



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2024 – 10:03 AM EDT

PDB ID : 8THW
Title : Cac1 PIP motif bound to PCNA
Authors : Veltri, E.; Hoitsma, N.M.; Dieckman, L.
Deposited on : 2023-07-18
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

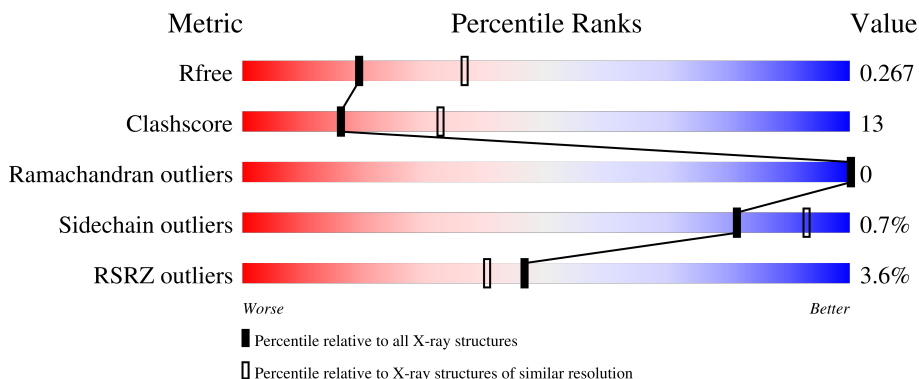
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	289	 2% 70% 23% 8%
1	B	289	 4% 63% 29% 8%
1	C	289	 4% 63% 29% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6315 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,Chromatin assembly factor 1 subunit p90.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	2105	1348	337	410	10	0	0	0
1	B	267	2105	1348	337	410	10	0	0	0
1	C	267	2105	1348	337	410	10	0	0	0

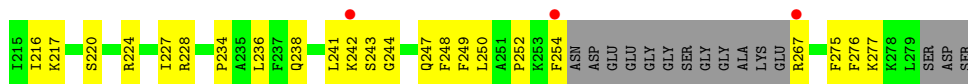
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P15873
A	-5	HIS	-	expression tag	UNP P15873
A	-4	HIS	-	expression tag	UNP P15873
A	-3	HIS	-	expression tag	UNP P15873
A	-2	HIS	-	expression tag	UNP P15873
A	-1	HIS	-	expression tag	UNP P15873
A	0	HIS	-	expression tag	UNP P15873
A	259	GLY	-	linker	UNP P15873
A	260	GLY	-	linker	UNP P15873
A	261	SER	-	linker	UNP P15873
A	262	GLY	-	linker	UNP P15873
A	263	GLY	-	linker	UNP P15873
B	-6	MET	-	expression tag	UNP P15873
B	-5	HIS	-	expression tag	UNP P15873
B	-4	HIS	-	expression tag	UNP P15873
B	-3	HIS	-	expression tag	UNP P15873
B	-2	HIS	-	expression tag	UNP P15873
B	-1	HIS	-	expression tag	UNP P15873
B	0	HIS	-	expression tag	UNP P15873
B	259	GLY	-	linker	UNP P15873
B	260	GLY	-	linker	UNP P15873
B	261	SER	-	linker	UNP P15873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	262	GLY	-	linker	UNP P15873
B	263	GLY	-	linker	UNP P15873
C	-6	MET	-	expression tag	UNP P15873
C	-5	HIS	-	expression tag	UNP P15873
C	-4	HIS	-	expression tag	UNP P15873
C	-3	HIS	-	expression tag	UNP P15873
C	-2	HIS	-	expression tag	UNP P15873
C	-1	HIS	-	expression tag	UNP P15873
C	0	HIS	-	expression tag	UNP P15873
C	259	GLY	-	linker	UNP P15873
C	260	GLY	-	linker	UNP P15873
C	261	SER	-	linker	UNP P15873
C	262	GLY	-	linker	UNP P15873
C	263	GLY	-	linker	UNP P15873



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.62Å 87.36Å 76.51Å 90.00° 108.33° 90.00°	Depositor
Resolution (Å)	24.89 – 2.60 24.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	61.2 (24.89-2.60) 76.9 (24.89-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.60Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.267 0.216 , 0.267	Depositor DCC
R_{free} test set	27291 reflections (8.18%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6315	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.45	0/2136	0.69	0/2875
1	B	0.46	0/2136	0.70	0/2875
1	C	0.44	0/2136	0.69	0/2875
All	All	0.45	0/6408	0.69	0/8625

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	2105	0	2137	41	0
1	B	2105	0	2137	62	0
1	C	2105	0	2137	66	0
All	All	6315	0	6411	164	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 13.

