



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2025 – 01:19 AM JST

PDB ID : 9JG8 / pdb\_00009jg8  
EMDB ID : EMD-61458  
Title : Structure of cargo complex (BtpeA-BtaeB-BtapC) bound to the VgrG spike from the Type VI secretion system  
Authors : Zheng, S.N.; Li, W.X.; Chen, Z.; Gao, X.  
Deposited on : 2024-09-06  
Resolution : 3.06 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

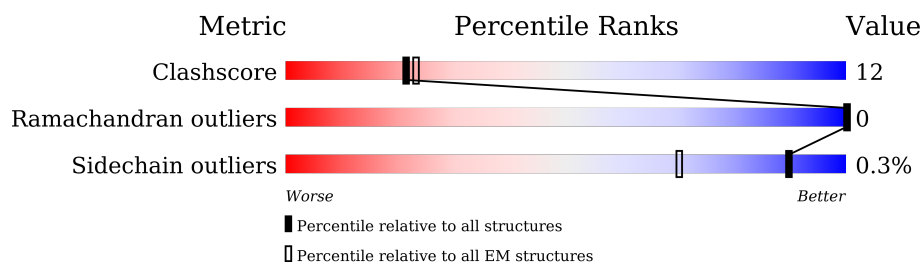
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.06 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	608	 17% 8% 75%
2	C	617	 30% 11% 59%
3	A	254	 67% 22% 11%
4	E	618	 6% 92%
4	F	618	 7% 92%
4	G	618	 6% 92%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6002 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 DUF3289 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	151	Total	C	N	O	S	0	0
			1118	704	187	210	17		

- Molecule 2 is a protein called Peptidase C39-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	253	Total	C	N	O	S	0	0
			1982	1264	330	377	11		

- Molecule 3 is a protein called Bacteroides T6SS Adapter Protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	226	Total	C	N	O	S	0	0
			1863	1196	296	361	10		

- Molecule 4 is a protein called Type VI secretion system spike protein VgrG.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	49	Total	C	N	O	S	0	0
			352	216	58	75	3		
4	E	48	Total	C	N	O	S	0	0
			343	211	56	73	3		
4	F	48	Total	C	N	O	S	0	0
			343	211	56	73	3		

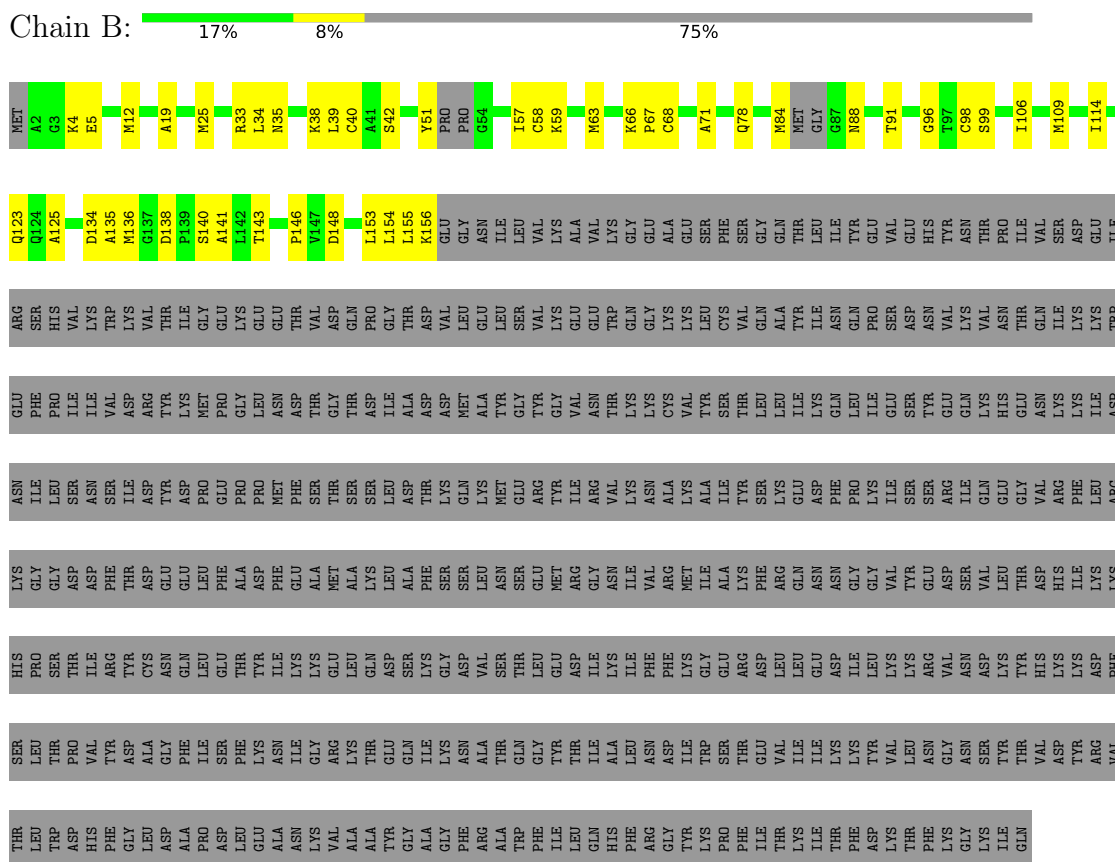
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	

