

Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 10:05 am BST

PDB ID	:	6T1F
Title	:	Crystal structure of the C-terminally truncated chromosome-partitioning
		protein ParB from Caulobacter crescentus complexed to the centromeric parS
		site
Authors	:	Jalal, A.S.B.; Pastrana, C.L.; Tran, N.T.; Stevenson, C.E.M.; Lawson, D.M.;
		Moreno-Herrero, F.; Le, T.B.K.
Deposited on	:	2019-10-04
Resolution	:	2.90 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:

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	257	^{2%} 61% 11%		26%
1	В	257	5% 65% 9	%•	26%
1	С	257	63% 12	%	24%
1	D	257	65% 7%		27%
2	Е	22	86%		14%



Mol	Chain	Length	Quality of chain	
2	F	22	77%	23%
2	G	22	82%	18%
2	Н	22	82%	18%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7163 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	Δ	101	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
	A	191	1376	858	251	264	3	0	0	0	
1	Р	100	Total	С	Ν	0	S	0	0	0	
	D	190	1312	820	234	256	2	0	0	0	
1	С	105	Total	С	Ν	0	S	0	0	0	
	U	195	1437	899	263	272	3	0	0	0	
1	П	197	Total	С	Ν	0	S	0	0	0	
		107	1246	772	232	240	2	0	0	0	

• Molecule 1 is a protein called Chromosome-partitioning protein ParB.

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	255	LYS	-	expression tag	UNP B8GW30
А	256	LEU	-	expression tag	UNP B8GW30
А	257	ALA	-	expression tag	UNP B8GW30
А	258	ALA	-	expression tag	UNP B8GW30
А	259	ALA	-	expression tag	UNP B8GW30
А	260	LEU	-	expression tag	UNP B8GW30
А	261	GLU	-	expression tag	UNP B8GW30
А	262	HIS	-	expression tag	UNP B8GW30
А	263	HIS	-	expression tag	UNP B8GW30
А	264	HIS	-	expression tag	UNP B8GW30
А	265	HIS	-	expression tag	UNP B8GW30
А	266	HIS	-	expression tag	UNP B8GW30
A	267	HIS	-	expression tag	UNP B8GW30
В	255	LYS	-	expression tag	UNP B8GW30
В	256	LEU	-	expression tag	UNP B8GW30
В	257	ALA	-	expression tag	UNP B8GW30
В	258	ALA	-	expression tag	UNP B8GW30
В	259	ALA	-	expression tag	UNP B8GW30
В	260	LEU	-	expression tag	UNP B8GW30
В	261	GLU	-	expression tag	UNP B8GW30
В	262	HIS	-	expression tag	UNP B8GW30



Chain	Residue	Modelled	Actual	Comment	Reference
В	263	HIS	-	expression tag	UNP B8GW30
В	264	HIS	-	expression tag	UNP B8GW30
В	265	HIS	-	expression tag	UNP B8GW30
В	266	HIS	-	expression tag	UNP B8GW30
В	267	HIS	-	expression tag	UNP B8GW30
С	255	LYS	-	expression tag	UNP B8GW30
С	256	LEU	-	expression tag	UNP B8GW30
С	257	ALA	-	expression tag	UNP B8GW30
С	258	ALA	-	expression tag	UNP B8GW30
С	259	ALA	-	expression tag	UNP B8GW30
С	260	LEU	-	expression tag	UNP B8GW30
С	261	GLU	-	expression tag	UNP B8GW30
С	262	HIS	-	expression tag	UNP B8GW30
С	263	HIS	-	expression tag	UNP B8GW30
С	264	HIS	-	expression tag	UNP B8GW30
С	265	HIS	-	expression tag	UNP B8GW30
С	266	HIS	-	expression tag	UNP B8GW30
С	267	HIS	-	expression tag	UNP B8GW30
D	255	LYS	-	expression tag	UNP B8GW30
D	256	LEU	-	expression tag	UNP B8GW30
D	257	ALA	-	expression tag	UNP B8GW30
D	258	ALA	-	expression tag	UNP B8GW30
D	259	ALA	-	expression tag	UNP B8GW30
D	260	LEU	-	expression tag	UNP B8GW30
D	261	GLU	-	expression tag	UNP B8GW30
D	262	HIS	-	expression tag	UNP B8GW30
D	263	HIS	-	expression tag	UNP B8GW30
D	264	HIS	-	expression tag	UNP B8GW30
D	265	HIS	-	expression tag	UNP B8GW30
D	266	HIS	-	expression tag	UNP B8GW30
D	267	HIS	-	expression tag	UNP B8GW30

• Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*AP*TP*GP*TP*TP*TP*CP*AP* CP*GP*TP*GP*AP*AP*AP*CP*AP*TP*CP*C)-3').