All (164) 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:B:129:GLU:HG2	1:B:276:PHE:HE1	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:OG1	1:C:267:ARG:NH1	2.07	0.86
1:B:129:GLU:HG2	1:B:276:PHE:CE1	2.26	0.65
1:C:54:VAL:HG13	1:C:60:TYR:HB3	1.81	0.62
1:C:252:PRO:HG2	1:C:254:PHE:CE2	2.37	0.59
1:B:168:LYS:HG3	1:B:181:ILE:HG13	1.84	0.59
1:A:49:SER:OG	1:A:247:GLN:HG3	2.02	0.59
1:B:90:LEU:HG	1:B:99:ILE:HD11	1.83	0.59
1:A:162:ILE:HD11	1:A:229:LEU:HD12	1.85	0.59
1:B:54:VAL:HG13	1:B:60:TYR:HB3	1.84	0.58
1:A:22:CYS:SG	1:A:214:ASP:HB3	2.44	0.57
1:B:49:SER:HB3	1:B:247:GLN:HG3	1.85	0.57
1:C:135:SER:HB3	1:C:162:ILE:HG21	1.87	0.57
1:C:70:MET:HE3	1:C:99:ILE:HD11	1.87	0.56
1:C:78:ILE:HG21	1:C:101:LEU:HD13	1.87	0.56
1:C:236:LEU:HD11	1:C:247:GLN:HG2	1.87	0.56
1:B:33:ASP:OD1	1:B:33:ASP:N	2.35	0.56
1:B:182:ILE:HG22	1:C:110:ARG:HE	1.71	0.56
1:C:70:MET:HE3	1:C:99:ILE:CD1	2.36	0.56
1:C:168:LYS:HE2	1:C:170:VAL:HG21	1.87	0.56
1:B:36:ILE:HG22	1:B:51:GLU:HG3	1.87	0.56
1:B:136:THR:HB	1:B:228:ARG:HG2	1.88	0.55
1:B:228:ARG:HB2	1:B:236:LEU:HB3	1.86	0.55
1:B:165:GLU:HA	1:B:197:LEU:HD23	1.89	0.55
1:C:55:GLU:OE1	1:C:243:SER:OG	2.16	0.55
1:B:70:MET:HE3	1:B:99:ILE:HG21	1.89	0.55
1:B:234:PRO:HD3	1:B:275:PHE:CD2	2.41	0.55
1:B:128:ILE:HG22	1:B:130:GLU:HG3	1.88	0.55
1:A:168:LYS:HG3	1:A:181:ILE:HG12	1.89	0.55
1:C:131:LEU:HD11	1:C:133:TYR:CE1	2.42	0.54
1:B:83:ASN:HB2	1:B:86:ASP:OD1	2.08	0.54
1:C:137:LEU:HD23	1:C:162:ILE:HD11	1.89	0.54
1:A:195:ILE:HD12	1:B:108:LYS:NZ	2.21	0.54
1:B:188:MET:O	1:B:189:GLU:C	2.44	0.54
1:C:131:LEU:HD12	1:C:131:LEU:C	2.29	0.54
1:B:78:ILE:HG21	1:B:101:LEU:HD13	1.90	0.53
1:A:10:SER:O	1:A:14:ARG:HG3	2.08	0.53
1:B:252:PRO:HB2	1:B:254:PHE:HD2	1.73	0.53
1:A:4:ALA:HB1	1:A:57:PHE:CE2	2.44	0.53
1:C:131:LEU:HD11	1:C:133:TYR:CZ	2.43	0.53
1:C:87:THR:HB	1:C:104:GLU:HB3	1.90	0.53
1:A:205:LEU:HD12	1:A:229:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:SER:HA	1:C:118:LEU:HG	1.91	0.53
1:B:108:LYS:HG2	1:B:109:ASP:N	2.25	0.52
1:C:20:LYS:O	1:C:21:ASP:HB2	2.09	0.52
1:B:29:GLN:HB2	1:B:36:ILE:HG13	1.92	0.52
1:A:78:ILE:HG21	1:A:101:LEU:HD13	1.92	0.51
1:A:47:LEU:HD12	1:A:126:LEU:HD12	1.92	0.51