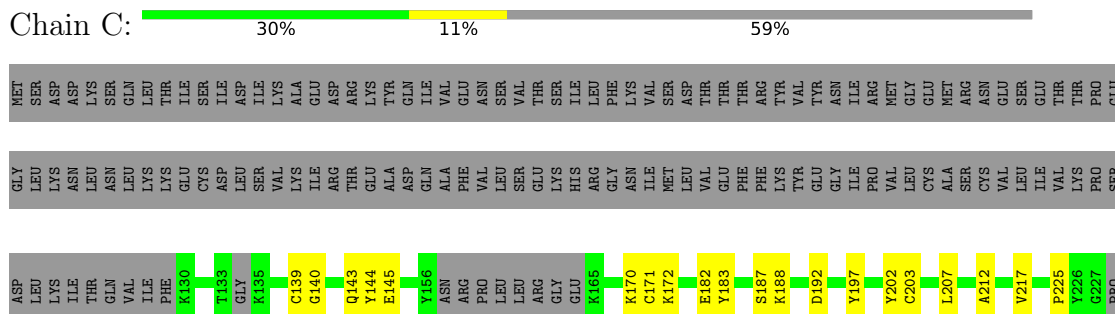
### 3 Residue-property plots

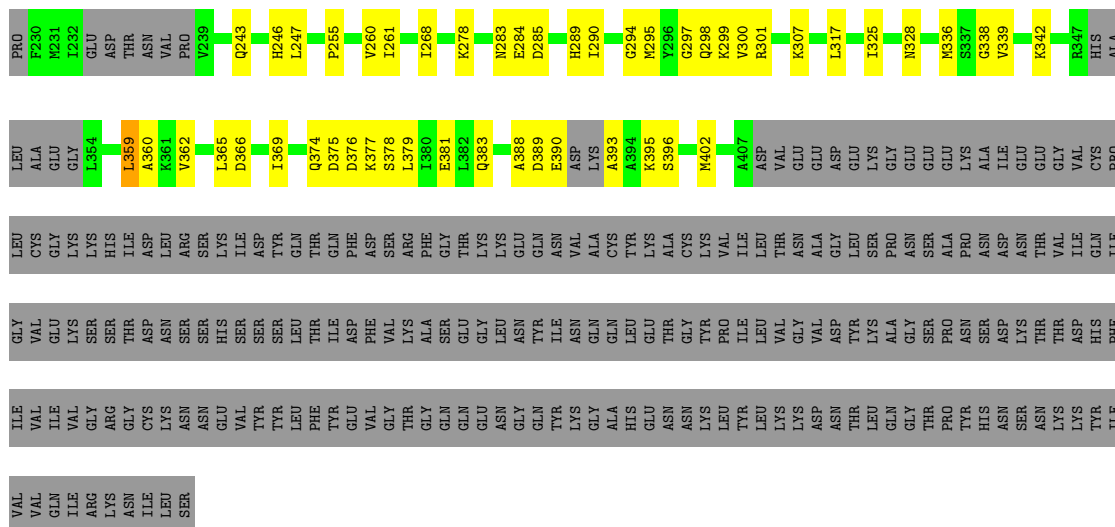
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: DUF3289 family protein

