

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7PJE
Title	:	Inhibiting parasite proliferation using a rationally designed anti-tubulin agent
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Deposited on	:	2021-08-24
Resolution	:	1.75 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
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.75 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	2340(1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	А	449	% 8 7%	6% • 6%					
1	С	449	% 8 5%	8% 6%					
2	В	443	2% 90%	5%••					
2	D	443	86%	9% • •					
3	Е	155	75% 6%	19%					



Mol	Chain	Length	Quality of chain						
3	F	155	79%	•	19%				



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31317 atoms, of which 14958 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	А	422	Total 6574	C 2096	Н 3265	N 561	O 628	S 24	0	9	0
1	С	424	Total 6551	C 2089	Н 3250	N 561	O 629	S 22	0	2	0

• Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	В	425	Total 6673	C 2124	Н 3295	N 582	O 643	S 29	0	11	0
2	D	424	Total 6553	C 2091	Н 3227	N 570	O 637	S 28	0	4	0

• Molecule 3 is a protein called Darpin D1.

Mol	Chain	Residues		Atoms						AltConf	Trace
3	F	126	Total 1867	C 588	Н 937	N 161	0 178	${ m S} { m 3}$	0	0	0
3	Е	125	Total 1877	C 589	Н 946	N 162	0 177	${ m S} { m 3}$	0	2	0

• Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
4 A	1	Total	С	Η	Ν	0	Р	0	0		
		41	10	9	5	14	3	0	0		
4	A B	1	Total	С	Η	Ν	Ο	Р	0	0	
4 D	D		42	10	10	5	14	3			
4	С	1	Total	С	Η	Ν	Ο	Р	0	0	
4 0		1	42	10	10	5	14	3	0	0	
4	Л	1	Total	С	Η	Ν	0	Р	0	0	
	D		41	10	9	5	14	3	0	0	

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Mg 1 1	0	0
5	В	1	Total Mg 1 1	0	0
5	С	1	Total Mg 1 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	241	Total O 241 241	0	0
6	В	280	Total O 280 280	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	\mathbf{F}	67	Total O 67 67	0	0
6	С	228	Total O 228 228	0	0
6	D	160	Total O 160 160	0	0
6	Ε	77	Total O 77 77	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: Tubulin alpha chain



• Molecule 3: Darpin D1

Chain F:	79%	·	19%
D13 E94 V98 W112	D138 VAL ALA ALA ALA ALA ALA ALA ALA ALA ASP ASP ASP ASP ASP ASP ASP ASP ASP AS		
• Molecule	3: Darpin D1		
Chain E:	75%	6%	19%
D13 K16 K17 L18 L18 L19 D44	M79 L89 K101 K101 T111 T111 T111 A137 A137 A137 A137 A137 A137 A137 A	ALA GLU ILE LEU GLN LYS	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	52.13Å 183.92Å 118.32Å	Deperitor
a, b, c, α , β , γ	90.00° 92.44° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	46.83 - 1.75	Depositor
Resolution (A)	46.83 - 1.75	EDS
% Data completeness	98.4 (46.83-1.75)	Depositor
(in resolution range)	98.4(46.83-1.75)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.33 (at 1.75 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.181 , 0.213	Depositor
Π, Π_{free}	0.182 , 0.214	DCC
R_{free} test set	10973 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	30.5	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31317	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.07% 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: MG, GTP

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	Bo	ond lengths	Bond angles	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.66	3/3429~(0.1%)	0.70	1/4642~(0.0%)
1	С	0.61	3/3380~(0.1%)	0.69	1/4577~(0.0%)
2	В	0.73	9/3495~(0.3%)	0.80	3/4728~(0.1%)
2	D	0.71	6/3417~(0.2%)	0.78	10/4625~(0.2%)
3	Е	0.51	0/953	0.66	1/1298~(0.1%)
3	F	0.47	0/944	0.64	0/1286
All	All	0.66	21/15618~(0.1%)	0.74	16/21156~(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
2	D	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	175	PRO	N-CA	13.16	1.69	1.47
2	D	175	PRO	N-CA	12.90	1.69	1.47
2	В	348	PRO	N-CA	12.87	1.69	1.47
1	А	175	PRO	N-CA	12.51	1.68	1.47
2	D	162	PRO	N-CA	12.44	1.68	1.47
2	В	222	PRO	N-CA	12.35	1.68	1.47
2	D	244	PHE	C-N	9.41	1.52	1.34
1	С	62	VAL	C-N	8.89	1.51	1.34
2	В	221	THR	C-N	6.17	1.46	1.34
2	D	161	TYR	C-N	5.78	1.45	1.34
1	А	174	SER	C-N	5.59	1.44	1.34
1	С	174	SER	C-N	5.58	1.44	1.34



