Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:32 AM GMT

PDB ID	:	2HIK
Title	:	heterotrimeric PCNA sliding clamp
Authors	:	Pascal, J.M.; Tsodikov, O.V.; Ellenberger, T.
Deposited on	:	2006-06-29
Resolution	:	3.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

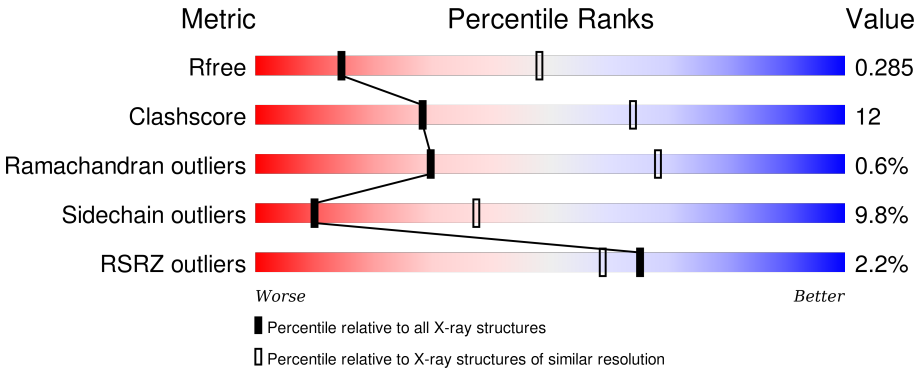
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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. 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	257	68% 25%
1	L	257	4% 73% 22%
1	X	257	2% 65% 30%
2	B	257	64% 29% 6%
2	M	245	% 62% 32% 6%

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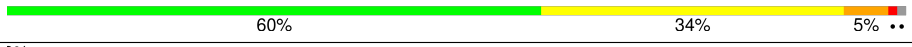
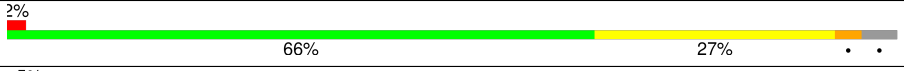
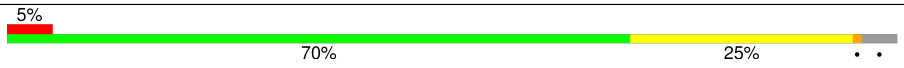
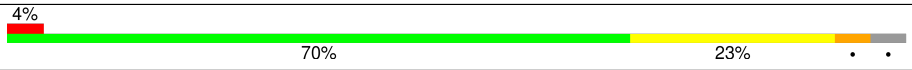
Mol	Chain	Length	Quality of chain
2	Y	245	
3	C	252	
3	N	252	
3	Z	252	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17311 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 PCNA1 (SSO0397).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	Se	0	0	0
			1924	1226	309	381	8			
1	L	248	Total	C	N	O	Se	0	0	0
			1919	1223	308	380	8			
1	X	248	Total	C	N	O	Se	0	0	0
			1919	1223	308	380	8			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	47	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	50	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	157	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	182	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	204	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	220	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	229	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	241	MSE	MET	MODIFIED RESIDUE	UNP P57766
A	250	LEU	-	CLONING ARTIFACT	UNP P57766
A	251	GLU	-	CLONING ARTIFACT	UNP P57766
A	252	HIS	-	EXPRESSION TAG	UNP P57766
A	253	HIS	-	EXPRESSION TAG	UNP P57766
A	254	HIS	-	EXPRESSION TAG	UNP P57766
A	255	HIS	-	EXPRESSION TAG	UNP P57766
A	256	HIS	-	EXPRESSION TAG	UNP P57766
A	257	HIS	-	EXPRESSION TAG	UNP P57766
L	1	MSE	MET	MODIFIED RESIDUE	UNP P57766
L	47	MSE	MET	MODIFIED RESIDUE	UNP P57766
L	50	MSE	MET	MODIFIED RESIDUE	UNP P57766
L	157	MSE	MET	MODIFIED RESIDUE	UNP P57766
L	182	MSE	MET	MODIFIED RESIDUE	UNP P57766
L	204	MSE	MET	MODIFIED RESIDUE	UNP P57766

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Chain	Residue	Modelled	Actual	Comment	Reference
L	220	MSE	MET	MODIFIED RESIDUE	UNP P57766
L	229	MSE	MET	MODIFIED RESIDUE	UNP P57766
L	241	MSE	MET	MODIFIED RESIDUE	UNP P57766
L	250	LEU	-	CLONING ARTIFACT	UNP P57766
L	251	GLU	-	CLONING ARTIFACT	UNP P57766
L	252	HIS	-	EXPRESSION TAG	UNP P57766
L	253	HIS	-	EXPRESSION TAG	UNP P57766
L	254	HIS	-	EXPRESSION TAG	UNP P57766
L	255	HIS	-	EXPRESSION TAG	UNP P57766
L	256	HIS	-	EXPRESSION TAG	UNP P57766
L	257	HIS	-	EXPRESSION TAG	UNP P57766
X	1	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	47	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	50	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	157	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	182	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	204	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	220	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	229	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	241	MSE	MET	MODIFIED RESIDUE	UNP P57766
X	250	LEU	-	CLONING ARTIFACT	UNP P57766
X	251	GLU	-	CLONING ARTIFACT	UNP P57766
X	252	HIS	-	EXPRESSION TAG	UNP P57766
X	253	HIS	-	EXPRESSION TAG	UNP P57766
X	254	HIS	-	EXPRESSION TAG	UNP P57766
X	255	HIS	-	EXPRESSION TAG	UNP P57766
X	256	HIS	-	EXPRESSION TAG	UNP P57766
X	257	HIS	-	EXPRESSION TAG	UNP P57766

- Molecule 2 is a protein called PCNA2 (SSO1047).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	Se	0	0	0
			1927	1240	302	381	4			
2	M	243	Total	C	N	O	Se	0	0	0
			1922	1237	301	380	4			
2	Y	243	Total	C	N	O	Se	0	0	0
			1922	1237	301	380	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
B	199	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
B	208	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
B	215	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
M	2	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
M	199	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
M	208	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
M	215	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
Y	2	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
Y	199	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
Y	208	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84
Y	215	MSE	MET	MODIFIED RESIDUE	UNP Q97Z84

- Molecule 3 is a protein called PCNA3 (SSO0405).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	243	Total	C	N	O	Se	0	0	0
			1926	1224	311	387	4			
3	N	243	Total	C	N	O	Se	0	0	0
			1926	1224	311	387	4			
3	Z	243	Total	C	N	O	Se	0	0	0
			1926	1224	311	387	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	MET	MODIFIED RESIDUE	UNP P57765
C	55	MSE	MET	MODIFIED RESIDUE	UNP P57765
C	75	MSE	MET	MODIFIED RESIDUE	UNP P57765
C	230	MSE	MET	MODIFIED RESIDUE	UNP P57765
C	245	LEU	-	CLONING ARTIFACT	UNP P57765
C	246	GLU	-	CLONING ARTIFACT	UNP P57765
C	247	HIS	-	EXPRESSION TAG	UNP P57765
C	248	HIS	-	EXPRESSION TAG	UNP P57765
C	249	HIS	-	EXPRESSION TAG	UNP P57765
C	250	HIS	-	EXPRESSION TAG	UNP P57765
C	251	HIS	-	EXPRESSION TAG	UNP P57765
C	252	HIS	-	EXPRESSION TAG	UNP P57765
N	1	MSE	MET	MODIFIED RESIDUE	UNP P57765
N	55	MSE	MET	MODIFIED RESIDUE	UNP P57765
N	75	MSE	MET	MODIFIED RESIDUE	UNP P57765
N	230	MSE	MET	MODIFIED RESIDUE	UNP P57765
N	245	LEU	-	CLONING ARTIFACT	UNP P57765

