



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:02 am BST

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 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

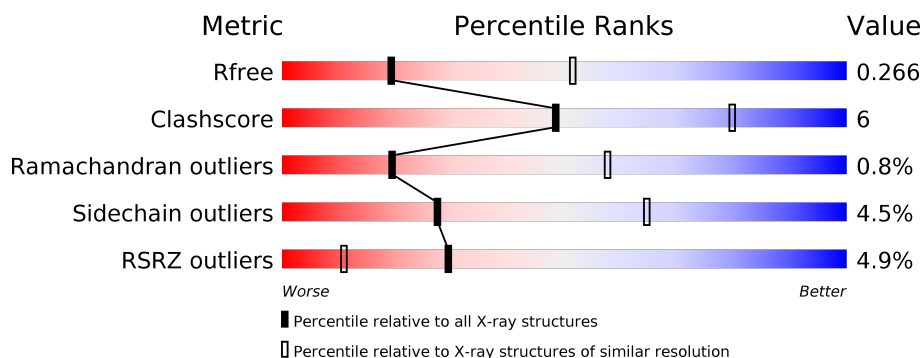
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 ≥ 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	261	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>6%</div> </div> </div>
1	B	261	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>6%</div> </div> </div>
1	C	261	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>6%</div> </div> </div>
1	D	261	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>6%</div> </div> </div>
1	E	261	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>6%</div> </div> </div>
1	F	261	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	23	<div> <div>4%</div> <div>35%</div> <div>13%</div> <div>52%</div> </div>
2	H	23	<div> <div>9%</div> <div>39%</div> <div>13%</div> <div>48%</div> </div>
2	I	23	<div> <div>9%</div> <div>39%</div> <div>13%</div> <div>48%</div> </div>
2	J	23	<div> <div>4%</div> <div>35%</div> <div>13%</div> <div>52%</div> </div>
2	K	23	<div> <div>9%</div> <div>43%</div> <div>9%</div> <div>48%</div> </div>
2	L	23	<div> <div>4%</div> <div>39%</div> <div>9%</div> <div>52%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11486 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 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			

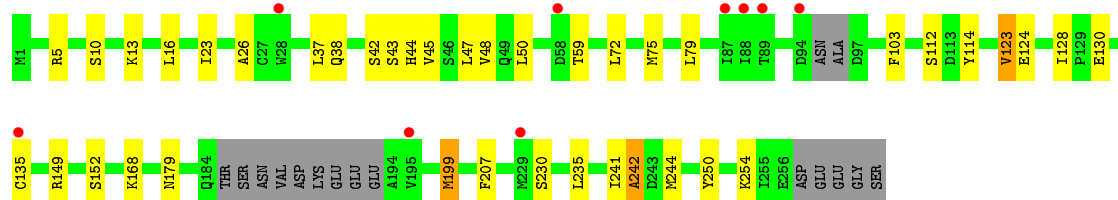
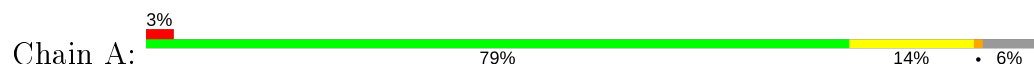
- Molecule 2 is a protein called Ribonuclease H2 subunit B.

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			

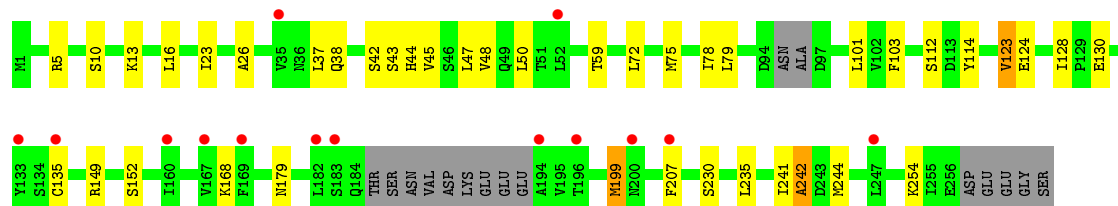
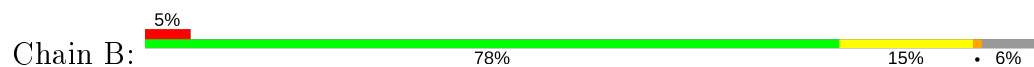
3 Residue-property plots [i](#)

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.