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Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	164[A]	ARG	C-O	5.51	1.33	1.23
2	В	164[B]	ARG	C-O	5.51	1.33	1.23
1	А	241	SER	CA-CB	-5.47	1.44	1.52
2	D	174	SER	C-N	5.27	1.44	1.34
2	В	351[A]	ILE	C-N	-5.13	1.22	1.34
2	В	351[B]	ILE	C-N	-5.13	1.22	1.34
2	В	253[A]	ARG	C-O	5.02	1.32	1.23
2	В	253[B]	ARG	C-O	5.02	1.32	1.23
2	D	303	CYS	CB-SG	-5.00	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	360	PRO	O-C-N	-10.01	106.69	122.70
2	В	222	PRO	CA-N-CD	-9.85	97.71	111.50
2	D	162	PRO	CA-N-CD	-7.75	100.65	111.50
2	D	360	PRO	CA-C-N	7.39	133.46	117.20
2	D	243	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	А	175	PRO	CA-N-CD	-7.28	101.30	111.50
1	С	175	PRO	CA-N-CD	-6.59	102.28	111.50
2	D	175	PRO	CA-N-CD	-6.44	102.48	111.50
3	Е	44	ASP	CB-CG-OD1	5.98	123.68	118.30
2	D	164[A]	ARG	CD-NE-CZ	5.50	131.30	123.60
2	D	164[B]	ARG	CD-NE-CZ	5.50	131.30	123.60
2	D	164[A]	ARG	C-N-CA	-5.41	108.17	121.70
2	D	164[B]	ARG	C-N-CA	-5.41	108.17	121.70
2	В	400	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	В	123	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	D	202	MET	CG-SD-CE	5.10	108.36	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	360	PRO	Mainchain

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3309	3265	3215	20	0
1	С	3301	3250	3234	29	0
2	В	3378	3295	3248	23	0
2	D	3326	3227	3200	35	0
3	Е	931	946	940	8	0
3	F	930	937	940	2	0
4	А	32	9	12	0	0
4	В	32	10	12	1	0
4	С	32	10	12	0	0
4	D	32	9	12	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
5	С	1	0	0	0	0
6	А	241	0	0	1	0
6	В	280	0	0	5	0
6	С	228	0	0	3	0
6	D	160	0	0	2	0
6	E	77	0	0	1	0
6	F	67	0	0	0	0
All	All	16359	14958	14825	114	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 4.

All (114) 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)
2:B:348:PRO:CA	2:B:348:PRO:N	1.69	1.46
1:C:175:PRO:CA	1:C:175:PRO:N	1.69	1.43
2:B:222:PRO:CA	2:B:222:PRO:N	1.68	1.41
1:A:175:PRO:N	1:A:175:PRO:CA	1.68	1.38
2:D:175:PRO:N	2:D:175:PRO:CA	1.69	1.32
2:D:162:PRO:N	2:D:162:PRO:CA	1.68	1.29
1:A:203[B]:MET:HG3	1:A:384:ILE:HD11	1.54	0.90
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.59	0.82
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.73	0.70
1:C:124:LYS:NZ	6:C:601:HOH:O	2.25	0.69
2:D:202:MET:CE	2:D:270:ILE:HD11	2.29	0.63
1:A:175:PRO:N	1:A:175:PRO:C	2.49	0.63
2:B:222:PRO:N	2:B:222:PRO:C	2.50	0.61



