



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:21 PM UTC

PDB ID : 3ZXU / pdb_00003zxu
Title : Crystal structure of the Ctf19-Mcm21 kinetochore heterodimer from yeast
Authors : Schmitzberger, F.; Harrison, S.C.
Deposited on : 2011-08-15
Resolution : 3.70 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

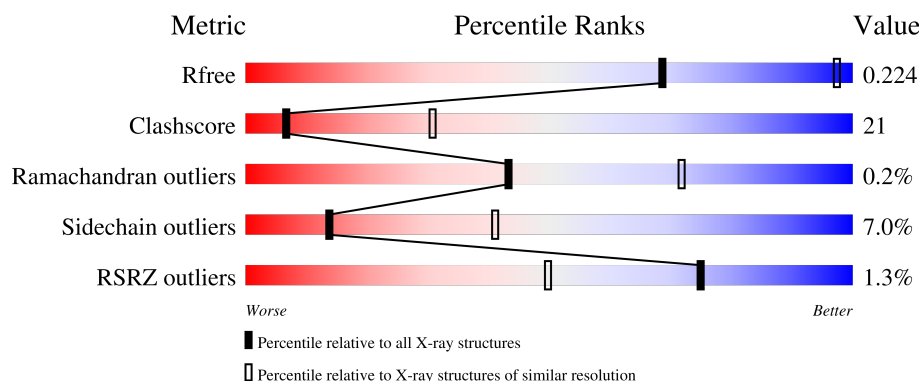
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	296	% 40% 25% 6% 29%
1	C	296	40% 25% 6% 29%
2	B	270	% 43% 27% • 27%
2	D	270	% 43% 26% • 27%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13474 atoms, of which 6763 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 MCM21.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	211	Total	C	H	N	O	S	0	0	0
			3487	1127	1745	290	318	7			
1	C	211	Total	C	H	N	O	S	0	0	0
			3488	1127	1746	290	318	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q6CVQ9
A	-1	ASN	-	expression tag	UNP Q6CVQ9
A	0	ALA	-	expression tag	UNP Q6CVQ9
C	-2	SER	-	expression tag	UNP Q6CVQ9
C	-1	ASN	-	expression tag	UNP Q6CVQ9
C	0	ALA	-	expression tag	UNP Q6CVQ9

- Molecule 2 is a protein called CTF19.

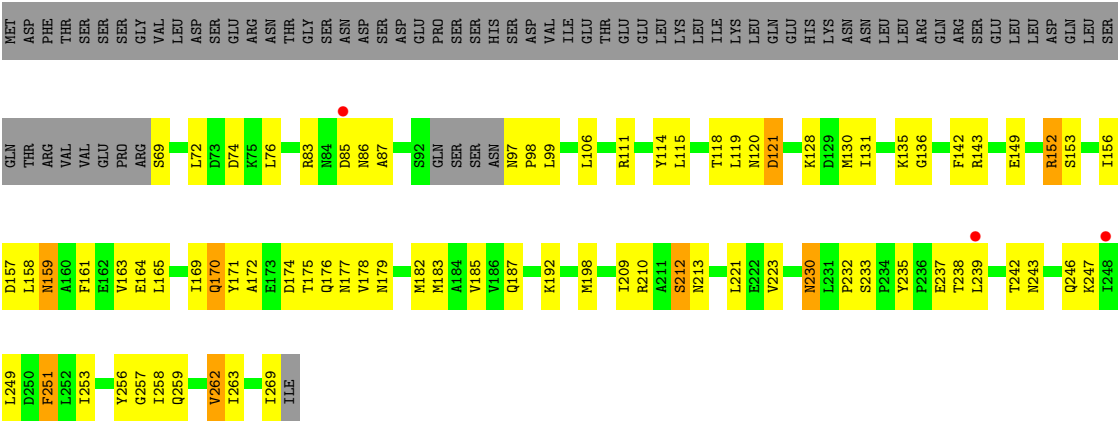
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	197	Total	C	H	N	O	S	0	0	0
			3216	1013	1632	265	299	7			
2	D	198	Total	C	H	N	O	S	0	0	0
			3230	1017	1638	267	301	7			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	13	Total	O		0	0
			13	13			
4	B	6	Total	O		0	0
			6	6			
4	C	18	Total	O		0	0
			18	18			
4	D	11	Total	H	O	0	0
			13	2	11		



