



## Full wwPDB EM Validation Report ⓘ

Nov 18, 2025 – 04:59 PM JST

PDB ID : 9KYE / pdb\_00009kye  
EMDB ID : EMD-62646  
Title : PltBd2 homopentameric holotoxin from E. coli  
Authors : Chen, Z.; Wang, D.D.; Gao, X.  
Deposited on : 2024-12-08  
Resolution : 2.61 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

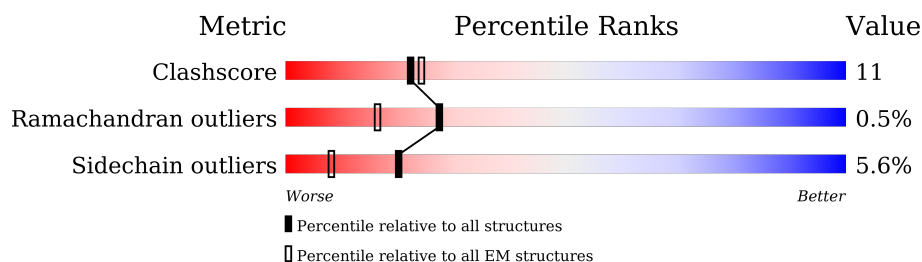
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.61 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	B	243	
2	C	116	
2	D	116	
2	E	116	
2	F	116	
2	G	116	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6290 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Pertussis toxin-like subunit ArtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	225	Total	C	N	O	S	0	0
			1780	1128	301	346	5		

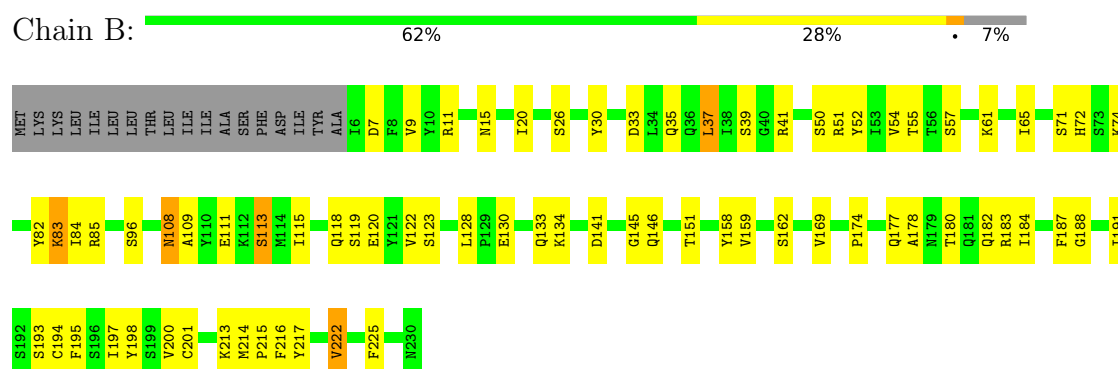
- Molecule 2 is a protein called Subtilase cytotoxin subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	115	Total	C	N	O	S	0	0
			902	575	149	173	5		
2	D	115	Total	C	N	O	S	0	0
			902	575	149	173	5		
2	E	115	Total	C	N	O	S	0	0
			902	575	149	173	5		
2	F	115	Total	C	N	O	S	0	0
			902	575	149	173	5		
2	G	115	Total	C	N	O	S	0	0
			902	575	149	173	5		

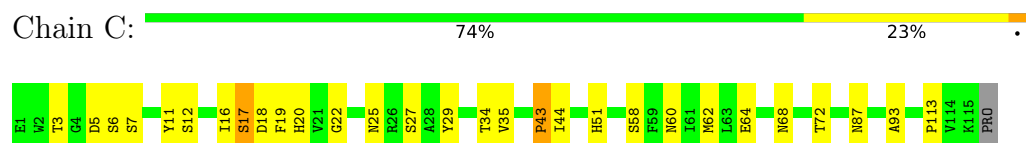
### 3 Residue-property plots [i](#)

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. 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. 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.

