Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 08:42 am GMT

PDB ID	:	4AKR
Title	:	Crystal Structure of the cytoplasmic actin capping protein Cap32_34 from Dictyostelium discoideum
Authors	:	Eckert, C.; Goretzki, A.; Faberova, M.; Kollmar, M.
Deposited on	:	2012-02-28
Resolution	:	2.20 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:

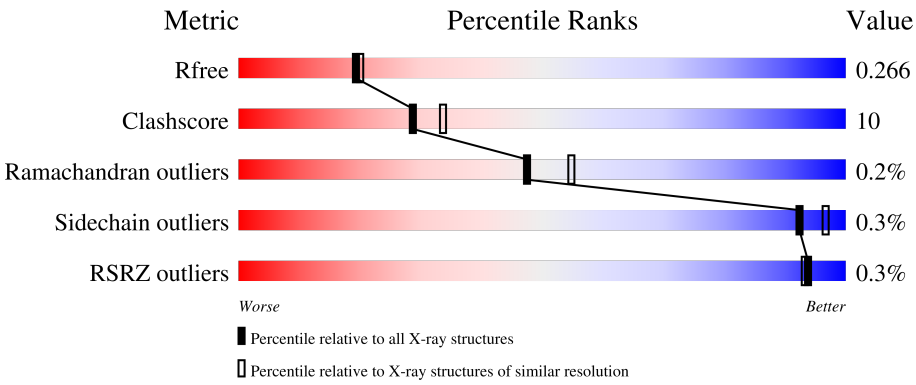
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	281	% 78% 18% •
1	C	281	80% 16% •
2	B	290	64% 20% • 16%
2	D	290	62% 22% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8399 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 F-ACTIN-CAPPING PROTEIN SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	2090	1303	358	421	8	0	0	0
1	C	271	2107	1313	362	424	8	0	0	0

- Molecule 2 is a protein called F-ACTIN-CAPPING PROTEIN SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	245	1943	1219	319	393	12	0	0	0
2	D	243	1929	1212	316	389	12	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	expression tag	UNP P13021
B	-16	ASP	-	expression tag	UNP P13021
B	-15	HIS	-	expression tag	UNP P13021
B	-14	HIS	-	expression tag	UNP P13021
B	-13	HIS	-	expression tag	UNP P13021
B	-12	HIS	-	expression tag	UNP P13021
B	-11	HIS	-	expression tag	UNP P13021
B	-10	HIS	-	expression tag	UNP P13021
B	-9	HIS	-	expression tag	UNP P13021
B	-8	HIS	-	expression tag	UNP P13021
B	-7	THR	-	expression tag	UNP P13021
B	-6	SER	-	expression tag	UNP P13021
B	-5	GLU	-	expression tag	UNP P13021
B	-4	THR	-	expression tag	UNP P13021
B	-3	GLY	-	expression tag	UNP P13021
B	-2	TYR	-	expression tag	UNP P13021

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	VAL	-	expression tag	UNP P13021
B	0	GLN	-	expression tag	UNP P13021
B	1	GLY	-	expression tag	UNP P13021
D	-17	MET	-	expression tag	UNP P13021
D	-16	ASP	-	expression tag	UNP P13021
D	-15	HIS	-	expression tag	UNP P13021
D	-14	HIS	-	expression tag	UNP P13021
D	-13	HIS	-	expression tag	UNP P13021
D	-12	HIS	-	expression tag	UNP P13021
D	-11	HIS	-	expression tag	UNP P13021
D	-10	HIS	-	expression tag	UNP P13021
D	-9	HIS	-	expression tag	UNP P13021
D	-8	HIS	-	expression tag	UNP P13021
D	-7	THR	-	expression tag	UNP P13021
D	-6	SER	-	expression tag	UNP P13021
D	-5	GLU	-	expression tag	UNP P13021
D	-4	THR	-	expression tag	UNP P13021
D	-3	GLY	-	expression tag	UNP P13021
D	-2	TYR	-	expression tag	UNP P13021
D	-1	VAL	-	expression tag	UNP P13021
D	0	GLN	-	expression tag	UNP P13021
D	1	GLY	-	expression tag	UNP P13021

- Molecule 3 is water.