• Molecule 2: CTF19



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	239.04Å 239.04Å 179.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.49 – 3.70 47.49 – 3.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.49-3.70) 96.5 (47.49-3.70)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.67Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.209 (Not available) , 0.224	Depositor DCC
R_{free} test set	2215 reflections (6.76%)	wwPDB-VP
Wilson B-factor (Å ²)	158.3	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 242.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13474	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.68	0/1779	1.09	8/2396 (0.3%)
1	C	0.66	0/1779	1.13	10/2396 (0.4%)
2	B	0.63	0/1607	1.12	10/2176 (0.5%)
2	D	0.65	0/1615	1.13	11/2187 (0.5%)
All	All	0.65	0/6780	1.12	39/9155 (0.4%)

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	0	3
1	C	0	4
2	B	0	1
2	D	0	1
All	All	0	9

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	PHE	CA-C-N	7.90	129.05	120.13
1	A	125	PHE	C-N-CA	7.90	129.05	120.13
2	B	233	SER	CA-C-N	7.89	127.55	119.82
2	B	233	SER	C-N-CA	7.89	127.55	119.82
2	D	233	SER	CA-C-N	7.80	127.46	119.82
2	D	233	SER	C-N-CA	7.80	127.46	119.82
1	C	164	LEU	N-CA-C	7.65	119.41	111.14
1	C	125	PHE	CA-C-N	7.58	128.69	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	PHE	C-N-CA	7.58	128.69	120.13
1	A	164	LEU	N-CA-C	7.53	119.27	111.14
2	D	170	GLN	N-CA-C	-7.17	102.27	111.02
2	B	170	GLN	N-CA-C	-7.12	102.33	111.02
1	C	291	ILE	N-CA-C	-6.99	99.61	110.09
1	A	146	SER	N-CA-C	-6.62	98.84	109.96
2	D	248	ILE	CB-CA-C	-6.44	103.61	112.04
2	D	74	ASP	N-CA-C	-6.15	103.70	112.13
2	B	121	ASP	N-CA-CB	-6.12	107.98	114.10
2	D	121	ASP	N-CA-CB	-6.05	108.05	114.10
1	C	211	LYS	N-CA-C	-6.05	104.25	111.69
1	C	146	SER	N-CA-C	-5.99	99.90	109.96
1	A	211	LYS	N-CA-C	-5.95	104.88	111.36
1	C	117	VAL	CB-CA-C	-5.87	104.35	112.04
2	B	74	ASP	N-CA-C	-5.83	104.14	112.13
2	D	212	SER	CB-CA-C	-5.82	108.21	115.89
1	A	252	ILE	CB-CA-C	-5.75	103.94	111.25
2	D	76	LEU	N-CA-C	-5.65	103.99	111.96
2	B	212	SER	CB-CA-C	-5.65	108.43	115.89
1	C	276	SER	CA-CB-OG	5.62	122.34	111.10
1	C	292	ILE	N-CA-C	5.50	120.78	109.34
2	B	76	LEU	N-CA-C	-5.48	104.24	111.96
2	B	69	SER	CA-CB-OG	5.41	121.92	111.10
2	D	85	ASP	N-CA-C	-5.40	105.40	111.28
2	B	85	ASP	N-CA-C	-5.29	105.52	111.28
1	A	252	ILE	N-CA-C	5.28	115.97	107.73
2	B	212	SER	N-CA-C	5.25	117.83	109.02
1	C	262	ASP	N-CA-C	-5.24	104.41	111.54
2	D	156	ILE	N-CA-C	5.17	115.82	108.42
2	D	213	ASN	N-CA-C	-5.07	105.45	111.69
1	A	193	THR	CB-CA-C	-5.00	102.61	111.22

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	LEU	Peptide
1	A	163	ARG	Peptide
1	A	57	MET	Peptide
2	B	230	ASN	Peptide
1	C	145	LEU	Peptide
1	C	163	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	C	291	ILE	Peptide
1	C	57	MET	Peptide
2	D	230	ASN	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	1742	1745	1741	84	1
1	C	1742	1746	1741	79	1
2	B	1584	1632	1631	73	1
2	D	1592	1638	1637	85	3
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	13	0	0	3	0
4	B	6	0	0	0	0
4	C	18	0	0	1	0
4	D	11	2	0	0	0
All	All	6711	6763	6750	288	4

