1.87	0.56
1:B:16:LEU:HD23	1:B:79:LEU:HD12	1.86	0.56
1:E:44:HIS:HE1	2:L:294:MET:O	1.89	0.55
1:D:16:LEU:HD23	1:D:79:LEU:HD12	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:16:LEU:HD21	1:F:75:MET:HB3	1.88	0.55
1:C:16:LEU:HD23	1:C:79:LEU:HD12	1.89	0.55
1:A:16:LEU:CD2	1:A:79:LEU:HD12	2.37	0.55
1:A:23:ILE:HG13	1:A:72:LEU:HD12	1.89	0.54
1:D:16:LEU:HD21	1:D:75:MET:HB3	1.89	0.54
2:G:294:MET:O	1:D:44:HIS:HE1	1.90	0.54
1:E:16:LEU:HD21	1:E:75:MET:HB3	1.88	0.54
1:C:16:LEU:HD21	1:C:75:MET:HB3	1.89	0.54
1:E:16:LEU:HD23	1:E:79:LEU:HD12	1.89	0.54
1:F:23:ILE:HG13	1:F:72:LEU:HD12	1.90	0.54
1:B:16:LEU:HD21	1:B:75:MET:HB3	1.89	0.54
1:A:16:LEU:HD21	1:A:75:MET:HB3	1.89	0.54
1:B:23:ILE:HG13	1:B:72:LEU:HD12	1.89	0.54
1:F:16:LEU:CD2	1:F:79:LEU:HD12	2.39	0.53
1:E:23:ILE:HG13	1:E:72:LEU:HD12	1.91	0.53
1:D:16:LEU:CD2	1:D:79:LEU:HD12	2.39	0.53
1:D:23:ILE:HG13	1:D:72:LEU:HD12	1.91	0.53
1:C:16:LEU:CD2	1:C:79:LEU:HD12	2.39	0.52
1:B:16:LEU:CD2	1:B:79:LEU:HD12	2.39	0.52
1:B:38:GLN:HG3	1:B:47:LEU:HD21	1.92	0.52
1:A:123:VAL:HG13	2:J:293:GLY:HA3	1.92	0.52
1:E:16:LEU:CD2	1:E:79:LEU:HD12	2.40	0.52
1:C:23:ILE:HG13	1:C:72:LEU:HD12	1.90	0.52
1:B:23:ILE:HD12	1:B:26:ALA:HB2	1.93	0.51
1:C:38:GLN:HG3	1:C:47:LEU:HD21	1.93	0.51
1:D:23:ILE:HD12	1:D:26:ALA:HB2	1.92	0.51
1:B:43:SER:HA	1:C:43:SER:HA	1.92	0.50
1:F:38:GLN:HG3	1:F:47:LEU:HD21	1.93	0.50
2:H:293:GLY:HA3	1:C:123:VAL:HG13	1.93	0.50
1:A:38:GLN:HG3	1:A:47:LEU:HD21	1.92	0.50
1:C:23:ILE:HD12	1:C:26:ALA:HB2	1.94	0.50
1:C:242:ALA:C	1:C:244:MET:H	2.16	0.50
2:G:293:GLY:HA3	1:D:123:VAL:HG13	1.94	0.50
1:D:38:GLN:HG3	1:D:47:LEU:HD21	1.92	0.49
1:E:242:ALA:C	1:E:244:MET:H	2.16	0.49
1:A:207:PHE:CZ	1:A:235:LEU:HB2	2.47	0.49
1:F:23:ILE:HD12	1:F:26:ALA:HB2	1.93	0.49
2:H:294:MET:O	1:C:44:HIS:HE1	1.95	0.49
1:E:23:ILE:HD12	1:E:26:ALA:HB2	1.93	0.49
1:A:242:ALA:C	1:A:244:MET:H	2.15	0.49
1:D:242:ALA:C	1:D:244:MET:H	2.15	0.49
1:E:38:GLN:HG3	1:E:47:LEU:HD21	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:242:ALA:C	1:F:244:MET:H	2.15	0.49
1:A:10:SER:HA	1:A:13:LYS:HD3	1.95	0.48
1:C:103:PHE:HB2	1:C:112:SER:HB2	1.95	0.48