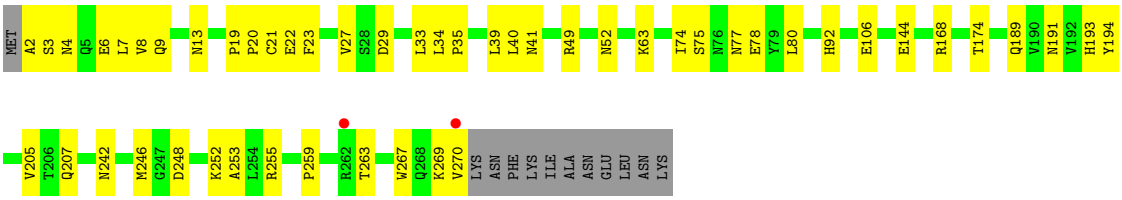
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	94	94	94	0	0
			Total	O		
3	B	55	55	55	0	0
			Total	O		
3	C	101	101	101	0	0
			Total	O		
3	D	80	80	80	0	0

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.

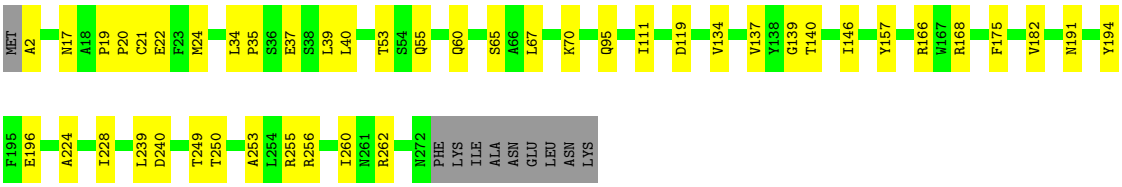
• Molecule 1: F-ACTIN-CAPPING PROTEIN SUBUNIT ALPHA

Chain A:



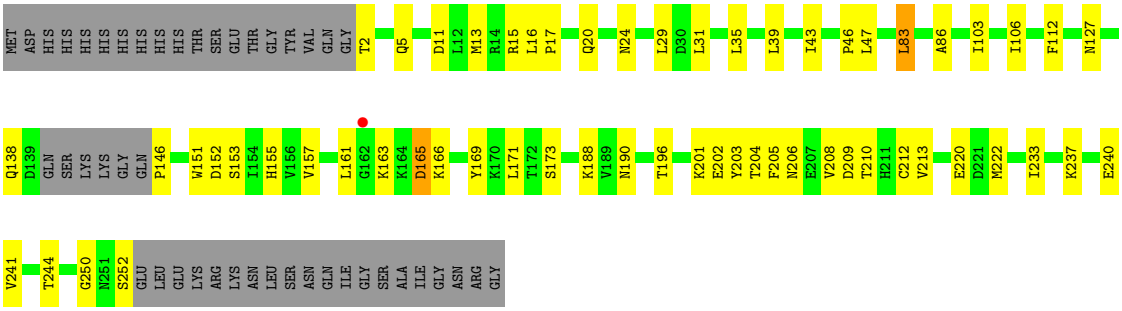
• Molecule 1: F-ACTIN-CAPPING PROTEIN SUBUNIT ALPHA

Chain C:



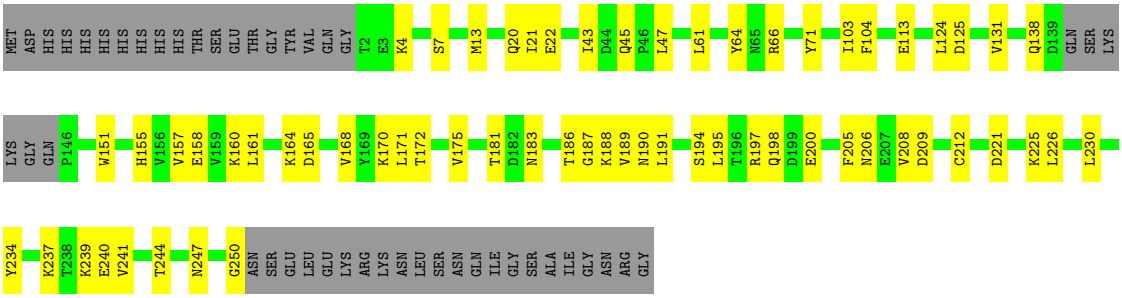
• Molecule 2: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA

Chain B:



• Molecule 2: F-ACTIN-CAPPING PROTEIN SUBUNIT BETA

Chain D:


MET ASP HIS HIS HIS HIS HIS HIS HIS THR SER GLU THR GLY TYR VAL GLN GLY T2 E3 K4 S7 M13 Q20 I21 E22 I43 D44 Q45 P46 L47 L61 Y64 N65 R66 Y71 I103 F104 E113 L124 D125 V131 Q138 D139 GLN SER LYS
LYS GLY GLN P146 W151 H155 V156 V157 E158 V159 K160 L161 K164 D165 V168 Y169 K170 L171 T172 V175 T181 D182 N183 T186 G187 K188 V189 N190 L191 S194 L195 T196 R197 Q198 D199 E200 F205 N206 E207 V208 D209 C212 D221 K225 L226 L230
Y234 K237 T238 K239 E240 V241 T244 N247 G250 ASN SER GLU LEU GLU LYS ARG LYS ASN LEU SER ASN GLN ILE GLY SER ALA ILE GLY ASN ARG GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	124.46Å 124.46Å 77.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 65.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.20) 99.8 (65.79-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.226 , 0.265 0.226 , 0.266	Depositor DCC
R_{free} test set	2991 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8399	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0730e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.34	0/2128	0.58	0/2889
1	C	0.36	0/2145	0.58	0/2911
2	B	0.35	0/1975	0.59	0/2674
2	D	0.35	0/1961	0.59	0/2655
All	All	0.35	0/8209	0.59	0/11129

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	2090	0	2037	39	0
1	C	2107	0	2056	33	0
2	B	1943	0	1912	48	0
2	D	1929	0	1901	49	0
3	A	94	0	0	4	0
3	B	55	0	0	3	0
3	C	101	0	0	1	0
3	D	80	0	0	1	0
All	All	8399	0	7906	155	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 10.