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 (288) 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:54:SER:OG	2:B:149:GLU:OE1	1.89	0.91
2:D:198:MET:SD	2:D:258:ILE:CD1	2.59	0.89
2:D:198:MET:SD	2:D:258:ILE:HD13	2.20	0.81
2:B:72:LEU:HD21	2:B:106:LEU:HD12	1.63	0.80
1:A:49:GLU:O	1:A:118:ARG:NH2	2.15	0.79
2:D:72:LEU:HD21	2:D:106:LEU:HD12	1.63	0.79
1:C:49:GLU:O	1:C:118:ARG:NH2	2.17	0.76
2:B:130:MET:HE3	2:B:143:ARG:NH2	2.02	0.75
2:D:178:VAL:HG12	2:D:182:MET:CE	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:VAL:HG12	2:B:182:MET:CE	2.17	0.74
1:C:54:SER:OG	2:D:149:GLU:OE1	2.04	0.74
2:B:72:LEU:HD21	2:B:106:LEU:CD1	2.17	0.73
2:D:72:LEU:HD21	2:D:106:LEU:CD1	2.17	0.73
1:C:51:ILE:O	1:C:51:ILE:HG12	1.90	0.72
1:A:161:VAL:O	1:A:162:LYS:CG	2.38	0.71
1:A:169:LEU:HD11	1:A:184:TRP:CG	2.25	0.71
1:A:161:VAL:O	1:A:162:LYS:HG2	1.91	0.71
2:B:97:ASN:N	2:B:98:PRO:HD3	2.06	0.70
2:B:251:PHE:C	2:B:251:PHE:CD1	2.68	0.70
2:D:97:ASN:N	2:D:98:PRO:HD3	2.07	0.70
1:C:169:LEU:HD11	1:C:184:TRP:CG	2.27	0.69
1:A:51:ILE:HG12	1:A:51:ILE:O	1.93	0.69
2:D:72:LEU:HD11	2:D:106:LEU:HD12	1.74	0.69
2:D:83:ARG:HG3	2:D:84:ASN:N	2.09	0.68
2:B:72:LEU:HD11	2:B:106:LEU:HD12	1.76	0.67
2:B:192:LYS:CD	2:B:213:ASN:ND2	2.59	0.66
2:B:120:ASN:O	2:B:121:ASP:CB	2.43	0.66
2:B:183:MET:HE2	2:B:235:TYR:OH	1.96	0.66
1:C:161:VAL:O	1:C:162:LYS:CG	2.45	0.65
1:A:170:PHE:CE1	1:C:161:VAL:HG11	2.30	0.65
1:A:114:GLU:OE2	2:B:111:ARG:NH1	2.30	0.65
2:D:198:MET:SD	2:D:258:ILE:HD11	2.35	0.65
1:A:161:VAL:HG11	1:C:170:PHE:CE1	2.31	0.65
1:A:169:LEU:HD11	1:A:184:TRP:CD2	2.31	0.65
1:C:114:GLU:OE2	2:D:111:ARG:NH1	2.31	0.65
1:C:169:LEU:HD11	1:C:184:TRP:CD2	2.33	0.63
2:D:131:ILE:HG13	2:D:131:ILE:O	1.98	0.63
2:B:120:ASN:O	2:B:121:ASP:HB3	1.99	0.63
2:D:120:ASN:O	2:D:121:ASP:CB	2.46	0.62
1:C:206:TYR:CE2	1:C:210:LEU:HD11	2.33	0.62
1:C:222:LEU:HB2	1:C:232:TYR:CE1	2.34	0.62
1:C:161:VAL:O	1:C:162:LYS:HG2	1.99	0.62
2:D:212:SER:OG	2:D:213:ASN:N	2.33	0.62
1:A:101:VAL:O	1:A:102:ALA:HB3	2.00	0.62
1:A:44:LYS:HG3	1:A:107:ILE:HD12	1.81	0.62
2:D:198:MET:CE	2:D:258:ILE:HD13	2.29	0.61
2:B:72:LEU:CD2	2:B:106:LEU:HD12	2.30	0.61
1:A:170:PHE:CZ	1:C:161:VAL:HG11	2.34	0.61
2:B:183:MET:HE2	2:B:235:TYR:CZ	2.36	0.61
2:D:72:LEU:CD2	2:D:106:LEU:HD12	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:PHE:CE2	2:D:182:MET:HG3	2.36	0.61
1:C:113:TRP:O	1:C:117:VAL:HG23	2.00	0.60
2:D:183:MET:HE2	2:D:235:TYR:OH	2.01	0.60
1:C:192:ASP:OD1	1:C:192:ASP:O	2.20	0.59
2:B:212:SER:OG	2:B:213:ASN:N	2.35	0.59
2:B:142:PHE:CE2	2:B:182:MET:HG3	2.38	0.58
2:D:120:ASN:O	2:D:121:ASP:HB3	2.02	0.58
1:A:161:VAL:CG1	1:C:170:PHE:CZ	2.85	0.58
1:A:44:LYS:HG3	1:A:107:ILE:CD1	2.34	0.58
1:A:173:ASN:O	1:A:173:ASN:CG	2.47	0.57
1:C:147:LEU:HB3	2:D:151:ILE:CG2	2.35	0.57
1:A:222:LEU:HB2	1:A:232:TYR:CE1	2.39	0.57
1:C:173:ASN:CG	1:C:173:ASN:O	2.46	0.57
2:D:209:ILE:HG22	2:D:210:ARG:N	2.20	0.57
2:D:244:LYS:HB3	2:D:245:VAL:HA	1.85	0.57
2:B:192:LYS:HD2	2:B:213:ASN:ND2	2.20	0.57
2:D:262:VAL:O	2:D:262:VAL:CG1	2.53	0.56
1:A:206:TYR:CE2	1:A:210:LEU:HD11	2.40	0.56
1:C:249:GLY:O	1:C:250:ALA:HB3	2.07	0.55
