Full wwPDB X-ray Structure Validation Report (i)

Jan 11, 2017 – 04:01 PM EST

PDB ID	:	5L7C
Title	:	Structural basis of human clamp sliding on DNA
Authors	:	De March, M.; Merino, N.; Barrera-Vilarmau, S.; Crehuet, R.; Onesti, S.; Blanco, F.J.; De Biasio, A.
Deposited on	:	2016-06-03
Resolution	:	2.82 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 (i)) were used in the production of this report:

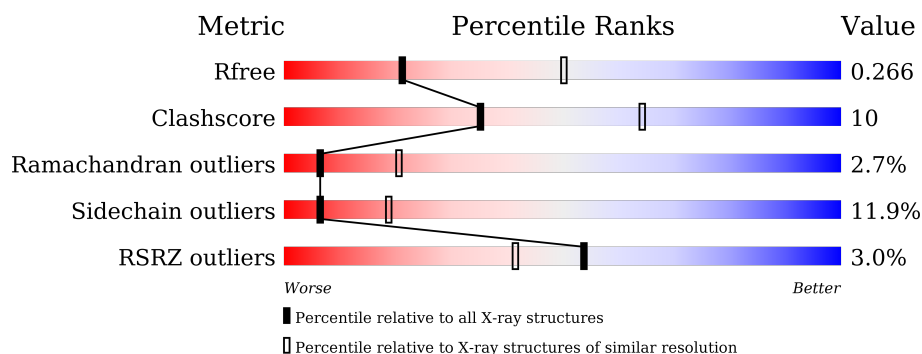|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		10
Ramachandran outliers		2.7%
Sidechain outliers		11.9%
RSRZ outliers		3.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	264	2% 67% 23% • 6%
1	B	264	69% 21% • 5%
1	C	264	2% 75% 14% 5% 7%
2	D	10	40% 100%
3	E	10	80% 80% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5743 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	248	Total	C	N	O	S	0	0	0
			1770	1131	297	328	14			
1	B	250	Total	C	N	O	S	0	0	0
			1772	1129	293	335	15			
1	C	246	Total	C	N	O	S	0	0	0
			1751	1116	287	333	15			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P12004
A	-1	PRO	-	expression tag	UNP P12004
A	0	HIS	-	expression tag	UNP P12004
B	-2	GLY	-	expression tag	UNP P12004
B	-1	PRO	-	expression tag	UNP P12004
B	0	HIS	-	expression tag	UNP P12004
C	-2	GLY	-	expression tag	UNP P12004
C	-1	PRO	-	expression tag	UNP P12004
C	0	HIS	-	expression tag	UNP P12004

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*TP*AP*CP*GP*AP*TP*GP*GP*G) -3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	P	0	0	0
			210	99	42	59	10			

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*CP*CP*AP*TP*CP*GP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	10	200	96	33	61	10	0	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	18	Total	O	0	0
			18	18		
4	C	9	Total	O	0	0
			9	9		

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.
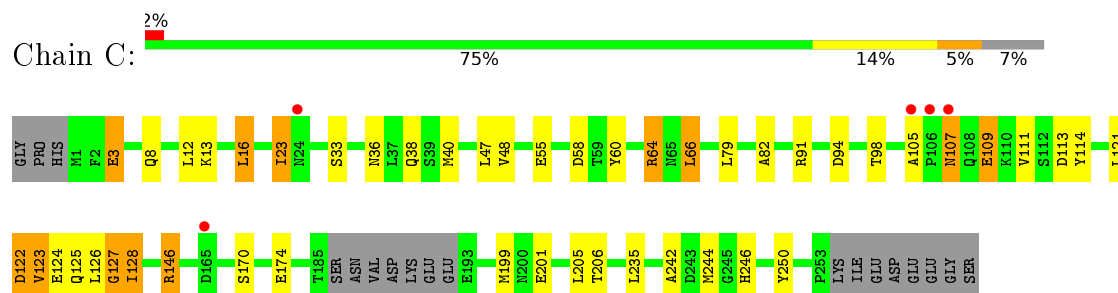
- Molecule 1: Proliferating cell nuclear antigen
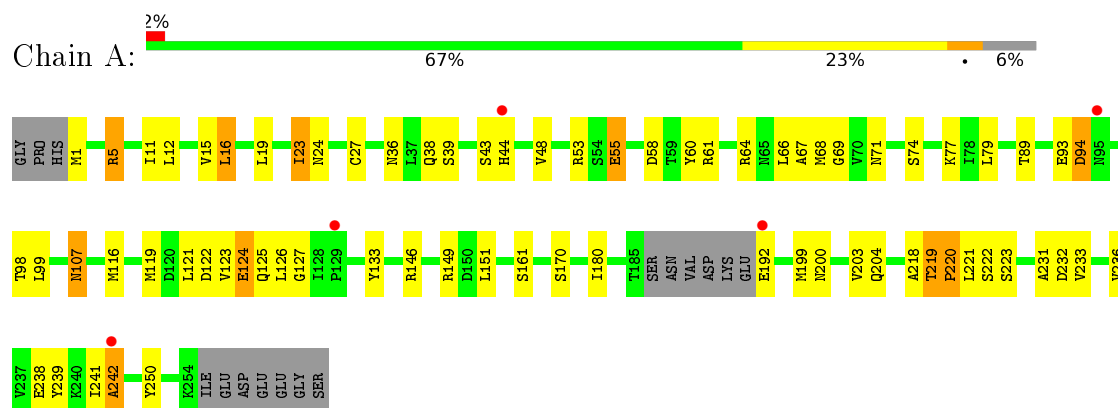
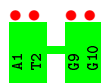Chain A:

- Molecule 1: Proliferating cell nuclear antigen
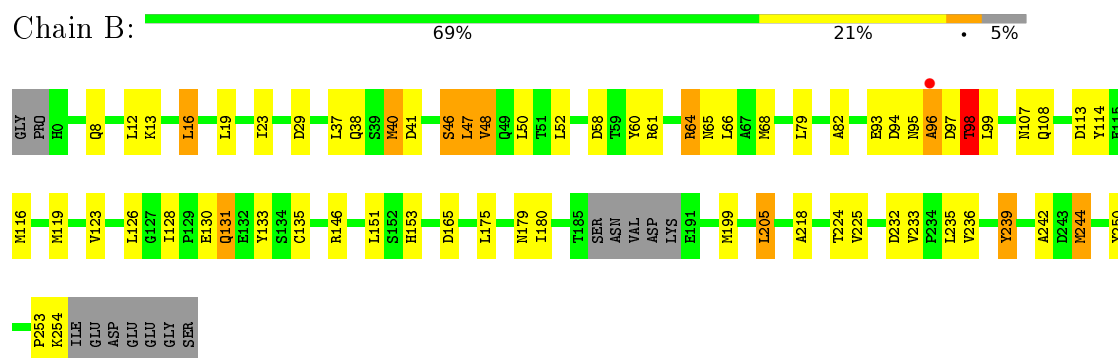
Chain B:

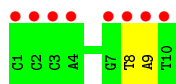- Molecule 1: Proliferating cell nuclear antigen

Chain C:

- Molecule 2: DNA (5'-D(P*AP*TP*AP*CP*GP*AP*TP*GP*GP*G)-3')

Chain D:

40%

100%

A1 T2 G9 G10

● Molecule 3: DNA (5'-D(P*CP*CP*CP*AP*TP*CP*GP*TP*AP*T)-3')

Chain E:

80%

80%

20%

C1 C2 C3 A4 G7 T8 A9 T10

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	180.19Å 180.19Å 76.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.09 – 2.82 90.09 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (90.09-2.82) 99.6 (90.09-2.82)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.97 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.252 , 0.292 0.228 , 0.266	Depositor DCC
R_{free} test set	1134 reflections (5.35%)	DCC
Wilson B-factor (Å²)	60.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.24 , 63.8	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5743	wwPDB-VP
Average B, all atoms (Å²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (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	1.05	10/1794 (0.6%)	1.11	12/2435 (0.5%)
1	B	1.23	15/1797 (0.8%)	1.09	8/2446 (0.3%)
1	C	0.96	3/1776 (0.2%)	0.98	5/2415 (0.2%)
2	D	0.28	0/236	0.87	0/363
3	E	0.25	0/222	0.87	0/339
All	All	1.04	28/5825 (0.5%)	1.05	25/7998 (0.3%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	TYR	CE1-CZ	-10.71	1.24	1.38
1	B	239	TYR	CE1-CZ	-10.36	1.25	1.38
1	A	60	TYR	CG-CD2	-10.09	1.26	1.39
1	B	114	TYR	CG-CD2	-9.93	1.26	1.39
1	B	133	TYR	CE2-CZ	-9.83	1.25	1.38
1	B	239	TYR	CG-CD2	-9.82	1.26	1.39
1	B	64	ARG	CZ-NH1	-9.42	1.20	1.33
1	B	133	TYR	CE1-CZ	-8.63	1.27	1.38
1	B	133	TYR	CG-CD2	-8.43	1.28	1.39
1	A	60	TYR	CE1-CZ	-8.27	1.27	1.38
1	B	114	TYR	CE2-CZ	-8.26	1.27	1.38
1	B	133	TYR	CG-CD1	-8.26	1.28	1.39
1	A	239	TYR	CE1-CZ	-7.73	1.28	1.38
1	C	60	TYR	CE1-CZ	-7.65	1.28	1.38
1	B	239	TYR	CG-CD1	-7.50	1.29	1.39
1	A	60	TYR	CG-CD1	-7.39	1.29	1.39
1	B	60	TYR	CE1-CZ	-6.83	1.29	1.38
1	B	114	TYR	CG-CD1	-6.34	1.30	1.39
1	B	239	TYR	CE2-CZ	-6.07	1.30	1.38
1	C	114	TYR	CE1-CZ	-5.81	1.30	1.38
1	B	113	ASP	CB-CG	-5.76	1.39	1.51
1	A	133	TYR	CG-CD2	-5.71	1.31	1.39
1	A	238	GLU	CD-OE2	-5.70	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	TYR	CE2-CZ	-5.69	1.31	1.38
1	A	133	TYR	CE1-CZ	-5.46	1.31	1.38
1	C	60	TYR	CG-CD2	-5.37	1.32	1.39
1	A	239	TYR	CG-CD2	-5.23	1.32	1.39
1	A	55	GLU	CD-OE2	-5.19	1.20	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	NE-CZ-NH1	12.60	126.60	120.30
1	B	64	ARG	NE-CZ-NH1	-11.84	114.38	120.30
1	A	219	THR	C-N-CD	-11.45	95.41	120.60
1	C	125	GLN	N-CA-C	-9.34	85.79	111.00
1	A	238	GLU	OE1-CD-OE2	-8.76	112.79	123.30
1	C	3	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	A	12	LEU	CA-CB-CG	7.41	132.35	115.30
1	A	12	LEU	CB-CG-CD2	-7.40	98.43	111.00
1	A	12	LEU	CB-CG-CD1	7.26	123.34	111.00
1	B	205	LEU	CB-CG-CD1	7.11	123.08	111.00
1	B	113	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	C	12	LEU	CA-CB-CG	6.61	130.50	115.30
1	C	47	LEU	CB-CG-CD1	6.60	122.23	111.00
1	A	55	GLU	OE1-CD-OE2	-6.42	115.60	123.30
1	B	12	LEU	CA-CB-CG	6.07	129.26	115.30
1	A	192	GLU	N-CA-C	-5.92	95.01	111.00
1	B	68	MET	CG-SD-CE	5.89	109.63	100.20
1	A	61	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	113	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	53	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	5	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	68	MET	CG-SD-CE	5.47	108.95	100.20
1	B	119	MET	CB-CA-C	-5.42	99.55	110.40
1	B	61	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	C	170	SER	N-CA-CB	-5.05	102.93	110.50

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	1770	0	1695	45	1
1	B	1772	0	1665	33	2
1	C	1751	0	1640	30	2
2	D	210	0	113	0	0
3	E	200	0	114	1	0
4	A	13	0	0	3	0
4	B	18	0	0	0	1
4	C	9	0	0	0	0
All	All	5743	0	5227	107	3

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 10.