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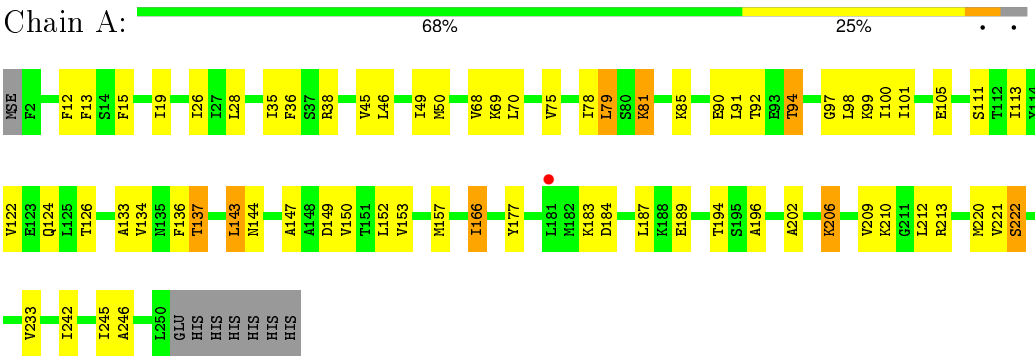
Chain	Residue	Modelled	Actual	Comment	Reference
N	246	GLU	-	CLONING ARTIFACT	UNP P57765
N	247	HIS	-	EXPRESSION TAG	UNP P57765
N	248	HIS	-	EXPRESSION TAG	UNP P57765
N	249	HIS	-	EXPRESSION TAG	UNP P57765
N	250	HIS	-	EXPRESSION TAG	UNP P57765
N	251	HIS	-	EXPRESSION TAG	UNP P57765
N	252	HIS	-	EXPRESSION TAG	UNP P57765
Z	1	MSE	MET	MODIFIED RESIDUE	UNP P57765
Z	55	MSE	MET	MODIFIED RESIDUE	UNP P57765
Z	75	MSE	MET	MODIFIED RESIDUE	UNP P57765
Z	230	MSE	MET	MODIFIED RESIDUE	UNP P57765
Z	245	LEU	-	CLONING ARTIFACT	UNP P57765
Z	246	GLU	-	CLONING ARTIFACT	UNP P57765
Z	247	HIS	-	EXPRESSION TAG	UNP P57765
Z	248	HIS	-	EXPRESSION TAG	UNP P57765
Z	249	HIS	-	EXPRESSION TAG	UNP P57765
Z	250	HIS	-	EXPRESSION TAG	UNP P57765
Z	251	HIS	-	EXPRESSION TAG	UNP P57765
Z	252	HIS	-	EXPRESSION TAG	UNP P57765

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 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.

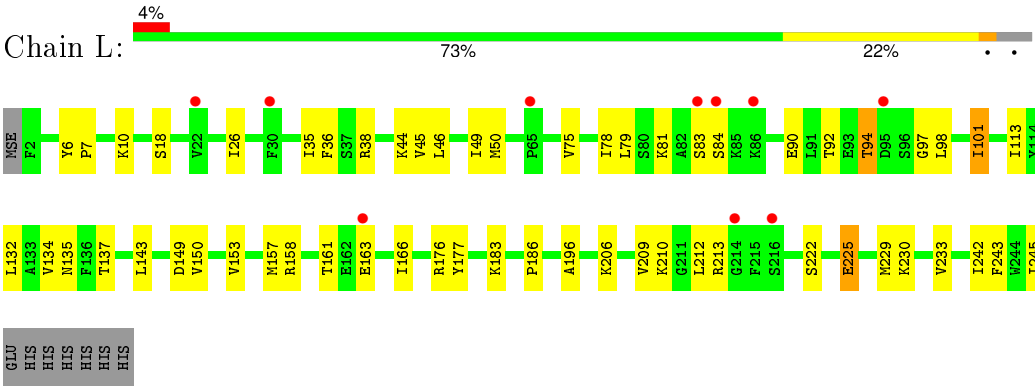
- Molecule 1: PCNA1 (SSO0397)

Chain A:



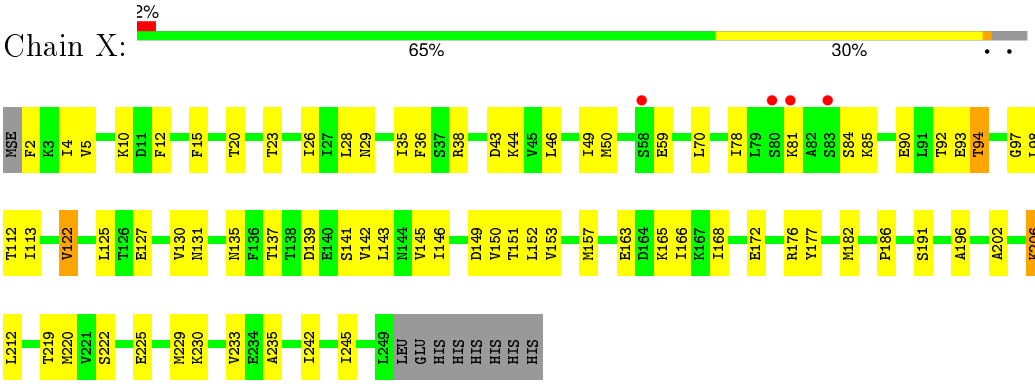
- Molecule 1: PCNA1 (SSO0397)

Chain L:



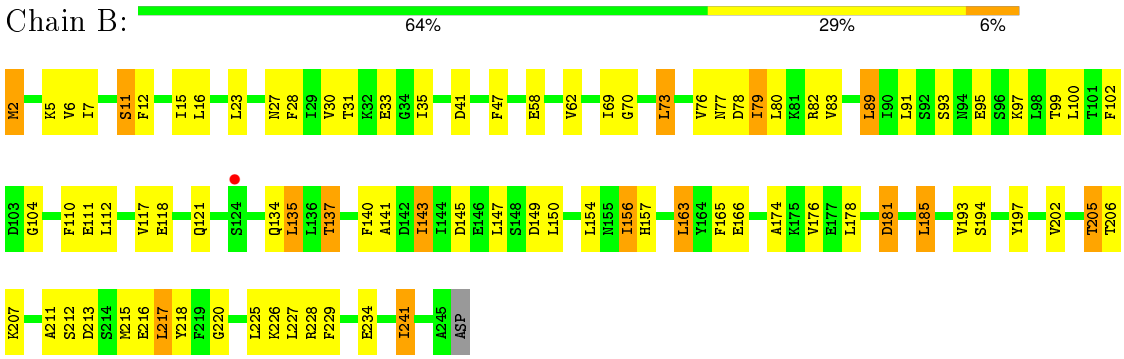
- Molecule 1: PCNA1 (SSO0397)

Chain X:



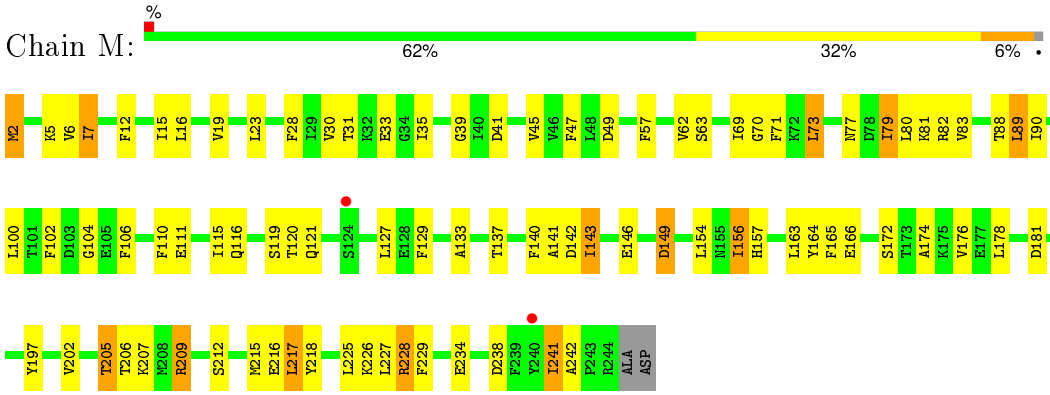
- Molecule 2: PCNA2 (SSO1047)

Chain B:



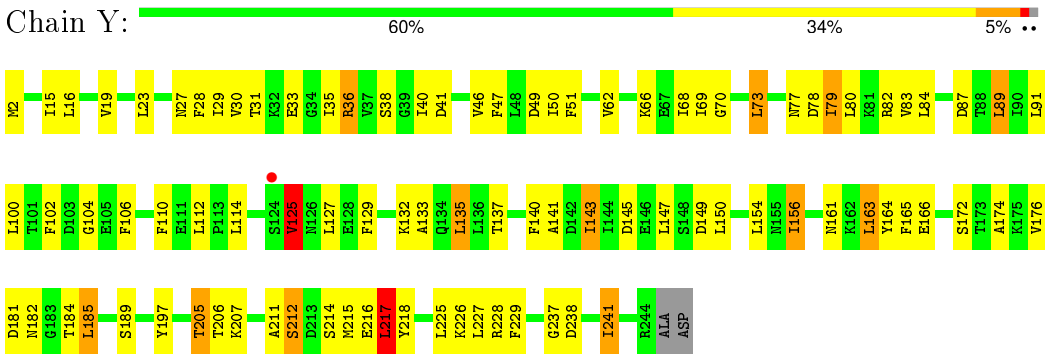
- Molecule 2: PCNA2 (SSO1047)

