

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2WPV
Title	:	Crystal structure of S. cerevisiae Get4-Get5 complex
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		CD.; Wang, C.
Deposited on	:	2009-08-11
Resolution	:	1.99 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 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	:	2.11
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)	:	2.11

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 1.99 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	$8085\ (2.00-2.00)$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	А	312	% • 75%	13%	• 10%
1	С	312	3% 71%	19%	• 10%
1	Е	312	^{2%} 78%	12%	10%
1	G	312	^{2%} 74%	14%	• 10%
2	В	59	3% 66% 1	15%	19%
2	D	59	3% 73%	7% •	19%



Mol	Chain	Length	Quality of chain				
2	F	59	2% 71%	8%	20%		
2	Н	59	3% 64%	17%	19%		



$2 \mathrm{WPV}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12001 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	1 1	201	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	281	2334	1521	369	439	5	0	0	0	
1	1 C	C 282	Total	С	Ν	Ο	\mathbf{S}	0	0	0
			2318	1512	366	435	5	0	0	0
1	Б	200	Total	С	Ν	Ο	S	0	0	0
	280	2303	1502	360	436	5	0	0	0	
1 G	281	Total	С	Ν	Ο	S	0	0	0	
	281	2329	1519	367	438	5	0	0	0	

• Molecule 1 is a protein called UPF0363 PROTEIN YOR164C.

• Molecule 2 is a protein called UBIQUITIN-LIKE PROTEIN MDY2.

Mol	Chain	Residues		Aton	ns		ZeroOcc	AltConf	Trace
2 B	48	Total	С	Ν	Ο	0	0	0	
	40	374	249	58	67	0	0	0	
9	2 D	19	Total	С	Ν	Ο	0	0	0
	40	382	254	59	69	0	0	0	
0	9 F	E 47	Total	С	Ν	Ο	0	0	0
	41	373	249	57	67	0	0	0	
2 H	48	Total	С	Ν	Ο	0	0	0	
	48	382	254	59	69	0	0		

• Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Hg 1 1	0	0
3	А	1	Total Hg 1 1	0	0
3	С	1	Total Hg 1 1	0	0
3	Е	1	Total Hg 1 1	0	0



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	254	Total O 254 254	0	0
4	В	44	$\begin{array}{cc} \text{Total} & \text{O} \\ 44 & 44 \end{array}$	0	0
4	С	237	Total O 237 237	0	0
4	D	55	Total O 55 55	0	0
4	Е	253	Total O 253 253	0	0
4	F	56	Total O 56 56	0	0
4	G	265	Total O 265 265	0	0
4	Н	38	Total O 38 38	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: UPF0363 PROTEIN YOR164C



MET VAL PRO GLU GLU SER ASN ASN ALA GLN GLN PHE LEU GLN ASP MET MET NET CLY GLY GLY GLY CLY SER CLY • Molecule 2: UBIQUITIN-LIKE PROTEIN MDY2 Chain B: 66% 15% 19% ASN ARG ALA LYS LYS MET THR THR SER ALA SER SER <u>25225</u> • Molecule 2: UBIQUITIN-LIKE PROTEIN MDY2 Chain D: 73% 19% 7% MET SER THR SER ALA SER ALA ALA LYS LYS • Molecule 2: UBIQUITIN-LIKE PROTEIN MDY2 Chain F: 71% 8% 20% MET SER THR SER ALA SER GLN ASN ARG ALA LYS LYS • Molecule 2: UBIQUITIN-LIKE PROTEIN MDY2 Chain H: 64% 17% 19% MET SER SER SER SER ARG ALA LYS LYS SI



