Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 06:00 am GMT

PDB ID	:	4CS5
Title	:	Crystal Structure of PCNA from Litopenaeus vannamei
Authors	:	Carrasco-Miranda, J.S.; Lopez-Zavala, A.A.; De-La-Mora, E.; Rudino-Pinera, E.; Brieba, L.G.; Sotelo-Mundo, R.R.
Deposited on	:	2014-03-04
Resolution	:	3.00 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:

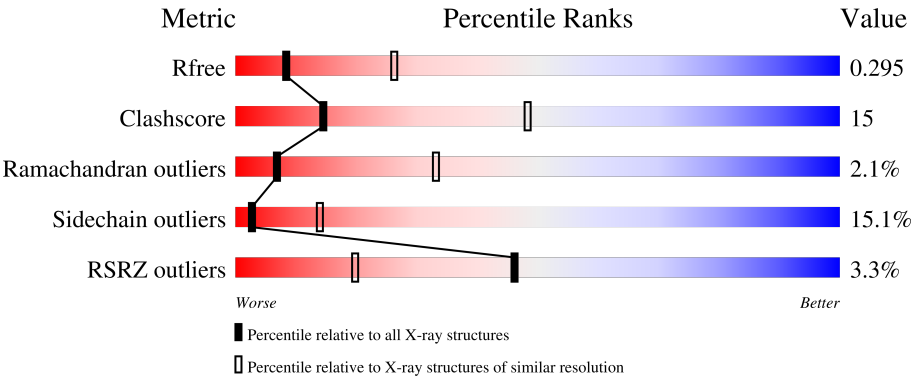
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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 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 <=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	260	3% 55% 38% 5% ·
1	B	260	3% 56% 36% 5% ·
1	C	260	3% 55% 38% · ·

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5877 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	255	Total	C	N	O	S	0	0	0
			1962	1239	324	380	19			
1	B	254	Total	C	N	O	S	0	0	0
			1960	1236	323	383	18			
1	C	254	Total	C	N	O	S	0	0	0
			1955	1233	321	382	19			

There are 3 discrepancies between the modelled and reference sequences:

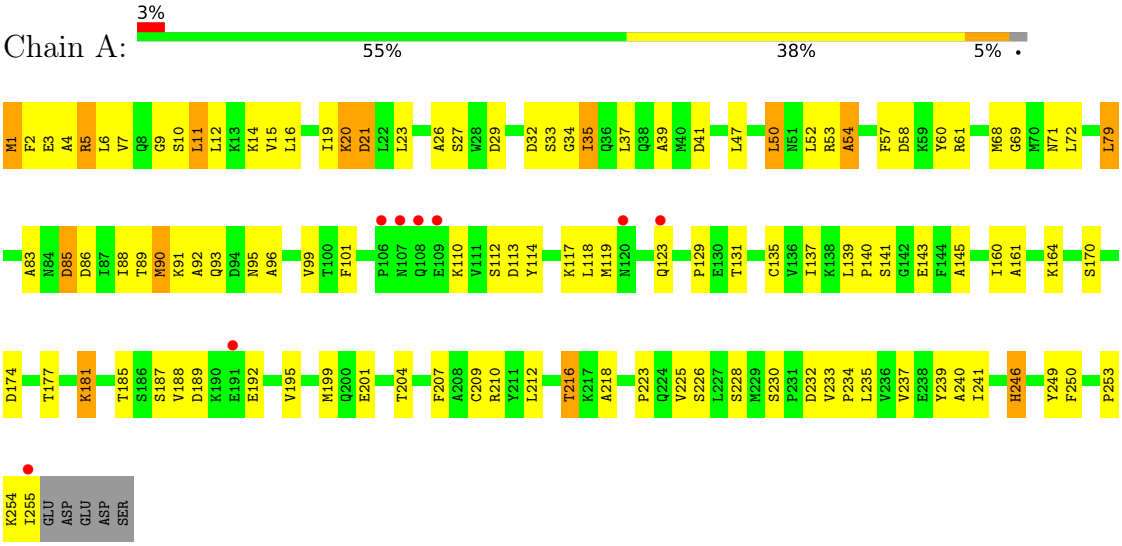
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	LYS	GLU	conflict	UNP G1E6N7
B	55	LYS	GLU	conflict	UNP G1E6N7
C	55	LYS	GLU	conflict	UNP G1E6N7