All (107) 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:64:ARG:NH2	1:A:94:ASP:CB	2.14	1.11
1:B:97:ASP:O	1:B:98:THR:HG22	1.55	1.06
1:C:38:GLN:NE2	1:C:127:GLY:HA2	1.71	1.05
1:C:64:ARG:HD3	1:C:94:ASP:OD1	1.61	1.00
1:C:107:ASN:HD22	1:C:107:ASN:H	1.04	0.96
1:C:64:ARG:CG	1:C:94:ASP:OD1	2.14	0.95
1:C:64:ARG:CD	1:C:94:ASP:OD1	2.15	0.94
1:C:38:GLN:HE22	1:C:127:GLY:HA2	1.30	0.93
1:C:107:ASN:ND2	1:C:107:ASN:H	1.70	0.90
1:A:220:PRO:CG	4:A:304:HOH:O	2.21	0.89
1:A:64:ARG:HH22	1:A:94:ASP:CB	1.86	0.87
1:A:27:CYS:HA	1:A:69:GLY:HA2	1.58	0.84
1:B:97:ASP:O	1:B:98:THR:CG2	2.26	0.84
1:A:220:PRO:HG2	4:A:304:HOH:O	1.77	0.83
1:A:122:ASP:O	1:A:124:GLU:N	2.12	0.82
1:A:218:ALA:C	1:A:220:PRO:HD2	2.00	0.82
1:A:231:ALA:O	1:A:233:VAL:N	2.14	0.81
1:C:105:ALA:HB1	1:C:107:ASN:HD21	1.44	0.81
1:B:93:GLU:O	1:B:95:ASN:N	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:O	1:A:221:LEU:N	2.16	0.78
1:C:107:ASN:HD22	1:C:107:ASN:N	1.83	0.77
1:C:105:ALA:HB1	1:C:107:ASN:ND2	1.98	0.77
1:B:38:GLN:HE22	1:B:128:ILE:HG12	1.52	0.74
1:A:218:ALA:O	1:A:220:PRO:HD2	1.88	0.72
1:C:23:ILE:HD11	1:C:48:VAL:CG1	2.19	0.72
1:B:97:ASP:C	1:B:98:THR:HG22	2.09	0.70
1:A:93:GLU:O	1:A:94:ASP:O	2.08	0.70
1:B:97:ASP:O	1:B:98:THR:CB	2.40	0.70
1:C:126:LEU:O	1:C:127:GLY:O	2.10	0.70
1:A:64:ARG:HH21	1:A:94:ASP:CB	2.06	0.69
1:C:64:ARG:HG3	1:C:94:ASP:OD1	1.92	0.68
1:B:165:ASP:OD1	1:B:165:ASP:O	2.14	0.65
1:B:64:ARG:NH1	1:B:65:ASN:O	2.27	0.64
1:A:219:THR:N	1:A:220:PRO:CD	2.61	0.64
1:C:23:ILE:HD11	1:C:48:VAL:HG11	1.81	0.63
1:A:23:ILE:HD11	1:A:48:VAL:CG1	2.28	0.63
1:C:146:ARG:HH11	1:C:146:ARG:CG	2.14	0.61
1:A:236:VAL:HG22	1:A:250:TYR:CD2	2.36	0.60
1:C:146:ARG:HH11	1:C:146:ARG:HG3	1.67	0.59
1:B:218:ALA:HB3	1:B:239:TYR:CE2	2.38	0.59
1:A:218:ALA:C	1:A:220:PRO:CD	2.71	0.59
1:C:64:ARG:O	1:C:66:LEU:HD23	2.03	0.58
1:A:119:MET:CE	1:A:121:LEU:HD11	2.34	0.58
1:C:121:LEU:O	1:C:122:ASP:O	2.22	0.58
1:A:161:SER:OG	1:A:204:GLN:OE1	2.16	0.58
1:B:41:ASP:OD1	1:B:46:SER:N	2.24	0.56
1:A:23:ILE:HD11	1:A:48:VAL:HG11	1.87	0.56
1:A:74:SER:HA	1:B:175:LEU:HD22	1.86	0.56
1:B:95:ASN:O	1:B:96:ALA:HB3	2.05	0.56
1:B:64:ARG:HD2	1:B:65:ASN:O	2.06	0.56
1:C:16:LEU:HD13	1:C:79:LEU:CD1	2.37	0.54
1:C:13:LYS:NZ	1:C:82:ALA:O	2.40	0.54
1:A:93:GLU:O	1:A:94:ASP:C	2.46	0.54
1:B:97:ASP:O	1:B:98:THR:HB	2.10	0.52
1:A:219:THR:C	1:A:221:LEU:H	2.13	0.52
1:A:218:ALA:O	1:A:221:LEU:HB2	2.11	0.51