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	48.27Å 118.77Å 168.38Å	Depositor
a, b, c, α , β , γ	90.00° 95.17° 90.00°	Depositor
$\mathbf{B}_{\mathrm{esolution}}(\mathbf{\hat{A}})$	25.59 - 1.99	Depositor
Resolution (A)	25.59 - 1.99	EDS
% Data completeness	80.0 (25.59-1.99)	Depositor
(in resolution range $)$	97.5(25.59-1.99)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.65 (at 1.99 \text{\AA})$	Xtriage
Refinement program	CNS 1.2	Depositor
R R.	0.175 , 0.206	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.190 , 0.220	DCC
R_{free} test set	11529 reflections (4.81%)	wwPDB-VP
Wilson B-factor $(Å^2)$	18.4	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 53.3	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12001	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.35% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Chain	Bond	lengths	Bond angles		
10101	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.34	0/2390	0.54	1/3226~(0.0%)	
1	С	0.33	0/2375	0.49	0/3213	
1	Е	0.34	0/2360	0.49	0/3193	
1	G	0.33	0/2386	0.50	0/3224	
2	В	0.32	0/385	0.58	0/526	
2	D	0.32	0/393	0.60	0/535	
2	F	0.33	0/384	0.58	0/523	
2	Н	0.31	0/393	0.58	0/535	
All	All	0.33	0/11066	0.52	1/14975~(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	A	181	ASP	CB-CG-OD1	8.12	125.61	118.30

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	А	2334	0	2275	36	0
1	С	2318	0	2231	57	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Е	2303	0	2206	27	0
1	G	2329	0	2256	37	0
2	В	374	0	385	10	0
2	D	382	0	400	10	0
2	F	373	0	392	7	0
2	Н	382	0	400	8	0
3	А	1	0	0	0	0
3	С	1	0	0	0	0
3	Е	1	0	0	0	0
3	G	1	0	0	0	0
4	А	254	0	0	6	0
4	В	44	0	0	2	0
4	С	237	0	0	3	0
4	D	55	0	0	0	0
4	Е	253	0	0	3	0
4	F	56	0	0	0	0
4	G	265	0	0	4	0
4	Н	38	0	0	1	0
All	All	12001	0	10545	166	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 8.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:258:LYS:HD3	2:F:26:LYS:HD3	1.50	0.91
1:E:113:LYS:HE2	1:E:152:GLU:HG3	1.57	0.87
1:C:193:ARG:NH2	2:D:46:PRO:O	2.08	0.87
1:C:205:SER:O	1:C:209:GLU:HG2	1.80	0.81
1:C:113:LYS:HE2	1:C:152:GLU:HG2	1.62	0.80
2:D:24:GLU:CD	2:D:24:GLU:H	1.91	0.72
1:G:113:LYS:HE2	1:G:152:GLU:HG2	1.70	0.71
1:A:260:LYS:HG2	1:A:291:ILE:HD11	1.73	0.70
1:C:116:ILE:HD12	1:C:140:ILE:HD12	1.71	0.70
1:A:290:ASN:HB2	4:A:2253:HOH:O	1.96	0.66
1:G:253:ILE:N	1:G:253:ILE:HD12	2.12	0.64
2:H:53:LYS:O	2:H:54:GLN:HB2	1.97	0.64
1:E:175:TRP:O	1:E:178:GLN:HB2	1.98	0.63
2:H:11:GLU:O	2:H:15:LYS:HG2	1.97	0.63
1:A:175:TRP:CH2	2:B:48:LEU:HD12	2.33	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:15:LYS:O	1:C:19:ARG:HG2	2.00	0.62
1:A:177:CYS:HB3	4:A:2193:HOH:O	2.00	0.61
1:G:193:ARG:NH2	2:H:46:PRO:O	2.34	0.60
1:E:278:LYS:HD2	4:E:2243:HOH:O	2.01	0.59
1:G:41:ASN:O	1:G:45:ARG:HG3	2.01	0.59
4:A:2150:HOH:O	2:B:36:LYS:HD3	2.02	0.59
1:G:61:LEU:HD22	1:G:65:LYS:HE2	1.85	0.58
1:A:175:TRP:O	1:A:178:GLN:HB2	2.04	0.58
1:G:286:GLN:OE1	1:G:292:VAL:HA	2.03	0.58
1:C:291:ILE:HG22	1:C:292:VAL:N	2.18	0.58
2:F:35:LEU:O	2:F:35:LEU:HD23	2.04	0.57
1:G:35:THR:O	1:G:39:ILE:HG12	2.05	0.57
1:E:89:LYS:NZ	4:E:2077:HOH:O	2.37	0.56
1:A:283:PHE:CZ	2:B:42:GLY:HA2	2.41	0.56
1:E:283:PHE:CZ	2:F:42:GLY:HA2	2.41	0.56
1:E:171:LEU:HD23	1:E:171:LEU:C	2.27	0.56
1:G:182:ILE:HG23	1:G:182:ILE:O	2.06	0.55
1:C:102:ILE:HD11	1:C:119:MET:SD	2.45	0.55
1:G:128:GLU:HG3	2:H:36:LYS:HB2	1.87	0.55
1:E:144:LEU:HD13	1:E:152:GLU:HB3	1.88	0.55
1:E:50:GLU:HG2	1:E:51:HIS:N	2.21	0.55
1:C:165:MET:HE3	1:C:169:VAL:HG23	1.89	0.55
1:G:171:LEU:C	1:G:171:LEU:HD23	2.27	0.55
1:C:191:PHE:CE1	1:C:215:LEU:HD11	2.42	0.54
1:A:175:TRP:CZ3	2:B:48:LEU:HD12	2.43	0.54
1:C:171:LEU:C	1:C:171:LEU:HD23	2.28	0.54
1:G:253:ILE:H	1:G:253:ILE:HD12	1.72	0.54
1:A:171:LEU:C	1:A:171:LEU:HD23	2.29	0.54
1:A:283:PHE:O	1:A:286:GLN:HG2	2.07	0.54
1:C:113:LYS:CE	1:C:152:GLU:HG2	2.34	0.53
1:G:203:ASN:ND2	1:G:206:PHE:H	2.05	0.53
1:G:45:ARG:HD3	4:G:2045:HOH:O	2.09	0.53
1:A:61:LEU:HD12	1:A:65:LYS:HE2	1.90	0.53
2:F:11:GLU:OE2	2:F:15:LYS:HG3	2.10	0.52
1:A:23:LYS:HG2	1:E:182:ILE:HD11	1.92	0.51
1:G:283:PHE:CZ	2:H:42:GLY:HA2	2.45	0.51
1:C:253:ILE:HD11	4:C:2195:HOH:O	2.08	0.51
1:A:225:LYS:HA	1:A:225:LYS:HE3	1.91	0.51
1:G:203:ASN:C	1:G:203:ASN:HD22	2.13	0.51
1:C:260:LYS:NZ	1:C:260:LYS:HB3	2.26	0.51
1:C:291:ILE:HG22	1:C:292:VAL:H	1.76	0.51



