Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 12:35 AM EDT

PDB ID	:	6QC0
Title	:	PCNA complex with Cdt2 C-terminal PIP-box peptide
Authors	:	Perrakis, A.P.; von Castelmur, E.
Deposited on	:	2018-12-25
Resolution	:	3.50 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 (i) 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 (1)) were used in the production of this report:

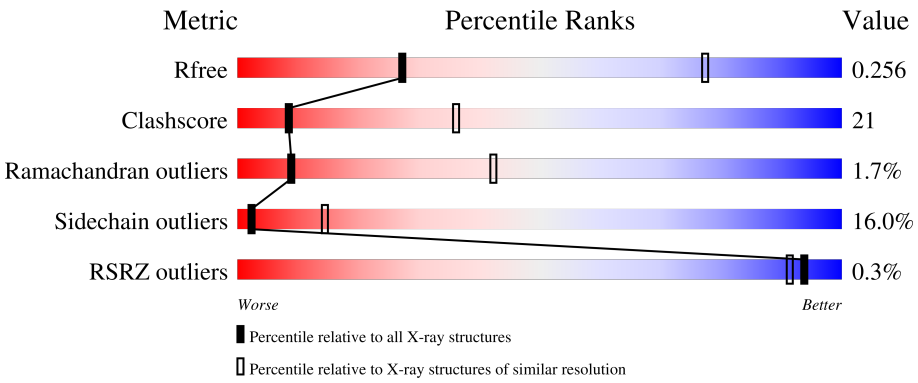
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	263	55% 35% 6% •
1	C	263	% 60% 31% 6% •
1	E	263	51% 40% 6% •
2	B	14	14% 36% 29% 21%
2	D	14	36% 29% 14% 21%

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Mol	Chain	Length	Quality of chain
2	F	14	14% 21% 43% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6173 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
			Total	C	N	O	S			
1	A	254	1950	1225	320	389	16	0	0	0
1	C	255	1963	1233	322	392	16	0	0	0
1	E	255	1963	1233	322	392	16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Denticleless protein homolog.

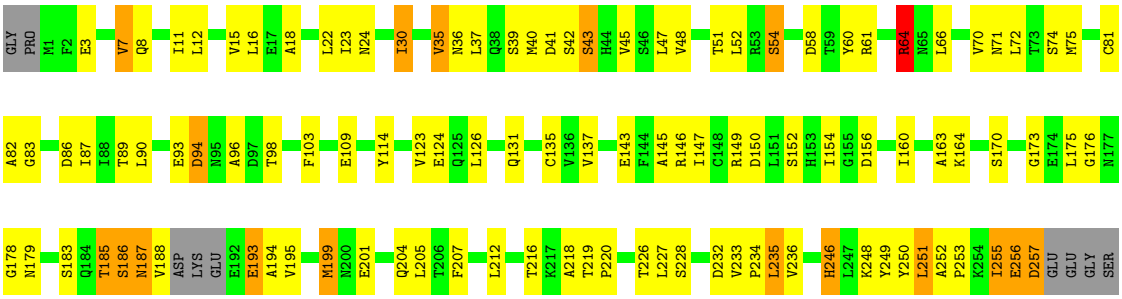
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	11	99	63	20	14	2	0	0	0
2	D	11	99	63	20	14	2	0	0	0
2	F	11	99	63	20	14	2	0	0	0

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.

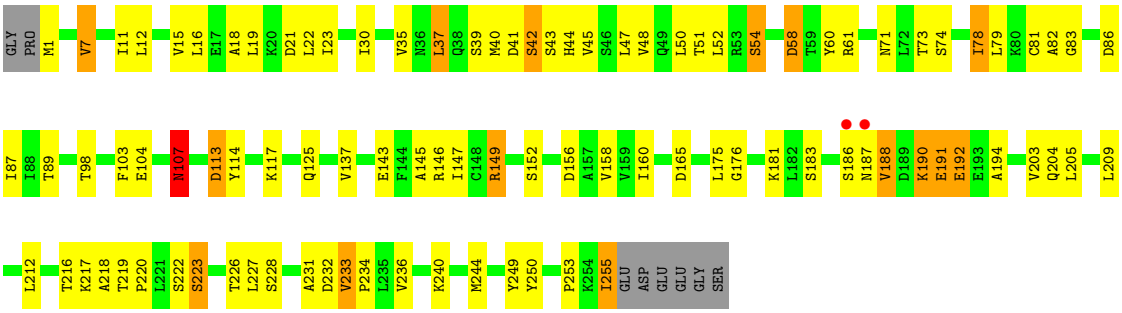
• Molecule 1: Proliferating cell nuclear antigen