1:A:249:GLY:O	1:A:250:ALA:HB3	2.06	0.55
2:B:192:LYS:HD3	2:B:213:ASN:ND2	2.21	0.55
1:C:282:TYR:CE2	2:D:232:PRO:HG3	2.42	0.55
1:A:192:ASP:OD1	1:A:192:ASP:O	2.25	0.55
1:A:288:PHE:CD1	1:A:288:PHE:O	2.60	0.55
1:A:176:LYS:HE2	4:A:2006:HOH:O	2.07	0.54
1:A:169:LEU:CD1	1:A:184:TRP:CG	2.90	0.54
1:A:170:PHE:CZ	1:C:161:VAL:CG1	2.90	0.54
2:D:142:PHE:HE2	2:D:182:MET:HG3	1.70	0.54
2:B:209:ILE:HG22	2:B:210:ARG:N	2.23	0.54
2:D:175:THR:OG1	2:D:177:ASN:CB	2.56	0.54
2:B:142:PHE:HE2	2:B:182:MET:HG3	1.73	0.54
1:C:155:VAL:HG22	1:C:172:HIS:HB2	1.89	0.54
2:D:157:ASP:C	2:D:158:LEU:HD12	2.33	0.53
2:D:175:THR:OG1	2:D:177:ASN:HB2	2.08	0.53
2:B:175:THR:OG1	2:B:177:ASN:HB2	2.09	0.53
1:C:192:ASP:OD1	1:C:197:ASN:ND2	2.41	0.53
1:C:128:ASN:HB3	4:C:2003:HOH:O	2.08	0.52
1:C:276:SER:O	1:C:288:PHE:CE1	2.62	0.52
1:C:206:TYR:CE2	1:C:210:LEU:CD1	2.93	0.52
2:B:175:THR:OG1	2:B:177:ASN:CB	2.57	0.52
1:A:123:SER:HB3	1:A:138:ARG:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ALA:O	1:A:205:CYS:N	2.43	0.51
1:C:110:PHE:CD1	1:C:110:PHE:C	2.88	0.51
1:A:187:ILE:HG22	1:A:188:THR:N	2.26	0.51
1:A:192:ASP:OD1	1:A:197:ASN:ND2	2.43	0.51
1:A:182:GLN:NE2	4:A:2008:HOH:O	2.44	0.51
1:C:169:LEU:CD1	1:C:184:TRP:CG	2.92	0.51
2:D:183:MET:HE2	2:D:235:TYR:CZ	2.46	0.51
2:D:72:LEU:CD1	2:D:106:LEU:HD12	2.39	0.51
2:B:165:LEU:HB3	2:B:169:ILE:CD1	2.41	0.51
2:B:157:ASP:C	2:B:158:LEU:HD12	2.36	0.50
1:C:246:PHE:CE1	1:C:253:ILE:HB	2.46	0.50
2:D:106:LEU:C	2:D:106:LEU:HD23	2.36	0.50
2:D:194:LEU:CD2	2:D:198:MET:CE	2.90	0.50
2:B:72:LEU:CD1	2:B:106:LEU:HD12	2.39	0.50
2:B:182:MET:O	2:B:185:VAL:HG12	2.11	0.50
1:C:188:THR:C	1:C:190:ASP:N	2.69	0.50
2:D:166:GLN:HG2	2:D:170:GLN:NE2	2.26	0.50
2:D:170:GLN:OE1	2:D:170:GLN:HA	2.11	0.50
1:A:155:VAL:HG22	1:A:172:HIS:HB2	1.93	0.50
2:D:182:MET:O	2:D:185:VAL:HG12	2.11	0.50
1:A:110:PHE:CD1	1:A:110:PHE:C	2.90	0.49
1:A:114:GLU:HG3	2:B:115:LEU:CD1	2.42	0.49
2:B:183:MET:HE3	2:B:187:GLN:HG3	1.94	0.49
2:D:83:ARG:O	2:D:87:ALA:N	2.45	0.49
2:D:119:LEU:O	2:D:120:ASN:C	2.55	0.49
2:B:221:LEU:CD2	2:B:223:VAL:HG23	2.42	0.49
1:C:156:ILE:HD12	2:D:80:LEU:CD2	2.43	0.49
1:C:188:THR:C	1:C:190:ASP:H	2.21	0.49
2:B:131:ILE:O	2:B:131:ILE:HG13	2.12	0.49
2:D:163:VAL:HG13	2:D:164:GLU:N	2.27	0.48
2:B:72:LEU:CG	2:B:106:LEU:HD12	2.43	0.48
1:C:259:ASP:OD1	1:C:259:ASP:N	2.45	0.48
2:D:156:ILE:HG22	2:D:157:ASP:N	2.28	0.48
2:B:221:LEU:CD2	2:B:223:VAL:CG2	2.92	0.48
2:B:159:ASN:C	2:B:161:PHE:H	2.22	0.48
1:C:123:SER:HB3	1:C:138:ARG:HB2	1.95	0.48
1:A:187:ILE:CD1	1:A:201:PHE:HA	2.43	0.48
2:B:253:ILE:O	2:B:257:GLY:CA	2.62	0.48
1:C:156:ILE:HD12	2:D:80:LEU:HD23	1.96	0.48
1:C:147:LEU:HB3	2:D:151:ILE:HG22	1.95	0.47
2:B:183:MET:HE3	2:B:187:GLN:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:244:LYS:CB	2:D:245:VAL:HA	2.43	0.47
2:D:166:GLN:NE2	2:D:170:GLN:HE21	2.12	0.47
1:A:169:LEU:CD1	1:A:184:TRP:CD2	2.96	0.47
1:A:252:ILE:HG13	1:A:252:ILE:O	2.13	0.47
1:C:169:LEU:CD1	1:C:184:TRP:CD2	2.98	0.47
1:A:280:SER:OG	1:A:281:ILE:N	2.47	0.47
2:B:163:VAL:HG13	2:B:164:GLU:N	2.29	0.47
2:B:253:ILE:O	2:B:257:GLY:HA2	2.15	0.47
2:D:259:GLN:O	2:D:263:ILE:HG12	2.14	0.47