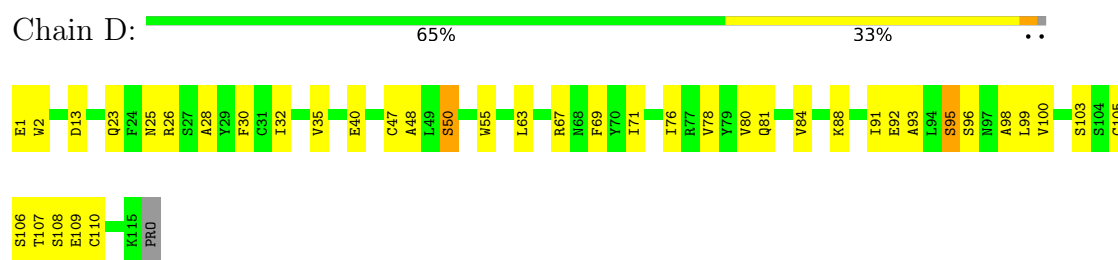
- Molecule 1: Pertussis toxin-like subunit ArtA



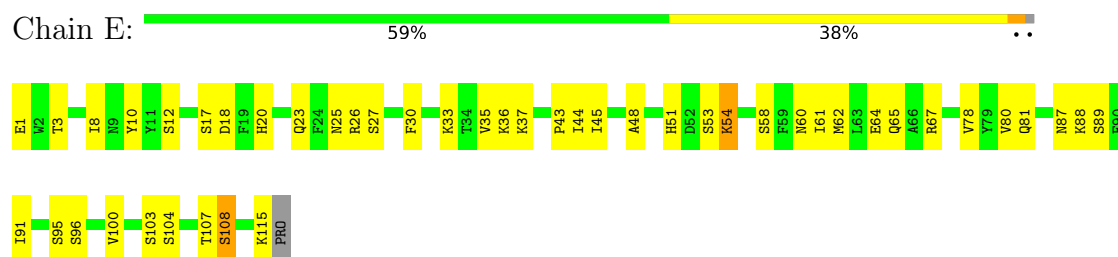
- Molecule 2: Subtilase cytotoxin subunit B



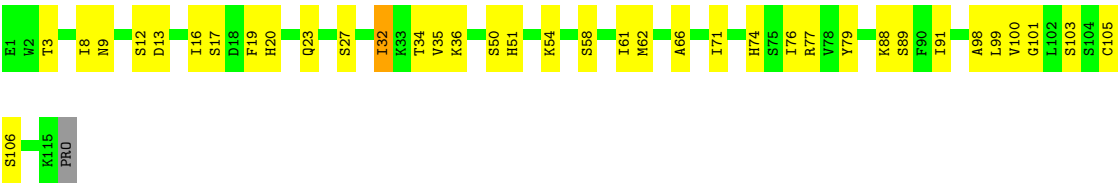
- Molecule 2: Subtilase cytotoxin subunit B



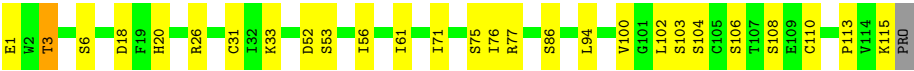
- Molecule 2: Subtilase cytotoxin subunit B



● Molecule 2: Subtilase cytotoxin subunit B



● Molecule 2: Subtilase cytotoxin subunit B



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 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	B	0.12	0/1821	0.34	0/2471
2	C	0.16	0/926	0.39	1/1256 (0.1%)
2	D	0.15	0/926	0.39	0/1256
2	E	0.19	0/926	0.42	0/1256
2	F	0.14	0/926	0.35	0/1256
2	G	0.14	0/926	0.36	0/1256
All	All	0.15	0/6451	0.37	1/8751 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	43	PRO	CA-N-CD	-5.32	104.55	112.00

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	B	1780	0	1730	48	0
2	C	902	0	862	17	0
2	D	902	0	862	26	0
2	E	902	0	862	29	0
2	F	902	0	862	22	0
2	G	902	0	862	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6290	0	6040	138	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 11.