Chain A: 55% 35% 6% •



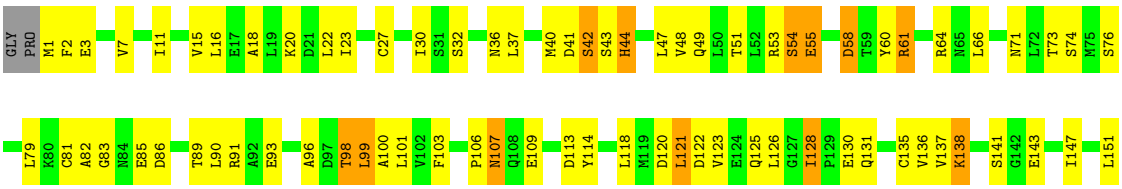
• Molecule 1: Proliferating cell nuclear antigen

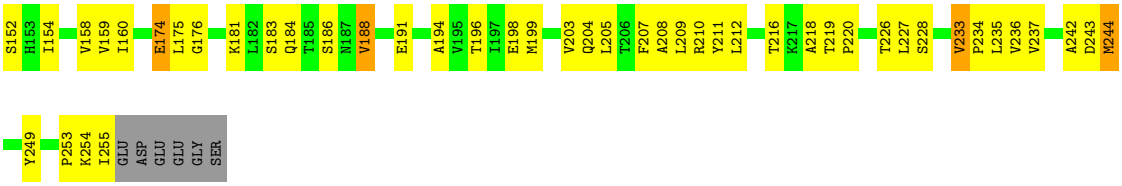
Chain C: % 60% 31% 6% •



• Molecule 1: Proliferating cell nuclear antigen

Chain E: 51% 40% 6% •



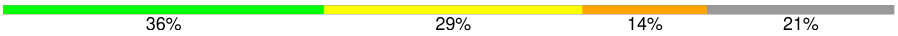


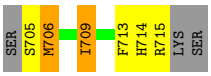
- Molecule 2: Denticleless protein homolog

Chain B:

- Molecule 2: Denticleless protein homolog

Chain D:





- Molecule 2: Denticleless protein homolog

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	151.37Å 151.37Å 91.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.73 – 3.50 43.70 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.73-3.50) 97.3 (43.70-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.196 , 0.252 0.203 , 0.256	Depositor DCC
R_{free} test set	748 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 12.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6173	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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 (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	0.77	1/1975 (0.1%)	0.97	3/2668 (0.1%)
1	C	0.72	0/1989	0.97	2/2687 (0.1%)
1	E	0.73	0/1989	1.01	1/2687 (0.0%)
2	B	0.87	0/101	1.19	0/132
2	D	0.91	0/101	1.30	0/132
2	F	0.91	0/101	1.29	0/132
All	All	0.75	1/6256 (0.0%)	1.00	6/8438 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	C	0	4
1	E	2	0
All	All	3	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ARG	CZ-NH2	12.35	1.49	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	122	ASP	CB-CA-C	10.53	131.46	110.40
1	C	156	ASP	CB-CA-C	-6.44	97.52	110.40
1	A	64	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A	156	ASP	CB-CA-C	-6.02	98.36	110.40
1	C	107	ASN	CB-CA-C	5.52	121.44	110.40
1	A	186	SER	N-CA-CB	5.26	118.40	110.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	186	SER	CA
1	E	122	ASP	CA
1	E	188	VAL	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	GLU	Peptide
1	A	185	THR	Peptide
1	A	193	GLU	Peptide
1	C	107	ASN	Peptide
1	C	187	ASN	Peptide
1	C	188	VAL	Peptide
1	C	190	LYS	Peptide

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	1950	0	1955	79	0
1	C	1963	0	1973	58	0
1	E	1963	0	1973	100	0
2	B	99	0	100	16	0
2	D	99	0	100	8	0
2	F	99	0	100	21	0
All	All	6173	0	6201	257	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 21.