All (155) 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)
2:D:21:ILE:HD12	2:D:22:GLU:N	1.85	0.91
2:D:103:ILE:HD13	2:D:212:CYS:HB3	1.56	0.87
2:B:157:VAL:HG22	2:B:171:LEU:HD13	1.55	0.87
1:A:22:GLU:OE2	1:A:193:HIS:HD2	1.60	0.85
1:C:60:GLN:HE22	1:C:65:SER:HB3	1.48	0.78
2:D:13:MET:HG3	2:D:43:ILE:HD13	1.68	0.76
2:B:13:MET:HG3	2:B:43:ILE:HD13	1.68	0.75
2:D:21:ILE:HD12	2:D:22:GLU:H	1.49	0.75
1:C:168:ARG:HH21	1:C:191:ASN:HD21	1.40	0.70
2:B:13:MET:HE2	2:B:16:LEU:HD12	1.75	0.69
2:D:197:ARG:NH2	2:D:225:LYS:HD2	2.08	0.68
1:A:269:LYS:O	1:A:270:VAL:HB	1.93	0.68
2:D:21:ILE:HD13	2:D:45:GLN:HB2	1.75	0.67
1:A:168:ARG:HH21	1:A:191:ASN:HD21	1.44	0.66
2:B:240:GLU:O	2:B:244:THR:HG23	1.96	0.66
1:C:253:ALA:HB1	2:D:138:GLN:HG2	1.78	0.64
2:D:240:GLU:O	2:D:244:THR:HG23	1.97	0.64
1:C:260:ILE:HD11	2:D:113:GLU:OE2	1.98	0.63
2:B:220:GLU:HB3	3:B:2051:HOH:O	1.99	0.63
1:A:20:PRO:HD3	3:A:2008:HOH:O	1.98	0.63
1:C:55:GLN:NE2	1:C:166:ARG:HE	1.97	0.62
2:B:206:ASN:HB2	2:B:208:VAL:HG12	1.80	0.62
2:B:173:SER:OG	2:B:222:MET:HG2	1.99	0.62
1:A:270:VAL:HG13	2:B:106:ILE:HG21	1.82	0.62
2:D:195:LEU:HD12	2:D:230:LEU:HD23	1.82	0.62
2:B:155:HIS:HB3	2:B:171:LEU:HD11	1.81	0.61
2:B:13:MET:CE	2:B:16:LEU:HD12	2.30	0.61
2:D:61:LEU:HD22	2:D:71:TYR:CG	2.36	0.61
1:C:168:ARG:HH21	1:C:191:ASN:ND2	1.99	0.60
1:C:262:ARG:HG2	1:C:262:ARG:HH11	1.65	0.60
2:D:157:VAL:HG12	2:D:171:LEU:HD13	1.84	0.60
2:B:127:ASN:ND2	2:B:161:LEU:H	2.00	0.59
1:C:17:ASN:ND2	2:D:20:GLN:HE22	2.00	0.59
1:A:52:ASN:HD22	1:A:92:HIS:HD2	1.50	0.59
1:C:240:ASP:OD1	2:D:239:LYS:HE3	2.02	0.59
2:D:205:PHE:HA	2:D:209:ASP:O	2.02	0.58
1:A:255:ARG:HB2	2:B:112:PHE:CE1	2.39	0.58
2:D:160:LYS:HB2	2:D:168:VAL:CG1	2.34	0.57
1:A:29:ASP:O	1:A:33:LEU:HG	2.05	0.56
1:A:35:PRO:HG2	1:A:39:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASP:HA	1:A:252:LYS:HE2	1.87	0.56
1:A:7:LEU:HD22	2:B:31:LEU:HD23	1.86	0.56
1:A:189:GLN:HG2	1:A:205:VAL:HG22	1.86	0.56
2:D:103:ILE:CD1	2:D:212:CYS:HB3	2.33	0.55
2:B:29:LEU:HD23	2:B:39:LEU:HD12	1.87	0.55
1:C:255:ARG:HD3	1:C:256:ARG:O	2.06	0.55
1:A:267:TRP:HB3	2:B:213:VAL:HG13	1.89	0.55
2:D:206:ASN:OD1	2:D:208:VAL:HG12	2.07	0.54
2:B:165:ASP:O	2:B:204:THR:HA	2.07	0.54
1:C:35:PRO:HG2	1:C:39:LEU:HD11	1.91	0.53
1:C:55:GLN:HE21	1:C:166:ARG:HE	1.56	0.52
1:C:19:PRO:HG2	1:C:22:GLU:HB2	1.92	0.52
1:A:77:ASN:ND2	3:A:2034:HOH:O	2.43	0.52
1:A:49:ARG:HA	1:A:92:HIS:CD2	2.44	0.52
2:B:17:PRO:HB2	2:B:20:GLN:HG3	1.91	0.52
1:C:60:GLN:NE2	1:C:65:SER:HB3	2.23	0.52
1:C:37:GLU:N	1:C:37:GLU:CD	2.63	0.52
1:A:3:SER:OG	1:A:6:GLU:HG3	2.09	0.51
1:A:168:ARG:HH21	1:A:191:ASN:ND2	2.07	0.51
1:C:253:ALA:CB	2:D:138:GLN:HG2	2.40	0.51
2:D:64:TYR:CD2	2:D:131:VAL:HG11	2.44	0.51
1:A:74:ILE:HD13	1:A:106:GLU:HG2	1.93	0.51
1:A:52:ASN:HD22	1:A:92:HIS:CD2	2.29	0.51
1:C:262:ARG:HG2	1:C:262:ARG:NH1	2.27	0.50
2:B:83:LEU:HD13	2:B:86:ALA:HB2	1.93	0.50
1:C:224:ALA:O	1:C:228:ILE:HG13	2.12	0.50
2:B:146:PRO:HA	3:B:2043:HOH:O	2.12	0.50
2:B:208:VAL:HG13	2:B:209:ASP:N	2.27	0.50
2:B:173:SER:O	2:B:196:THR:HG23	2.12	0.49
1:C:34:LEU:HD11	1:C:40:LEU:CD1	2.42	0.49
2:B:47:LEU:HD12	3:B:2042:HOH:O	2.12	0.49
1:C:175:PHE:HB3	1:C:182:VAL:HA	1.94	0.49
2:B:46:PRO:HA	2:B:152:ASP:OD2	2.13	0.49
2:D:186:THR:HG23	2:D:187:GLY:O	2.12	0.49
1:C:53:THR:HB	1:C:70:LYS:HG3	1.95	0.49
1:C:67:LEU:HD21	1:C:134:VAL:HB	1.94	0.49
2:D:103:ILE:HG13	2:D:104:PHE:N	2.27	0.49
2:B:169:TYR:HE1	2:B:203:TYR:HB2	1.79	0.48
2:B:210:THR:OG1	2:B:213:VAL:HG23	2.13	0.48
2:D:188:LYS:HE3	2:D:190:ASN:HD21	1.78	0.48