All (138) 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:B:118:GLN:HB3	1:B:120:GLU:HG3	1.67	0.76
2:F:3:THR:HG23	2:F:100:VAL:HG23	1.70	0.73
2:D:40:GLU:OE1	2:D:40:GLU:N	2.20	0.72
2:C:64:GLU:OE1	2:D:67:ARG:NH1	2.20	0.72
1:B:177:GLN:NE2	1:B:178:ALA:O	2.25	0.69
1:B:83:LYS:HE3	1:B:134:LYS:HE3	1.74	0.69
2:D:103:SER:OG	2:E:20:HIS:ND1	2.28	0.66
2:F:91:ILE:HD12	2:F:91:ILE:H	1.61	0.65
2:F:27:SER:HB2	2:F:51:HIS:H	1.61	0.64
2:E:36:LYS:HD2	2:E:43:PRO:HD3	1.79	0.64
1:B:109:ALA:HB3	2:G:71:ILE:HG23	1.79	0.63
2:D:25:ASN:O	2:D:26:ARG:NH1	2.21	0.61
2:E:27:SER:HB2	2:E:51:HIS:H	1.65	0.61
2:D:84:VAL:HG21	2:D:98:ALA:HB2	1.83	0.61
2:F:13:ASP:HB2	2:F:36:LYS:HE2	1.83	0.60
2:E:18:ASP:HB2	2:E:33:LYS:HB3	1.83	0.60
1:B:85:ARG:HD3	1:B:158:TYR:HE1	1.66	0.60
2:C:16:ILE:HA	2:C:34:THR:HG22	1.84	0.60
2:E:45:ILE:HB	2:E:95:SER:HB3	1.83	0.60
2:E:103:SER:OG	2:F:20:HIS:ND1	2.34	0.60
2:C:58:SER:HB3	2:D:23:GLN:HB2	1.84	0.59
2:F:8:ILE:HD12	2:F:100:VAL:HG21	1.85	0.58
1:B:72:HIS:CE1	1:B:74:LYS:HG2	2.39	0.57
2:C:68:ASN:O	2:C:72:THR:HG23	2.04	0.57
2:E:104:SER:HB2	2:F:19:PHE:H	1.69	0.57
1:B:30:TYR:HA	1:B:51:ARG:HG2	1.87	0.56
2:D:25:ASN:O	2:D:26:ARG:HD3	2.06	0.56
1:B:141:ASP:O	1:B:145:GLY:N	2.36	0.55
2:E:8:ILE:HD12	2:E:100:VAL:HG21	1.89	0.55
1:B:54:VAL:HG22	1:B:122:VAL:HG12	1.88	0.55
1:B:11:ARG:HB2	1:B:55:THR:HG22	1.89	0.55
1:B:146:GLN:NE2	2:E:37:LYS:O	2.39	0.55
2:F:103:SER:OG	2:G:20:HIS:ND1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:58:SER:HB3	2:F:23:GLN:HB2	1.90	0.54
1:B:39:SER:HA	1:B:184:ILE:HG23	1.89	0.54
2:E:1:GLU:OE1	2:E:54:LYS:NZ	2.36	0.53
2:D:1:GLU:O	2:E:25:ASN:N	2.32	0.53
2:D:106:SER:O	2:D:108:SER:N	2.42	0.53
2:C:22:GLY:HA3	2:G:3:THR:HG21	1.91	0.52
1:B:65:ILE:HG12	1:B:191:ILE:HG21	1.91	0.52
1:B:113:SER:HB3	2:F:71:ILE:HG22	1.91	0.52
2:E:91:ILE:HG12	2:E:96:SER:HB3	1.92	0.52
2:C:20:HIS:ND1	2:G:103:SER:OG	2.44	0.51
1:B:96:SER:HA	1:B:169:VAL:HG12	1.93	0.51
2:F:16:ILE:HA	2:F:34:THR:HG22	1.92	0.51
1:B:37:LEU:HD13	1:B:52:TYR:HB2	1.93	0.51
2:D:95:SER:OG	2:D:96:SER:N	2.44	0.51
2:C:35:VAL:HG23	2:C:43:PRO:HB3	1.93	0.50
2:E:35:VAL:HG12	2:E:37:LYS:H	1.75	0.50
2:G:18:ASP:HB2	2:G:33:LYS:HB3	1.93	0.50
2:D:67:ARG:O	2:D:71:ILE:HG12	2.12	0.49
1:B:193:SER:OG	1:B:194:CYS:N	2.45	0.49
1:B:15:ASN:O	1:B:82:TYR:OH	2.27	0.49
1:B:61:LYS:HE2	1:B:118:GLN:HE21	1.77	0.49
2:C:60:ASN:O	2:C:64:GLU:HG3	2.12	0.48
1:B:180:THR:HB	1:B:182:GLN:HG2	1.95	0.48
2:D:63:LEU:O	2:D:67:ARG:HG3	2.13	0.48
1:B:71:SER:HB2	2:D:106:SER:HB2	1.95	0.48
2:E:60:ASN:O	2:E:64:GLU:HG3	2.13	0.48
2:F:54:LYS:HB2	2:G:26:ARG:HH22	1.78	0.48
1:B:52:TYR:HB3	1:B:122:VAL:HB	1.95	0.48
2:G:106:SER:OG	2:G:108:SER:OG	2.31	0.48
1:B:214:MET:HE3	1:B:215:PRO:HD2	1.96	0.47
2:D:55:TRP:NE1	2:D:81:GLN:OE1	2.40	0.47
2:G:52:ASP:O	2:G:53:SER:OG	2.22	0.47
2:E:17:SER:HB3	2:E:35:VAL:HG22	1.97	0.47
2:F:77:ARG:HB2	2:F:105:CYS:SG	2.55	0.47
2:D:91:ILE:HG12	2:D:96:SER:HB3	1.97	0.46
1:B:162:SER:O	1:B:162:SER:OG	2.33	0.46
2:G:56:ILE:HD12	2:G:56:ILE:H	1.81	0.46