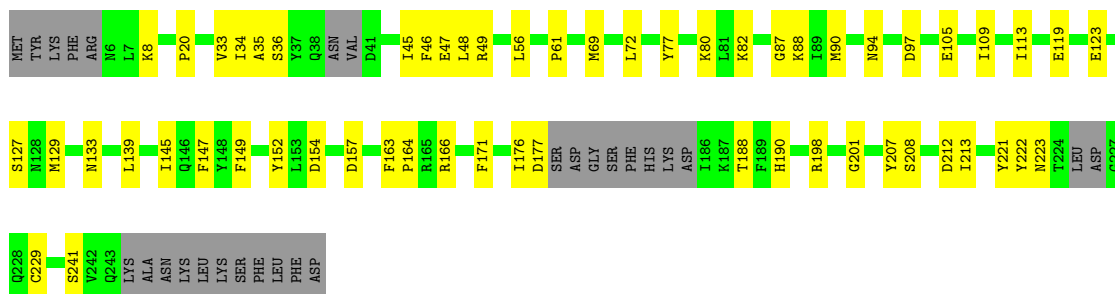


- Molecule 2: Peptidase C39-like domain-containing protein

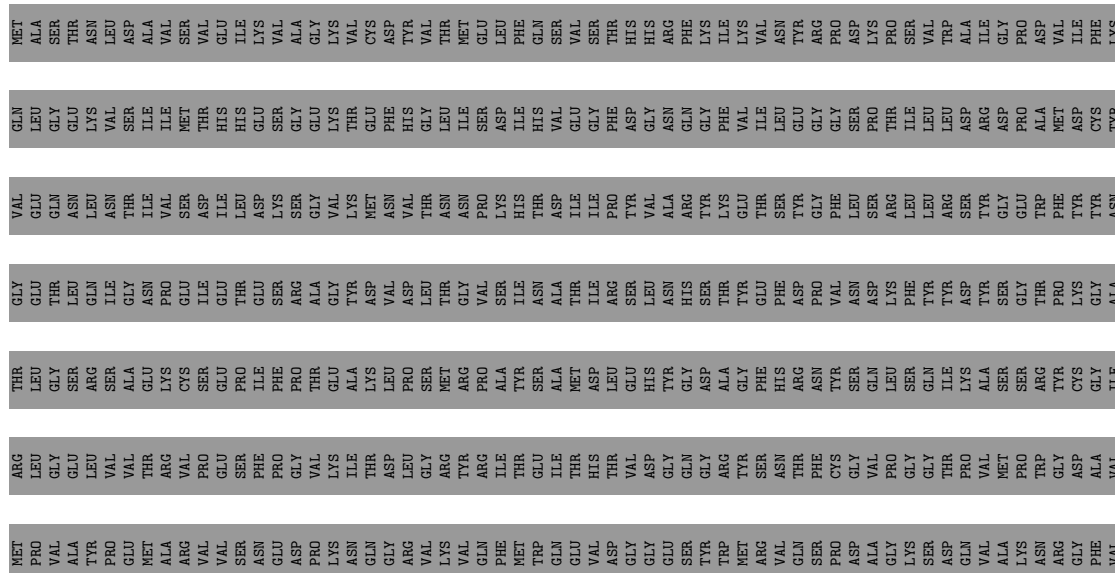




- Molecule 3: Bacteroides T6SS Adapter Protein C

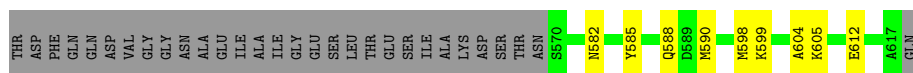


- Molecule 4: Type VI secretion system spike protein VgrG





- Molecule 4: Type VI secretion system spike protein VgrG



- Molecule 4: Type VI secretion system spike protein VgrG



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106021	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)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor



## 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: ZN

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	0.18	0/1140	0.34	0/1536
2	C	0.29	0/2012	0.42	0/2695
3	A	0.24	0/1899	0.37	0/2556
4	E	0.11	0/343	0.27	0/461
4	F	0.09	0/343	0.26	0/461
4	G	0.10	0/352	0.27	0/473
All	All	0.23	0/6089	0.37	0/8182

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	B	1118	0	1116	33	0
2	C	1982	0	1989	59	0
3	A	1863	0	1820	37	0
4	E	343	0	348	9	0
4	F	343	0	348	8	0
4	G	352	0	356	12	0
5	B	1	0	0	0	0
All	All	6002	0	5977	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 12.

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:42:SER:HB3	1:B:84:MET:HE2	1.66	0.76
2:C:336:MET:HE2	2:C:339:VAL:HG21	1.70	0.72
3:A:154:ASP:HB3	3:A:176:ILE:HG22	1.77	0.66
3:A:20:PRO:HD3	3:A:229:CYS:SG	2.34	0.66
3:A:119:GLU:O	3:A:123:GLU:HG2	1.96	0.66
2:C:285:ASP:HB3	2:C:395:LYS:HA	1.76	0.66
3:A:35:ALA:HA	3:A:46:PHE:HA	1.77	0.66
2:C:284:GLU:HG2	2:C:393:ALA:HA	1.77	0.65
2:C:336:MET:CE	2:C:339:VAL:HG21	2.28	0.63
2:C:139:CYS:SG	2:C:140:GLY:N	2.72	0.62
1:B:19:ALA:HB2	1:B:59:LYS:HZ1	1.65	0.61
2:C:395:LYS:HG2	2:C:396:SER:N	2.15	0.61
1:B:96:GLY:H	1:B:106:ILE:HB	1.66	0.60
2:C:183:TYR:CE2	2:C:217:VAL:HG21	2.37	0.60
1:B:58:CYS:N	1:B:66:LYS:O	2.33	0.60
2:C:255:PRO:HB3	2:C:295:MET:HG2	1.83	0.60
2:C:376:ASP:HA	2:C:379:LEU:HD22	1.82	0.60
2:C:207:LEU:HD23	2:C:247:LEU:HD21	1.82	0.60
3:A:129:MET:O	3:A:129:MET:HG3	2.01	0.59
2:C:188:LYS:NZ	3:A:127:SER:OG	2.33	0.58
2:C:300:VAL:HG11	2:C:362:VAL:HG13	1.85	0.58
2:C:395:LYS:HG2	2:C:396:SER:H	1.67	0.58
1:B:12:MET:HA	1:B:12:MET:HE2	1.85	0.58
1:B:34:LEU:HD13	1:B:40:CYS:HB2	1.85	0.57
1:B:63:MET:SD	1:B:63:MET:N	2.77	0.57
3:A:34:ILE:HD12	3:A:49:ARG:HE	1.69	0.57
1:B:125:ALA:O	3:A:166:ARG:NH1	2.38	0.57
1:B:155:LEU:HD21	2:C:197:TYR:HA	1.87	0.57
1:B:57:ILE:O	1:B:59:LYS:NZ	2.39	0.56
4:F:587:ALA:HB3	4:F:590:MET:HE2	1.88	0.56
2:C:172:LYS:HD2	2:C:225:PRO:HD2	1.86	0.56
2:C:143:GLN:HG2	2:C:246:HIS:HB3	1.88	0.55