2:B:106:LEU:HD23	2:B:106:LEU:C	2.40	0.47
1:A:167:TRP:HB2	1:A:193:THR:HG21	1.96	0.47
2:D:198:MET:HE1	2:D:258:ILE:HD13	1.97	0.46
1:A:135:MET:HE1	1:A:198:ILE:HD13	1.98	0.46
1:A:206:TYR:CE2	1:A:210:LEU:CD1	2.98	0.46
1:A:281:ILE:CG2	1:A:282:TYR:CE2	2.99	0.46
2:B:83:ARG:O	2:B:86:ASN:N	2.49	0.46
1:C:187:ILE:CD1	1:C:201:PHE:HA	2.45	0.46
1:C:202:ALA:O	1:C:205:CYS:N	2.48	0.46
2:B:251:PHE:CD1	2:B:251:PHE:O	2.68	0.46
1:C:171:LYS:HE3	2:D:84:ASN:CB	2.46	0.46
2:D:72:LEU:CG	2:D:106:LEU:HD12	2.45	0.46
1:A:135:MET:HE1	1:A:198:ILE:CD1	2.45	0.46
2:B:119:LEU:O	2:B:120:ASN:C	2.58	0.46
1:A:170:PHE:HZ	1:C:161:VAL:CG1	2.29	0.46
1:A:268:THR:CG2	1:A:271:GLY:HA2	2.46	0.46
2:B:135:LYS:O	2:B:136:GLY:C	2.58	0.46
1:C:135:MET:HE1	1:C:198:ILE:CD1	2.46	0.46
1:A:176:LYS:CE	4:A:2006:HOH:O	2.64	0.46
1:A:188:THR:C	1:A:190:ASP:N	2.71	0.46
2:B:170:GLN:O	2:B:174:ASP:HB2	2.15	0.46
2:D:159:ASN:C	2:D:161:PHE:H	2.23	0.46
2:D:135:LYS:O	2:D:136:GLY:C	2.58	0.46
1:A:248:LEU:HD22	1:A:289:GLN:NE2	2.31	0.46
1:C:261:ASP:OD1	1:C:261:ASP:N	2.48	0.46
2:D:130:MET:HE2	2:D:141:SER:HB3	1.98	0.46
1:A:246:PHE:CE1	1:A:253:ILE:HB	2.50	0.46
2:B:221:LEU:HD21	2:B:223:VAL:CG2	2.46	0.46
1:C:101:VAL:O	1:C:102:ALA:HB3	2.15	0.46
1:C:187:ILE:HG22	1:C:188:THR:N	2.30	0.45
2:D:209:ILE:CG2	2:D:210:ARG:N	2.78	0.45
2:D:166:GLN:CG	2:D:170:GLN:NE2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:LEU:O	2:B:169:ILE:HD12	2.16	0.45
1:A:161:VAL:HG11	1:C:170:PHE:CZ	2.52	0.45
2:B:159:ASN:O	2:B:161:PHE:N	2.50	0.45
2:B:230:ASN:C	2:B:232:PRO:HD2	2.41	0.45
2:D:159:ASN:O	2:D:161:PHE:N	2.50	0.45
1:A:259:ASP:N	1:A:259:ASP:OD1	2.49	0.45
2:D:165:LEU:HB3	2:D:169:ILE:CD1	2.47	0.45
2:D:268:THR:OG1	2:D:269:ILE:N	2.50	0.45
1:A:252:ILE:O	1:A:252:ILE:CG1	2.64	0.45
1:C:125:PHE:CE1	1:C:136:GLY:HA3	2.52	0.45
1:A:108:THR:HG23	1:A:109:ASP:N	2.32	0.44
1:C:238:ASP:O	1:C:239:ASN:C	2.59	0.44
2:D:244:LYS:HD3	2:D:245:VAL:HA	1.99	0.44
1:A:180:ILE:HG23	1:A:181:HIS:N	2.32	0.44
2:B:115:LEU:HA	2:B:118:THR:HG22	1.99	0.44
1:C:212:VAL:HG12	1:C:213:HIS:N	2.32	0.44
1:C:277:LEU:HD11	1:C:293:MET:O	2.16	0.44
2:D:159:ASN:N	2:D:159:ASN:OD1	2.51	0.44
1:C:167:TRP:HB2	1:C:193:THR:HG21	1.99	0.44
2:D:127:GLU:O	2:D:128:LYS:C	2.61	0.44
2:B:192:LYS:HD3	2:B:213:ASN:HD21	1.80	0.44
1:C:44:LYS:HG3	1:C:44:LYS:O	2.17	0.44
1:C:135:MET:HE1	1:C:198:ILE:HD13	1.99	0.44
2:D:169:ILE:O	2:D:170:GLN:C	2.60	0.44
1:A:126:PRO:HG3	2:B:111:ARG:HA	2.00	0.44
2:B:83:ARG:O	2:B:87:ALA:N	2.50	0.44
1:C:171:LYS:HE3	2:D:84:ASN:HB3	1.99	0.44
1:C:194:SER:O	1:C:197:ASN:N	2.51	0.44
2:B:259:GLN:O	2:B:263:ILE:HG12	2.17	0.44
1:A:162:LYS:O	2:D:98:PRO:HB3	2.18	0.44
1:C:118:ARG:HG2	1:C:140:GLU:OE2	2.17	0.44
2:D:115:LEU:HA	2:D:118:THR:HG22	1.98	0.44
1:A:125:PHE:CE1	1:A:136:GLY:HA3	2.53	0.43
1:C:255:ILE:HD11	1:C:264:ILE:HG12	2.00	0.43
1:A:144:GLU:HA	1:A:147:LEU:CD2	2.48	0.43
2:B:171:TYR:CD1	2:B:171:TYR:C	2.96	0.43
1:A:194:SER:O	1:A:197:ASN:N	2.52	0.43
1:A:291:ILE:HG22	1:A:292:ILE:N	2.33	0.43
1:C:108:THR:HG23	1:C:109:ASP:N	2.32	0.43
1:A:161:VAL:CG1	1:C:170:PHE:CE1	3.01	0.43
2:B:209:ILE:CG2	2:B:210:ARG:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ARG:O	2:D:86:ASN:N	2.50	0.43