2:F:88:LYS:HD2	2:F:88:LYS:N	2.30	0.46
2:G:6:SER:O	2:G:115:LYS:NZ	2.48	0.46
2:E:26:ARG:HH12	2:E:51:HIS:HB3	1.79	0.46
1:B:187:PHE:HB3	1:B:216:PHE:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:ARG:HG2	2:F:79:TYR:CE1	2.50	0.46
2:C:19:PHE:H	2:G:104:SER:HB2	1.81	0.45
1:B:37:LEU:HD21	1:B:122:VAL:HG11	1.98	0.45
2:C:27:SER:HB2	2:C:51:HIS:H	1.82	0.45
1:B:52:TYR:HA	1:B:123:SER:O	2.17	0.45
1:B:130:GLU:HB2	1:B:159:VAL:HG23	1.98	0.45
2:C:25:ASN:N	2:G:1:GLU:O	2.44	0.45
2:F:58:SER:O	2:F:61:ILE:HG22	2.17	0.45
2:D:69:PHE:CG	2:D:76:ILE:HG21	2.52	0.45
2:F:3:THR:HG21	2:F:101:GLY:HA3	1.98	0.45
2:E:44:ILE:HD12	2:E:44:ILE:N	2.32	0.45
2:C:113:PRO:HB3	2:D:93:ALA:HB1	1.99	0.44
2:G:56:ILE:HD12	2:G:56:ILE:N	2.33	0.44
2:F:62:MET:HG2	2:F:99:LEU:HG	1.98	0.44
2:D:30:PHE:CE1	2:D:48:ALA:HB3	2.53	0.44
2:E:30:PHE:CE1	2:E:48:ALA:HB3	2.53	0.44
2:C:20:HIS:NE2	2:C:29:TYR:OH	2.50	0.44
1:B:108:ASN:OD1	1:B:108:ASN:N	2.39	0.43
2:D:47:CYS:O	2:D:98:ALA:HA	2.18	0.43
2:E:1:GLU:OE2	2:E:81:GLN:NE2	2.47	0.43
1:B:35:GLN:NE2	1:B:111:GLU:OE2	2.52	0.43
1:B:115:ILE:H	1:B:115:ILE:HG13	1.62	0.43
1:B:72:HIS:NE2	1:B:74:LYS:HE2	2.33	0.43
2:E:87:ASN:OD1	2:E:89:SER:OG	2.29	0.43
2:G:26:ARG:N	2:G:26:ARG:HD2	2.34	0.43
2:C:17:SER:OG	2:C:18:ASP:OD2	2.36	0.43
2:D:32:ILE:HG12	2:D:99:LEU:HD22	2.00	0.43
2:F:74:HIS:O	2:F:76:ILE:HG23	2.19	0.43
2:F:98:ALA:O	2:F:100:VAL:HG13	2.19	0.43
1:B:26:SER:HB2	1:B:201:CYS:HB2	2.01	0.43
2:D:2:TRP:HA	2:E:23:GLN:O	2.19	0.43
2:E:30:PHE:HZ	2:E:62:MET:HB3	1.82	0.43
1:B:7:ASP:OD1	1:B:7:ASP:N	2.43	0.43
2:F:17:SER:HB3	2:F:35:VAL:HG12	2.00	0.42
2:G:77:ARG:NH2	2:G:110:CYS:HB2	2.34	0.42
1:B:41:ARG:NH1	1:B:183:ARG:O	2.52	0.42
1:B:225:PHE:HE1	2:E:67:ARG:HD2	1.85	0.42
1:B:133:GLN:HG3	1:B:158:TYR:CD2	2.54	0.42
2:F:32:ILE:HG21	2:F:66:ALA:HB1	2.01	0.42
1:B:54:VAL:HG12	1:B:195:PHE:CE1	2.55	0.42
2:C:58:SER:O	2:C:62:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:TYR:HA	2:E:78:VAL:O	2.19	0.42
2:D:88:LYS:HD2	2:D:92:GLU:HG2	2.02	0.42
2:E:88:LYS:HD2	2:E:88:LYS:O	2.19	0.42
1:B:9:VAL:HG23	1:B:84:ILE:HB	2.02	0.42
1:B:198:TYR:CD2	1:B:213:LYS:HD3	2.55	0.42
1:B:72:HIS:HE2	1:B:74:LYS:HE2	1.84	0.41
1:B:33:ASP:HA	1:B:174:PRO:HG2	2.01	0.41
2:G:31:CYS:SG	2:G:94:LEU:HD13	2.60	0.41
1:B:20:ILE:HG13	1:B:82:TYR:OH	2.20	0.41
1:B:61:LYS:HD3	1:B:118:GLN:HA	2.02	0.41
2:D:28:ALA:O	2:D:50:SER:N	2.47	0.41
2:E:61:ILE:O	2:E:65:GLN:HB2	2.20	0.41
2:E:115:LYS:HE2	2:E:115:LYS:HB2	1.96	0.41
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.93	0.41
2:D:78:VAL:HG12	2:D:80:VAL:HG13	2.03	0.41
1:B:188:GLY:HA3	1:B:191:ILE:HD12	2.02	0.41
2:G:76:ILE:HD13	2:G:102:LEU:HD22	2.03	0.41
1:B:217:TYR:CE1	1:B:222:VAL:HG21	2.56	0.41
1:B:222:VAL:HA	2:D:71:ILE:HD12	2.03	0.41
2:C:11:TYR:CD2	2:C:44:ILE:HD13	2.56	0.41
2:E:107:THR:O	2:E:108:SER:C	2.63	0.41
2:C:93:ALA:HB1	2:G:113:PRO:HA	2.02	0.40
2:D:30:PHE:CE2	2:D:99:LEU:HD23	2.57	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 PDB entries followed by that with respect to all EM entries.