2:C:297:GLY:HA2	2:C:325:ILE:O	2.06	0.55
3:A:163:PHE:HB3	3:A:164:PRO:HD3	1.89	0.55
2:C:212:ALA:HA	2:C:247:LEU:HB3	1.89	0.54
2:C:389:ASP:O	2:C:390:GLU:HB2	2.06	0.54
1:B:98:CYS:HB2	1:B:106:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:56:LEU:HD12	3:A:61:PRO:HB3	1.89	0.54
3:A:157:ASP:OD1	3:A:157:ASP:N	2.39	0.54
3:A:48:LEU:HD12	3:A:77:TYR:HE1	1.72	0.54
2:C:295:MET:HB3	2:C:298:GLN:HG3	1.90	0.53
2:C:278:LYS:HZ2	2:C:379:LEU:HD23	1.74	0.53
1:B:148:ASP:OD1	2:C:188:LYS:NZ	2.31	0.53
2:C:300:VAL:CG1	2:C:362:VAL:HG13	2.39	0.53
1:B:138:ASP:OD2	1:B:140:SER:HB3	2.08	0.53
4:G:588:GLN:O	4:F:596:GLY:N	2.41	0.53
4:F:579:VAL:HG21	4:F:583:LEU:HD12	1.91	0.52
1:B:57:ILE:HA	1:B:67:PRO:HA	1.91	0.52
2:C:297:GLY:CA	2:C:325:ILE:O	2.58	0.52
3:A:36:SER:N	3:A:45:ILE:O	2.43	0.51
1:B:123:GLN:O	3:A:166:ARG:NH1	2.44	0.51
2:C:375:ASP:OD1	2:C:375:ASP:N	2.43	0.51
4:G:602:ALA:HB2	4:E:598:MET:HE3	1.93	0.51
1:B:141:ALA:HA	1:B:146:PRO:HB3	1.93	0.51
3:A:47:GLU:HA	3:A:80:LYS:HA	1.93	0.50
2:C:360:ALA:H	2:C:374:GLN:HB2	1.75	0.50
2:C:278:LYS:NZ	2:C:379:LEU:O	2.40	0.50
2:C:317:LEU:HD12	2:C:339:VAL:HG12	1.94	0.50
4:G:579:VAL:HG12	4:G:581:GLU:H	1.75	0.50
2:C:284:GLU:HG3	2:C:388:ALA:HB2	1.93	0.50
3:A:139:LEU:HG	3:A:145:ILE:HD13	1.94	0.49
4:E:604:ALA:N	4:F:596:GLY:O	2.46	0.49
4:G:583:LEU:HD11	4:G:585:TYR:HE1	1.78	0.49
2:C:260:VAL:HG22	2:C:290:ILE:HG23	1.94	0.48
1:B:78:GLN:HG3	1:B:88:ASN:HB2	1.95	0.48
3:A:33:VAL:HG22	3:A:48:LEU:HA	1.96	0.48
1:B:71:ALA:HB3	1:B:99:SER:HB3	1.95	0.48
4:G:589:ASP:HB2	4:E:582:ASN:HB3	1.95	0.48
2:C:366:ASP:HB3	2:C:369:ILE:HD12	1.96	0.47
2:C:171:CYS:SG	2:C:172:LYS:N	2.87	0.47
2:C:301:ARG:HB3	2:C:301:ARG:NH1	2.30	0.47
1:B:138:ASP:OD1	2:C:187:SER:OG	2.33	0.47
1:B:153:LEU:HD12	2:C:203:CYS:HB2	1.95	0.47
2:C:336:MET:O	2:C:339:VAL:HG22	2.16	0.46
1:B:33:ARG:HG3	1:B:39:LEU:HD23	1.97	0.46
3:A:147:PHE:O	3:A:152:TYR:OH	2.31	0.46
2:C:307:LYS:HB2	2:C:359:LEU:HD11	1.97	0.46
2:C:317:LEU:HD12	2:C:339:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:177:ASP:O	3:A:190:HIS:ND1	2.33	0.45