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
3:E:101:LYS:NZ	6:E:201:HOH:O	2.34	0.61
2:D:175:PRO:N	2:D:175:PRO:C	2.53	0.61
1:C:27:GLU:OE1	1:C:243:ARG:NH2	2.35	0.59
1:A:203[B]:MET:HG3	1:A:384:ILE:CD1	2.29	0.59
2:D:360:PRO:HG2	2:D:371:LEU:HD12	1.85	0.59
2:D:19:LYS:NZ	6:D:605:HOH:O	2.35	0.59
2:D:162:PRO:N	2:D:162:PRO:C	2.52	0.59
3:E:79:MET:CE	3:E:111:THR:HG21	2.34	0.58
1:A:205:ASP:HB3	1:A:303:ALA:HA	1.85	0.58
2:D:57:THR:O	2:D:57:THR:HG23	2.04	0.57
2:D:396:THR:O	2:D:400:ARG:HG3	2.03	0.57
2:D:202:MET:HE2	2:D:270:ILE:HD11	1.87	0.56
1:C:239:THR:OG1	1:C:243:ARG:NH1	2.38	0.56
1:C:175:PRO:N	1:C:175:PRO:C	2.54	0.56
2:D:295:MET:CE	2:D:375:VAL:HG21	2.36	0.56
2:B:315:ALA:HB3	2:B:351[A]:ILE:HD12	1.89	0.55
2:B:348:PRO:N	2:B:348:PRO:C	2.54	0.55
3:E:79:MET:O	3:E:111:THR:HG22	2.06	0.55
2:B:396:THR:O	2:B:400:ARG:HG3	2.07	0.54
2:B:400:ARG:HD3	6:B:752:HOH:O	2.06	0.54
1:C:205:ASP:HB3	1:C:303:ALA:HA	1.91	0.53
1:A:48:ALA:O	1:A:51:THR:HG23	2.09	0.53
2:D:400:ARG:HD2	3:E:112:TRP:NE1	2.24	0.53
1:C:241:SER:HB2	6:C:602:HOH:O	2.08	0.53
2:B:343:PHE:CD1	2:B:351[A]:ILE:HD11	2.44	0.52
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.91	0.52
1:C:133:GLN:OE1	1:C:251:ASP:HB2	2.10	0.52
3:E:79:MET:HE2	3:E:111:THR:HG21	1.90	0.52
1:C:62:VAL:HG13	1:C:86:LEU:O	2.10	0.51
1:C:296:PHE:CE1	1:C:341:ILE:HD11	2.46	0.51
2:D:202:MET:HE3	2:D:270:ILE:CG1	2.41	0.51
3:E:16:LYS:HA	3:E:19:LEU:HD12	1.93	0.51
2:D:123:ARG:NH2	2:D:160:GLU:OE1	2.42	0.51
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.93	0.51
2:D:295:MET:HE3	2:D:375:VAL:HG21	1.92	0.51
1:C:265:ILE:HD11	1:C:431:ASP:HB3	1.93	0.50
2:B:350:ASN:O	2:B:351[A]:ILE:HD13	2.10	0.50
2:D:202:MET:HE3	2:D:270:ILE:HD11	1.94	0.49
2:B:104:ALA:HB2	2:B:413:MET:HE3	1.95	0.48
2:B:213:CYS:HB3	2:B:222:PRO:HB3	1.95	0.48
2:B:60:ARG:NH2	6:B:611:HOH:O	2.47	0.48