All (257) 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:30:ILE:CD1	1:A:66:LEU:HB2	1.85	1.06
1:C:255:ILE:HG23	2:D:705:SER:HB2	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG23	1:A:52:LEU:HB2	1.46	0.97
1:C:192:GLU:HG3	1:C:223:SER:HB2	1.49	0.93
1:C:255:ILE:CG2	2:D:705:SER:HB2	2.01	0.90
1:A:36:ASN:HD21	1:A:51:THR:HG23	1.35	0.90
2:F:715:ARG:CZ	2:F:715:ARG:HA	2.03	0.89
2:F:707:ARG:HA	2:F:707:ARG:NE	1.85	0.89
1:A:233:VAL:HG22	1:A:234:PRO:HD2	1.54	0.88
1:A:30:ILE:HD11	1:A:66:LEU:HB2	1.56	0.87
2:B:707:ARG:NE	2:B:707:ARG:HA	1.87	0.86
1:E:120:ASP:O	1:E:121:LEU:HD23	1.76	0.85
1:A:7:VAL:HA	1:A:87:ILE:CD1	2.10	0.82
1:E:120:ASP:C	1:E:121:LEU:HD23	2.04	0.78
2:B:705:SER:OG	2:B:706:MET:N	2.17	0.77
1:A:36:ASN:ND2	1:A:51:THR:HG23	2.01	0.75
1:E:138:LYS:HG2	1:E:226:THR:HG22	1.69	0.73
1:C:18:ALA:HB1	1:C:249:TYR:OH	1.91	0.70
1:A:7:VAL:HA	1:A:87:ILE:HD13	1.71	0.70
1:E:235:LEU:CD2	1:E:237:VAL:HG23	2.21	0.70
1:A:18:ALA:HB1	1:A:249:TYR:OH	1.91	0.69
1:A:219:THR:N	1:A:220:PRO:HD2	2.08	0.69
1:C:50:LEU:HD11	1:C:52:LEU:HD11	1.75	0.69
2:B:709:ILE:HD13	2:B:709:ILE:H	1.57	0.69
1:C:219:THR:N	1:C:220:PRO:HD2	2.08	0.69
1:E:141:SER:HB2	1:E:219:THR:HG23	1.74	0.68
1:C:145:ALA:HB2	1:C:219:THR:HG21	1.75	0.68
1:A:23:ILE:HD12	1:A:72:LEU:CD1	2.25	0.67
1:E:174:GLU:N	1:E:174:GLU:OE1	2.27	0.67
1:E:219:THR:N	1:E:220:PRO:HD2	2.10	0.67
1:E:128:ILE:HD13	1:E:128:ILE:H	1.60	0.66
1:E:18:ALA:HB1	1:E:249:TYR:OH	1.95	0.66
1:E:141:SER:CB	1:E:219:THR:HG23	2.25	0.66
1:E:235:LEU:HD23	1:E:236:VAL:N	2.11	0.66
1:C:192:GLU:HG3	1:C:223:SER:CB	2.25	0.64
1:A:37:LEU:C	1:A:37:LEU:HD23	2.18	0.64
1:A:30:ILE:HD13	1:A:66:LEU:H	1.63	0.63
1:C:37:LEU:C	1:C:37:LEU:HD23	2.19	0.63
1:E:254:LYS:HE3	2:F:706:MET:CE	2.28	0.63
1:E:82:ALA:HB2	1:E:103:PHE:CE2	2.34	0.63
1:C:52:LEU:HD23	1:C:244:MET:CE	2.29	0.62
1:E:37:LEU:HD23	1:E:37:LEU:C	2.19	0.62
1:A:45:VAL:HG11	2:B:706:MET:SD	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:MET:HG2	2:F:709:ILE:HD11	1.82	0.61
2:F:715:ARG:HA	2:F:715:ARG:NE	2.15	0.61
1:C:82:ALA:HB2	1:C:103:PHE:CE2	2.37	0.60
1:E:254:LYS:O	1:E:255:ILE:HG12	2.01	0.60
1:A:235:LEU:HD23	1:A:236:VAL:N	2.17	0.59
1:A:7:VAL:O	1:A:87:ILE:HD13	2.02	0.59
1:C:52:LEU:HD23	1:C:244:MET:HE1	1.85	0.59
1:E:204:GLN:O	1:E:205:LEU:HD12	2.03	0.58
1:E:53:ARG:HB3	1:E:55:GLU:OE2	2.03	0.58
1:A:82:ALA:HB2	1:A:103:PHE:CE2	2.37	0.58
1:A:30:ILE:CD1	1:A:66:LEU:CB	2.73	0.58
1:E:255:ILE:C	2:F:705:SER:HB2	2.23	0.58
1:C:7:VAL:CG2	1:C:58:ASP:OD1	2.52	0.58
1:C:40:MET:HE2	1:C:44:HIS:HA	1.86	0.58
1:A:145:ALA:HB2	1:A:219:THR:HG21	1.85	0.57
1:E:1:MET:CE	1:E:91:ARG:HD3	2.35	0.57
1:E:40:MET:HE2	1:E:44:HIS:HA	1.86	0.57
1:A:256:GLU:HB2	1:A:257:ASP:OD1	2.04	0.57
1:E:203:VAL:HG13	1:E:205:LEU:HD13	1.86	0.57
1:A:218:ALA:C	1:A:220:PRO:HD2	2.26	0.56
1:A:188:VAL:O	1:A:193:GLU:OE2	2.24	0.56
1:C:212:LEU:O	1:C:216:THR:HG23	2.06	0.56