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	B	223/243 (92%)	213 (96%)	10 (4%)	0	100	100
2	C	113/116 (97%)	107 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	113/116 (97%)	100 (88%)	12 (11%)	1 (1%)	14	29
2	E	113/116 (97%)	103 (91%)	7 (6%)	3 (3%)	4	6
2	F	113/116 (97%)	102 (90%)	11 (10%)	0	100	100
2	G	113/116 (97%)	103 (91%)	10 (9%)	0	100	100
All	All	788/823 (96%)	728 (92%)	56 (7%)	4 (0%)	27	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	107	THR
2	E	53	SER
2	E	54	LYS
2	E	108	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	B	200/216 (93%)	189 (94%)	11 (6%)	18	37
2	C	102/103 (99%)	95 (93%)	7 (7%)	13	26
2	D	102/103 (99%)	94 (92%)	8 (8%)	10	21
2	E	102/103 (99%)	99 (97%)	3 (3%)	37	62
2	F	102/103 (99%)	96 (94%)	6 (6%)	16	33
2	G	102/103 (99%)	97 (95%)	5 (5%)	21	41
All	All	710/731 (97%)	670 (94%)	40 (6%)	20	36

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	LEU
1	B	50	SER
1	B	57	SER

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Mol	Chain	Res	Type
1	B	83	LYS
1	B	108	ASN
1	B	113	SER
1	B	119	SER
1	B	151	THR
1	B	197	ILE
1	B	200	VAL
1	B	222	VAL
2	C	3	THR
2	C	5	ASP
2	C	6	SER
2	C	7	SER
2	C	12	SER
2	C	17	SER
2	C	87	ASN
2	D	13	ASP
2	D	35	VAL
2	D	50	SER
2	D	95	SER
2	D	100	VAL
2	D	105	CYS
2	D	109	GLU
2	D	110	CYS
2	E	3	THR
2	E	12	SER
2	E	80	VAL
2	F	9	ASN
2	F	12	SER
2	F	32	ILE
2	F	50	SER
2	F	89	SER
2	F	106	SER
2	G	3	THR
2	G	61	ILE
2	G	75	SER
2	G	86	SER
2	G	100	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN

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Mol	Chain	Res	Type
2	C	9	ASN
2	D	68	ASN
2	D	83	ASN
2	G	23	GLN
2	G	51	HIS

### 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 oligosaccharides 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.