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:D:33:THR:OG1	2:D:35:THR:HG23	2.13	0.48	
1:C:296:PHE:CD1	1:C:341:ILE:HD11	2.48	0.48	
2:B:400:ARG:HD2	3:F:112:TRP:NE1	2.29	0.48	
1:A:147:SER:HB2	1:A:190:SER:OG	2.14	0.47	
2:B:293:GLN:NE2	6:B:612:HOH:O	2.47	0.47	
2:B:71:GLU:HG2	6:B:657:HOH:O	2.14	0.47	
2:B:69:ASP:O	2:B:94:PHE:HA	2.14	0.47	
1:C:351:PHE:CE2	1:C:353:VAL:HG23	2.49	0.47	
1:C:3:GLU:O	1:C:133:GLN:HG2	2.15	0.47	
2:D:60:ARG:HB2	2:D:60:ARG:NH1	2.30	0.47	
2:D:35:THR:HG22	2:D:60:ARG:HG2	1.96	0.47	
2:D:60:ARG:CZ	2:D:60:ARG:CB	2.93	0.46	
1:C:68:LEU:CD2	1:C:93:ILE:HD12	2.46	0.46	
1:A:166:LYS:HE2	1:A:197:HIS:O	2.16	0.46	
3:F:94:GLU:O	3:F:98:VAL:HG23	2.16	0.46	
1:C:296:PHE:CZ	1:C:341:ILE:HD11	2.51	0.45	
2:D:69:ASP:O	2:D:94:PHE:HA	2.16	0.45	
1:C:257:THR:HG23	6:C:697:HOH:O	2.16	0.45	
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.97	0.45	
2:B:99:ALA:HB3	4:B:501:GTP:O2G	2.17	0.45	
1:C:362:VAL:HG21	1:C:370:LYS:HD2	1.99	0.45	
1:A:343:PHE:HD2	6:A:717:HOH:O	2.00	0.44	
3:E:79:MET:HE3	3:E:111:THR:HG21	1.99	0.44	
1:A:351:PHE:CE2	1:A:353:VAL:HG23	2.53	0.43	
2:D:1:MET:SD	2:D:133:GLN:HG3	2.58	0.43	
2:D:382:THR:O	2:D:385:GLN:HG2	2.18	0.43	
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.37	0.43	
2:D:109:THR:HG21	2:D:411:GLU:OE1	2.19	0.43	
2:D:202:MET:CE	2:D:270:ILE:CD1	2.96	0.43	
1:A:170:THR:HG21	1:A:194:LEU:HD11	2.01	0.42	
2:B:350:ASN:C	2:B:351[A]:ILE:HD13	2.40	0.42	
1:C:4:VAL:HG23	1:C:133:GLN:HE21	1.84	0.42	
1:C:106:GLY:O	1:C:111:GLY:HA3	2.20	0.42	
2:D:295:MET:HE1	2:D:317:ALA:HB1	2.01	0.42	
1:C:183:GLU:HB2	1:C:184:PRO:HD3	2.02	0.42	
2:D:126:ALA:C	2:D:128:GLY:N	2.72	0.42	
2:D:401:ARG:HD3	3:E:89:LEU:HD22	2.02	0.42	
2:D:218:LYS:NZ	6:D:615:HOH:O	2.49	0.42	
1:C:124:LYS:HA	1:C:124:LYS:HD3	1.94	0.42	
2:D:202:MET:HE3	2:D:270:ILE:HG12	2.02	0.42	
2:B:104:ALA:HB2	2:B:413:MET:CE	2.51	0.41	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:60:ARG:HB2	2:D:60:ARG:CZ	2.50	0.41
2:B:343:PHE:CE1	2:B:351[A]:ILE:HG13	2.55	0.41
2:D:126:ALA:C	2:D:128:GLY:H	2.23	0.41
1:A:220:GLU:HG3	1:A:221:ARG:N	2.36	0.41
2:D:66:ILE:HG12	2:D:121:VAL:HG12	2.02	0.41
1:C:105:ARG:HG3	1:C:411:GLU:HG3	2.03	0.41
1:A:351:PHE:CE2	1:A:353:VAL:CG2	3.03	0.41
1:C:3:GLU:HG2	1:C:64:ARG:CZ	2.50	0.41
1:C:296:PHE:CE1	1:C:341:ILE:CD1	3.04	0.41
1:C:335:ILE:HG21	1:C:341:ILE:HD12	2.03	0.41
2:D:295:MET:HE1	2:D:375:VAL:HG21	2.02	0.41
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.94	0.41
2:B:164[B]:ARG:HE	2:B:164[B]:ARG:HA	1.86	0.41
2:B:343:PHE:CE1	2:B:351[A]:ILE:CD1	3.04	0.41
2:B:318:LEU:HB3	6:B:764:HOH:O	2.21	0.40
1:C:29:GLY:O	1:C:36:MET:HB2	2.21	0.40
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.95	0.40
1:A:2:ARG:HA	1:A:2:ARG:HD2	1.75	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	Perce	\mathbf{ntiles}
1	А	425/449~(95%)	413 (97%)	12 (3%)	0	100	100
1	С	420/449~(94%)	406 (97%)	14 (3%)	0	100	100
2	В	432/443~(98%)	424 (98%)	8 (2%)	0	100	100
2	D	424/443~(96%)	415 (98%)	9~(2%)	0	100	100
3	Ε	125/155~(81%)	125 (100%)	0	0	100	100
3	F	124/155~(80%)	124 (100%)	0	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1950/2094~(93%)	1907~(98%)	43 (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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	366/376~(97%)	362~(99%)	4 (1%)	73 60
1	С	361/376~(96%)	357~(99%)	4 (1%)	73 60
2	В	372/376~(99%)	367~(99%)	5 (1%)	69 54
2	D	363/376~(96%)	357~(98%)	6 (2%)	60 42
3	Ε	97/120~(81%)	96~(99%)	1 (1%)	76 63
3	F	96/120~(80%)	96 (100%)	0	100 100
All	All	1655/1744~(95%)	1635 (99%)	20 (1%)	71 56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	33	ASP
1	А	71	GLU
1	А	241	SER
1	А	320	ARG
2	В	2	ARG
2	В	139	HIS
2	В	167	GLU
2	В	293	GLN
2	В	372	LYS
1	С	71	GLU
1	С	175	PRO
1	С	241	SER
1	С	339	ARG
2	D	26	ASP