1:E:235:LEU:HD22	1:E:237:VAL:HG23	1.87	0.56
1:A:204:GLN:O	1:A:205:LEU:HD23	2.06	0.56
1:E:1:MET:HE2	1:E:91:ARG:HD3	1.87	0.56
1:E:212:LEU:O	1:E:216:THR:HG23	2.06	0.55
1:E:7:VAL:CG2	1:E:58:ASP:OD1	2.54	0.55
1:A:207:PHE:CE2	1:A:235:LEU:HB2	2.41	0.55
1:E:99:LEU:C	1:E:99:LEU:CD2	2.74	0.55
1:E:41:ASP:OD1	1:E:43:SER:OG	2.19	0.55
1:C:78:ILE:HD11	1:E:175:LEU:CD1	2.36	0.55
1:C:125:GLN:O	2:D:715:ARG:C	2.45	0.55
1:E:188:VAL:HG21	1:E:194:ALA:HB1	1.88	0.55
2:D:709:ILE:HD13	2:D:709:ILE:H	1.72	0.54
1:A:150:ASP:HB3	1:E:81:CYS:SG	2.46	0.54
1:E:218:ALA:C	1:E:220:PRO:HD2	2.28	0.54
1:A:93:GLU:HB2	1:A:96:ALA:HB2	1.90	0.54
1:A:40:MET:HE3	2:B:709:ILE:HD11	1.89	0.54
1:A:212:LEU:O	1:A:216:THR:HG23	2.07	0.54
1:C:52:LEU:HD12	1:C:52:LEU:N	2.23	0.54
1:E:16:LEU:HG	1:E:79:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HD13	1:A:154:ILE:N	2.23	0.53
1:C:219:THR:N	1:C:220:PRO:CD	2.72	0.53
1:C:233:VAL:HG22	1:C:234:PRO:HD2	1.91	0.53
1:E:7:VAL:HG22	1:E:58:ASP:CG	2.28	0.53
1:C:45:VAL:HG11	2:D:706:MET:SD	2.49	0.53
1:C:137:VAL:O	1:C:226:THR:HA	2.08	0.53
2:F:707:ARG:HA	2:F:707:ARG:CZ	2.38	0.53
1:A:146:ARG:NH1	1:A:149:ARG:HH22	2.07	0.53
1:E:99:LEU:HD23	1:E:100:ALA:N	2.23	0.53
1:E:254:LYS:CE	2:F:706:MET:HE2	2.39	0.53
2:F:715:ARG:HA	2:F:715:ARG:NH1	2.23	0.53
1:A:219:THR:N	1:A:220:PRO:CD	2.72	0.53
1:A:23:ILE:CD1	1:A:72:LEU:CD1	2.86	0.53
1:A:185:THR:HG21	1:A:194:ALA:HA	1.92	0.52
1:C:30:ILE:N	1:C:30:ILE:HD12	2.24	0.52
1:E:137:VAL:O	1:E:226:THR:HA	2.09	0.52
2:B:705:SER:HG	2:B:706:MET:H	1.55	0.52
1:C:218:ALA:C	1:C:220:PRO:HD2	2.30	0.52
1:E:135:CYS:SG	1:E:199:MET:HG2	2.50	0.52
1:A:124:GLU:HG3	1:A:124:GLU:O	2.10	0.52
1:A:124:GLU:O	1:A:126:LEU:HD12	2.09	0.52
1:C:191:GLU:HA	1:C:194:ALA:HB3	1.91	0.51
1:E:219:THR:N	1:E:220:PRO:CD	2.72	0.51
1:C:47:LEU:HD23	1:C:47:LEU:C	2.31	0.51
1:E:30:ILE:N	1:E:30:ILE:HD12	2.25	0.51
1:C:16:LEU:HG	1:C:79:LEU:HD12	1.93	0.51
1:A:47:LEU:C	1:A:47:LEU:HD23	2.31	0.51
1:A:257:ASP:OD1	1:A:257:ASP:N	2.43	0.51
1:C:47:LEU:HD23	1:C:48:VAL:N	2.26	0.51
1:A:246:HIS:NE2	1:A:248:LYS:HD2	2.26	0.51
1:E:208:ALA:HB2	2:F:706:MET:HE1	1.93	0.51
2:B:707:ARG:HA	2:B:707:ARG:CZ	2.40	0.51
1:C:7:VAL:HG22	1:C:58:ASP:OD1	2.11	0.51
1:E:128:ILE:HG12	1:E:128:ILE:O	2.11	0.51
1:E:27:CYS:CB	1:E:123:VAL:HG11	2.41	0.50
1:E:128:ILE:H	1:E:128:ILE:CD1	2.23	0.50
1:A:137:VAL:O	1:A:226:THR:HA	2.12	0.50
1:A:23:ILE:HD12	1:A:72:LEU:HD12	1.93	0.50
1:A:204:GLN:C	1:A:205:LEU:HD23	2.31	0.50
1:A:126:LEU:HD21	2:B:710:CYS:HA	1.93	0.50
1:A:170:SER:HB3	1:A:179:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:VAL:HG22	1:E:234:PRO:HD2	1.93	0.50
1:A:40:MET:HE3	2:B:709:ILE:CD1	2.42	0.50
1:C:51:THR:C	1:C:52:LEU:HD12	2.33	0.49
1:E:47:LEU:HD23	1:E:47:LEU:C	2.32	0.49
1:A:185:THR:CG2	1:A:194:ALA:HB1	2.42	0.49
1:E:254:LYS:HE3	2:F:706:MET:HE2	1.94	0.49
1:C:175:LEU:HD12	1:C:176:GLY:N	2.26	0.49