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	F	22	Total	С	Ν	Ο	Р	0	0	0
2	Ľ		448	215	82	130	21	0	0	0
0	Б	22	Total	С	Ν	Ο	Р	0	0	0
	Г		448	215	82	130	21	0	0	0
0	С	22	Total	С	Ν	0	Р	0	0	0
	G		448	215	82	130	21	0	0	0



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	Н	22	Total 448	C 215	N 82	O 130	Р 21	0	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Chromosome-partitioning protein ParB



SIH SIH SIH SIH SIH

• Molecule 1: Chromosome-partitioning protein ParB



• Molecule 2: DNA (5'-D(*GP*GP*AP*TP*GP*TP*TP*TP*CP*AP*CP*GP*TP*GP*AP*AP *AP*CP*AP*TP*CP*C)-3')

Chain E:	86%	14%
<mark>2 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 12 11 </mark>		

• Molecule 2: DNA (5'-D(*GP*GP*AP*TP*GP*TP*TP*TP*CP*AP*CP*GP*TP*GP*AP*AP *AP*CP*AP*TP*CP*C)-3')

C	ha	in	1]	7:	•				77%	23%	
<u>G1</u>	<mark>ду</mark>		C11 210	617 113		# T	A19	C22			

• Molecule 2: DNA (5'-D(*GP*GP*AP*TP*GP*TP*TP*TP*CP*AP*CP*GP*TP*GP*AP*AP *AP*CP*AP*TP*CP*C)-3')

Chain G:	82%	18%
11 21 113 22 22 22		

• Molecule 2: DNA (5'-D(*GP*GP*AP*TP*GP*TP*TP*TP*CP*AP*CP*GP*TP*GP*AP*AP *AP*CP*AP*TP*CP*C)-3')

Chain	H:	82%	18%
G <mark>1</mark> G5 G5	6 1 1 8 0 1 2 8 0 1 1 8 0 1 1 9 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	54.25Å 172.93Å 72.85Å	Deperitor
a, b, c, α , β , γ	90.00° 90.54° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	72.96 - 2.90	Depositor
Resolution (A)	72.85 - 2.90	EDS
% Data completeness	99.6 (72.96-2.90)	Depositor
(in resolution range)	97.2 (72.85-2.90)	EDS
R_{merge}	0.14	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.50 (at 2.91 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
D D.	0.239 , 0.263	Depositor
Π, Π_{free}	0.241 , 0.265	DCC
R_{free} test set	1466 reflections (4.95%)	wwPDB-VP
Wilson B-factor $(Å^2)$	78.6	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.108 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7163	wwPDB-VP
Average B, all atoms $(Å^2)$	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.83% 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)

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	А	0.37	0/1391	0.55	0/1892
1	В	0.36	0/1329	0.53	0/1820
1	С	0.36	0/1454	0.55	0/1975
1	D	0.35	0/1261	0.53	0/1731
2	Ε	0.45	0/502	0.82	0/773
2	F	0.54	0/502	0.82	0/773
2	G	0.50	0/502	0.84	0/773
2	Н	0.46	0/502	0.83	0/773
All	All	0.40	0/7443	0.64	0/10510

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	А	0	4
1	В	0	2
1	С	0	2
1	D	0	4
All	All	0	12

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12)) planarity	outliers	are listed	below:
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Mol	Chain	Res	Type	Group
1	А	139	ARG	Sidechain
1	А	160	ARG	Sidechain
1	А	173	ARG	Sidechain



Mol	Chain	Res	Type	Group
1	А	54	ARG	Sidechain
1	В	104	ARG	Sidechain
1	В	173	ARG	Sidechain
1	С	160	ARG	Sidechain
1	С	173	ARG	Sidechain
1	D	104	ARG	Sidechain
1	D	160	ARG	Sidechain
1	D	173	ARG	Sidechain
1	D	227	ARG	Sidechain

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	1376	0	1317	14	0
1	В	1312	0	1171	16	0
1	С	1437	0	1418	22	0
1	D	1246	0	1077	12	0
2	Е	448	0	250	3	0
2	F	448	0	250	4	0
2	G	448	0	250	3	0
2	Н	448	0	250	3	0
All	All	7163	0	5983	68	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 5.