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

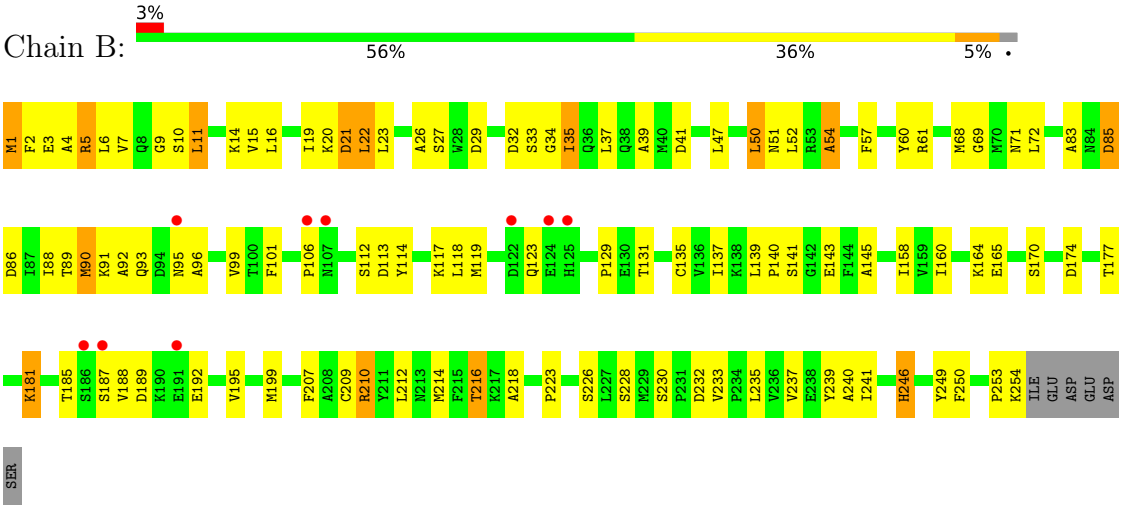
• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

Chain A:



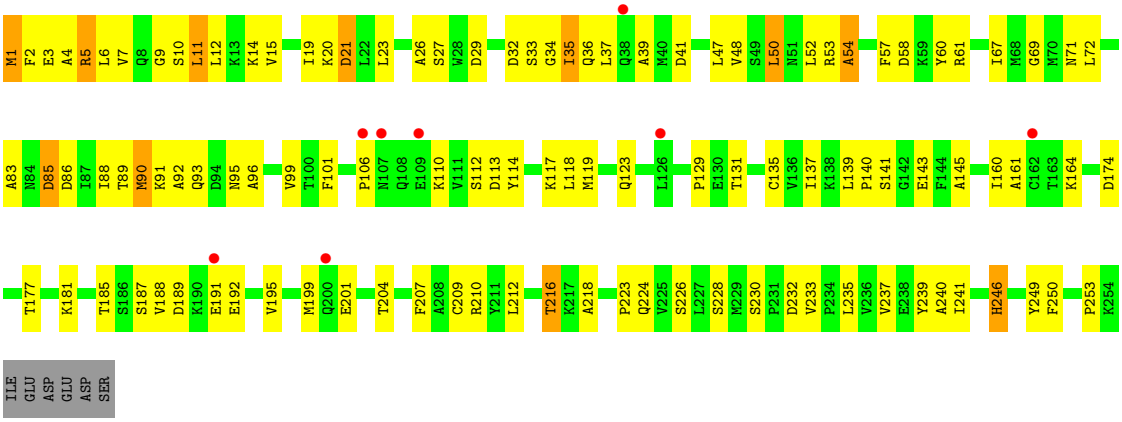
• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

Chain B:



• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

Chain C:


M1 F2 E3 A4 R5 L6 V7 Q8 G9 S10 L11 L12 K13 K14 V15 I19 K20 D21 L22 L23 A26 S27 W28 D29 D32 S33 G34 I35 Q36 L37 Q38 A39 M40 D41 L47 V48 S49 L50 N51 L52 R53 A54 F57 D58 K59 Y60 R61 I67 M68 G69 M70 N71 L72
A83 N84 D85 D86 I87 I88 T89 M90 K91 A92 Q93 D94 N95 A96 V99 T100 F101 P106 N107 Q108 E109 K110 V111 S112 D113 Y114 K117 L118 M119 Q123 L126 P129 E130 T131 C135 V136 I137 K138 L139 P140 S141 G142 E143 F144 A145 I160 A161 C162 T163 K164 D174
T177 K181 T185 S186 S187 V188 D189 K190 E191 E192 V195 M199 Q200 E201 T204 F207 A208 C209 R210 Y211 L212 T216 K217 A218 P223 Q224 V225 S226 L227 S228 M229 S230 P231 D232 V233 P234 L235 V236 V237 E238 Y239 A240 I241 H246 Y249 F250 P253 K254
ILE GLU ASP GLU ASP SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.57Å 83.38Å 74.31Å 90.00° 117.65° 90.00°	Depositor
Resolution (Å)	28.06 – 3.00 28.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (28.06-3.00) 93.7 (28.06-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.265 , 0.311 0.246 , 0.295	Depositor DCC
R_{free} test set	736 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5877	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.51	0/1991	0.74	0/2688
1	B	0.50	0/1989	0.75	1/2685 (0.0%)
1	C	0.49	0/1983	0.72	0/2676
All	All	0.50	0/5963	0.74	1/8049 (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})
1	B	22	LEU	CA-CB-CG	5.67	128.34	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	1962	0	1980	65	0
1	B	1960	0	1972	60	0
1	C	1955	0	1960	59	0
All	All	5877	0	5912	182	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 15.