1:A:143:GLU:O	1:A:147:ILE:HG13	2.13	0.49
1:A:146:ARG:HD2	1:A:150:ASP:OD2	2.13	0.49
2:F:708:LYS:O	2:F:711:THR:HG23	2.12	0.49
1:A:47:LEU:HD23	1:A:48:VAL:N	2.28	0.49
1:A:233:VAL:CG2	1:A:234:PRO:HD2	2.36	0.49
1:C:78:ILE:CD1	1:E:175:LEU:HD13	2.43	0.49
1:E:85:GLU:HB3	1:E:106:PRO:HG3	1.96	0.48
1:A:22:LEU:HG	1:A:23:ILE:HG23	1.94	0.48
1:A:175:LEU:HD12	1:A:176:GLY:N	2.29	0.48
1:A:236:VAL:HG22	1:A:250:TYR:CE2	2.49	0.48
1:A:178:GLY:HA2	1:E:114:TYR:HA	1.95	0.48
2:F:706:MET:HE2	2:F:706:MET:HB2	1.81	0.48
1:A:94:ASP:OD1	1:A:94:ASP:N	2.46	0.48
1:E:207:PHE:CE2	1:E:235:LEU:HB2	2.48	0.48
1:A:41:ASP:OD1	1:A:43:SER:N	2.37	0.48
1:C:107:ASN:O	1:C:107:ASN:ND2	2.47	0.48
1:C:21:ASP:OD2	1:C:217:LYS:HE2	2.13	0.48
1:A:135:CYS:SG	1:A:199:MET:HG2	2.54	0.48
2:B:707:ARG:NE	2:B:707:ARG:CA	2.70	0.47
1:E:158:VAL:HB	1:E:209:LEU:HD21	1.97	0.47
1:A:163:ALA:HA	1:A:199:MET:HE2	1.95	0.47
1:C:233:VAL:HG22	1:C:234:PRO:CD	2.44	0.47
1:C:52:LEU:HD23	1:C:244:MET:HE3	1.96	0.47
2:D:713:PHE:O	2:D:714:HIS:CD2	2.67	0.47
1:A:30:ILE:HD13	1:A:66:LEU:HB2	1.88	0.47
1:C:22:LEU:HD23	1:C:48:VAL:CG2	2.44	0.47
1:E:233:VAL:HG22	1:E:234:PRO:CD	2.44	0.47
1:C:40:MET:CE	1:C:44:HIS:HB3	2.45	0.47
1:A:185:THR:HG22	1:A:195:VAL:H	1.79	0.47
2:B:708:LYS:O	2:B:711:THR:HG23	2.15	0.46
2:B:707:ARG:HG3	2:B:711:THR:HG21	1.96	0.46
1:E:174:GLU:OE2	1:E:175:LEU:HD23	2.16	0.46
1:A:81:CYS:HB3	1:A:114:TYR:OH	2.16	0.46
1:A:83:GLY:O	1:A:86:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HE	1:A:94:ASP:HB3	1.80	0.46
1:E:41:ASP:OD2	1:E:211:TYR:CE1	2.68	0.46
1:E:125:GLN:O	2:F:715:ARG:NH2	2.49	0.46
1:E:235:LEU:HD21	1:E:237:VAL:HG23	1.96	0.46
1:E:41:ASP:OD1	1:E:43:SER:N	2.36	0.45
1:A:11:ILE:O	1:A:15:VAL:HG23	2.17	0.45
1:C:222:SER:HB2	1:C:240:LYS:O	2.16	0.45
1:E:154:ILE:N	1:E:154:ILE:HD12	2.30	0.45
1:E:174:GLU:N	1:E:174:GLU:CD	2.70	0.45
1:E:120:ASP:O	1:E:121:LEU:CD2	2.55	0.45
1:E:126:LEU:HD23	2:F:713:PHE:HB2	1.99	0.45
1:C:19:LEU:CD2	1:C:48:VAL:HG11	2.46	0.45
1:E:175:LEU:HD12	1:E:176:GLY:N	2.31	0.45
1:E:235:LEU:HD23	1:E:235:LEU:C	2.37	0.45
1:A:16:LEU:HD21	1:A:75:MET:CG	2.46	0.45
1:E:7:VAL:CG2	1:E:58:ASP:CG	2.85	0.45
1:E:22:LEU:HG	1:E:23:ILE:HG23	1.98	0.45
2:B:709:ILE:HD13	2:B:709:ILE:N	2.30	0.45
1:C:83:GLY:O	1:C:86:ASP:HB2	2.17	0.45
1:A:71:ASN:O	1:A:74:SER:HB2	2.17	0.45
1:C:54:SER:HB3	1:C:60:TYR:CD2	2.52	0.45
1:E:188:VAL:HG21	1:E:194:ALA:CB	2.47	0.45
1:E:83:GLY:O	1:E:86:ASP:HB2	2.16	0.45
1:E:141:SER:OG	1:E:219:THR:HG23	2.17	0.45
1:E:235:LEU:HD21	1:E:237:VAL:CG2	2.47	0.45
1:A:3:GLU:HA	1:A:90:LEU:O	2.18	0.44
1:E:41:ASP:OD2	1:E:211:TYR:HE1	2.00	0.44
1:C:160:ILE:O	1:C:204:GLN:HA	2.16	0.44
1:E:143:GLU:O	1:E:147:ILE:HG13	2.17	0.44
1:C:11:ILE:O	1:C:15:VAL:HG23	2.17	0.44
1:E:54:SER:HB3	1:E:60:TYR:CD2	2.52	0.44
1:E:242:ALA:O	1:E:243:ASP:HB2	2.17	0.44
1:C:22:LEU:HG	1:C:23:ILE:HG23	2.00	0.44