Interstomic Clash						
Atom-1	Atom-2	distance $(Å)$	overlan (Å)			
1:E:129:TYR:CD1	2:F:35:LEU:HD22	2.46	0.51			
1:A:190:PHE:CE1	2:B:48:LEU:HD13	2.46	0.50			
1:A:234:TYB:CD1	1:A:253:ILE:HD12	2.46	0.50			
1:G:195:VAL:O	1:G:199:LEU:HD13	2.13	0.50			
1:E:47:LYS:NZ	1:E:47:LYS:HB2	2.26	0.50			
1:A:179:VAL:O	1:A:180:ASP:C	2.50	0.50			
1:A:35:THR:HG21	4:A:2015:HOH:O	2.11	0.50			
1:G:208:HIS:O	1:G:211:LYS:HG3	2.12	0.50			
1:A:87:GLU:OE2	1:C:278:LYS:HD2	2.11	0.50			
1:C:179:VAL:HG12	1:C:180:ASP:N	2.27	0.50			
1:C:283:PHE:CZ	2:D:42:GLY:HA2	2.46	0.50			
1:G:140:ILE:HG21	1:G:156:TYR:CE2	2.47	0.50			
1:G:89:LYS:HA	1:G:89:LYS:HE3	1.92	0.49			
1:G:176:LEU:O	1:G:179:VAL:HG22	2.12	0.49			
1:C:41:ASN:O	1:C:45:ABG:HG2	2.12	0.49			
1.G.36.LEU.C	1.G.36.LEU.HD23	2.33	0.49			
1:A:203:ASN:HD22	1:A:203:ASN:C	2.00	0.49			
1:G:128:GLU:O	1:G:128:GLU:HG3	2.13	0.49			
1:G:253:ILE:HD11	4:G:2230:HOH:O	2.12	0.49			
$1 \cdot E \cdot 113 \cdot LYS \cdot CE$	1.E.152.GLU.HG3	2.37	0.49			
1:A:41:ASN:ND2	1:A:78:TYB:OH	2.46	0.49			
1:C:283:PHE:O	1:C:286:GLN:HG2	2.13	0.49			
1:C:116:ILE:HG23	1:C:140:ILE:HG23	1.96	0.48			
1:G:15:LYS:O	1:G:19:ARG:HG3	2.13	0.48			
1:A:31:GLU:O	1:A:35:THR:HG22	2.13	0.48			
1:A:84:ASP:CG	2:D:46:PRO:HB3	2.34	0.48			
1:C:190:PHE:CE1	2:D:48:LEU:HD23	2.49	0.48			
1:C:175:TRP:CH2	2:D:48:LEU:HD22	2.49	0.48			
1:C:17:LEU:O	1:C:21:GLU:HG2	2.14	0.48			
1:C:46:SER:O	1:C:47:LYS:HB2	2.13	0.48			
1:A:203:ASN:ND2	1:A:206:PHE:H	2.12	0.47			
1:C:148:ASP:HB2	2:D:54:GLN:NE2	2.28	0.47			
1:C:239:PHE:CB	1:C:242:TYR:HB2	2.44	0.47			
1:C:260:LYS:HG3	4:C:2211:HOH:O	2.14	0.47			
1:C:36:LEU:HD23	1:C:36:LEU:C	2.35	0.47			
1:G:50:GLU:O	1:G:54:GLU:HG3	2.15	0.47			
1:C:154:GLU:OE1	1:C:193:ARG:NH1	2.48	0.47			
2:B:46:PRO:HB3	1:C:84:ASP:CG	2.35	0.47			
1:C:230:ASP:OD1	1:C:235:GLU:HB2	2.15	0.47			
1:C:90:VAL:HG21	1:C:127:SER:HB3	1.97	0.47			
1:E:20:PHE:CZ	1:E:24:ILE:HD11	2.50	0.47			