All (68) 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:C:51:ILE:HG22	1:C:95:GLU:HA	1.46	0.92
1:B:199:THR:HG22	1:B:202:HIS:ND1	1.88	0.89
1:D:199:THR:HG22	1:D:202:HIS:ND1	1.87	0.88
1:B:219:ILE:HG12	1:B:229:THR:HG22	1.59	0.83
1:D:219:ILE:HG12	1:D:229:THR:HG22	1.67	0.75
1:B:218:GLN:NE2	1:B:232:LEU:HD13	2.07	0.70



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1:B:219:ILE:HG12	1:B:229:THR:CG2	2.22	0.69		
1:A:81:LEU:H	1:A:167:GLN:HE22	1.39	0.68		
1:D:199:THR:CG2	1:D:202:HIS:ND1	2.58	0.66		
1:D:219:ILE:HG12	1:D:229:THR:CG2	2.25	0.65		
1:B:199:THR:CG2	1:B:202:HIS:ND1	2.59	0.65		
1:C:173:ARG:NH2	2:G:5:DG:O6	2.31	0.63		
1:C:51:ILE:CG2	1:C:95:GLU:HA	2.27	0.63		
1:A:130:GLU:OE1	1:A:160:ARG:NH1	2.33	0.60		
1:D:226:VAL:HG12	1:D:227:ARG:HH11	1.67	0.59		
1:D:173:ARG:NH2	2:H:5:DG:O6	2.36	0.58		
1:C:82:GLN:HB2	1:C:164:ASN:HD21	1.70	0.57		
1:B:218:GLN:HE22	1:B:232:LEU:HD13	1.70	0.56		
1:D:55:ASN:ND2	1:D:128:VAL:HG11	2.21	0.55		
1:A:82:GLN:HB2	1:A:164:ASN:HD21	1.73	0.54		
1:C:151:TYR:CE1	1:C:169:ILE:HD13	2.43	0.54		
1:A:215:LEU:HD22	1:A:232:LEU:HD13	1.90	0.54		
1:A:64:ARG:HH11	1:B:66:GLU:CB	2.20	0.53		
1:C:136:ASN:HD21	1:C:142:LEU:HD21	1.73	0.53		
1:B:173:ARG:NH2	2:F:5:DG:O6	2.42	0.51		
1:A:173:ARG:NH2	2:E:5:DG:O6	2.44	0.51		
1:D:158:PHE:O	1:D:160:ARG:NH1	2.37	0.51		
1:D:173:ARG:HD2	2:H:4:DT:H73	1.93	0.50		
1:B:125:ASP:O	1:B:128:VAL:HG22	2.12	0.50		
2:H:11:DC:H2'	2:H:12:DG:C8	2.47	0.49		
2:E:11:DC:H2'	2:E:12:DG:C8	2.49	0.47		
1:C:75:ILE:HD12	1:C:80:VAL:HA	1.97	0.47		
2:F:11:DC:H2'	2:F:12:DG:C8	2.49	0.47		
2:G:11:DC:H2'	2:G:12:DG:C8	2.50	0.47		
1:A:204:ARG:NH2	2:F:14:DG:O6	2.49	0.46		
1:C:87:ARG:CZ	1:C:99:VAL:HG12	2.45	0.46		
1:C:219:ILE:HD11	1:C:229:THR:HG23	1.99	0.45		
1:D:199:THR:OG1	2:G:13:DT:OP2	2.33	0.44		
1:A:211:ASP:N	1:A:212:PRO:HD3	2.32	0.44		
1:C:211:ASP:N	1:C:212:PRO:HD3	2.32	0.44		
1:A:219:ILE:HD11	1:A:229:THR:CG2	2.48	0.44		
1:C:151:TYR:OH	1:C:169:ILE:CD1	2.66	0.44		
1:B:211:ASP:N	1:B:212:PRO:HD3	2.33	0.43		
1:C:139:ARG:O	1:C:140:ALA:HB3	2.19	0.43		
1:D:211:ASP:N	1:D:212:PRO:HD3	2.33	0.43		
1:C:84:ILE:CD1	1:C:116:VAL:HG11	2.49	0.43		
1:A:85:LEU:O	1:A:99:VAL:HG12	2.18	0.43		