1:C:3:GLU:OE1	1:C:91:ARG:NE	2.44	0.50
1:C:146:ARG:NH1	1:C:146:ARG:CG	2.73	0.50
1:A:219:THR:N	1:A:220:PRO:HD3	2.27	0.50
1:A:69:GLY:HA3	1:A:121:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:VAL:HG22	1:B:250:TYR:CE2	2.47	0.50
1:A:23:ILE:HD13	1:A:39:SER:HB3	1.94	0.49
1:B:218:ALA:HB3	1:B:239:TYR:CD2	2.48	0.49
1:B:40:MET:HG3	1:B:47:LEU:HD12	1.93	0.49
1:B:13:LYS:NZ	1:B:82:ALA:O	2.42	0.49
1:B:38:GLN:NE2	1:B:128:ILE:HG12	2.26	0.48
1:C:127:GLY:C	1:C:128:ILE:HG12	2.33	0.48
1:B:16:LEU:HD13	1:B:79:LEU:CD1	2.43	0.48
1:A:236:VAL:HG22	1:A:250:TYR:CE2	2.48	0.48
1:A:220:PRO:HG3	4:A:304:HOH:O	1.99	0.48
1:A:119:MET:HE3	1:A:121:LEU:HD11	1.94	0.48
1:A:38:GLN:HG2	1:A:125:GLN:CB	2.44	0.48
1:A:27:CYS:SG	1:A:67:ALA:HB1	2.54	0.47
1:B:165:ASP:C	1:B:165:ASP:OD1	2.52	0.47
1:A:74:SER:HA	1:B:175:LEU:CD2	2.45	0.47
1:C:235:LEU:O	1:C:250:TYR:HA	2.15	0.47
1:C:38:GLN:CD	1:C:127:GLY:HA2	2.34	0.46
1:A:16:LEU:HD13	1:A:79:LEU:CD1	2.45	0.46
1:A:151:LEU:HD11	1:A:180:ILE:HD12	1.98	0.46
1:C:23:ILE:HD11	1:C:48:VAL:HG13	1.94	0.46
1:B:151:LEU:HD11	1:B:180:ILE:HD12	1.97	0.45
1:A:43:SER:O	1:A:44:HIS:HB2	2.17	0.45
1:A:99:LEU:HD23	1:A:116:MET:HE2	1.98	0.45
1:B:52:LEU:HD22	1:B:244:MET:SD	2.57	0.45
1:B:235:LEU:O	1:B:250:TYR:HA	2.16	0.45
1:B:99:LEU:HD23	1:B:116:MET:HE2	1.99	0.45
3:E:8:DT:H2"	3:E:9:DA:C8	2.51	0.45
1:C:109:GLU:O	1:C:111:VAL:HG23	2.17	0.44
1:B:225:VAL:HG23	1:B:239:TYR:CE1	2.53	0.44
1:B:64:ARG:CD	1:B:65:ASN:O	2.66	0.44
1:A:19:LEU:CD2	1:A:48:VAL:HG21	2.47	0.44
1:A:241:ILE:HG22	1:A:242:ALA:N	2.33	0.44
1:A:16:LEU:HD13	1:A:79:LEU:HD11	2.00	0.43
1:C:105:ALA:CB	1:C:107:ASN:ND2	2.78	0.43
1:C:16:LEU:HD13	1:C:79:LEU:HD11	1.99	0.43
1:A:107:ASN:ND2	1:A:107:ASN:H	2.17	0.42
1:B:19:LEU:CD2	1:B:48:VAL:HG21	2.49	0.42
1:A:11:ILE:O	1:A:15:VAL:HG23	2.20	0.42
1:A:24:ASN:O	1:A:71:ASN:OD1	2.37	0.42
1:B:130:GLU:C	1:B:131:GLN:HG2	2.39	0.42
1:B:37:LEU:HB3	1:B:50:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD23	1:A:116:MET:CE	2.51	0.41
1:A:5:ARG:HG3	1:A:89:THR:OG1	2.20	0.41
1:A:27:CYS:HA	1:A:69:GLY:CA	2.39	0.40
1:C:122:ASP:O	1:C:123:VAL:CB	2.69	0.40
1:B:107:ASN:O	1:B:108:GLN:CB	2.68	0.40
1:B:253:PRO:O	1:B:254:LYS:CB	2.68	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:CB	4:B:315:HOH:O[8_655]	1.92	0.28
1:B:96:ALA:O	1:C:124:GLU:O[5_554]	2.15	0.05
1:B:97:ASP:CB	1:C:124:GLU:CB[5_554]	2.16	0.04