1:E:82:ALA:HB2	1:E:103:PHE:CD2	2.53	0.44
1:C:40:MET:CE	1:C:44:HIS:CB	2.96	0.43
1:E:27:CYS:HB2	1:E:123:VAL:HG11	2.00	0.43
1:C:71:ASN:O	1:C:74:SER:HB2	2.18	0.43
1:C:143:GLU:O	1:C:147:ILE:HG13	2.18	0.43
1:E:160:ILE:O	1:E:204:GLN:HA	2.18	0.43
2:F:709:ILE:HD13	2:F:709:ILE:H	1.83	0.43
1:A:154:ILE:O	1:A:173:GLY:HA3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ILE:O	1:E:15:VAL:HG23	2.18	0.43
1:A:7:VAL:CG2	1:A:8:GLN:N	2.81	0.43
1:A:188:VAL:C	1:A:193:GLU:OE2	2.57	0.43
1:E:7:VAL:HG23	1:E:58:ASP:OD1	2.18	0.43
1:C:30:ILE:HG13	1:C:35:VAL:HG22	2.00	0.43
1:C:158:VAL:HB	1:C:209:LEU:HD21	2.00	0.43
2:D:713:PHE:O	2:D:714:HIS:CG	2.70	0.43
1:A:160:ILE:O	1:A:204:GLN:HA	2.18	0.43
1:A:54:SER:HB3	1:A:60:TYR:CD2	2.54	0.43
1:C:113:ASP:OD1	1:C:113:ASP:O	2.36	0.43
2:B:709:ILE:H	2:B:709:ILE:CD1	2.29	0.43
1:E:40:MET:CE	1:E:44:HIS:CB	2.96	0.43
1:E:99:LEU:CD2	1:E:100:ALA:O	2.67	0.42
1:E:40:MET:CE	1:E:44:HIS:HB3	2.49	0.42
1:E:93:GLU:HB2	1:E:96:ALA:HB2	2.01	0.42
1:E:208:ALA:HB2	2:F:706:MET:CE	2.49	0.42
1:E:3:GLU:HA	1:E:90:LEU:O	2.19	0.42
1:C:81:CYS:HB3	1:C:114:TYR:OH	2.19	0.42
1:E:107:ASN:HB3	1:E:109:GLU:H	1.84	0.42
1:E:244:MET:HE3	1:E:244:MET:HB3	1.96	0.42
2:F:707:ARG:HG3	2:F:711:THR:HG21	2.02	0.42
1:E:44:HIS:O	2:F:708:LYS:HG3	2.20	0.42
1:E:101:LEU:HD12	1:E:101:LEU:N	2.34	0.42
1:A:235:LEU:HD23	1:A:236:VAL:H	1.84	0.41
1:C:82:ALA:HB2	1:C:103:PHE:CD2	2.54	0.41
1:E:23:ILE:HG22	1:E:41:ASP:HA	2.01	0.41
1:A:235:LEU:CD2	1:A:236:VAL:N	2.83	0.41
1:E:36:ASN:OD1	1:E:51:THR:HG23	2.19	0.41
1:E:47:LEU:HD23	1:E:48:VAL:N	2.34	0.41
1:E:98:THR:HA	1:E:118:LEU:HD23	2.02	0.41
1:C:205:LEU:HD21	1:C:231:ALA:HA	2.03	0.41
1:E:71:ASN:O	1:E:74:SER:HB2	2.20	0.41
1:E:81:CYS:HB3	1:E:114:TYR:OH	2.20	0.41
1:E:235:LEU:HD23	1:E:236:VAL:C	2.41	0.41
1:A:251:LEU:HD22	1:A:252:ALA:O	2.20	0.41
1:A:40:MET:CE	2:B:709:ILE:CD1	2.99	0.41
1:A:256:GLU:H	1:A:256:GLU:HG2	1.74	0.41
1:C:236:VAL:HG22	1:C:250:TYR:CE2	2.56	0.41
1:E:2:PHE:HA	1:E:61:ARG:O	2.20	0.41
1:A:82:ALA:HB2	1:A:103:PHE:CD2	2.56	0.41
2:D:715:ARG:HA	2:D:715:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD23	2:B:713:PHE:HB2	2.01	0.40
1:E:184:GLN:HG3	1:E:196:THR:HA	2.04	0.40
2:F:709:ILE:H	2:F:709:ILE:CD1	2.33	0.40
1:C:87:ILE:HB	1:C:104:GLU:HB2	2.04	0.40
1:E:20:LYS:HD3	1:E:76:SER:CB	2.51	0.40
1:A:131:GLN:HE22	1:A:233:VAL:HG11	1.86	0.40
1:C:23:ILE:HG22	1:C:41:ASP:HA	2.03	0.40
1:C:146:ARG:HH11	1:C:149:ARG:HH21	1.68	0.40
1:E:254:LYS:CE	2:F:706:MET:CE	2.96	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	250/263 (95%)	215 (86%)	30 (12%)	5 (2%)	7 39
1	C	253/263 (96%)	227 (90%)	23 (9%)	3 (1%)	13 50
1	E	253/263 (96%)	225 (89%)	25 (10%)	3 (1%)	13 50
2	B	9/14 (64%)	6 (67%)	2 (22%)	1 (11%)	0 6
2	D	9/14 (64%)	5 (56%)	3 (33%)	1 (11%)	0 6
2	F	9/14 (64%)	7 (78%)	2 (22%)	0	100 100
All	All	783/831 (94%)	685 (88%)	85 (11%)	13 (2%)	9 42