2:B:169:TYR:CE1	2:B:203:TYR:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ALA:N	1:A:6:GLU:OE1	2.46	0.48
2:D:237:LYS:O	2:D:241:VAL:HG23	2.14	0.48
2:B:11:ASP:O	2:B:15:ARG:HG3	2.13	0.47
1:A:194:TYR:CE1	2:B:233:ILE:HD13	2.48	0.47
2:D:181:THR:HG22	2:D:189:VAL:HB	1.97	0.47
1:A:19:PRO:HG2	1:A:22:GLU:HB2	1.96	0.47
1:A:144:GLU:HG3	1:A:174:THR:HG21	1.96	0.47
1:A:269:LYS:O	1:A:270:VAL:CB	2.62	0.47
1:A:34:LEU:HD11	1:A:40:LEU:HD22	1.95	0.47
2:B:35:LEU:O	2:B:39:LEU:HG	2.14	0.47
2:D:160:LYS:HB2	2:D:168:VAL:HG13	1.96	0.47
2:D:183:ASN:OD1	2:D:186:THR:HG22	2.15	0.47
1:A:74:ILE:HD11	1:A:80:LEU:HB2	1.96	0.47
1:C:111:ILE:HG21	1:C:146:ILE:HD12	1.96	0.46
2:D:170:LYS:NZ	2:D:198:GLN:NE2	2.63	0.46
1:C:2:ALA:N	3:C:2001:HOH:O	2.49	0.46
2:D:247:ASN:ND2	2:D:250:GLY:H	2.14	0.45
2:D:175:VAL:O	2:D:194:SER:HA	2.16	0.45
2:D:155:HIS:HB3	2:D:171:LEU:HD11	1.99	0.45
2:B:2:THR:HG21	2:B:5:GLN:HG3	1.99	0.45
2:D:13:MET:HG3	2:D:43:ILE:CD1	2.44	0.45
2:B:165:ASP:O	2:B:204:THR:HG23	2.17	0.44
1:A:75:SER:HB3	1:A:78:GLU:HB2	1.98	0.44
2:B:237:LYS:O	2:B:241:VAL:HG23	2.17	0.44
2:B:250:GLY:O	2:B:252:SER:N	2.48	0.44
1:A:63:LYS:HD3	3:A:2028:HOH:O	2.17	0.44
1:C:139:GLY:O	1:C:140:THR:HG23	2.17	0.44
1:A:22:GLU:OE2	1:A:193:HIS:CD2	2.52	0.44
1:A:20:PRO:O	1:A:21:CYS:HB2	2.18	0.44
2:B:188:LYS:NZ	2:B:190:ASN:HD21	2.16	0.44
2:D:170:LYS:HD3	2:D:200:GLU:OE1	2.18	0.44
1:A:242:ASN:ND2	1:A:246:MET:CE	2.81	0.43
2:D:47:LEU:HD12	3:D:2058:HOH:O	2.18	0.43
2:B:103:ILE:CD1	2:B:212:CYS:HB3	2.48	0.43
1:C:194:TYR:OH	1:C:196:GLU:OE1	2.36	0.43
2:D:161:LEU:HD22	2:D:205:PHE:CZ	2.53	0.43
2:B:205:PHE:HA	2:B:209:ASP:O	2.19	0.43
1:C:20:PRO:O	1:C:21:CYS:HB2	2.19	0.43
1:A:4:ASN:O	1:A:8:VAL:HG23	2.19	0.43
1:A:9:GLN:HE21	1:A:13:ASN:ND2	2.16	0.43
1:C:249:THR:HG22	1:C:250:THR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLU:CD	1:C:37:GLU:H	2.22	0.43
1:A:259:PRO:HG3	1:A:263:THR:O	2.19	0.43
1:A:270:VAL:CG1	2:B:106:ILE:HG21	2.48	0.43
2:D:124:LEU:O	2:D:125:ASP:HB2	2.19	0.43
2:B:20:GLN:HB2	2:B:24:ASN:ND2	2.34	0.42
2:D:164:LYS:HB3	2:D:165:ASP:H	1.57	0.42
2:D:151:TRP:C	2:D:151:TRP:CD1	2.93	0.42
2:D:171:LEU:HD12	2:D:172:THR:N	2.34	0.42
2:B:103:ILE:HD13	2:B:212:CYS:HB3	2.01	0.42
2:D:158:GLU:HB2	2:D:170:LYS:HB3	2.02	0.42
2:D:191:LEU:HG	2:D:234:TYR:CD2	2.55	0.42
1:C:119:ASP:HA	1:C:137:VAL:HG21	2.01	0.42
2:D:221:ASP:OD2	2:D:225:LYS:NZ	2.52	0.42
2:B:157:VAL:HG22	2:B:171:LEU:CD1	2.39	0.42
1:C:21:CYS:HB3	1:C:157:TYR:HB2	2.02	0.42
1:A:267:TRP:CB	2:B:213:VAL:HG13	2.50	0.41
2:D:175:VAL:HG23	2:D:226:LEU:HD13	2.01	0.41
1:A:23:PHE:O	1:A:27:VAL:HG23	2.20	0.41
2:D:206:ASN:OD1	2:D:208:VAL:CG1	2.68	0.41
2:B:127:ASN:HD21	2:B:161:LEU:H	1.65	0.41
2:B:166:LYS:HE3	2:B:202:GLU:OE1	2.19	0.41
2:B:155:HIS:HD2	2:B:173:SER:OG	2.04	0.41
1:A:253:ALA:CB	2:B:138:GLN:HG2	2.50	0.41
2:B:151:TRP:NE1	2:B:153:SER:OG	2.40	0.41
2:D:66:ARG:HB2	2:D:71:TYR:CE1	2.55	0.41
1:C:24:MET:CE	1:C:95:GLN:OE1	2.69	0.40
1:A:20:PRO:HB3	3:A:2008:HOH:O	2.21	0.40
2:B:83:LEU:CD1	2:B:86:ALA:HB2	2.51	0.40
2:B:201:LYS:HB2	2:B:201:LYS:HE3	1.82	0.40
2:D:4:LYS:O	2:D:7:SER:HB3	2.22	0.40
1:C:239:LEU:HD23	2:D:186:THR:OG1	2.22	0.40
2:D:175:VAL:HG11	2:D:230:LEU:HD11	2.04	0.40
2:D:226:LEU:HD23	2:D:226:LEU:HA	1.84	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	267/281 (95%)	253 (95%)	14 (5%)	0	100	100
1	C	269/281 (96%)	258 (96%)	11 (4%)	0	100	100
2	B	241/290 (83%)	230 (95%)	9 (4%)	2 (1%)	19	19
2	D	239/290 (82%)	228 (95%)	11 (5%)	0	100	100
All	All	1016/1142 (89%)	969 (95%)	45 (4%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	163	LYS
2	B	165	ASP