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:61:LEU:CD1	1:A:65:LYS:HE2	2.45	0.47
2:B:23:THR:HG22	4:B:2006:HOH:O	2.15	0.47
1:A:90:VAL:HG21	1:A:123:SER:HA	1.97	0.46
1:A:46:SER:O	1:A:47:LYS:HB2	2.16	0.46
1:G:253:ILE:H	1:G:253:ILE:CD1	2.28	0.46
1:G:253:ILE:N	1:G:253:ILE:CD1	2.78	0.46
1:C:112:LEU:O	1:C:116:ILE:HG12	2.15	0.46
1:C:219:ILE:HD11	1:C:239:PHE:CE1	2.50	0.46
1:E:102:ILE:HD13	1:E:140:ILE:HG22	1.98	0.46
1:C:180:ASP:HA	1:G:19:ARG:HD3	1.97	0.45
4:B:2040:HOH:O	1:C:37:ARG:HD3	2.17	0.45
1:G:219:ILE:HA	1:G:224:PRO:HD2	1.99	0.45
1:C:260:LYS:HG2	1:C:289:PHE:HB3	1.99	0.45
1:C:165:MET:HE2	1:C:166:ILE:HA	1.99	0.45
1:A:114:ASP:OD2	1:C:150:VAL:HG12	2.17	0.45
1:C:260:LYS:HB3	1:C:260:LYS:HZ3	1.81	0.45
1:A:14:ALA:HB3	4:A:2001:HOH:O	2.16	0.45
1:E:46:SER:O	1:E:47:LYS:HB2	2.17	0.44
2:B:24:GLU:HA	2:B:25:PRO:HD3	1.89	0.44
1:C:179:VAL:HG12	1:C:181:ASP:H	1.82	0.44
2:F:11:GLU:O	2:F:15:LYS:HG2	2.18	0.44
1:E:154:GLU:HG3	1:E:168:TYR:CE1	2.53	0.44
1:C:260:LYS:HE2	1:C:291:ILE:HG12	2.00	0.43
2:H:15:LYS:NZ	2:H:15:LYS:HB3	2.33	0.43
1:C:175:TRP:CZ2	2:D:48:LEU:HD22	2.53	0.43
1:G:260:LYS:HG2	4:G:2238:HOH:O	2.18	0.43
1:E:23:LYS:HB3	1:E:32:ALA:HB2	2.01	0.43
1:A:263:PHE:HB2	1:A:289:PHE:CE2	2.53	0.43
1:G:17:LEU:O	1:G:21:GLU:HG2	2.19	0.43
1:G:98:LEU:O	1:G:102:ILE:HG13	2.19	0.43
1:E:155:ARG:HA	1:E:158:MET:HE2	2.01	0.43
1:E:205:SER:O	1:E:209:GLU:HG3	2.19	0.43
2:H:7:GLY:N	2:H:8:PRO:HD2	2.34	0.43
2:H:8:PRO:HG2	4:H:2002:HOH:O	2.19	0.42
1:E:239:PHE:CB	1:E:242:TYR:HB2	2.49	0.42
1:C:211:LYS:O	1:C:215:LEU:HD13	2.20	0.42
1:E:17:LEU:O	1:E:21:GLU:HG2	2.19	0.42
1:G:260:LYS:HB2	4:G:2239:HOH:O	2.19	0.42
1:A:175:TRP:CZ2	2:B:48:LEU:HD12	2.54	0.42
1:C:50:GLU:H	1:C:50:GLU:CD	2.22	0.42
1:C:242:TYR:HB3	1:C:245:LEU:HB2	2.02	0.42