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	244/264 (92%)	221 (91%)	16 (7%)	7 (3%)	6	19
1	B	246/264 (93%)	227 (92%)	12 (5%)	7 (3%)	6	20
1	C	242/264 (92%)	227 (94%)	9 (4%)	6 (2%)	7	23
All	All	732/792 (92%)	675 (92%)	37 (5%)	20 (3%)	6	20

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	123	VAL
1	A	124	GLU
1	A	127	GLY

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Mol	Chain	Res	Type
1	A	220	PRO
1	A	232	ASP
1	B	94	ASP
1	B	98	THR
1	B	123	VAL
1	C	122	ASP
1	C	123	VAL
1	C	127	GLY
1	C	242	ALA
1	B	242	ALA
1	B	96	ALA
1	B	126	LEU
1	B	232	ASP
1	C	244	MET
1	A	242	ALA
1	C	109	GLU

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	170/230 (74%)	152 (89%)	18 (11%)	8	24
1	B	170/230 (74%)	149 (88%)	21 (12%)	6	17
1	C	166/230 (72%)	145 (87%)	21 (13%)	5	16
All	All	506/690 (73%)	446 (88%)	60 (12%)	6	19

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	LEU
1	A	23	ILE
1	A	36	ASN
1	A	55	GLU
1	A	58	ASP

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Mol	Chain	Res	Type
1	A	66	LEU
1	A	77	LYS
1	A	98	THR
1	A	107	ASN
1	A	146	ARG
1	A	149	ARG
1	A	170	SER
1	A	199	MET
1	A	200	ASN
1	A	203	VAL
1	A	222	SER
1	A	223	SER
1	B	8	GLN
1	B	16	LEU
1	B	23	ILE
1	B	29	ASP
1	B	40	MET
1	B	46	SER
1	B	47	LEU
1	B	48	VAL
1	B	58	ASP
1	B	66	LEU
1	B	98	THR
1	B	131	GLN
1	B	135	CYS
1	B	146	ARG
1	B	153	HIS
1	B	179	ASN
1	B	199	MET
1	B	205	LEU
1	B	224	THR
1	B	233	VAL
1	B	244	MET
1	C	8	GLN
1	C	16	LEU
1	C	23	ILE
1	C	33	SER
1	C	36	ASN
1	C	40	MET
1	C	55	GLU
1	C	58	ASP
1	C	64	ARG

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Mol	Chain	Res	Type
1	C	66	LEU
1	C	98	THR
1	C	107	ASN
1	C	113	ASP
1	C	128	ILE
1	C	146	ARG
1	C	174	GLU
1	C	199	MET
1	C	201	GLU
1	C	205	LEU
1	C	206	THR
1	C	246	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	107	ASN
1	B	36	ASN
1	B	38	GLN
1	B	179	ASN
1	B	204	GLN
1	C	38	GLN
1	C	107	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 (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	248/264 (93%)	-0.16	5 (2%)	68	58	39, 60, 92, 134	12 (4%)
1	B	250/264 (94%)	-0.23	1 (0%)	93	90	41, 59, 93, 153	9 (3%)
1	C	246/264 (93%)	-0.17	5 (2%)	68	58	39, 63, 109, 176	13 (5%)
2	D	10/10 (100%)	4.28	4 (40%)	0	0	420, 472, 563, 611	0
3	E	10/10 (100%)	5.84	8 (80%)	0	0	458, 471, 506, 517	0
All	All	764/812 (94%)	-0.05	23 (3%)	54	41	39, 61, 118, 611	34 (4%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	1	DC	16.5
3	E	2	DC	15.5
2	D	1	DA	13.0
2	D	10	DG	11.7
3	E	3	DC	8.4
2	D	9	DG	5.8
2	D	2	DT	5.2
1	B	96	ALA	4.8
1	A	95	ASN	4.1
3	E	8	DT	4.0
3	E	9	DA	3.1
1	A	44	HIS	3.0
3	E	10	DT	3.0
1	C	106	PRO	2.8
1	A	242	ALA	2.5
1	C	107	ASN	2.5
1	C	105	ALA	2.3
1	A	192	GLU	2.2
1	C	165	ASP	2.2
3	E	7	DG	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	4	DA	2.1
1	C	24	ASN	2.1
1	A	129	PRO	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.