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	232/243 (96%)	230 (99%)	2 (1%)	78	88
1	C	234/243 (96%)	234 (100%)	0	100	100
2	B	223/261 (85%)	222 (100%)	1 (0%)	91	96
2	D	221/261 (85%)	221 (100%)	0	100	100
All	All	910/1008 (90%)	907 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	207	GLN
2	B	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	84	ASN
1	A	86	GLN
1	A	92	HIS
1	A	95	GLN
1	A	113	GLN
1	A	160	ASN
1	A	181	ASN
1	A	185	ASN
1	A	189	GLN
1	A	191	ASN
1	A	193	HIS
1	A	201	GLN
1	A	207	GLN
1	A	209	GLN
1	A	241	ASN
1	A	242	ASN
2	B	99	GLN
2	B	109	ASN
2	B	127	ASN
2	B	138	GLN
2	B	155	HIS
2	B	190	ASN
1	C	17	ASN
1	C	55	GLN
1	C	60	GLN
1	C	77	ASN
1	C	113	GLN
1	C	132	ASN
1	C	185	ASN
1	C	191	ASN
1	C	203	ASN
1	C	223	ASN
1	C	241	ASN
2	D	190	ASN
2	D	198	GLN

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Mol	Chain	Res	Type
2	D	247	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no 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	269/281 (95%)	-0.39	2 (0%) 87 86	10, 23, 43, 60	0
1	C	271/281 (96%)	-0.48	0 100 100	10, 22, 33, 45	0
2	B	245/290 (84%)	-0.23	1 (0%) 92 91	13, 26, 47, 59	0
2	D	243/290 (83%)	-0.39	0 100 100	10, 21, 41, 56	0
All	All	1028/1142 (90%)	-0.38	3 (0%) 94 93	10, 23, 43, 60	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	162	GLY	2.6
1	A	270	VAL	2.5
1	A	262	ARG	2.4

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.