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	188	VAL
1	E	188	VAL
2	B	706	MET

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Mol	Chain	Res	Type
2	D	706	MET
1	A	187	ASN
1	A	255	ILE
1	C	42	SER
1	A	42	SER
1	C	253	PRO
1	E	42	SER
1	A	253	PRO
1	A	256	GLU
1	E	253	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	221/229 (96%)	190 (86%)	31 (14%)	3 19
1	C	223/229 (97%)	190 (85%)	33 (15%)	3 17
1	E	223/229 (97%)	187 (84%)	36 (16%)	2 14
2	B	11/14 (79%)	7 (64%)	4 (36%)	0 1
2	D	11/14 (79%)	10 (91%)	1 (9%)	9 36
2	F	11/14 (79%)	4 (36%)	7 (64%)	0 0
All	All	700/729 (96%)	588 (84%)	112 (16%)	2 14

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	12	LEU
1	A	24	ASN
1	A	30	ILE
1	A	35	VAL
1	A	39	SER
1	A	43	SER
1	A	54	SER

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Mol	Chain	Res	Type
1	A	58	ASP
1	A	61	ARG
1	A	64	ARG
1	A	70	VAL
1	A	89	THR
1	A	94	ASP
1	A	98	THR
1	A	123	VAL
1	A	152	SER
1	A	164	LYS
1	A	183	SER
1	A	186	SER
1	A	187	ASN
1	A	199	MET
1	A	201	GLU
1	A	227	LEU
1	A	228	SER
1	A	232	ASP
1	A	235	LEU
1	A	246	HIS
1	A	251	LEU
1	A	255	ILE
1	A	257	ASP
1	C	1	MET
1	C	7	VAL
1	C	12	LEU
1	C	37	LEU
1	C	39	SER
1	C	42	SER
1	C	43	SER
1	C	54	SER
1	C	58	ASP
1	C	61	ARG
1	C	73	THR
1	C	78	ILE
1	C	89	THR
1	C	98	THR
1	C	107	ASN
1	C	113	ASP
1	C	117	LYS
1	C	149	ARG
1	C	152	SER