Chain M:



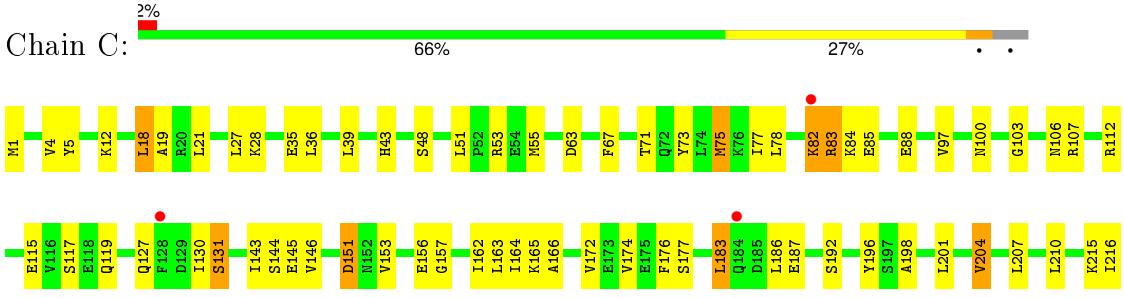
- Molecule 2: PCNA2 (SSO1047)

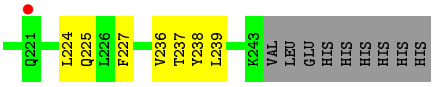
Chain Y:



- Molecule 3: PCNA3 (SSO0405)

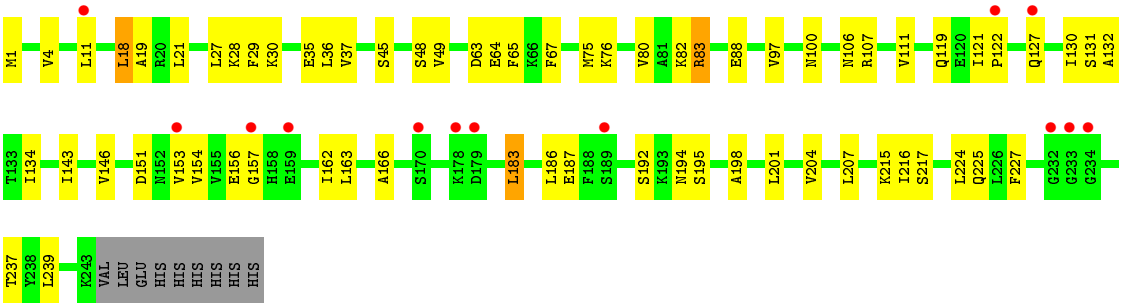
Chain C:





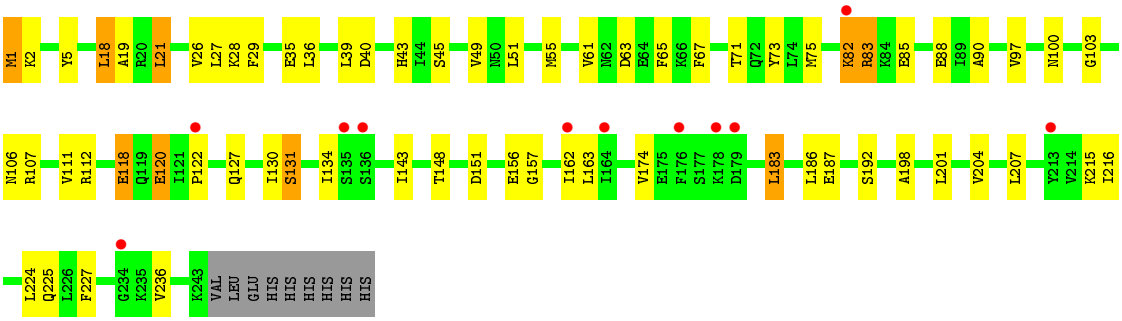
- Molecule 3: PCNA3 (SSO0405)

Chain N:



- Molecule 3: PCNA3 (SSO0405)

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	142.28Å 223.09Å 79.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 47.80 – 3.22	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-3.30) 84.9 (47.80-3.22)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.299 0.226 , 0.285	Depositor DCC
R_{free} test set	1750 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 35279 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17311	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/1944	0.53	0/2607
1	L	0.34	0/1939	0.51	0/2600
1	X	0.34	0/1939	0.52	0/2600
2	B	0.36	0/1959	0.58	0/2643
2	M	0.34	0/1954	0.56	0/2636
2	Y	0.36	0/1954	0.58	1/2636 (0.0%)
3	C	0.36	0/1949	0.53	0/2622
3	N	0.33	0/1949	0.51	0/2622
3	Z	0.33	0/1949	0.51	0/2622
All	All	0.35	0/17536	0.54	1/23588 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	217	LEU	CA-CB-CG	5.33	127.56	115.30

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	A	1924	0	1966	49	0
1	L	1919	0	1964	28	0
1	X	1919	0	1964	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1927	0	1925	56	0
2	M	1922	0	1920	66	0
2	Y	1922	0	1920	68	0
3	C	1926	0	1936	42	0
3	N	1926	0	1936	36	0
3	Z	1926	0	1936	40	0
All	All	17311	0	17467	402	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 12.