A 4 1	A +	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:198:LEU:HD22	1:C:202:HIS:HB3	2.00	0.42
1:D:197:GLU:O	1:D:198:LEU:HD12	2.19	0.42
1:A:198:LEU:HD22	1:A:202:HIS:HB3	2.01	0.42
1:B:162:GLN:OE1	1:B:173:ARG:NH1	2.52	0.42
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.94	0.42
1:C:85:LEU:O	1:C:99:VAL:HG22	2.20	0.42
1:B:142:LEU:HG	1:B:146:GLU:HB3	2.02	0.41
1:A:227:ARG:HA	1:A:227:ARG:HE	1.84	0.41
1:C:51:ILE:HG22	1:C:95:GLU:CA	2.34	0.41
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.95	0.41
1:C:151:TYR:HE1	1:C:169:ILE:HD13	1.86	0.41
1:C:219:ILE:HD11	1:C:229:THR:CG2	2.50	0.41
1:B:125:ASP:HA	1:B:128:VAL:HG22	2.02	0.41
1:B:198:LEU:HD22	1:B:202:HIS:HB3	2.03	0.41
1:C:84:ILE:HD12	1:C:116:VAL:HG11	2.03	0.41
2:E:5:DG:C2	2:F:19:DA:C2	3.09	0.41
1:C:162:GLN:OE1	1:C:173:ARG:NH1	2.53	0.41
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.93	0.40
1:A:139:ARG:O	1:A:140:ALA:HB3	2.20	0.40
1:B:199:THR:HG22	1:B:202:HIS:CE1	2.52	0.40
1:B:142:LEU:HG	1:B:146:GLU:CB	2.52	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	ntiles
1	А	187/257~(73%)	177~(95%)	10 (5%)	0	100	100
1	В	186/257~(72%)	179 (96%)	7 (4%)	0	100	100
1	С	193/257~(75%)	182 (94%)	11 (6%)	0	100	100
1	D	183/257~(71%)	175 (96%)	8 (4%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	749/1028~(73%)	713~(95%)	36~(5%)	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	126/203~(62%)	114 (90%)	12 (10%)	8 26
1	В	108/203~(53%)	100~(93%)	8 (7%)	13 38
1	С	137/203~(68%)	133~(97%)	4 (3%)	42 76
1	D	95/203~(47%)	90~(95%)	5(5%)	22 54
All	All	466/812~(57%)	437 (94%)	29~(6%)	18 47

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	68	LEU
1	А	73	ASN
1	А	104	ARG
1	А	123	LEU
1	А	142	LEU
1	А	159	GLU
1	А	161	THR
1	А	169	ILE
1	А	171	LYS
1	А	227	ARG
1	А	232	LEU
1	А	238	ASN
1	В	57	ASP
1	В	122	GLU
1	В	123	LEU
1	В	156	GLU
1	В	161	THR



Mol	Chain	Res	Type
1	В	193	LEU
1	В	218	GLN
1	В	227	ARG
1	С	62	THR
1	С	76	ARG
1	С	104	ARG
1	С	238	ASN
1	D	54	ARG
1	D	82	GLN
1	D	161	THR
1	D	164	ASN
1	D	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	73	ASN
1	А	167	GLN
1	В	218	GLN
1	С	136	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, 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	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	191/257~(74%)	0.04	6 (3%) 49 44	64, 92, 126, 147	0
1	В	190/257~(73%)	0.26	13 (6%) 17 13	67, 100, 130, 136	0
1	С	195/257~(75%)	0.01	1 (0%) 91 91	59, 85, 123, 140	0
1	D	187/257~(72%)	0.36	21 (11%) 5 4	88, 115, 138, 149	0
2	Е	22/22~(100%)	-0.68	0 100 100	58, 68, 89, 92	0
2	F	22/22~(100%)	-0.70	0 100 100	59,69,84,90	0
2	G	22/22~(100%)	-0.63	0 100 100	62,71,93,98	0
2	Н	22/22~(100%)	-0.63	0 100 100	56, 75, 92, 104	0
All	All	851/1116 (76%)	0.08	41 (4%) 30 27	56, 95, 132, 149	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	94	GLY	5.0
1	D	113	LEU	4.3
1	D	119	MET	4.1
1	А	91	ASP	3.9
1	D	107	ALA	3.8
1	D	120	VAL	3.7
1	D	105	TRP	3.6
1	D	112	GLY	3.6
1	D	84	ILE	3.5
1	А	88	PRO	3.4
1	В	49	ILE	3.2
1	В	84	ILE	3.2
1	А	96	TYR	3.1
1	В	105	TRP	3.1
1	В	193	LEU	3.1
1	D	206	ILE	3.0



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Mol	Chain	Res	Type	RSRZ
1	В	83	PRO	3.0
1	А	123	LEU	2.9
1	D	122	GLU	2.9
1	D	151	TYR	2.9
1	В	63	PHE	2.8
1	D	207	ALA	2.8
1	В	151	TYR	2.8
1	D	149	LEU	2.7
1	D	98	ILE	2.7
1	В	99	VAL	2.7
1	D	114	LYS	2.6
1	А	97	GLN	2.6
1	D	83	PRO	2.5
1	А	105	TRP	2.5
1	D	121	ARG	2.5
1	D	57	ASP	2.4
1	D	165	ILE	2.2
1	В	59	PRO	2.2
1	В	96	TYR	2.2
1	В	85	LEU	2.1
1	С	123	LEU	2.1
1	В	206	ILE	2.1
1	D	99	VAL	2.1
1	В	98	ILE	2.0
1	D	130	GLU	2.0

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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.