All (182) 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:140:PRO:HB2	1:A:143:GLU:HB2	1.70	0.73
1:B:140:PRO:HB2	1:B:143:GLU:HB2	1.70	0.73
1:C:140:PRO:HB2	1:C:143:GLU:HB2	1.72	0.72
1:A:99:VAL:HG12	1:A:118:LEU:HD11	1.72	0.72
1:C:99:VAL:HG12	1:C:118:LEU:HD11	1.72	0.71
1:A:33:SER:O	1:A:54:ALA:N	2.19	0.71
1:B:33:SER:O	1:B:54:ALA:N	2.18	0.69
1:A:21:ASP:OD1	1:A:21:ASP:N	2.23	0.68
1:B:21:ASP:N	1:B:21:ASP:OD1	2.27	0.68
1:C:145:ALA:HA	1:C:216:THR:HG21	1.77	0.67
1:B:2:PHE:HE2	1:B:90:MET:HB3	1.59	0.67
1:B:240:ALA:HA	1:B:246:HIS:HB3	1.78	0.66
1:B:145:ALA:HA	1:B:216:THR:HG21	1.77	0.65
1:B:83:ALA:N	1:B:86:ASP:OD2	2.25	0.65
1:A:145:ALA:HA	1:A:216:THR:HG21	1.79	0.65
1:A:240:ALA:HA	1:A:246:HIS:HB3	1.78	0.65
1:A:7:VAL:HG22	1:A:58:ASP:HB2	1.80	0.63
1:B:99:VAL:HG12	1:B:118:LEU:HD11	1.79	0.63
1:C:33:SER:O	1:C:54:ALA:N	2.24	0.62
1:A:2:PHE:HE2	1:A:90:MET:HB3	1.63	0.62
1:C:7:VAL:HG22	1:C:58:ASP:HB2	1.80	0.61
1:C:2:PHE:HE2	1:C:90:MET:HB3	1.65	0.61
1:C:23:LEU:HD23	1:C:41:ASP:HA	1.82	0.61
1:C:5:ARG:HG3	1:C:89:THR:OG1	2.00	0.61
1:A:241:ILE:HG13	1:A:246:HIS:HA	1.82	0.61
1:C:240:ALA:HA	1:C:246:HIS:HB3	1.82	0.61
1:B:241:ILE:HG13	1:B:246:HIS:HA	1.81	0.61
1:A:23:LEU:HD23	1:A:41:ASP:HA	1.83	0.60
1:B:23:LEU:HD23	1:B:41:ASP:HA	1.83	0.60
1:C:241:ILE:HG13	1:C:246:HIS:HA	1.82	0.60
1:C:21:ASP:OD1	1:C:21:ASP:N	2.26	0.60
1:C:50:LEU:HD11	1:C:52:LEU:HG	1.84	0.59
1:C:83:ALA:N	1:C:86:ASP:OD2	2.29	0.59
1:A:141:SER:HB2	1:A:239:TYR:HE1	1.68	0.59
1:B:26:ALA:HB3	1:B:72:LEU:HD21	1.85	0.59
1:C:141:SER:HB2	1:C:239:TYR:HE1	1.68	0.58
1:B:185:THR:OG1	1:B:195:VAL:N	2.37	0.58
1:A:85:ASP:N	1:A:85:ASP:OD1	2.37	0.58
1:B:141:SER:HB2	1:B:239:TYR:HE1	1.68	0.57
1:B:85:ASP:N	1:B:85:ASP:OD1	2.36	0.57
1:B:5:ARG:HG3	1:B:89:THR:OG1	2.05	0.57
1:B:23:LEU:HD13	1:B:39:ALA:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LEU:HD13	1:C:39:ALA:HB3	1.86	0.57
1:B:207:PHE:HE1	1:B:253:PRO:HG3	1.70	0.56
1:C:185:THR:OG1	1:C:195:VAL:N	2.38	0.55
1:A:83:ALA:N	1:A:86:ASP:OD2	2.27	0.54
1:A:23:LEU:HD13	1:A:39:ALA:HB3	1.89	0.54
1:A:29:ASP:O	1:A:35:ILE:HA	2.07	0.54
1:A:50:LEU:HD11	1:A:52:LEU:HG	1.89	0.54
1:A:181:LYS:O	1:C:110:LYS:HA	2.07	0.54
1:B:3:GLU:HG3	1:B:91:LYS:HG2	1.88	0.54
1:A:3:GLU:HG3	1:A:91:LYS:HG2	1.90	0.54
1:C:3:GLU:HG3	1:C:91:LYS:HG2	1.88	0.53
1:C:19:ILE:O	1:C:21:ASP:N	2.42	0.53
1:A:5:ARG:HG3	1:A:89:THR:OG1	2.08	0.53
1:A:192:GLU:HG3	1:A:223:PRO:HB2	1.90	0.53
1:A:207:PHE:HE1	1:A:253:PRO:HG3	1.74	0.52
1:B:37:LEU:HB3	1:B:50:LEU:HB3	1.91	0.52
1:C:90:MET:HG2	1:C:99:VAL:HG21	1.92	0.52
1:B:192:GLU:HG3	1:B:223:PRO:HB2	1.92	0.52
1:A:2:PHE:O	1:A:91:LYS:HA	2.10	0.52
1:A:185:THR:OG1	1:A:195:VAL:N	2.39	0.52