All (402) 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)
2:M:137:THR:HA	2:M:215:MSE:HE3	1.37	1.06
2:Y:137:THR:HA	2:Y:215:MSE:HE3	1.43	0.97
1:A:149:ASP:HB3	2:B:82:ARG:HE	1.29	0.97
2:B:137:THR:HA	2:B:215:MSE:HE3	1.45	0.96
2:B:218:TYR:HB2	2:B:226:LYS:HB3	1.54	0.90
1:A:69:LYS:HB3	1:A:118:GLU:HB3	1.59	0.83
2:B:80:LEU:O	2:B:83:VAL:HG23	1.77	0.82
2:Y:16:LEU:HD21	2:Y:28:PHE:HZ	1.46	0.81
2:Y:218:TYR:HB2	2:Y:226:LYS:HB3	1.64	0.79
1:A:229:MSE:HE3	1:A:245:ILE:HD12	1.66	0.78
3:Z:51:LEU:HD22	3:Z:55:MSE:HE1	1.63	0.78
2:Y:205:THR:HG21	2:Y:227:LEU:HD13	1.65	0.78
1:X:149:ASP:HB3	2:Y:82:ARG:HE	1.48	0.78
1:L:229:MSE:HE3	1:L:245:ILE:HD12	1.65	0.78
3:Z:215:LYS:HB3	3:Z:227:PHE:HB3	1.66	0.77
2:M:16:LEU:HD21	2:M:28:PHE:HZ	1.50	0.76
1:A:149:ASP:HB2	2:B:110:PHE:HZ	1.50	0.76
3:Z:130:ILE:HD13	3:Z:157:GLY:HA3	1.66	0.76
3:C:156:GLU:HB3	3:C:163:LEU:HB2	1.67	0.76
1:X:229:MSE:HE3	1:X:245:ILE:HD12	1.68	0.75
2:M:197:TYR:HB3	2:M:241:ILE:HD11	1.70	0.74
2:M:116:GLN:HE21	2:Y:29:ILE:HG21	1.53	0.73
3:C:130:ILE:HD13	3:C:157:GLY:HA3	1.71	0.73
2:B:137:THR:HG21	2:B:212:SER:O	1.90	0.72
3:N:130:ILE:O	3:N:217:SER:HA	1.90	0.72
1:X:149:ASP:HB2	2:Y:110:PHE:CZ	2.26	0.70
2:M:172:SER:CB	3:N:111:VAL:HA	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HB3	1:A:101:ILE:HG12	1.71	0.70
2:Y:205:THR:HG23	2:Y:229:PHE:CZ	2.26	0.70
2:Y:16:LEU:HD21	2:Y:28:PHE:CZ	2.27	0.70
3:N:204:VAL:HG13	3:N:207:LEU:HD12	1.73	0.70
2:Y:205:THR:HG23	2:Y:229:PHE:HZ	1.56	0.69
2:M:16:LEU:HD21	2:M:28:PHE:CZ	2.27	0.69
2:Y:30:VAL:HG22	2:Y:35:ILE:HG12	1.73	0.69
1:L:90:GLU:HB3	1:L:101:ILE:HG12	1.74	0.68
1:X:90:GLU:HB3	1:X:101:ILE:HG12	1.75	0.68
2:B:215:MSE:HE2	2:B:229:PHE:CE2	2.28	0.67
3:N:130:ILE:HD13	3:N:157:GLY:HA3	1.74	0.67
2:B:205:THR:HG21	2:B:227:LEU:HD13	1.75	0.67
2:Y:143:ILE:HG21	2:Y:176:VAL:HG11	1.75	0.67
2:Y:215:MSE:HE2	2:Y:229:PHE:CE2	2.28	0.67
1:X:152:LEU:HD11	2:Y:78:ASP:HB3	1.75	0.66
3:N:19:ALA:HB3	3:N:75:MSE:HE3	1.78	0.66
2:M:172:SER:HB3	3:N:111:VAL:HA	1.78	0.65
1:A:149:ASP:HB2	2:B:110:PHE:CZ	2.31	0.65
2:M:218:TYR:HB2	2:M:226:LYS:HB3	1.77	0.65
2:B:202:VAL:O	2:B:205:THR:HG22	1.96	0.65
3:C:204:VAL:HG13	3:C:207:LEU:HD12	1.78	0.64
2:B:156:ILE:HD12	2:B:165:PHE:HE2	1.62	0.64
3:C:183:LEU:HD11	3:C:186:LEU:HB2	1.79	0.64
1:X:153:VAL:HG21	1:X:177:TYR:HB2	1.79	0.63
2:M:15:ILE:O	2:M:19:VAL:HG23	1.99	0.63
3:Z:183:LEU:HD11	3:Z:186:LEU:HB2	1.79	0.62
3:N:4:VAL:HG22	3:N:88:GLU:HG3	1.81	0.62
1:L:10:LYS:HG2	1:L:84:SER:HB2	1.83	0.61
3:N:156:GLU:HB3	3:N:163:LEU:HB2	1.82	0.61
3:C:215:LYS:HB3	3:C:227:PHE:HB3	1.82	0.61
2:B:16:LEU:HD21	2:B:28:PHE:HZ	1.64	0.61
3:Z:162:ILE:HD13	3:Z:183:LEU:HG	1.83	0.61
2:B:30:VAL:HG22	2:B:35:ILE:HG12	1.83	0.61
1:A:36:PHE:HA	1:A:50:MSE:O	2.01	0.61
2:Y:137:THR:HG21	2:Y:212:SER:O	2.00	0.61
2:B:147:LEU:HA	2:B:150:LEU:HD12	1.83	0.60
3:N:162:ILE:HD13	3:N:183:LEU:HG	1.82	0.60
2:Y:28:PHE:HB2	2:Y:69:ILE:HB	1.82	0.60
1:X:153:VAL:HG21	1:X:177:TYR:CB	2.32	0.60
1:A:137:THR:CG2	1:A:189:GLU:HB3	2.32	0.60
2:M:205:THR:HG21	2:M:227:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:137:THR:HG22	1:X:220:MSE:HB3	1.84	0.60
2:B:166:GLU:HA	2:B:174:ALA:O	2.01	0.59
3:C:210:LEU:HD13	3:C:236:VAL:HG21	1.83	0.59
2:M:28:PHE:HB2	2:M:69:ILE:HB	1.84	0.59
2:M:6:VAL:HG22	2:M:57:PHE:CD2	2.38	0.59
1:L:38:ARG:HG3	1:L:49:ILE:HG12	1.85	0.59
1:A:153:VAL:HG21	1:A:177:TYR:HB3	1.85	0.59
1:A:147:ALA:HB1	1:A:206:LYS:HA	1.85	0.59
2:B:157:HIS:HB2	2:B:194:SER:HB3	1.85	0.58
3:C:143:ILE:HD12	3:C:201:LEU:HD13	1.83	0.58
2:Y:147:LEU:HA	2:Y:150:LEU:HD12	1.85	0.58
3:N:215:LYS:HB3	3:N:227:PHE:HB3	1.84	0.58
2:M:172:SER:HB2	3:N:111:VAL:HA	1.83	0.58
2:Y:133:ALA:HB3	2:Y:217:LEU:HB3	1.86	0.58
2:M:137:THR:HA	2:M:215:MSE:CE	2.24	0.58
2:M:23:LEU:HB2	2:M:73:LEU:HD13	1.85	0.58
3:Z:88:GLU:HB3	3:Z:100:ASN:HB2	1.86	0.58
1:X:149:ASP:HB2	2:Y:110:PHE:HZ	1.67	0.57
3:C:67:PHE:CD2	3:C:97:VAL:HG21	2.39	0.57
2:M:80:LEU:O	2:M:83:VAL:HG23	2.05	0.57
1:X:78:ILE:HG22	3:Z:148:THR:OG1	2.05	0.57
2:B:83:VAL:HG22	2:B:102:PHE:CE2	2.40	0.57
1:A:81:LYS:HG2	3:C:144:SER:HB3	1.87	0.57
2:Y:141:ALA:HB1	2:Y:206:THR:HG23	1.86	0.57
3:Z:85:GLU:OE1	3:Z:103:GLY:HA3	2.05	0.57
2:M:166:GLU:HA	2:M:174:ALA:O	2.05	0.57
3:N:27:LEU:HG	3:N:36:LEU:HD12	1.87	0.57
1:X:10:LYS:HG2	1:X:84:SER:HB2	1.87	0.57
1:A:152:LEU:HD11	2:B:78:ASP:HB3	1.86	0.57
1:A:28:LEU:HD12	1:A:70:LEU:HD21	1.86	0.56
2:M:137:THR:HG21	2:M:212:SER:O	2.04	0.56
3:N:134:ILE:HG22	3:N:183:LEU:HA	1.88	0.56
1:A:196:ALA:HA	1:A:225:GLU:HG2	1.87	0.56
3:C:146:VAL:HG13	3:C:166:ALA:HB2	1.87	0.56