1:C:241:LEU:HB2	1:C:244:GLY:C	2.31	0.51
1:B:222:SER:OG	1:B:224:ARG:O	2.28	0.51
1:A:133:TYR:HA	1:A:230:SER:HB3	1.91	0.50
1:C:137:LEU:HD12	1:C:137:LEU:C	2.31	0.50
1:A:162:ILE:CD1	1:A:229:LEU:HD12	2.42	0.50
1:C:70:MET:HE2	1:C:75:LEU:HD13	1.94	0.50
1:C:214:ASP:HA	1:C:217:LYS:HD2	1.93	0.50
1:B:133:TYR:HA	1:B:230:SER:HB2	1.93	0.49
1:C:137:LEU:HD11	1:C:227:ILE:HD12	1.94	0.49
1:A:135:SER:OG	1:A:162:ILE:HG21	2.11	0.49
1:A:145:SER:HB3	1:A:216:ILE:HB	1.94	0.49
1:A:23:VAL:HG21	1:A:39:ALA:HB3	1.95	0.49
1:A:137:LEU:HD13	1:A:139:LEU:HD22	1.94	0.49
1:B:46:LEU:HD23	1:B:48:VAL:HG23	1.94	0.49
1:C:51:GLU:O	1:C:244:GLY:HA3	2.12	0.49
1:A:230:SER:OG	1:A:233:ALA:HB3	2.13	0.49
1:C:46:LEU:HD11	1:C:248:PHE:HB3	1.93	0.48
1:C:228:ARG:HG3	1:C:236:LEU:HD23	1.95	0.48
1:A:155:SER:OG	1:A:157:SER:O	2.31	0.48
1:A:254:PHE:O	1:A:267:ARG:N	2.47	0.48
1:C:14:ARG:HD2	1:C:220:SER:O	2.12	0.48
1:C:128:ILE:HG21	1:C:249:PHE:CZ	2.47	0.48
1:C:127:LYS:HE2	1:C:277:LYS:HB2	1.95	0.48
1:C:162:ILE:HG21	1:C:197:LEU:HD11	1.96	0.47
1:B:155:SER:OG	1:B:157:SER:O	2.32	0.47
1:A:76:SER:O	1:A:80:ARG:HG3	2.14	0.47
1:A:154:LEU:O	1:A:173:GLY:HA3	2.14	0.47
1:B:163:THR:HB	1:B:164:LYS:HE2	1.97	0.47
1:C:145:SER:HB3	1:C:216:ILE:HB	1.95	0.47
1:C:19:PHE:CG	1:C:48:VAL:HG11	2.49	0.47
1:C:46:LEU:HD13	1:C:250:LEU:HD13	1.97	0.47
1:B:13:LYS:NZ	1:B:80:ARG:HG3	2.29	0.47
1:B:137:LEU:HD22	1:B:162:ILE:HD11	1.96	0.47
1:B:252:PRO:HB2	1:B:254:PHE:CD2	2.49	0.47
1:C:5:LYS:HE2	1:C:89:THR:OG1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:O	1:A:96:PRO:HD3	2.16	0.46
1:B:37:ALA:HB3	1:B:50:LEU:HB3	1.98	0.46
1:B:46:LEU:CD2	1:B:48:VAL:HG23	2.45	0.46
1:B:154:LEU:O	1:B:173:GLY:HA3	2.15	0.46
1:C:238:GLN:HG3	1:C:247:GLN:HG3	1.97	0.46
1:A:167:ILE:HB	1:A:182:ILE:HG13	1.96	0.46
1:B:54:VAL:HG22	1:B:60:TYR:CD2	2.51	0.46
1:B:254:PHE:CZ	1:B:275:PHE:HZ	2.34	0.46
1:A:99:ILE:CG2	1:A:116:LEU:HB3	2.46	0.46
1:B:145:SER:HB3	1:B:216:ILE:HB	1.97	0.46
1:C:131:LEU:HD12	1:C:131:LEU:O	2.16	0.46
1:C:188:MET:O	1:C:191:PRO:HD3	2.15	0.46
1:B:126:LEU:HB3	1:B:276:PHE:HB3	1.96	0.45
1:A:50:LEU:HD11	1:A:52:ILE:HD11	1.99	0.45
1:C:137:LEU:HD11	1:C:227:ILE:HB	1.97	0.45