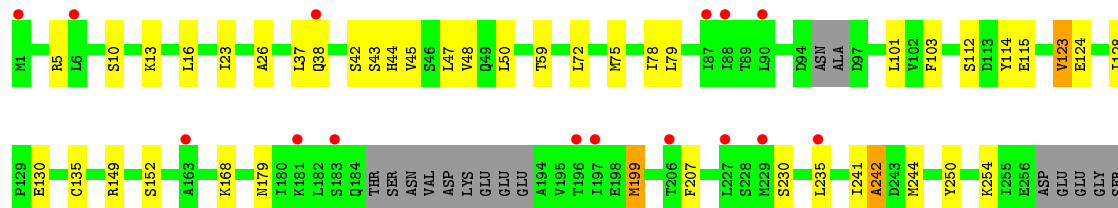
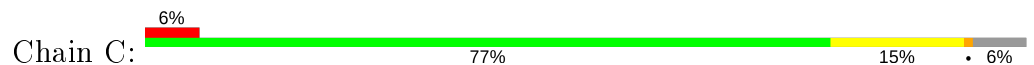
- Molecule 1: Proliferating cell nuclear antigen



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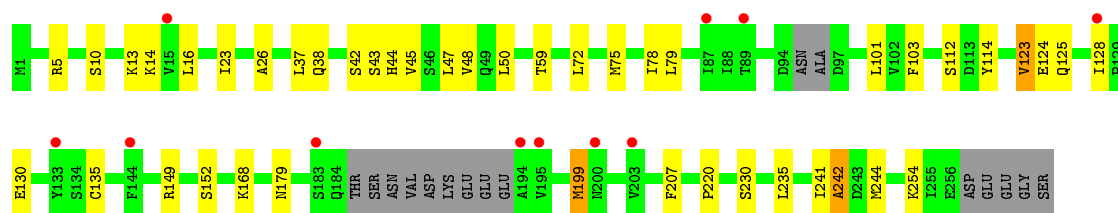


- Molecule 1: Proliferating cell nuclear antigen

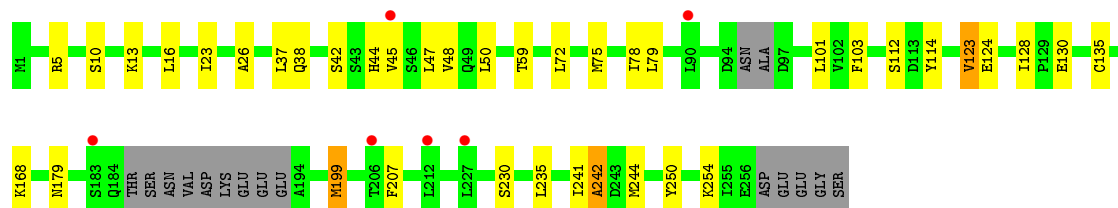
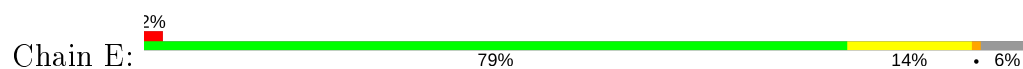


- Molecule 1: Proliferating cell nuclear antigen

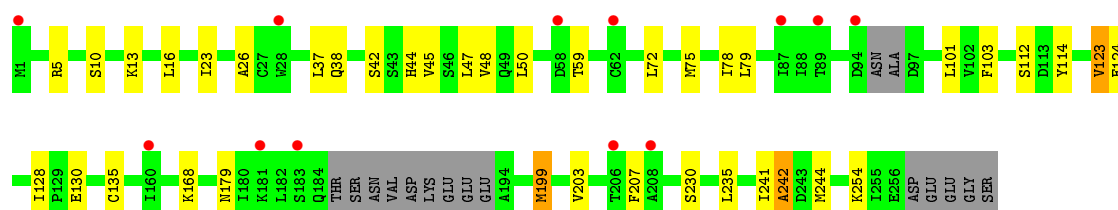
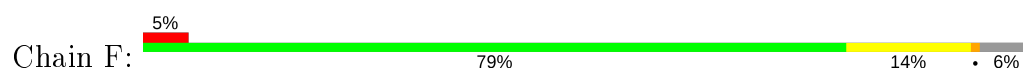