3:C:162:ILE:HD13	3:C:183:LEU:HG	1.88	0.56
2:M:156:ILE:HD12	2:M:165:PHE:HE2	1.71	0.56
1:L:36:PHE:HA	1:L:50:MSE:O	2.06	0.56
3:Z:130:ILE:HD12	3:Z:192:SER:HB2	1.87	0.55
1:A:49:ILE:HB	1:A:242:ILE:HG23	1.87	0.55
1:X:172:GLU:O	1:X:176:ARG:HG3	2.06	0.55
3:Z:134:ILE:HG22	3:Z:183:LEU:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2:MSE:N	2:M:63:SER:HG	2.04	0.55
1:X:78:ILE:HD12	1:X:113:ILE:HD12	1.89	0.55
1:X:36:PHE:HA	1:X:50:MSE:O	2.06	0.55
1:X:149:ASP:HB3	2:Y:82:ARG:NE	2.20	0.55
3:C:88:GLU:HB3	3:C:100:ASN:HB2	1.89	0.55
3:Z:21:LEU:HD21	3:Z:204:VAL:HG23	1.87	0.55
2:Y:140:PHE:CD2	2:Y:215:MSE:HE1	2.42	0.54
3:N:36:LEU:HB3	3:N:49:VAL:HB	1.89	0.54
2:Y:140:PHE:HA	2:Y:143:ILE:HD11	1.90	0.54
1:A:78:ILE:HG22	3:C:145:GLU:O	2.08	0.54
3:C:18:LEU:HD11	3:C:36:LEU:HD11	1.90	0.54
1:L:153:VAL:HG21	1:L:177:TYR:HB3	1.90	0.54
2:Y:89:LEU:HD13	2:Y:91:LEU:HD22	1.89	0.54
2:B:178:LEU:HB3	2:B:185:LEU:HD13	1.90	0.54
1:L:209:VAL:HA	1:L:212:LEU:HG	1.90	0.54
3:N:67:PHE:CD2	3:N:97:VAL:HG21	2.43	0.53
3:C:48:SER:HB2	3:C:237:THR:HB	1.89	0.53
3:C:51:LEU:HD22	3:C:55:MSE:HE1	1.89	0.53
3:Z:2:LYS:HG3	3:Z:90:ALA:HB2	1.89	0.53
3:Z:83:ARG:H	3:Z:83:ARG:HH11	1.57	0.53
2:B:2:MSE:HG2	2:B:30:VAL:HG21	1.90	0.53
2:Y:166:GLU:HA	2:Y:174:ALA:O	2.09	0.53
2:B:215:MSE:HG2	2:B:216:GLU:N	2.24	0.53
2:M:39:GLY:HA2	2:M:120:THR:OG1	2.07	0.53
2:Y:83:VAL:HG22	2:Y:102:PHE:CE2	2.43	0.53
1:A:137:THR:HG23	1:A:189:GLU:HB3	1.90	0.52
2:B:181:ASP:OD2	2:B:181:ASP:N	2.38	0.52
2:M:178:LEU:HB3	2:M:185:LEU:HD13	1.91	0.52
3:N:143:ILE:HD12	3:N:201:LEU:HD13	1.91	0.52
1:L:153:VAL:HG21	1:L:177:TYR:CB	2.39	0.52
3:Z:82:LYS:HG2	3:Z:83:ARG:HD3	1.91	0.52
1:A:45:VAL:HG23	1:A:246:ALA:HB3	1.91	0.52
3:N:83:ARG:H	3:N:83:ARG:HH11	1.56	0.52
1:A:149:ASP:HB3	2:B:82:ARG:NE	2.11	0.52
1:X:149:ASP:HB2	2:Y:110:PHE:CE2	2.43	0.52
3:C:19:ALA:HB3	3:C:75:MSE:HE3	1.91	0.52
2:Y:27:ASN:ND2	2:Y:70:GLY:HA2	2.25	0.52
3:Z:36:LEU:HB3	3:Z:49:VAL:HB	1.92	0.52
3:Z:156:GLU:HB3	3:Z:163:LEU:HB2	1.92	0.52
2:M:140:PHE:CD2	2:M:215:MSE:HE1	2.45	0.51
2:B:135:LEU:HD21	2:B:140:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:129:PHE:CG	2:Y:218:TYR:HB3	2.45	0.51
1:L:230:LYS:HE3	1:L:242:ILE:HD12	1.92	0.51
2:Y:215:MSE:HG2	2:Y:216:GLU:N	2.25	0.51
1:X:209:VAL:HA	1:X:212:LEU:HG	1.91	0.51
2:M:89:LEU:HD21	2:M:100:LEU:HB3	1.93	0.51
1:A:153:VAL:HG21	1:A:177:TYR:CB	2.41	0.51
3:Z:216:ILE:HG13	3:Z:224:LEU:HD11	1.92	0.51
3:N:30:LYS:HG2	3:N:64:GLU:HG3	1.91	0.51
2:B:79:ILE:HD11	2:B:100:LEU:HD22	1.93	0.51
3:Z:131:SER:OG	3:Z:187:GLU:HB3	2.11	0.51
2:M:154:LEU:HD22	2:M:156:ILE:HG22	1.93	0.51
2:Y:197:TYR:HB3	2:Y:241:ILE:HD11	1.92	0.51
1:A:111:SER:HA	3:C:174:VAL:HA	1.93	0.51
2:M:70:GLY:HA3	2:M:115:ILE:O	2.11	0.51
3:C:131:SER:OG	3:C:187:GLU:HB3	2.11	0.51
2:B:12:PHE:HA	2:B:15:ILE:HD12	1.94	0.50
1:X:20:THR:HG22	1:X:23:THR:HG23	1.92	0.50
1:A:137:THR:HB	1:A:220:MSE:HG3	1.92	0.50
1:L:78:ILE:HD12	1:L:113:ILE:HD12	1.92	0.50
2:Y:84:LEU:HB2	2:Y:87:ASP:OD2	2.11	0.50
3:Z:151:ASP:HA	3:Z:198:ALA:HB3	1.94	0.50
2:M:83:VAL:HG22	2:M:102:PHE:CE2	2.47	0.50
2:Y:172:SER:HG	3:Z:73:TYR:HH	1.54	0.50
3:C:39:LEU:HD13	3:C:43:HIS:HD2	1.77	0.50
2:M:202:VAL:O	2:M:205:THR:HG22	2.12	0.50
2:B:89:LEU:HD13	2:B:91:LEU:HD22	1.94	0.50
3:N:153:VAL:HG23	3:N:198:ALA:HB2	1.94	0.50
2:B:6:VAL:HG11	2:B:12:PHE:HB2	1.94	0.50
2:Y:164:TYR:HA	2:Y:176:VAL:O	2.12	0.49
2:B:143:ILE:HG21	2:B:176:VAL:HG11	1.93	0.49
3:N:88:GLU:HB3	3:N:100:ASN:HB2	1.93	0.49
1:X:186:PRO:HD3	2:Y:106:PHE:HB3	1.93	0.49
1:X:196:ALA:HA	1:X:225:GLU:HG2	1.94	0.49
1:L:149:ASP:HB3	2:M:82:ARG:HE	1.77	0.49
1:X:94:THR:HB	1:X:97:GLY:H	1.77	0.49
1:A:209:VAL:HA	1:A:212:LEU:HG	1.93	0.49
3:Z:28:LYS:HB2	3:Z:35:GLU:HB2	1.95	0.49
2:Y:156:ILE:HB	2:Y:165:PHE:HD2	1.76	0.49
3:C:165:LYS:HB2	3:C:172:VAL:O	2.12	0.49
1:A:134:VAL:O	1:A:222:SER:HA	2.12	0.49
2:B:134:GLN:HG2	2:B:216:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:151:ASP:HA	3:N:198:ALA:HB3	1.95	0.49
1:A:143:LEU:HD11	1:A:221:VAL:HG21	1.94	0.49
1:A:94:THR:HB	1:A:97:GLY:H	1.78	0.49
2:Y:49:ASP:HB3	2:Y:238:ASP:HB2	1.94	0.49
2:M:30:VAL:HG22	2:M:35:ILE:HG12	1.95	0.49
1:A:230:LYS:HE3	1:A:242:ILE:HD12	1.95	0.49
2:Y:89:LEU:HD21	2:Y:100:LEU:HB3	1.95	0.49
3:C:151:ASP:HA	3:C:198:ALA:HB3	1.94	0.49
1:L:186:PRO:HG3	2:M:106:PHE:CD2	2.47	0.49
2:M:79:ILE:HD11	2:M:100:LEU:HD22	1.94	0.48
2:B:89:LEU:HD21	2:B:100:LEU:HB3	1.93	0.48
2:Y:135:LEU:HD21	2:Y:140:PHE:HB2	1.95	0.48
1:L:158:ARG:HH12	1:L:176:ARG:HH12	1.59	0.48
3:N:216:ILE:HG13	3:N:224:LEU:HD11	1.94	0.48
2:Y:156:ILE:HB	2:Y:165:PHE:CD2	2.48	0.48