1:C:55:GLU:H	1:C:55:GLU:CD	2.19	0.45
1:A:46:LEU:HD11	1:A:248:PHE:HB3	1.98	0.45
1:A:234:PRO:HD3	1:A:275:PHE:CD2	2.52	0.44
1:B:124:ASP:OD1	1:B:278:LYS:HE2	2.17	0.44
1:C:134:ASP:HB3	1:C:201:GLN:HB2	1.98	0.44
1:A:83:ASN:C	1:A:85:THR:H	2.21	0.44
1:C:252:PRO:HG2	1:C:254:PHE:CZ	2.53	0.44
1:B:30:CYS:HB2	1:B:66:VAL:HG13	2.00	0.44
1:B:253:LYS:HA	1:B:268:ALA:O	2.16	0.44
1:C:189:GLU:H	1:C:189:GLU:HG3	1.57	0.44
1:B:91:ILE:HD12	1:B:102:LEU:HD12	2.00	0.44
1:A:228:ARG:HD2	1:A:236:LEU:HD23	2.00	0.44
1:C:162:ILE:HD12	1:C:197:LEU:HD13	2.00	0.44
1:C:20:LYS:O	1:C:21:ASP:CB	2.61	0.43
1:B:192:GLU:HG2	1:B:193:THR:N	2.33	0.43
1:C:141:SER:H	1:C:224:ARG:HA	1.84	0.43
1:C:162:ILE:HG23	1:C:197:LEU:HD21	1.99	0.43
1:A:10:SER:OG	1:A:14:ARG:NH1	2.51	0.43
1:A:166:THR:HG23	1:A:181:ILE:CG2	2.48	0.43
1:C:148:VAL:O	1:C:152:SER:OG	2.32	0.43
1:C:234:PRO:HD3	1:C:275:PHE:CD2	2.54	0.43
1:C:238:GLN:HG3	1:C:247:GLN:CG	2.49	0.43
1:C:22:CYS:SG	1:C:214:ASP:HB3	2.59	0.43
1:A:137:LEU:C	1:A:137:LEU:HD12	2.38	0.43
1:B:119:MET:HE3	1:B:119:MET:HB3	1.74	0.43
1:C:3:GLU:HG2	1:C:91:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HD23	1:B:72:LEU:HA	1.76	0.43
1:C:129:GLU:HB2	1:C:276:PHE:HE1	1.83	0.42
1:C:162:ILE:HD13	1:C:167:ILE:HG12	2.00	0.42
1:C:194:SER:OG	1:C:196:LYS:HE3	2.18	0.42
1:C:11:LEU:HD22	1:C:242:LYS:NZ	2.33	0.42
1:C:68:LEU:HD22	1:C:99:ILE:CG2	2.48	0.42
1:B:15:ILE:HA	1:B:221:LEU:HD21	2.00	0.42
1:B:154:LEU:HD11	1:C:114:TYR:HD2	1.85	0.42
1:B:254:PHE:HZ	1:B:275:PHE:HZ	1.66	0.42
1:C:31:LYS:HB2	1:C:31:LYS:HE3	1.88	0.42
1:A:31:LYS:HE3	1:A:36:ILE:HD11	2.01	0.42
1:B:46:LEU:HD21	1:B:248:PHE:HD2	1.84	0.42
1:B:164:LYS:HA	1:B:199:MET:HE1	2.02	0.42
1:C:210:LYS:HE3	1:C:211:TYR:CZ	2.55	0.42
1:A:90:LEU:HD22	1:A:99:ILE:HD11	2.02	0.41
1:A:238:GLN:HG3	1:A:247:GLN:HB3	2.00	0.41
1:C:4:ALA:HB1	1:C:57:PHE:CE2	2.54	0.41
1:A:154:LEU:HD11	1:B:114:TYR:HD2	1.85	0.41
1:B:7:GLU:HB3	1:B:58:GLN:HB2	2.02	0.41
1:A:184:PRO:HG3	1:A:197:LEU:HB3	2.03	0.41
1:B:23:VAL:HG21	1:B:39:ALA:HB3	2.03	0.41
1:C:47:LEU:HB3	1:C:249:PHE:HB2	2.02	0.41
1:A:160:ILE:HD13	1:A:169:PHE:HE1	1.86	0.41
1:B:154:LEU:HD11	1:C:114:TYR:CD2	2.55	0.41
1:A:134:ASP:HB2	1:A:203:VAL:CG1	2.51	0.41