1:B:29:ASP:O	1:B:35:ILE:HA	2.10	0.52
1:C:11:LEU:O	1:C:15:VAL:HG23	2.10	0.51
1:A:26:ALA:HB3	1:A:72:LEU:HD21	1.92	0.51
1:A:69:GLY:O	1:A:119:MET:HE2	2.11	0.51
1:C:85:ASP:OD1	1:C:85:ASP:N	2.43	0.51
1:C:207:PHE:HE1	1:C:253:PRO:HG3	1.75	0.51
1:B:137:ILE:HG22	1:B:139:LEU:HD22	1.93	0.51
1:A:137:ILE:HG22	1:A:139:LEU:HD22	1.93	0.50
1:C:29:ASP:O	1:C:35:ILE:HA	2.11	0.50
1:C:164:LYS:HD2	1:C:199:MET:HB3	1.93	0.50
1:B:164:LYS:HD2	1:B:199:MET:HB3	1.93	0.50
1:C:192:GLU:HG3	1:C:223:PRO:HB2	1.92	0.50
1:C:26:ALA:HB3	1:C:72:LEU:HD21	1.93	0.50
1:B:218:ALA:HB3	1:B:239:TYR:CD2	2.47	0.49
1:C:37:LEU:HB3	1:C:50:LEU:HB3	1.94	0.49
1:A:90:MET:HG2	1:A:99:VAL:HG21	1.95	0.49
1:B:93:GLN:H	1:B:96:ALA:HB2	1.76	0.49
1:A:12:LEU:HG	1:A:79:LEU:HD21	1.93	0.49
1:B:19:ILE:O	1:B:21:ASP:N	2.46	0.49
1:A:164:LYS:HD2	1:A:199:MET:HB3	1.95	0.48
1:C:2:PHE:O	1:C:91:LYS:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ASN:HB2	1:B:119:MET:SD	2.54	0.48
1:A:11:LEU:HD22	1:A:11:LEU:HA	1.72	0.48
1:A:19:ILE:O	1:A:21:ASP:N	2.46	0.48
1:B:34:GLY:HA2	1:B:60:TYR:CZ	2.49	0.48
1:A:218:ALA:HB3	1:A:239:TYR:CD2	2.49	0.47
1:A:10:SER:O	1:A:14:LYS:HG3	2.15	0.47
1:C:218:ALA:HB3	1:C:239:TYR:CD2	2.50	0.47
1:B:90:MET:HG2	1:B:99:VAL:HG21	1.96	0.47
1:B:93:GLN:N	1:B:96:ALA:HB2	2.30	0.47
1:A:93:GLN:H	1:A:96:ALA:HB2	1.79	0.47
1:A:11:LEU:O	1:A:15:VAL:HG23	2.15	0.47
1:C:4:ALA:HB1	1:C:57:PHE:CD2	2.50	0.47
1:C:246:HIS:N	1:C:246:HIS:ND1	2.61	0.47
1:B:9:GLY:HA2	1:B:88:ILE:HG12	1.97	0.47
1:C:93:GLN:H	1:C:96:ALA:HB2	1.80	0.46
1:B:11:LEU:O	1:B:15:VAL:HG23	2.15	0.46
1:A:53:ARG:HE	1:A:53:ARG:HB2	1.33	0.46
1:C:93:GLN:N	1:C:96:ALA:HB2	2.31	0.46
1:B:2:PHE:HA	1:B:61:ARG:O	2.16	0.46
1:A:161:ALA:HB2	1:A:204:THR:HG23	1.98	0.46
1:B:2:PHE:O	1:B:91:LYS:HA	2.15	0.46
1:B:160:ILE:HD12	1:B:207:PHE:CE2	2.50	0.46
1:B:246:HIS:ND1	1:B:246:HIS:N	2.63	0.46
1:C:160:ILE:HD12	1:C:207:PHE:CE2	2.51	0.45
1:A:71:ASN:HB2	1:A:119:MET:SD	2.56	0.45
1:A:93:GLN:N	1:A:96:ALA:HB2	2.32	0.45
1:A:112:SER:HB3	1:A:114:TYR:CE1	2.52	0.45
1:B:4:ALA:HB1	1:B:57:PHE:CD2	2.51	0.45
1:B:27:SER:HB2	1:B:123:GLN:NE2	2.30	0.45
1:B:27:SER:HA	1:B:68:MET:O	2.17	0.45
1:C:112:SER:HB3	1:C:114:TYR:CE1	2.51	0.45
1:C:137:ILE:HG22	1:C:139:LEU:HD22	1.98	0.45
1:A:2:PHE:HA	1:A:61:ARG:O	2.17	0.45
1:C:69:GLY:O	1:C:119:MET:HE2	2.16	0.45
1:B:11:LEU:HD22	1:B:11:LEU:HA	1.72	0.44
1:C:10:SER:O	1:C:14:LYS:HG3	2.17	0.44
1:A:27:SER:HA	1:A:68:MET:O	2.18	0.44
1:A:37:LEU:HB3	1:A:50:LEU:HB3	1.99	0.44
1:C:2:PHE:HA	1:C:61:ARG:O	2.18	0.44
1:A:135:CYS:SG	1:A:199:MET:HG2	2.57	0.44
1:A:4:ALA:HB1	1:A:57:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD13	1:A:16:LEU:HA	1.74	0.44