3:N:45:SER:HA	3:N:239:LEU:O	2.13	0.48
2:B:16:LEU:HD21	2:B:28:PHE:CZ	2.46	0.48
2:B:2:MSE:N	2:B:93:SER:HG	2.11	0.48
2:B:5:LYS:HB3	2:B:58:GLU:O	2.13	0.48
2:M:129:PHE:CG	2:M:218:TYR:HB3	2.48	0.48
2:B:215:MSE:HE2	2:B:229:PHE:HE2	1.76	0.48
1:A:150:VAL:HG11	1:A:157:MSE:HB2	1.94	0.48
1:X:229:MSE:CE	1:X:245:ILE:HD12	2.40	0.48
1:A:212:LEU:HD22	1:A:233:VAL:CG2	2.42	0.48
3:C:196:TYR:CZ	3:C:224:LEU:HB2	2.48	0.48
2:B:27:ASN:ND2	2:B:70:GLY:HA2	2.29	0.48
2:B:143:ILE:HG13	2:B:143:ILE:H	1.52	0.48
2:B:135:LEU:HB2	2:B:185:LEU:HD12	1.95	0.48
2:B:241:ILE:HG13	2:B:241:ILE:O	2.12	0.48
3:Z:73:TYR:HE2	3:Z:111:VAL:HG22	1.78	0.48
1:X:139:ASP:HB3	1:X:142:VAL:HG23	1.96	0.48
2:Y:80:LEU:O	2:Y:83:VAL:HG23	2.13	0.47
1:L:49:ILE:HB	1:L:242:ILE:HG23	1.96	0.47
1:X:151:THR:HG21	1:X:206:LYS:HE3	1.95	0.47
2:B:141:ALA:HB1	2:B:206:THR:HG23	1.96	0.47
3:C:4:VAL:HG22	3:C:88:GLU:HG3	1.96	0.47
1:A:100:ILE:HB	1:A:113:ILE:HB	1.97	0.47
2:B:28:PHE:HB2	2:B:69:ILE:HB	1.97	0.47
2:M:216:GLU:HB2	2:M:228:ARG:HB3	1.96	0.47
2:B:140:PHE:CD2	2:B:215:MSE:HE1	2.50	0.47
1:A:12:PHE:HA	1:A:15:PHE:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:111:SER:HB3	3:Z:174:VAL:HG22	1.96	0.47
1:A:124:GLN:HG3	1:A:126:THR:HG23	1.97	0.47
3:Z:26:VAL:HG11	3:Z:118:GLU:CD	2.34	0.47
1:X:135:ASN:HB2	1:X:191:SER:HB3	1.95	0.47
2:Y:50:ILE:HG13	2:Y:237:GLY:HA2	1.96	0.47
2:M:164:TYR:HA	2:M:176:VAL:O	2.14	0.47
3:Z:120:GLU:O	3:Z:122:PRO:HD3	2.14	0.47
2:M:140:PHE:HB3	2:M:215:MSE:HE1	1.98	0.47
3:C:130:ILE:HD12	3:C:192:SER:HB2	1.97	0.47
2:Y:36:ARG:HB2	2:Y:51:PHE:HD1	1.80	0.46
3:Z:39:LEU:HD13	3:Z:43:HIS:HD2	1.80	0.46
3:C:204:VAL:HG21	3:C:238:TYR:CD1	2.50	0.46
2:B:11:SER:HB2	2:B:211:ALA:HA	1.97	0.46
1:A:38:ARG:HG3	1:A:49:ILE:HG12	1.97	0.46
3:N:131:SER:OG	3:N:187:GLU:HB3	2.14	0.46
2:Y:143:ILE:H	2:Y:143:ILE:HG13	1.50	0.46
2:Y:79:ILE:HD11	2:Y:100:LEU:HD22	1.98	0.46
3:Z:29:PHE:HB2	3:Z:65:PHE:HB3	1.97	0.46
2:B:97:LYS:HD3	2:B:111:GLU:OE1	2.15	0.46
2:M:49:ASP:HB3	2:M:238:ASP:HB2	1.97	0.46
2:M:23:LEU:HB2	2:M:73:LEU:CD1	2.45	0.46
1:L:6:TYR:HA	1:L:7:PRO:HD3	1.84	0.46
2:Y:15:ILE:HG13	2:Y:211:ALA:HB1	1.97	0.46
3:N:132:ALA:HB2	3:N:162:ILE:HG12	1.98	0.46
3:C:82:LYS:HD3	3:C:82:LYS:H	1.81	0.46
2:Y:179:SER:H	2:Y:182:ASN:HB2	1.80	0.46
1:X:141:SER:O	1:X:145:VAL:HG23	2.15	0.46
2:M:226:LYS:HE2	2:M:228:ARG:HG2	1.98	0.45
3:N:130:ILE:HD12	3:N:192:SER:HB2	1.97	0.45
1:X:230:LYS:HE3	1:X:242:ILE:HD12	1.97	0.45
2:M:215:MSE:HG2	2:M:216:GLU:N	2.31	0.45
1:X:206:LYS:O	1:X:210:LYS:HB2	2.17	0.45
2:M:143:ILE:HG21	2:M:176:VAL:HG11	1.99	0.45
2:Y:145:ASP:OD2	2:Y:206:THR:HG21	2.16	0.45
1:A:133:ALA:HB1	1:A:194:THR:H	1.82	0.45
3:Z:18:LEU:HD11	3:Z:36:LEU:HD11	1.99	0.45
1:L:45:VAL:HG23	1:L:246:ALA:HB3	1.98	0.45
2:M:6:VAL:HG22	2:M:57:PHE:HD2	1.79	0.45
1:L:176:ARG:HB3	2:M:111:GLU:HB2	1.98	0.45
1:X:165:LYS:HG2	1:X:182:MSE:HB3	1.98	0.45
2:M:205:THR:HG23	2:M:229:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:133:ALA:HB3	2:M:217:LEU:HB3	1.99	0.45
2:Y:178:LEU:HB3	2:Y:185:LEU:HD13	1.99	0.45
2:Y:163:LEU:HD11	2:Y:217:LEU:HG	1.99	0.45
1:L:150:VAL:HG11	1:L:157:MSE:HB2	1.98	0.45
3:Z:143:ILE:HD12	3:Z:201:LEU:HD13	1.97	0.45
2:M:12:PHE:HA	2:M:15:ILE:HD12	1.99	0.45
2:M:149:ASP:O	3:N:76:LYS:HD3	2.17	0.45
1:X:15:PHE:CZ	1:X:235:ALA:HB2	2.52	0.44
2:Y:180:THR:HA	2:Y:185:LEU:O	2.18	0.44
1:X:101:ILE:HG22	1:X:112:THR:HB	1.98	0.44
2:B:197:TYR:HB3	2:B:241:ILE:HD11	1.99	0.44
3:C:82:LYS:HG2	3:C:83:ARG:HD3	1.98	0.44
1:L:196:ALA:HA	1:L:225:GLU:HG2	1.99	0.44
1:L:210:LYS:HG2	1:L:213:ARG:HH21	1.82	0.44
3:Z:19:ALA:HB3	3:Z:75:MSE:HE3	1.99	0.44
1:A:136:PHE:HD1	1:A:187:LEU:HD22	1.83	0.44
3:C:27:LEU:HG	3:C:36:LEU:HD12	1.98	0.44
1:A:183:LYS:O	1:A:184:ASP:HB2	2.18	0.44
3:Z:27:LEU:HD23	3:Z:36:LEU:HB2	1.99	0.44
1:A:143:LEU:C	1:A:209:VAL:HG11	2.38	0.44
2:Y:179:SER:HB2	2:Y:182:ASN:H	1.83	0.44
1:X:165:LYS:HE3	1:X:182:MSE:SE	2.67	0.44
3:Z:19:ALA:HA	3:Z:71:THR:HB	1.99	0.44
2:M:215:MSE:HE2	2:M:229:PHE:CE2	2.53	0.44
2:Y:135:LEU:HB2	2:Y:185:LEU:HD12	1.99	0.44
3:Z:5:TYR:OH	3:Z:55:MSE:HE3	2.18	0.43
1:X:212:LEU:HD13	1:X:219:THR:HG21	1.99	0.43
2:M:45:VAL:HG13	2:M:242:ALA:HB3	1.98	0.43
3:C:19:ALA:HA	3:C:71:THR:HB	1.99	0.43
2:M:47:PHE:HZ	2:M:121:GLN:O	2.01	0.43
2:Y:27:ASN:HB3	2:Y:68:ILE:HG23	2.01	0.43
1:X:212:LEU:HD22	1:X:233:VAL:CG2	2.48	0.43
3:C:216:ILE:HG13	3:C:224:LEU:HD11	1.99	0.43
2:B:145:ASP:OD2	2:B:206:THR:HG21	2.18	0.43
2:Y:15:ILE:O	2:Y:19:VAL:HG23	2.18	0.43
2:M:146:GLU:HB3	3:N:80:VAL:HB	2.00	0.43
2:M:143:ILE:H	2:M:143:ILE:HG13	1.48	0.43