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Mol	Chain	Res	Type
1	C	165	ASP
1	C	181	LYS
1	C	183	SER
1	C	186	SER
1	C	190	LYS
1	C	191	GLU
1	C	192	GLU
1	C	203	VAL
1	C	223	SER
1	C	227	LEU
1	C	228	SER
1	C	232	ASP
1	C	233	VAL
1	C	255	ILE
1	E	32	SER
1	E	42	SER
1	E	44	HIS
1	E	49	GLN
1	E	54	SER
1	E	55	GLU
1	E	58	ASP
1	E	61	ARG
1	E	64	ARG
1	E	66	LEU
1	E	73	THR
1	E	89	THR
1	E	98	THR
1	E	99	LEU
1	E	107	ASN
1	E	113	ASP
1	E	121	LEU
1	E	128	ILE
1	E	130	GLU
1	E	131	GLN
1	E	136	VAL
1	E	138	LYS
1	E	151	LEU
1	E	152	SER
1	E	159	VAL
1	E	174	GLU
1	E	181	LYS
1	E	183	SER

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Mol	Chain	Res	Type
1	E	186	SER
1	E	191	GLU
1	E	198	GLU
1	E	210	ARG
1	E	227	LEU
1	E	228	SER
1	E	233	VAL
1	E	244	MET
2	B	705	SER
2	B	707	ARG
2	B	709	ILE
2	B	714	HIS
2	D	709	ILE
2	F	705	SER
2	F	706	MET
2	F	707	ARG
2	F	709	ILE
2	F	711	THR
2	F	714	HIS
2	F	715	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	84	ASN
1	A	107	ASN
1	A	131	GLN
1	A	179	ASN
1	A	246	HIS
1	C	107	ASN
1	E	38	GLN
1	E	177	ASN
2	D	714	HIS

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 (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	254/263 (96%)	-0.48	0 100 100	51, 71, 102, 116	0
1	C	255/263 (96%)	-0.40	2 (0%) 86 81	48, 71, 112, 149	0
1	E	255/263 (96%)	-0.44	0 100 100	48, 70, 105, 138	0
2	B	11/14 (78%)	-0.34	0 100 100	76, 84, 103, 105	0
2	D	11/14 (78%)	-0.21	0 100 100	85, 95, 106, 115	0
2	F	11/14 (78%)	-0.08	0 100 100	78, 95, 107, 111	0
All	All	797/831 (95%)	-0.43	2 (0%) 94 91	48, 71, 106, 149	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	ASN	2.9
1	C	186	SER	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.