	1.0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:181:ASP:HB3	1:G:186:THR:HG21	2.01	0.42
1:G:154:GLU:OE1	1:G:193:ARG:NH1	2.52	0.42
1:A:102:ILE:HD13	1:A:140:ILE:HG22	2.01	0.41
1:C:140:ILE:HG21	1:C:156:TYR:CE2	2.55	0.41
1:C:190:PHE:CE1	2:D:48:LEU:CD2	3.03	0.41
1:E:20:PHE:CE1	1:E:32:ALA:HB1	2.55	0.41
1:C:175:TRP:CZ3	2:D:48:LEU:HD22	2.55	0.41
1:G:116:ILE:HG23	1:G:140:ILE:HG23	2.02	0.41
1:C:208:HIS:NE2	1:C:256:GLN:NE2	2.69	0.41
1:A:61:LEU:O	1:A:61:LEU:HD13	2.21	0.41
1:G:219:ILE:HD11	1:G:237:VAL:HG11	2.03	0.41
1:C:165:MET:HE2	1:C:165:MET:O	2.20	0.41
1:C:215:LEU:O	1:C:219:ILE:HG12	2.20	0.41
1:A:215:LEU:O	1:A:219:ILE:HG13	2.21	0.41
1:E:89:LYS:HD3	4:E:2082:HOH:O	2.20	0.41
1:A:12:LYS:N	4:A:2001:HOH:O	2.53	0.41
1:A:242:TYR:HB3	1:A:245:LEU:HD22	2.02	0.41
1:C:209:GLU:HG2	1:C:209:GLU:H	1.70	0.41
1:C:286:GLN:HB2	4:C:2237:HOH:O	2.20	0.40
1:C:197:ASN:HD22	1:C:197:ASN:HA	1.72	0.40
1:E:41:ASN:ND2	1:E:78:TYR:OH	2.53	0.40
1:C:13:LEU:HD21	1:C:55:LEU:HB2	2.04	0.40
2:F:35:LEU:HD23	2:F:35:LEU:C	2.42	0.40
1:A:144:LEU:HD11	1:A:156:TYR:CE2	2.57	0.40
1:C:116:ILE:HG23	1:C:140:ILE:CG2	2.52	0.40
1:A:130:LYS:HD3	2:B:39:THR:HA	2.04	0.40
1:E:23:LYS:HD2	1:E:32:ALA:HA	2.04	0.40
1:E:36:LEU:HD23	1:E:36:LEU:C	2.42	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	А	279/312~(89%)	272~(98%)	7 (2%)	0	100 100
1	С	280/312~(90%)	272~(97%)	8 (3%)	0	100 100
1	Ε	278/312~(89%)	270~(97%)	8 (3%)	0	100 100
1	G	279/312~(89%)	272~(98%)	7(2%)	0	100 100
2	В	46/59~(78%)	46 (100%)	0	0	100 100
2	D	46/59~(78%)	45~(98%)	1 (2%)	0	100 100
2	F	45/59~(76%)	45~(100%)	0	0	100 100
2	Н	46/59~(78%)	45 (98%)	1 (2%)	0	100 100
All	All	1299/1484~(88%)	1267 (98%)	32 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	254/279~(91%)	249~(98%)	5(2%)	55 58
1	С	248/279~(89%)	242 (98%)	6(2%)	49 51
1	Ε	247/279~(88%)	244 (99%)	3 (1%)	71 76
1	G	252/279~(90%)	243~(96%)	9 (4%)	35 34
2	В	42/54~(78%)	41 (98%)	1 (2%)	49 51
2	D	44/54~(82%)	43~(98%)	1 (2%)	50 53
2	F	43/54~(80%)	43~(100%)	0	100 100
2	Н	44/54~(82%)	43 (98%)	1 (2%)	50 53
All	All	1174/1332~(88%)	1148 (98%)	26(2%)	52 55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	61	LEU
1	А	83	TYR