3:Z:40:ASP:OD1	3:Z:45:SER:N	2.51	0.43
3:C:204:VAL:CG1	3:C:204:VAL:O	2.67	0.43
2:M:157:HIS:HB2	2:M:194:SER:HB3	2.01	0.43
2:M:142:ASP:OD1	2:M:209:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:VAL:HG22	2:B:102:PHE:HE2	1.82	0.43
3:N:154:VAL:HG22	3:N:195:SER:HB3	2.01	0.43
2:M:119:SER:HB2	2:Y:66:LYS:H	1.83	0.43
1:X:38:ARG:HG3	1:X:49:ILE:HG12	2.00	0.43
2:M:140:PHE:HA	2:M:143:ILE:HD11	2.01	0.43
3:C:85:GLU:OE1	3:C:103:GLY:HA3	2.19	0.43
3:N:183:LEU:HD11	3:N:186:LEU:HB2	2.01	0.43
3:Z:1:MSE:HB2	3:Z:61:VAL:HG22	2.01	0.43
1:A:78:ILE:HD12	3:C:172:VAL:HG22	2.00	0.43
1:A:136:PHE:CZ	1:A:221:VAL:HB	2.54	0.43
1:X:49:ILE:HB	1:X:242:ILE:HG23	2.01	0.43
2:Y:23:LEU:HB2	2:Y:73:LEU:HD13	1.99	0.43
1:X:150:VAL:HG12	1:X:202:ALA:HB1	1.99	0.43
3:N:146:VAL:HG13	3:N:166:ALA:HB2	1.99	0.43
2:B:143:ILE:O	2:B:147:LEU:N	2.49	0.42
1:A:91:LEU:HA	1:A:99:LYS:O	2.18	0.42
2:Y:161:ASN:OD1	2:Y:189:SER:HA	2.19	0.42
3:Z:5:TYR:CZ	3:Z:55:MSE:HE3	2.53	0.42
2:Y:40:ILE:HG13	2:Y:46:VAL:O	2.19	0.42
1:L:94:THR:HB	1:L:97:GLY:H	1.82	0.42
2:M:165:PHE:HB2	2:M:176:VAL:HB	2.02	0.42
1:A:19:ILE:HD13	1:A:50:MSE:HG2	2.01	0.42
1:A:134:VAL:CG1	1:A:166:ILE:HD11	2.48	0.42
3:Z:27:LEU:HG	3:Z:36:LEU:HD12	2.01	0.42
1:A:75:VAL:O	1:A:79:LEU:HB2	2.20	0.42
2:M:156:ILE:HB	2:M:165:PHE:CD2	2.54	0.42
2:Y:214:SER:OG	2:Y:215:MSE:N	2.52	0.42
3:C:153:VAL:HG23	3:C:198:ALA:HB2	2.01	0.42
3:N:28:LYS:N	3:N:35:GLU:O	2.51	0.42
3:C:28:LYS:HB2	3:C:35:GLU:HB2	2.00	0.42
3:N:48:SER:HB2	3:N:237:THR:HB	2.00	0.42
1:X:150:VAL:HG11	1:X:157:MSE:HB2	2.01	0.42
1:A:13:PHE:HB2	1:A:79:LEU:HD22	2.02	0.42
3:Z:28:LYS:N	3:Z:35:GLU:O	2.52	0.42
1:A:12:PHE:O	1:A:15:PHE:HB2	2.20	0.42
1:X:29:ASN:HB3	1:X:122:VAL:HG12	2.02	0.42
2:Y:73:LEU:O	2:Y:77:ASN:HB2	2.19	0.42
3:C:164:ILE:HD12	3:C:176:PHE:HE1	1.85	0.42
1:X:2:PHE:N	1:X:93:GLU:HB2	2.35	0.42
2:M:156:ILE:HB	2:M:165:PHE:HD2	1.85	0.41
2:B:140:PHE:HA	2:B:143:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:28:LEU:HD12	1:X:70:LEU:HD21	2.02	0.41
1:L:75:VAL:CG2	1:L:115:ILE:HG21	2.50	0.41
2:M:5:LYS:HG3	2:M:90:ILE:HG12	2.02	0.41
2:Y:125:VAL:HG12	2:Y:127:LEU:HG	2.02	0.41
2:Y:205:THR:CG2	2:Y:229:PHE:HZ	2.30	0.41
3:C:196:TYR:CE1	3:C:224:LEU:HB2	2.55	0.41
1:X:5:VAL:HB	1:X:59:GLU:HB3	2.02	0.41
1:X:101:ILE:O	1:X:101:ILE:HG13	2.19	0.41
2:M:71:PHE:CE1	2:M:73:LEU:HG	2.55	0.41
1:A:136:PHE:CD1	1:A:187:LEU:HD22	2.55	0.41
1:L:186:PRO:HD3	2:M:106:PHE:HB3	2.01	0.41
1:A:100:ILE:HD11	1:A:115:ILE:HD11	2.02	0.41
3:Z:67:PHE:CD2	3:Z:97:VAL:HG21	2.55	0.41
3:N:29:PHE:HB2	3:N:65:PHE:HB3	2.02	0.41
1:X:146:ILE:HG21	1:X:168:ILE:HD13	2.03	0.41
3:N:18:LEU:HD11	3:N:36:LEU:HD11	2.02	0.41
1:A:210:LYS:HG2	1:A:213:ARG:HH21	1.84	0.41
2:M:77:ASN:O	2:M:81:LYS:HG3	2.21	0.41
3:N:37:VAL:HG11	3:N:121:ILE:HD13	2.02	0.41
2:Y:29:ILE:CG2	2:Y:66:LYS:HD2	2.50	0.41
1:A:150:VAL:HG12	1:A:202:ALA:HB1	2.02	0.41
2:Y:182:ASN:HB3	2:Y:184:THR:HG23	2.03	0.41
1:L:18:SER:HB3	1:L:243:PHE:HZ	1.86	0.41
2:M:141:ALA:HB1	2:M:206:THR:HG23	2.03	0.41
1:L:134:VAL:HG21	1:L:161:THR:HG21	2.03	0.41
2:B:135:LEU:O	2:B:215:MSE:HB3	2.21	0.41
1:L:149:ASP:HB2	2:M:110:PHE:CZ	2.55	0.41
2:B:27:ASN:HD21	2:B:117:VAL:HB	1.86	0.41
1:X:12:PHE:HA	1:X:15:PHE:HD1	1.85	0.41
2:Y:165:PHE:HB2	2:Y:176:VAL:HB	2.03	0.41
2:B:77:ASN:HA	2:B:80:LEU:HB2	2.03	0.41
1:L:212:LEU:HD22	1:L:233:VAL:CG2	2.51	0.41
3:C:39:LEU:HD13	3:C:43:HIS:CD2	2.56	0.41
3:Z:207:LEU:HD22	3:Z:236:VAL:HG11	2.02	0.41
3:C:5:TYR:CZ	3:C:55:MSE:HE3	2.56	0.41
1:X:219:THR:HG23	1:X:233:VAL:HG22	2.02	0.40
3:C:12:LYS:HA	3:C:78:LEU:HD13	2.02	0.40
2:B:163:LEU:HD11	2:B:217:LEU:HG	2.03	0.40
2:M:7:ILE:O	2:M:88:THR:HG22	2.22	0.40
2:B:193:VAL:HG21	2:B:220:GLY:HA2	2.03	0.40
3:C:73:TYR:O	3:C:77:ILE:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:GLU:HB3	2:Y:132:LYS:HB3	2.02	0.40
1:L:130:VAL:HG13	1:L:132:LEU:HG	2.03	0.40
2:B:23:LEU:HB2	2:B:73:LEU:HD13	2.03	0.40
2:Y:140:PHE:HB3	2:Y:215:MSE:HE1	2.03	0.40
1:X:4:ILE:O	1:X:90:GLU:HA	2.22	0.40
1:X:43:ASP:O	1:X:44:LYS:HB2	2.20	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	247/257 (96%)	230 (93%)	15 (6%)	2 (1%)	24	62
1	L	246/257 (96%)	233 (95%)	10 (4%)	3 (1%)	16	54
1	X	246/257 (96%)	229 (93%)	15 (6%)	2 (1%)	24	62
2	B	242/245 (99%)	225 (93%)	16 (7%)	1 (0%)	39	76
2	M	241/245 (98%)	222 (92%)	18 (8%)	1 (0%)	39	76
2	Y	241/245 (98%)	225 (93%)	14 (6%)	2 (1%)	24	62
3	C	241/252 (96%)	226 (94%)	14 (6%)	1 (0%)	39	76
3	N	241/252 (96%)	232 (96%)	8 (3%)	1 (0%)	39	76
3	Z	241/252 (96%)	229 (95%)	12 (5%)	0	100	100
All	All	2186/2262 (97%)	2051 (94%)	122 (6%)	13 (1%)	30	68