1:C:47:LEU:HB3	1:C:250:PHE:HB2	1.99	0.44
1:A:246:HIS:ND1	1:A:246:HIS:N	2.64	0.44
1:B:1:MET:HB2	1:B:1:MET:HE2	1.85	0.44
1:B:112:SER:HB3	1:B:114:TYR:CE1	2.53	0.44
1:C:9:GLY:HA2	1:C:88:ILE:HG12	1.99	0.44
1:B:135:CYS:SG	1:B:199:MET:HG2	2.57	0.43
1:C:135:CYS:SG	1:C:199:MET:HG2	2.58	0.43
1:A:27:SER:HB2	1:A:123:GLN:NE2	2.32	0.43
1:A:241:ILE:HG22	1:A:241:ILE:O	2.18	0.43
1:C:27:SER:HB2	1:C:123:GLN:NE2	2.33	0.43
1:C:34:GLY:HA2	1:C:60:TYR:CZ	2.52	0.43
1:A:9:GLY:HA2	1:A:88:ILE:HG12	1.99	0.43
1:B:10:SER:O	1:B:14:LYS:HG3	2.19	0.43
1:C:1:MET:HB3	1:C:92:ALA:O	2.18	0.43
1:B:210:ARG:O	1:B:214:MET:HE2	2.19	0.43
1:A:1:MET:HB2	1:A:1:MET:HE3	1.89	0.43
1:B:47:LEU:HB3	1:B:250:PHE:HB2	2.00	0.43
1:B:50:LEU:HD22	1:B:51:ASN:N	2.34	0.43
1:C:53:ARG:HE	1:C:53:ARG:HB2	1.34	0.43
1:A:99:VAL:CG1	1:A:118:LEU:HD11	2.46	0.42
1:A:225:VAL:HB	1:A:239:TYR:CE1	2.54	0.42
1:C:161:ALA:HB2	1:C:204:THR:HG23	2.01	0.42
1:C:4:ALA:HB1	1:C:57:PHE:CE2	2.54	0.42
1:B:69:GLY:O	1:B:119:MET:HE2	2.19	0.42
1:A:110:LYS:HA	1:B:181:LYS:O	2.20	0.42
1:A:212:LEU:O	1:A:216:THR:OG1	2.38	0.42
1:A:34:GLY:HA2	1:A:60:TYR:CZ	2.55	0.42
1:A:1:MET:HB3	1:A:92:ALA:O	2.20	0.42
1:C:191:GLU:OE1	1:C:224:GLN:NE2	2.53	0.42
1:A:57:PHE:CD1	1:A:57:PHE:N	2.88	0.41
1:B:16:LEU:HD13	1:B:16:LEU:HA	1.74	0.41
1:B:19:ILE:HG23	1:B:23:LEU:HD12	2.01	0.41
1:B:1:MET:HB3	1:B:92:ALA:O	2.20	0.41
1:B:158:ILE:HD12	1:B:212:LEU:HD12	2.01	0.41
1:B:50:LEU:HD21	1:B:52:LEU:HG	2.01	0.41
1:C:71:ASN:HB2	1:C:119:MET:SD	2.61	0.41
1:C:241:ILE:O	1:C:241:ILE:HG22	2.21	0.41
1:A:47:LEU:HB3	1:A:250:PHE:HB2	2.03	0.41
1:C:12:LEU:O	1:C:15:VAL:HB	2.19	0.41
1:C:212:LEU:O	1:C:216:THR:OG1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HB	1:A:249:TYR:HB2	2.02	0.41
1:A:4:ALA:HB1	1:A:57:PHE:CE2	2.56	0.41
1:A:19:ILE:HB	1:A:20:LYS:H	1.71	0.41
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.85	0.41
1:A:141:SER:HA	1:A:225:VAL:HG12	2.03	0.41
1:B:4:ALA:HB1	1:B:57:PHE:CE2	2.55	0.41
1:B:57:PHE:CD1	1:B:57:PHE:N	2.89	0.41
1:B:237:VAL:HB	1:B:249:TYR:HB2	2.04	0.40
1:B:69:GLY:HA3	1:B:119:MET:O	2.21	0.40
1:B:85:ASP:HB2	1:B:106:PRO:HG3	2.04	0.40
1:B:160:ILE:HD12	1:B:207:PHE:HE2	1.85	0.40
1:C:67:ILE:O	1:C:67:ILE:HG22	2.20	0.40
1:C:160:ILE:HD12	1:C:207:PHE:HE2	1.85	0.40
1:C:237:VAL:HB	1:C:249:TYR:HB2	2.03	0.40
1:A:160:ILE:HD12	1:A:207:PHE:CE2	2.56	0.40
1:C:36:GLN:HA	1:C:50:LEU:O	2.22	0.40
1:C:85:ASP:HB2	1:C:106:PRO:HG3	2.03	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	253/260 (97%)	217 (86%)	30 (12%)	6 (2%)	6	29
1	B	252/260 (97%)	215 (85%)	32 (13%)	5 (2%)	7	34
1	C	252/260 (97%)	217 (86%)	30 (12%)	5 (2%)	7	34
All	All	757/780 (97%)	649 (86%)	92 (12%)	16 (2%)	7	33