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Mol	Chain	Res	Type
2	D	39	ASP
2	D	139	HIS
2	D	167	GLU
2	D	326	LYS
2	D	340	SER
3	Е	17	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	422/449~(93%)	-0.02	4 (0%) 84 89	26, 41, 69, 100	0
1	С	424/449~(94%)	-0.05	4 (0%) 84 89	28, 42, 75, 126	0
2	В	425/443~(95%)	-0.05	8 (1%) 66 74	25, 36, 60, 84	0
2	D	424/443~(95%)	0.01	13 (3%) 49 55	30, 46, 77, 117	0
3	Ε	125/155~(80%)	-0.14	0 100 100	32, 44, 62, 85	0
3	F	126/155~(81%)	-0.16	0 100 100	31, 41, 62, 78	0
All	All	1946/2094~(92%)	-0.04	29 (1%) 73 80	25, 42, 71, 126	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	322	ARG	4.7
2	D	221	THR	3.9
2	D	296	PHE	3.6
2	В	1	MET	3.5
2	D	58	GLY	3.0
2	D	220	THR	3.0
1	С	37	PRO	2.9
2	D	322	ARG	2.8
1	С	278	ALA	2.8
2	D	333	LEU	2.7
1	А	38	SER	2.6
2	В	97	THR	2.6
2	D	57	THR	2.6
2	В	219	LEU	2.6
2	D	56	ALA	2.5
1	A	339	ARG	2.4
1	С	58	ALA	2.4
1	А	163	LYS	2.3
2	D	$\overline{26}$	ASP	2.2



Mol	Chain	Res	Type	RSRZ
1	А	242	LEU	2.2
2	В	60	ARG	2.2
2	В	333	LEU	2.2
2	D	60	ARG	2.2
2	В	318	LEU	2.1
2	D	216	THR	2.1
1	С	280	LYS	2.1
2	D	215	ARG	2.0
2	D	78	VAL	2.0
2	В	2	ARG	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 monosaccharides 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
5	MG	В	502	1/1	0.82	0.11	$45,\!45,\!45,\!45$	0
4	GTP	D	501	32/32	0.96	0.10	31,39,66,77	0
5	MG	А	502	1/1	0.97	0.10	31,31,31,31	0
4	GTP	В	501	32/32	0.97	0.09	26,31,38,49	0
4	GTP	С	502	32/32	0.98	0.10	29,33,40,45	0
5	MG	С	501	1/1	0.98	0.14	37,37,37,37	0
4	GTP	А	501	32/32	0.99	0.10	26,30,35,38	0

6.5 Other polymers (i)

There are no such residues in this entry.