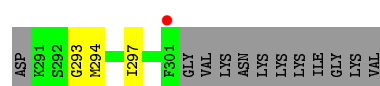
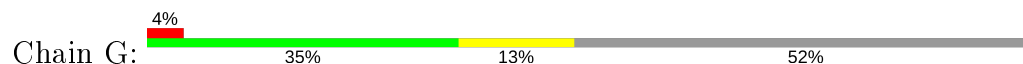
• Molecule 1: Proliferating cell nuclear antigen



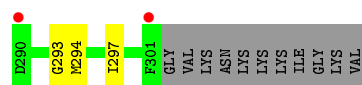
• Molecule 1: Proliferating cell nuclear antigen



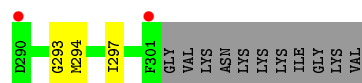
• Molecule 2: Ribonuclease H2 subunit B



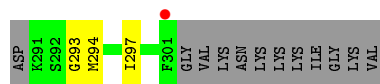
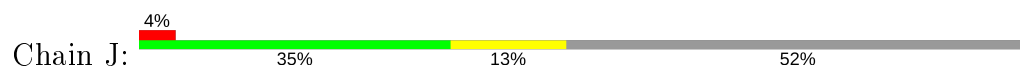
• Molecule 2: Ribonuclease H2 subunit B



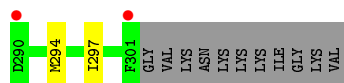
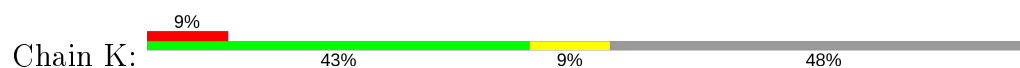
• Molecule 2: Ribonuclease H2 subunit B



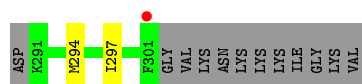
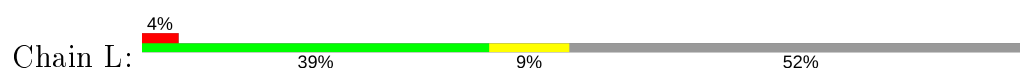
● Molecule 2: Ribonuclease H2 subunit B



● Molecule 2: Ribonuclease H2 subunit B



● Molecule 2: Ribonuclease H2 subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.223 , 0.248 0.250 , 0.266	Depositor DCC
R_{free} test set	1612 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.011 for -k,-h,-l 0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11486	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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 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	1834	0	1833	23	0
1	B	1827	0	1825	23	0
1	C	1834	0	1831	25	0
1	D	1834	0	1833	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 6.

All (137) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:242:ALA:C	1:C:244:MET:H	2.16	0.50
1:C:23:ILE:HD12	1:C:26:ALA:HB2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:GLN:HG3	1:E:47:LEU:HD21	1.94	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	19	57
1	B	239/261 (92%)	227 (95%)	10 (4%)	2 (1%)	19	57
1	C	239/261 (92%)	227 (95%)	10 (4%)	2 (1%)	19	57
1	D	239/261 (92%)	228 (95%)	9 (4%)	2 (1%)	19	57
1	E	239/261 (92%)	228 (95%)	9 (4%)	2 (1%)	19	57
1	F	239/261 (92%)	227 (95%)	10 (4%)	2 (1%)	19	57
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%)	19	57

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%)	31	68
1	B	198/228 (87%)	190 (96%)	8 (4%)	31	68
1	C	200/228 (88%)	191 (96%)	9 (4%)	27	64
1	D	200/228 (88%)	191 (96%)	9 (4%)	27	64
1	E	202/228 (89%)	194 (96%)	8 (4%)	31	68
1	F	198/228 (87%)	190 (96%)	8 (4%)	31	68
2	G	8/20 (40%)	7 (88%)	1 (12%)	4	20
2	H	8/20 (40%)	7 (88%)	1 (12%)	4	20
2	I	8/20 (40%)	7 (88%)	1 (12%)	4	20
2	J	8/20 (40%)	7 (88%)	1 (12%)	4	20
2	K	8/20 (40%)	7 (88%)	1 (12%)	4	20
2	L	8/20 (40%)	7 (88%)	1 (12%)	4	20
All	All	1246/1488 (84%)	1190 (96%)	56 (4%)	27	64