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	125	VAL
1	A	85	LYS

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Mol	Chain	Res	Type
1	X	163	GLU
3	C	117	SER
1	X	85	LYS
1	A	225	GLU
2	B	104	GLY
1	L	163	GLU
3	N	122	PRO
2	Y	104	GLY
1	L	83	SER
1	L	225	GLU
2	M	104	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/219 (100%)	200 (92%)	18 (8%)	14	47
1	L	218/219 (100%)	200 (92%)	18 (8%)	14	47
1	X	218/219 (100%)	202 (93%)	16 (7%)	17	53
2	B	218/215 (101%)	185 (85%)	33 (15%)	3	16
2	M	218/215 (101%)	192 (88%)	26 (12%)	6	27
2	Y	218/215 (101%)	187 (86%)	31 (14%)	4	19
3	C	219/224 (98%)	197 (90%)	22 (10%)	9	36
3	N	219/224 (98%)	205 (94%)	14 (6%)	22	60
3	Z	219/224 (98%)	204 (93%)	15 (7%)	20	57
All	All	1965/1974 (100%)	1772 (90%)	193 (10%)	10	37

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	35	ILE
1	A	46	LEU

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Mol	Chain	Res	Type
1	A	68	VAL
1	A	79	LEU
1	A	81	LYS
1	A	92	THR
1	A	94	THR
1	A	98	LEU
1	A	105	GLU
1	A	115	ILE
1	A	122	VAL
1	A	137	THR
1	A	143	LEU
1	A	144	ASN
1	A	166	ILE
1	A	206	LYS
1	A	222	SER
2	B	2	MSE
2	B	7	ILE
2	B	11	SER
2	B	31	THR
2	B	33	GLU
2	B	41	ASP
2	B	47	PHE
2	B	62	VAL
2	B	73	LEU
2	B	76	VAL
2	B	79	ILE
2	B	89	LEU
2	B	95	GLU
2	B	99	THR
2	B	112	LEU
2	B	121	GLN
2	B	135	LEU
2	B	137	THR
2	B	143	ILE
2	B	149	ASP
2	B	154	LEU
2	B	156	ILE
2	B	163	LEU
2	B	181	ASP
2	B	185	LEU
2	B	205	THR
2	B	207	LYS

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Mol	Chain	Res	Type
2	B	213	ASP
2	B	217	LEU
2	B	225	LEU
2	B	228	ARG
2	B	234	GLU
2	B	241	ILE
3	C	1	MSE
3	C	18	LEU
3	C	21	LEU
3	C	53	ARG
3	C	63	ASP
3	C	75	MSE
3	C	82	LYS
3	C	83	ARG
3	C	84	LYS
3	C	106	ASN
3	C	107	ARG
3	C	112	ARG
3	C	115	GLU
3	C	119	GLN
3	C	127	GLN
3	C	131	SER
3	C	151	ASP
3	C	177	SER
3	C	183	LEU
3	C	204	VAL
3	C	225	GLN
3	C	239	LEU
1	L	26	ILE
1	L	35	ILE
1	L	44	LYS
1	L	46	LEU
1	L	79	LEU
1	L	81	LYS
1	L	92	THR
1	L	94	THR
1	L	98	LEU
1	L	101	ILE
1	L	115	ILE
1	L	135	ASN
1	L	137	THR
1	L	143	LEU

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Mol	Chain	Res	Type
1	L	166	ILE
1	L	183	LYS
1	L	206	LYS
1	L	222	SER
2	M	2	MSE
2	M	7	ILE
2	M	31	THR
2	M	33	GLU
2	M	41	ASP
2	M	62	VAL
2	M	73	LEU
2	M	79	ILE
2	M	89	LEU
2	M	95	GLU
2	M	99	THR
2	M	127	LEU
2	M	143	ILE
2	M	149	ASP
2	M	156	ILE
2	M	163	LEU
2	M	181	ASP
2	M	185	LEU
2	M	205	THR
2	M	207	LYS
2	M	209	ARG
2	M	217	LEU
2	M	225	LEU
2	M	228	ARG
2	M	234	GLU
2	M	241	ILE
3	N	1	MSE
3	N	11	LEU
3	N	18	LEU
3	N	21	LEU
3	N	63	ASP
3	N	82	LYS
3	N	83	ARG
3	N	106	ASN
3	N	107	ARG
3	N	119	GLN
3	N	127	GLN
3	N	183	LEU

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Mol	Chain	Res	Type
3	N	194	ASN
3	N	225	GLN
1	X	26	ILE
1	X	35	ILE
1	X	46	LEU
1	X	81	LYS
1	X	92	THR
1	X	94	THR
1	X	98	LEU
1	X	122	VAL
1	X	125	LEU
1	X	127	GLU
1	X	130	VAL
1	X	131	ASN
1	X	143	LEU
1	X	166	ILE
1	X	206	LYS
1	X	222	SER
2	Y	2	MSE
2	Y	31	THR
2	Y	33	GLU
2	Y	36	ARG
2	Y	38	SER
2	Y	41	ASP
2	Y	47	PHE
2	Y	62	VAL
2	Y	73	LEU
2	Y	79	ILE
2	Y	89	LEU
2	Y	95	GLU
2	Y	99	THR
2	Y	112	LEU
2	Y	114	LEU
2	Y	125	VAL
2	Y	135	LEU
2	Y	143	ILE
2	Y	149	ASP
2	Y	154	LEU
2	Y	156	ILE
2	Y	163	LEU
2	Y	181	ASP
2	Y	185	LEU

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Mol	Chain	Res	Type
2	Y	205	THR
2	Y	207	LYS
2	Y	212	SER
2	Y	217	LEU
2	Y	225	LEU
2	Y	228	ARG
2	Y	241	ILE
3	Z	1	MSE
3	Z	18	LEU
3	Z	21	LEU
3	Z	63	ASP
3	Z	82	LYS
3	Z	83	ARG
3	Z	106	ASN
3	Z	107	ARG
3	Z	112	ARG
3	Z	118	GLU
3	Z	120	GLU
3	Z	127	GLN
3	Z	131	SER
3	Z	183	LEU
3	Z	225	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	27	ASN
2	B	116	GLN
3	C	70	ASN
3	C	100	ASN
3	C	106	ASN
3	C	110	ASN
2	M	116	GLN
3	N	100	ASN
3	N	106	ASN
3	N	158	HIS
2	Y	27	ASN
2	Y	121	GLN
3	Z	43	HIS
3	Z	100	ASN
3	Z	158	HIS

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

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	241/257 (93%)	0.07	1 (0%)	93 92	65, 71, 74, 76	0
1	L	240/257 (93%)	0.33	10 (4%)	40 33	65, 71, 74, 76	0
1	X	240/257 (93%)	0.16	4 (1%)	73 67	63, 71, 74, 76	0
2	B	240/245 (97%)	0.02	1 (0%)	93 92	69, 71, 75, 81	0
2	M	239/245 (97%)	0.12	2 (0%)	87 84	69, 71, 76, 82	0
2	Y	239/245 (97%)	0.03	1 (0%)	93 92	69, 71, 75, 83	0
3	C	239/252 (94%)	0.09	4 (1%)	73 67	69, 71, 79, 85	0
3	N	239/252 (94%)	0.37	13 (5%)	29 24	69, 71, 80, 85	0
3	Z	239/252 (94%)	0.25	11 (4%)	36 30	69, 71, 81, 86	0
All	All	2156/2262 (95%)	0.16	47 (2%)	65 59	63, 71, 75, 86	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	162	ILE	3.7
2	B	124	SER	3.6
3	C	128	PHE	3.4
3	Z	82	LYS	3.3
3	N	159	GLU	3.2
1	L	22	VAL	3.2
3	Z	136	SER	3.1
3	N	179	ASP	3.0
1	L	84	SER	2.9
3	N	233	GLY	2.9
3	Z	176	PHE	2.9
1	L	216	SER	2.9
1	L	30	PHE	2.8
1	L	83	SER	2.7
3	N	178	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	Z	178	LYS	2.6
1	X	80	SER	2.6
3	N	232	GLY	2.6
1	X	58	SER	2.6
3	Z	135	SER	2.6
1	L	214	GLY	2.5
1	L	163	GLU	2.5
3	N	153	VAL	2.5
1	L	65	PRO	2.4
2	Y	124	SER	2.4
3	C	221	GLN	2.4
1	L	86	LYS	2.4
3	Z	164	ILE	2.3
3	N	234	GLY	2.3
2	M	240	TYR	2.3
3	N	157	GLY	2.3
1	X	83	SER	2.2
3	Z	213	TYR	2.2
3	Z	179	ASP	2.1
3	N	122	PRO	2.1
3	C	82	LYS	2.1
3	Z	122	PRO	2.1
1	L	95	ASP	2.1
3	C	184	GLN	2.1
3	N	127	GLN	2.1
3	N	170	SER	2.1
1	A	181	LEU	2.1
3	N	11	LEU	2.0
1	X	81	LYS	2.0
2	M	124	SER	2.0
3	Z	234	GLY	2.0
3	N	189	SER	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.