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	129	PRO
1	A	188	VAL
1	B	20	LYS
1	B	129	PRO
1	B	188	VAL
1	C	20	LYS
1	C	129	PRO
1	C	188	VAL
1	C	54	ALA
1	A	187	SER
1	B	54	ALA
1	B	187	SER
1	C	187	SER
1	A	54	ALA
1	A	234	PRO

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	219/226 (97%)	185 (84%)	34 (16%)	2 13
1	B	219/226 (97%)	185 (84%)	34 (16%)	2 13
1	C	217/226 (96%)	186 (86%)	31 (14%)	3 15
All	All	655/678 (97%)	556 (85%)	99 (15%)	3 14

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	ARG
1	A	6	LEU
1	A	11	LEU
1	A	21	ASP
1	A	32	ASP
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	50	LEU
1	A	79	LEU
1	A	85	ASP
1	A	90	MET
1	A	95	ASN
1	A	101	PHE
1	A	113	ASP
1	A	117	LYS
1	A	131	THR
1	A	170	SER
1	A	174	ASP
1	A	177	THR
1	A	181	LYS
1	A	189	ASP
1	A	201	GLU
1	A	209	CYS
1	A	210	ARG
1	A	216	THR
1	A	226	SER
1	A	228	SER
1	A	230	SER
1	A	232	ASP
1	A	233	VAL
1	A	235	LEU
1	A	246	HIS
1	A	254	LYS
1	A	255	ILE
1	B	1	MET
1	B	5	ARG
1	B	6	LEU
1	B	7	VAL
1	B	11	LEU
1	B	21	ASP
1	B	22	LEU
1	B	32	ASP
1	B	35	ILE
1	B	50	LEU
1	B	85	ASP
1	B	90	MET
1	B	95	ASN
1	B	101	PHE
1	B	113	ASP

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Mol	Chain	Res	Type
1	B	117	LYS
1	B	131	THR
1	B	165	GLU
1	B	170	SER
1	B	174	ASP
1	B	177	THR
1	B	181	LYS
1	B	189	ASP
1	B	209	CYS
1	B	210	ARG
1	B	216	THR
1	B	226	SER
1	B	228	SER
1	B	230	SER
1	B	232	ASP
1	B	233	VAL
1	B	235	LEU
1	B	246	HIS
1	B	254	LYS
1	C	1	MET
1	C	5	ARG
1	C	6	LEU
1	C	11	LEU
1	C	21	ASP
1	C	32	ASP
1	C	35	ILE
1	C	48	VAL
1	C	50	LEU
1	C	85	ASP
1	C	90	MET
1	C	95	ASN
1	C	101	PHE
1	C	113	ASP
1	C	117	LYS
1	C	131	THR
1	C	174	ASP
1	C	177	THR
1	C	181	LYS
1	C	189	ASP
1	C	201	GLU
1	C	209	CYS
1	C	210	ARG

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Mol	Chain	Res	Type
1	C	216	THR
1	C	226	SER
1	C	228	SER
1	C	230	SER
1	C	232	ASP
1	C	233	VAL
1	C	235	LEU
1	C	246	HIS

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 monosaccharides 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, 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	255/260 (98%)	0.05	8 (3%)	49	21	43, 67, 114, 134	0
1	B	254/260 (97%)	0.10	9 (3%)	44	18	43, 67, 113, 135	0
1	C	254/260 (97%)	0.11	8 (3%)	49	21	42, 67, 114, 134	0
All	All	763/780 (97%)	0.09	25 (3%)	46	20	42, 67, 114, 135	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	HIS	4.4
1	A	123	GLN	4.3
1	B	107	ASN	4.2
1	B	187	SER	4.1
1	A	120	ASN	3.9
1	A	107	ASN	3.5
1	B	106	PRO	3.2
1	A	191	GLU	3.2
1	B	186	SER	3.2
1	C	126	LEU	3.0
1	C	38	GLN	2.8
1	B	95	ASN	2.7
1	C	162	CYS	2.6
1	B	124	GLU	2.6
1	C	200	GLN	2.6
1	C	191	GLU	2.5
1	C	109	GLU	2.5
1	A	106	PRO	2.4
1	C	107	ASN	2.3
1	A	255	ILE	2.3
1	C	106	PRO	2.3
1	A	109	GLU	2.1
1	B	191	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	108	GLN	2.1
1	B	122	ASP	2.1

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.