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

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Mol	Chain	Res	Type
1	C	45	VAL
1	C	48	VAL
1	C	115	GLU
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

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

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	245/261 (93%)	0.42	9 (3%)	41	17	28, 65, 100, 118	0
1	B	245/261 (93%)	0.58	14 (5%)	23	8	44, 70, 109, 130	0
1	C	245/261 (93%)	0.60	15 (6%)	21	7	43, 76, 116, 135	0
1	D	245/261 (93%)	0.54	11 (4%)	33	12	37, 69, 109, 126	0
1	E	245/261 (93%)	0.31	6 (2%)	59	30	30, 60, 102, 116	0
1	F	245/261 (93%)	0.55	12 (4%)	29	11	39, 72, 109, 128	0
2	G	11/23 (47%)	0.50	1 (9%)	9	3	56, 63, 78, 104	0
2	H	12/23 (52%)	0.68	2 (16%)	1	0	69, 79, 89, 98	0
2	I	12/23 (52%)	0.77	2 (16%)	1	0	72, 86, 98, 118	0
2	J	11/23 (47%)	0.44	1 (9%)	9	3	58, 69, 81, 112	0
2	K	12/23 (52%)	0.84	2 (16%)	1	0	63, 78, 89, 126	0
2	L	11/23 (47%)	0.37	1 (9%)	9	3	61, 72, 88, 106	0
All	All	1539/1704 (90%)	0.51	76 (4%)	29	11	28, 69, 108, 135	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	290	ASP	5.6
2	K	301	PHE	4.8
1	D	183	SER	4.4
2	J	301	PHE	4.3
1	A	87	ILE	4.3
2	L	301	PHE	4.0
2	H	301	PHE	3.9
2	H	290	ASP	3.8
1	C	206	THR	3.7
2	K	290	ASP	3.7
1	B	52	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	G	301	PHE	3.5
1	E	206	THR	3.4
1	C	183	SER	3.3
1	F	87	ILE	3.3
1	B	183	SER	3.2
1	D	87	ILE	3.1
1	B	182	LEU	3.1
2	I	301	PHE	2.9
1	C	227	LEU	2.9
1	A	135	CYS	2.8
1	F	62	CYS	2.8
1	E	227	LEU	2.8
1	E	183	SER	2.7
1	E	90	LEU	2.7
1	B	35	VAL	2.6
1	D	89	THR	2.6
1	C	90	LEU	2.6
1	F	183	SER	2.6
1	A	195	VAL	2.6
1	B	167	VAL	2.6
1	B	160	ILE	2.5
1	E	45	VAL	2.5
1	C	87	ILE	2.5
1	A	89	THR	2.5
1	C	163	ALA	2.4
1	C	196	THR	2.4
1	F	58	ASP	2.4
1	C	6	LEU	2.4
1	F	206	THR	2.4
1	D	200	ASN	2.4
1	B	196	THR	2.4
1	F	1	MET	2.4
1	D	128	ILE	2.4
1	E	212	LEU	2.4
1	B	169	PHE	2.3
1	B	194	ALA	2.3
1	C	181	LYS	2.3
1	C	88	ILE	2.3
1	D	15	VAL	2.3
1	D	133	TYR	2.3
1	F	208	ALA	2.3
1	B	247	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	229	MET	2.2
1	A	58	ASP	2.2
1	C	1	MET	2.2
1	D	144	PHE	2.2
1	F	181	LYS	2.2
1	C	197	ILE	2.2
1	B	135	CYS	2.2
1	F	94	ASP	2.2
1	A	94	ASP	2.2
1	B	133	TYR	2.2
1	C	235	LEU	2.1
1	B	207	PHE	2.1
1	C	38	GLN	2.1
1	D	194	ALA	2.1
1	F	89	THR	2.1
1	A	88	ILE	2.1
1	F	28	TRP	2.1
1	D	203	VAL	2.1
1	B	200	ASN	2.1
1	A	229	MET	2.0
1	D	195	VAL	2.0
1	F	160	ILE	2.0
1	A	28	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.