2:K:294:MET:O	1:F:44:HIS:HE1	1.96	0.48
1:B:103:PHE:HB2	1:B:112:SER:HB2	1.96	0.48
1:B:242:ALA:C	1:B:244:MET:H	2.16	0.48
1:C:207:PHE:CZ	1:C:235:LEU:HB2	2.48	0.48
1:D:207:PHE:CZ	1:D:235:LEU:HB2	2.49	0.48
1:F:103:PHE:HB2	1:F:112:SER:HB2	1.96	0.48
1:B:207:PHE:CZ	1:B:235:LEU:HB2	2.48	0.48
1:E:103:PHE:HB2	1:E:112:SER:HB2	1.95	0.47
1:A:103:PHE:HB2	1:A:112:SER:HB2	1.95	0.47
1:D:103:PHE:HB2	1:D:112:SER:HB2	1.96	0.47
1:D:168:LYS:HD2	1:D:179:ASN:HD21	1.80	0.47
1:F:10:SER:HA	1:F:13:LYS:HD3	1.97	0.47
1:D:37:LEU:HB3	1:D:50:LEU:HB3	1.97	0.47
1:E:207:PHE:CZ	1:E:235:LEU:HB2	2.49	0.47
1:F:207:PHE:CZ	1:F:235:LEU:HB2	2.49	0.47
1:A:23:ILE:HD12	1:A:26:ALA:HB2	1.95	0.47
1:B:37:LEU:HB3	1:B:50:LEU:HB3	1.97	0.47
1:C:37:LEU:HB3	1:C:50:LEU:HB3	1.97	0.46
1:B:168:LYS:HD2	1:B:179:ASN:HD21	1.80	0.46
1:C:168:LYS:HD2	1:C:179:ASN:HD21	1.80	0.46
1:D:10:SER:HA	1:D:13:LYS:HD3	1.97	0.46
1:F:168:LYS:HD2	1:F:179:ASN:HD21	1.80	0.46
1:C:112:SER:HB3	1:C:114:TYR:HE2	1.81	0.46
1:E:112:SER:HB3	1:E:114:TYR:HE2	1.80	0.46
1:E:168:LYS:HD2	1:E:179:ASN:HD21	1.80	0.46
1:A:168:LYS:HD2	1:A:179:ASN:HD21	1.81	0.46
1:B:44:HIS:HE1	2:I:294:MET:O	1.97	0.46
1:E:10:SER:HA	1:E:13:LYS:HD3	1.97	0.46
1:E:37:LEU:HB3	1:E:50:LEU:HB3	1.97	0.46
1:F:112:SER:HB3	1:F:114:TYR:HE2	1.81	0.46
1:A:37:LEU:HB3	1:A:50:LEU:HB3	1.98	0.45
1:B:10:SER:HA	1:B:13:LYS:HD3	1.98	0.45
1:C:10:SER:HA	1:C:13:LYS:HD3	1.97	0.45
1:F:37:LEU:HB3	1:F:50:LEU:HB3	1.97	0.45
1:A:112:SER:HB3	1:A:114:TYR:HE2	1.81	0.45
1:D:112:SER:HB3	1:D:114:TYR:HE2	1.82	0.45
1:B:112:SER:HB3	1:B:114:TYR:HE2	1.81	0.45
1:A:43:SER:HA	1:D:43:SER:HA	2.00	0.44
1:A:123:VAL:HG12	1:A:124:GLU:H	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:78:ILE:HG21	1:F:101:LEU:HD13	2.01	0.43
1:B:123:VAL:HG12	1:B:124:GLU:H	1.84	0.43
1:E:78:ILE:HG21	1:E:101:LEU:HD13	2.01	0.43
1:B:78:ILE:HG21	1:B:101:LEU:HD13	2.01	0.43
1:C:78:ILE:HG21	1:C:101:LEU:HD13	2.00	0.43
1:E:16:LEU:HD12	1:E:16:LEU:HA	1.85	0.43
1:D:78:ILE:HG21	1:D:101:LEU:HD13	2.01	0.42
1:A:149:ARG:O	1:A:152:SER:HB2	2.19	0.42
1:F:16:LEU:HD12	1:F:16:LEU:HA	1.84	0.42