1:B:35:ILE:HD12	1:B:57:PHE:HZ	1.86	0.41
1:B:99:ILE:CG2	1:B:116:LEU:HB3	2.50	0.41
1:B:163:THR:OG1	1:B:166:THR:HB	2.21	0.41
1:B:168:LYS:HE3	1:B:168:LYS:HB3	1.73	0.41
1:C:227:ILE:HA	1:C:236:LEU:O	2.20	0.41
1:C:243:SER:OG	1:C:243:SER:O	2.39	0.41
1:A:227:ILE:HA	1:A:236:LEU:O	2.21	0.41
1:B:164:LYS:H	1:B:164:LYS:HG3	1.47	0.41
1:B:169:PHE:O	1:B:179:SER:HA	2.21	0.41
1:B:278:LYS:HE3	1:B:278:LYS:HB2	1.82	0.40
1:B:236:LEU:HD13	1:B:249:PHE:CZ	2.55	0.40
1:C:45:VAL:HG21	1:C:211:TYR:CZ	2.57	0.40
1:A:183:LYS:HA	1:A:184:PRO:HD3	1.83	0.40
1:B:164:LYS:HD2	1:B:164:LYS:O	2.21	0.40
1:C:119:MET:HE3	1:C:119:MET:HB3	1.82	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	263/289 (91%)	247 (94%)	16 (6%)	0	100	100
1	B	263/289 (91%)	251 (95%)	12 (5%)	0	100	100
1	C	263/289 (91%)	249 (95%)	14 (5%)	0	100	100
All	All	789/867 (91%)	747 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	240/257 (93%)	239 (100%)	1 (0%)	89	96
1	B	240/257 (93%)	237 (99%)	3 (1%)	65	84
1	C	240/257 (93%)	239 (100%)	1 (0%)	89	96
All	All	720/771 (93%)	715 (99%)	5 (1%)	81	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	110	ARG
1	B	164	LYS
1	B	204	ASP
1	C	120	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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

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	267/289 (92%)	0.07	6 (2%) 62 57	19, 39, 69, 110	0
1	B	267/289 (92%)	0.14	11 (4%) 42 36	21, 41, 75, 94	0
1	C	267/289 (92%)	0.16	12 (4%) 39 33	17, 39, 77, 99	0
All	All	801/867 (92%)	0.12	29 (3%) 46 40	17, 40, 72, 110	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	GLU	3.7
1	B	107	LYS	3.7
1	A	186	VAL	3.4
1	C	110	ARG	3.1
1	B	125	PHE	3.1
1	B	124	ASP	3.0
1	B	129	GLU	2.9
1	B	254	PHE	2.8
1	B	131	LEU	2.8
1	C	124	ASP	2.8
1	C	242	LYS	2.6
1	C	109	ASP	2.5
1	B	106	THR	2.4
1	C	267	ARG	2.4
1	A	156	ASP	2.4
1	C	188	MET	2.3
1	B	190	HIS	2.3
1	C	106	THR	2.3
1	C	95	THR	2.3
1	C	254	PHE	2.3
1	B	188	MET	2.2
1	C	131	LEU	2.2
1	C	94	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	254	PHE	2.2
1	C	135	SER	2.1
1	A	188	MET	2.1
1	A	94	ASN	2.1
1	B	123	ALA	2.1
1	A	278	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.