1:A:114:GLU:HG3	2:B:115:LEU:HD11	2.01	0.43
1:A:178:ILE:O	1:A:178:ILE:HG22	2.19	0.43
1:A:202:ALA:O	1:A:203:ASN:C	2.61	0.43
1:A:284:ILE:O	1:A:288:PHE:HB3	2.19	0.43
1:C:144:GLU:HA	1:C:147:LEU:CD2	2.49	0.43
2:D:198:MET:SD	2:D:258:ILE:CG1	3.07	0.43
1:A:213:HIS:O	1:A:214:SER:C	2.62	0.43
1:A:261:ASP:N	1:A:261:ASP:OD1	2.51	0.43
1:A:119:LEU:O	2:B:179:ASN:CB	2.67	0.43
2:B:262:VAL:O	2:B:262:VAL:CG1	2.66	0.43
1:C:194:SER:O	1:C:195:ASP:C	2.62	0.43
2:B:238:THR:HG22	2:B:239:LEU:N	2.34	0.43
1:C:180:ILE:HG23	1:C:181:HIS:N	2.34	0.43
2:D:131:ILE:O	2:D:131:ILE:CG1	2.66	0.43
1:C:277:LEU:CD1	1:C:293:MET:O	2.66	0.43
2:D:148:ASN:HA	2:D:149:GLU:HA	1.79	0.42
2:D:198:MET:SD	2:D:258:ILE:HG12	2.59	0.42
1:A:118:ARG:HG2	1:A:140:GLU:OE2	2.19	0.42
1:C:128:ASN:O	2:D:105:SER:N	2.52	0.42
1:C:280:SER:OG	1:C:281:ILE:N	2.52	0.42
1:C:255:ILE:HD11	1:C:264:ILE:CD1	2.49	0.42
1:C:283:GLY:HA2	1:C:287:ARG:NH2	2.35	0.42
2:D:171:TYR:C	2:D:171:TYR:CD1	2.97	0.42
1:A:161:VAL:CG1	1:C:170:PHE:HZ	2.32	0.42
1:A:283:GLY:HA2	1:A:287:ARG:NH2	2.35	0.42
1:C:292:ILE:HG13	1:C:293:MET:HG3	2.01	0.42
1:A:126:PRO:HB3	2:B:114:TYR:CD2	2.55	0.42
1:A:156:ILE:O	1:A:170:PHE:HB3	2.19	0.42
2:B:198:MET:HE2	2:B:258:ILE:HG12	2.01	0.42
2:D:79:LYS:O	2:D:79:LYS:CG	2.66	0.42
1:C:281:ILE:CG2	1:C:282:TYR:CD2	3.02	0.42
1:A:161:VAL:O	1:A:162:LYS:HG3	2.17	0.42
1:A:194:SER:O	1:A:195:ASP:C	2.63	0.42
2:B:152:ARG:O	2:B:176:GLN:OE1	2.38	0.42
1:C:268:THR:CG2	1:C:271:GLY:HA2	2.50	0.42
2:D:108:ILE:O	2:D:109:GLU:C	2.63	0.41
2:B:97:ASN:N	2:B:98:PRO:CD	2.81	0.41
2:D:198:MET:CE	2:D:258:ILE:CD1	2.96	0.41
2:D:198:MET:HE1	2:D:258:ILE:CD1	2.51	0.41
2:B:159:ASN:OD1	2:B:159:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ILE:O	1:C:275:ILE:HG22	2.20	0.41
2:D:246:GLN:O	2:D:248:ILE:N	2.53	0.41
2:B:169:ILE:O	2:B:170:GLN:C	2.61	0.41
2:D:155:ALA:C	2:D:156:ILE:HG13	2.46	0.41
1:A:202:ALA:O	1:A:204:LEU:N	2.53	0.41
1:C:49:GLU:CD	2:D:74:ASP:O	2.64	0.41
1:C:117:VAL:HG13	2:D:119:LEU:HD21	2.03	0.41
1:C:244:VAL:HB	1:C:255:ILE:CG2	2.51	0.41
1:A:119:LEU:O	2:B:179:ASN:HB2	2.20	0.41
1:A:126:PRO:HB3	2:B:114:TYR:CE2	2.56	0.41
1:A:160:SER:OG	1:A:161:VAL:N	2.54	0.41
1:A:276:SER:O	1:A:288:PHE:CE1	2.74	0.41
2:B:156:ILE:HG22	2:B:157:ASP:N	2.36	0.41
1:A:135:MET:CE	1:A:198:ILE:HD13	2.51	0.41
1:A:169:LEU:HD12	1:A:184:TRP:CE2	2.56	0.41
1:C:114:GLU:HG3	2:D:115:LEU:CD1	2.51	0.41
1:A:101:VAL:O	1:A:102:ALA:CB	2.65	0.41
1:A:292:ILE:HG22	1:A:293:MET:N	2.35	0.41
2:B:249:LEU:C	2:B:249:LEU:HD23	2.45	0.41
2:D:183:MET:HE3	2:D:187:GLN:CG	2.51	0.41
2:D:194:LEU:HD23	2:D:198:MET:CE	2.50	0.41
2:D:170:GLN:O	2:D:174:ASP:HB2	2.21	0.41
2:B:171:TYR:O	2:B:172:ALA:C	2.64	0.40
1:C:244:VAL:HB	1:C:255:ILE:HG22	2.03	0.40
2:D:194:LEU:HD23	2:D:198:MET:HE3	2.03	0.40
2:B:242:THR:HG23	2:B:243:ASN:O	2.22	0.40
2:B:246:GLN:O	2:B:247:LYS:C	2.63	0.40
1:C:252:ILE:O	1:C:252:ILE:HG13	2.19	0.40
2:D:155:ALA:C	2:D:156:ILE:CG1	2.94	0.40
2:D:183:MET:HE3	2:D:187:GLN:HG3	2.03	0.40
1:A:117:VAL:HG13	2:B:119:LEU:HD21	2.03	0.40
1:A:177:TYR:CZ	1:A:212:VAL:HG11	2.56	0.40
1:C:177:TYR:CZ	1:C:212:VAL:HG11	2.57	0.40