1:A:235:LEU:O	1:A:250:TYR:HA	2.20	0.42
1:F:123:VAL:HG12	1:F:124:GLU:H	1.84	0.42
1:E:112:SER:HB3	1:E:114:TYR:CE2	2.55	0.42
1:C:123:VAL:HG12	1:C:124:GLU:H	1.85	0.42
1:C:16:LEU:HD12	1:C:16:LEU:HA	1.85	0.41
1:D:123:VAL:HG12	1:D:124:GLU:H	1.85	0.41
1:F:112:SER:HB3	1:F:114:TYR:CE2	2.56	0.41
1:C:235:LEU:O	1:C:250:TYR:HA	2.21	0.41
1:C:149:ARG:O	1:C:152:SER:HB2	2.21	0.41
1:D:149:ARG:O	1:D:152:SER:HB2	2.21	0.41
1:B:149:ARG:O	1:B:152:SER:HB2	2.21	0.41
1:D:47:LEU:HD22	1:D:128:ILE:CD1	2.51	0.41
1:A:112:SER:HB3	1:A:114:TYR:CE2	2.55	0.41
1:C:112:SER:HB3	1:C:114:TYR:CE2	2.56	0.41
1:E:235:LEU:O	1:E:250:TYR:HA	2.21	0.41
1:E:123:VAL:HG12	1:E:124:GLU:H	1.86	0.40
1:D:14:LYS:HD3	1:D:220:PRO:HB2	2.02	0.40
1:F:135:CYS:SG	1:F:203:VAL:HG23	2.62	0.40
1:B:112:SER:HB3	1:B:114:TYR:CE2	2.56	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	239/261 (92%)	227 (95%)	10 (4%)	2 (1%)	27 76

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	239/261 (92%)	227 (95%)	10 (4%)	2 (1%)	27	76
1	C	239/261 (92%)	227 (95%)	10 (4%)	2 (1%)	27	76
1	D	239/261 (92%)	228 (95%)	9 (4%)	2 (1%)	27	76
1	E	239/261 (92%)	228 (95%)	9 (4%)	2 (1%)	27	76
1	F	239/261 (92%)	227 (95%)	10 (4%)	2 (1%)	27	76
2	G	9/23 (39%)	9 (100%)	0	0	100	100
2	H	10/23 (44%)	10 (100%)	0	0	100	100
2	I	10/23 (44%)	10 (100%)	0	0	100	100
2	J	9/23 (39%)	9 (100%)	0	0	100	100
2	K	10/23 (44%)	10 (100%)	0	0	100	100
2	L	9/23 (39%)	9 (100%)	0	0	100	100
All	All	1491/1704 (88%)	1421 (95%)	58 (4%)	12 (1%)	27	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	242	ALA
1	F	242	ALA
1	A	242	ALA
1	B	242	ALA
1	C	242	ALA
1	D	242	ALA
1	A	241	ILE
1	B	241	ILE
1	D	241	ILE
1	E	241	ILE
1	C	241	ILE
1	F	241	ILE

### 5.3.2 Protein sidechains ⓘ

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	200/228 (88%)	192 (96%)	8 (4%)	42	84
1	B	198/228 (87%)	190 (96%)	8 (4%)	42	84
1	C	200/228 (88%)	191 (96%)	9 (4%)	38	81
1	D	200/228 (88%)	191 (96%)	9 (4%)	38	81
1	E	202/228 (89%)	194 (96%)	8 (4%)	42	84
1	F	198/228 (87%)	190 (96%)	8 (4%)	42	84
2	G	8/20 (40%)	7 (88%)	1 (12%)	7	28
2	H	8/20 (40%)	7 (88%)	1 (12%)	7	28