Mol	Chain	Res	Type
1	A	203	ASN
1	A	225	LYS
1	А	260	LYS
2	В	22	LEU
1	С	12	LYS
1	С	50	GLU
1	С	78	TYR
1	С	83	TYR
1	С	165	MET
1	С	245	LEU
2	D	24	GLU
1	Е	54	GLU
1	Е	83	TYR
1	Е	260	LYS
1	G	13	LEU
1	G	61	LEU
1	G	78	TYR
1	G	83	TYR
1	G	85	LEU
1	G	89	LYS
1	G	145	LEU
1	G	203	ASN
1	G	211	LYS
2	H	41	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	33	HIS
1	А	41	ASN
1	А	51	HIS
1	А	58	GLN
1	А	203	ASN
1	А	268	ASN
1	А	275	GLN
1	С	22	ASN
1	С	34	GLN
1	С	197	ASN
1	С	256	GLN
1	С	275	GLN
1	С	286	GLN
2	D	54	GLN



Mol	Chain	Res	Type
1	Е	33	HIS
1	Е	34	GLN
1	Е	41	ASN
1	Е	223	HIS
1	Е	232	ASN
1	G	58	GLN
1	G	138	ASN
1	G	203	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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, 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	А	281/312~(90%)	-0.05	3 (1%) 80 79	9, 20, 35, 48	0
1	С	282/312~(90%)	0.01	8 (2%) 53 51	11, 20, 37, 52	0
1	Ε	280/312~(89%)	-0.03	5 (1%) 68 66	9, 18, 42, 52	0
1	G	281/312~(90%)	-0.04	5 (1%) 68 66	8, 19, 33, 46	0
2	В	48/59~(81%)	0.19	2 (4%) 36 35	15, 24, 41, 49	0
2	D	48/59~(81%)	0.16	2 (4%) 36 35	14, 21, 37, 44	0
2	F	47/59~(79%)	-0.12	1 (2%) 63 62	11, 19, 34, 44	0
2	Η	48/59~(81%)	0.27	2 (4%) 36 35	13, 24, 38, 48	0
All	All	1315/1484 (88%)	-0.01	28 (2%) 63 62	8, 20, 37, 52	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	G	292	VAL	4.2	
1	С	135	TYR	4.0	
1	А	292	VAL	4.0	
1	С	292	VAL	4.0	
2	Н	54	GLN	3.1	
1	Ε	292	VAL	3.1	
1	С	290	ASN	3.1	
1	С	11	ALA	2.9	
1	G	251	LEU	2.8	
1	Ε	22	ASN	2.6	
2	Н	24	GLU	2.6	
1	Ε	24	ILE	2.5	
2	В	8	PRO	2.4	
2	D	54	GLN	2.4	
1	С	19	ARG	2.4	
1	G	290	ASN	2.4	



Mol	Chain	\mathbf{Res}	Type	RSRZ
1	Ε	135	TYR	2.3
2	D	22	LEU	2.2
1	С	286	GLN	2.2
2	В	7	GLY	2.2
1	G	223	HIS	2.2
1	А	223	HIS	2.1
1	С	45	ARG	2.1
1	G	135	TYR	2.1
2	F	7	GLY	2.1
1	А	286	GLN	2.1
1	Е	28	ASP	2.1
1	С	28	ASP	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 carbohydrates 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, 95^{th} 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	$\mathbf{B} extsf{-factors}(\mathbf{A}^2)$	Q<0.9
3	HG	С	1293	1/1	0.96	0.07	47,47,47,47	0
3	HG	А	1293	1/1	0.96	0.05	$53,\!53,\!53,\!53$	0
3	HG	Е	1293	1/1	0.97	0.06	44,44,44,44	0
3	HG	G	1293	1/1	0.98	0.07	51, 51, 51, 51	0

6.5 Other polymers (i)

There are no such residues in this entry.