All (4) 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)
2:D:173:GLU:OE2	2:D:176:GLN:NE2[11_655]	2.03	0.17
1:A:235:LEU:O	2:D:256:TYR:OH[4_665]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:TYR:OH	1:C:235:LEU:O[7_554]	2.08	0.12
2:D:173:GLU:OE2	2:D:176:GLN:HE21[11_655]	1.59	0.01

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	207/296 (70%)	185 (89%)	21 (10%)	1 (0%)	24	56
1	C	207/296 (70%)	184 (89%)	22 (11%)	1 (0%)	24	56
2	B	193/270 (72%)	173 (90%)	20 (10%)	0	100	100
2	D	194/270 (72%)	173 (89%)	21 (11%)	0	100	100
All	All	801/1132 (71%)	715 (89%)	84 (10%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ILE
1	C	51	ILE

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	197/269 (73%)	179 (91%)	18 (9%)	9	33
1	C	197/269 (73%)	179 (91%)	18 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	183/254 (72%)	174 (95%)	9 (5%)	22	48
2	D	184/254 (72%)	176 (96%)	8 (4%)	26	50
All	All	761/1046 (73%)	708 (93%)	53 (7%)	14	41

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	114	GLU
1	A	127	VAL
1	A	155	VAL
1	A	164	LEU
1	A	169	LEU
1	A	178	ILE
1	A	180	ILE
1	A	190	ASP
1	A	194	SER
1	A	212	VAL
1	A	213	HIS
1	A	244	VAL
1	A	252	ILE
1	A	253	ILE
1	A	259	ASP
1	A	261	ASP
1	A	278	LEU
2	B	99	LEU
2	B	128	LYS
2	B	152	ARG
2	B	153	SER
2	B	159	ASN
2	B	237	GLU
2	B	251	PHE
2	B	262	VAL
2	B	269	ILE
1	C	51	ILE
1	C	114	GLU
1	C	127	VAL
1	C	155	VAL
1	C	164	LEU
1	C	166	ILE
1	C	169	LEU