2	I	8/20 (40%)	7 (88%)	1 (12%)	7	28
2	J	8/20 (40%)	7 (88%)	1 (12%)	7	28
2	K	8/20 (40%)	7 (88%)	1 (12%)	7	28
2	L	8/20 (40%)	7 (88%)	1 (12%)	7	28
All	All	1246/1488 (84%)	1190 (96%)	56 (4%)	38	81

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	A	45	VAL
1	A	48	VAL
1	A	123	VAL
1	A	130	GLU
1	A	199	MET
1	A	230	SER
1	A	254	LYS
2	G	297	ILE
1	B	42	SER
1	B	45	VAL
1	B	48	VAL
1	B	123	VAL
1	B	130	GLU
1	B	199	MET
1	B	230	SER
1	B	254	LYS
2	H	297	ILE
1	C	42	SER
1	C	45	VAL
1	C	48	VAL
1	C	115	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	123	VAL
1	C	130	GLU
1	C	199	MET
1	C	230	SER
1	C	254	LYS
2	I	297	ILE
1	D	42	SER
1	D	45	VAL
1	D	48	VAL
1	D	123	VAL
1	D	125	GLN
1	D	130	GLU
1	D	199	MET
1	D	230	SER
1	D	254	LYS
2	J	297	ILE
1	E	42	SER
1	E	45	VAL
1	E	48	VAL
1	E	123	VAL
1	E	130	GLU
1	E	199	MET
1	E	230	SER
1	E	254	LYS
2	K	297	ILE
1	F	42	SER
1	F	45	VAL
1	F	48	VAL
1	F	123	VAL
1	F	130	GLU
1	F	199	MET
1	F	230	SER
1	F	254	LYS
2	L	297	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	44	HIS
1	A	65	ASN
1	B	38	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	44	HIS
1	B	65	ASN
1	C	38	GLN
1	C	44	HIS
1	C	65	ASN
1	D	38	GLN
1	D	44	HIS
1	D	65	ASN
1	E	38	GLN
1	E	44	HIS
1	E	65	ASN
1	F	38	GLN
1	F	44	HIS
1	F	65	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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(Å²)	Q<0.9
1	A	245/261 (93%)	0.53	15 (6%) 21 5	28, 65, 100, 118	0
1	B	245/261 (93%)	0.68	22 (8%) 10 2	44, 70, 109, 130	0
1	C	245/261 (93%)	0.75	25 (10%) 7 2	43, 76, 116, 135	0
1	D	245/261 (93%)	0.67	17 (6%) 17 4	37, 69, 109, 126	0
1	E	245/261 (93%)	0.39	7 (2%) 49 9	30, 60, 102, 116	0
1	F	245/261 (93%)	0.68	19 (7%) 13 3	39, 72, 109, 128	0
2	G	11/23 (47%)	0.57	2 (18%) 2 1	56, 63, 78, 104	0
2	H	12/23 (52%)	0.89	2 (16%) 2 1	69, 79, 89, 98	0
2	I	12/23 (52%)	0.82	2 (16%) 2 1	72, 86, 98, 118	0
2	J	11/23 (47%)	0.55	1 (9%) 9 2	58, 69, 81, 112	0
2	K	12/23 (52%)	1.03	3 (25%) 1 1	63, 78, 89, 126	0
2	L	11/23 (47%)	0.40	1 (9%) 9 2	61, 72, 88, 106	0
All	All	1539/1704 (90%)	0.62	116 (7%) 14 3	28, 69, 108, 135	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	301	PHE	6.1
2	I	290	ASP	5.4
1	A	87	ILE	5.2
2	J	301	PHE	5.1
2	H	301	PHE	5.0
2	L	301	PHE	4.6
1	D	183	SER	4.3
1	F	87	ILE	4.1
1	D	87	ILE	4.1
2	H	290	ASP	4.0
2	G	301	PHE	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	160	ILE	3.9
1	B	182	LEU	3.9
2	I	301	PHE	3.9
1	C	163	ALA	3.7
2	K	290	ASP	3.7
1	C	206	THR	3.5
1	C	229	MET	3.5
1	C	87	ILE	3.4
1	E	206	THR	3.4
1	B	166	GLY	3.4
1	C	227	LEU	3.4
1	F	160	ILE	3.2
1	C	160	ILE	3.2
1	C	88	ILE	3.2
1	B	183	SER	3.2
1	B	169	PHE	3.2
1	F	205	LEU	3.2
1	B	167	VAL	3.2
1	D	205	LEU	3.1
1	F	163	ALA	3.1
1	F	62	CYS	3.1
1	A	7	VAL	3.0
1	A	229	MET	3.0
1	B	52	LEU	3.0
1	D	203	VAL	3.0
1	C	205	LEU	3.0
1	C	38	GLN	2.9
1	C	90	LEU	2.9
1	C	183	SER	2.9
1	C	162	CYS	2.9
1	B	196	THR	2.8
1	D	15	VAL	2.8
1	C	196	THR	2.8
1	E	90	LEU	2.8
1	D	128	ILE	2.8
1	F	7	VAL	2.8
1	B	162	CYS	2.8
1	E	227	LEU	2.8
1	D	229	MET	2.7
1	C	235	LEU	2.7
1	B	194	ALA	2.7
1	D	89	THR	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	88	ILE	2.7
1	A	28	TRP	2.7
1	A	135	CYS	2.6
1	A	89	THR	2.6
1	F	1	MET	2.6
1	B	205	LEU	2.6
1	F	229	MET	2.6
1	B	207	PHE	2.6
1	F	227	LEU	2.6
1	F	28	TRP	2.5
1	A	195	VAL	2.5
1	C	1	MET	2.5
1	C	197	ILE	2.5
1	B	35	VAL	2.5
1	E	212	LEU	2.5
1	B	128	ILE	2.5
1	C	158	VAL	2.5
1	A	58	ASP	2.4
1	F	89	THR	2.4
1	F	58	ASP	2.4
1	E	38	GLN	2.4
1	D	144	PHE	2.4
1	D	1	MET	2.4
1	D	167	VAL	2.4
1	B	87	ILE	2.4
1	F	207	PHE	2.4
1	C	169	PHE	2.3
1	D	12	LEU	2.3
1	B	1	MET	2.3
1	B	12	LEU	2.3
1	C	250	TYR	2.3
1	C	6	LEU	2.3
1	C	7	VAL	2.3
1	F	183	SER	2.3
1	A	94	ASP	2.2
1	C	126	LEU	2.2
1	E	183	SER	2.2
1	D	194	ALA	2.2
1	C	181	LYS	2.2
1	D	195	VAL	2.2
1	A	227	LEU	2.2
1	B	135	CYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	99	LEU	2.1
1	A	235	LEU	2.1
1	D	163	ALA	2.1
1	E	45	VAL	2.1
1	F	167	VAL	2.1
1	A	72	LEU	2.1
1	B	247	LEU	2.1
1	F	94	ASP	2.1
1	C	133	TYR	2.1
1	B	126	LEU	2.1
2	K	297	ILE	2.1
1	A	126	LEU	2.1
1	F	206	THR	2.1
1	D	182	LEU	2.1
1	D	88	ILE	2.1
1	F	88	ILE	2.1
1	F	158	VAL	2.0
1	B	171	ALA	2.0
1	B	235	LEU	2.0
1	C	204	GLN	2.0
2	G	297	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.