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Mol	Chain	Res	Type
1	C	178	ILE
1	C	180	ILE
1	C	190	ASP
1	C	212	VAL
1	C	237	ILE
1	C	244	VAL
1	C	252	ILE
1	C	253	ILE
1	C	259	ASP
1	C	261	ASP
1	C	278	LEU
2	D	99	LEU
2	D	128	LYS
2	D	152	ARG
2	D	153	SER
2	D	159	ASN
2	D	170	GLN
2	D	237	GLU
2	D	262	VAL

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	50	ASN
1	A	172	HIS
1	A	289	GLN
2	B	84	ASN
2	B	213	ASN
1	C	50	ASN
1	C	172	HIS
1	C	231	GLN
1	C	243	ASN
2	D	166	GLN

5.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	211/296 (71%)	0.11	4 (1%) 66 42	83, 163, 267, 322	0
1	C	211/296 (71%)	0.16	0 100 100	85, 162, 256, 327	0
2	B	197/270 (72%)	0.06	3 (1%) 72 46	99, 169, 296, 389	0
2	D	198/270 (73%)	0.15	4 (2%) 65 41	95, 164, 297, 401	0
All	All	817/1132 (72%)	0.12	11 (1%) 75 50	83, 164, 283, 401	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	LYS	2.5
1	A	211	LYS	2.3
2	B	239	LEU	2.2
2	D	100	PRO	2.2
2	B	85	ASP	2.1
2	D	99	LEU	2.1
2	D	108	ILE	2.1
2	B	248	ILE	2.1
1	A	145	LEU	2.1
1	A	120	ILE	2.0
2	D	163	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	1294	1/1	0.87	0.20	199,199,199,199	0
3	CA	A	1294	1/1	0.91	0.27	184,184,184,184	0
3	CA	D	1270	1/1	0.97	0.10	217,217,217,217	0

6.5 Other polymers [i](#)

There are no such residues in this entry.