3:A:198:ARG:HA	3:A:223:ASN:HB2	1.98	0.45
1:B:154:LEU:HD22	2:C:192:ASP:HB2	1.99	0.45
2:C:268:ILE:HD12	2:C:289:HIS:CG	2.51	0.45
1:B:114:ILE:HG21	3:A:113:ILE:HD11	1.98	0.45
3:A:87:GLY:O	3:A:149:PHE:HB3	2.17	0.45
4:E:590:MET:HG2	4:F:583:LEU:HD22	1.99	0.45
3:A:207:TYR:CE1	3:A:213:ILE:HG12	2.51	0.44
4:G:583:LEU:HD11	4:G:585:TYR:CE1	2.52	0.44
3:A:8:LYS:HB2	3:A:34:ILE:HA	2.00	0.44
4:E:612:GLU:HB3	4:F:604:ALA:O	2.18	0.43
1:B:140:SER:O	1:B:143:THR:OG1	2.34	0.43
2:C:284:GLU:CG	2:C:388:ALA:HB2	2.48	0.43
1:B:35:ASN:HB3	1:B:38:LYS:HD2	2.00	0.43
1:B:25:MET:HG3	1:B:51:TYR:CE2	2.54	0.43
3:A:133:ASN:OD1	3:A:133:ASN:N	2.52	0.43
4:E:588:GLN:HA	4:E:588:GLN:OE1	2.19	0.43
2:C:383:GLN:N	2:C:383:GLN:OE1	2.52	0.43
3:A:72:LEU:HD23	3:A:72:LEU:HA	1.83	0.43
1:B:4:LYS:HB2	1:B:4:LYS:HE2	1.82	0.43
3:A:94:ASN:OD1	3:A:97:ASP:HB2	2.19	0.43
3:A:208:SER:HB2	3:A:212:ASP:HB2	2.01	0.43
4:G:579:VAL:HG12	4:G:581:GLU:O	2.18	0.43
1:B:134:ASP:HB2	3:A:69:MET:HB3	2.01	0.42
2:C:374:GLN:NE2	2:C:378:SER:O	2.52	0.42
3:A:105:GLU:O	3:A:109:ILE:HD12	2.19	0.42
4:G:571:ILE:H	4:G:571:ILE:HD12	1.84	0.42
2:C:261:ILE:HG13	2:C:289:HIS:HB2	2.01	0.42
4:G:609:LYS:HE3	4:G:609:LYS:HB3	1.89	0.42
3:A:8:LYS:O	3:A:241:SER:N	2.44	0.42
2:C:170:LYS:HB3	3:A:171:PHE:CD2	2.55	0.42
2:C:299:LYS:HB2	2:C:365:LEU:HD12	2.00	0.42
2:C:402:MET:HE3	2:C:402:MET:HB3	1.97	0.42
2:C:144:TYR:HD1	2:C:145:GLU:H	1.67	0.42
2:C:283:ASN:ND2	2:C:390:GLU:OE2	2.53	0.42
3:A:88:LYS:HE3	3:A:88:LYS:HB3	1.84	0.42
3:A:201:GLY:HA2	3:A:221:TYR:CE1	2.55	0.42
4:F:609:LYS:HB2	4:F:609:LYS:HE2	1.88	0.42
1:B:135:ALA:HB3	1:B:136:MET:HE2	2.02	0.42
3:A:177:ASP:OD1	3:A:188:THR:HG23	2.20	0.42
1:B:58:CYS:HB2	1:B:68:CYS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:GLU:O	1:B:91:THR:HG23	2.19	0.41
4:G:592:LEU:HD22	4:E:585:TYR:HB2	2.02	0.41
4:E:599:LYS:HE2	4:E:599:LYS:HB2	1.77	0.41
2:C:278:LYS:HD2	2:C:381:GLU:HG3	2.01	0.41
4:G:582:ASN:N	4:G:582:ASN:OD1	2.53	0.41
4:F:590:MET:HE3	4:F:590:MET:HB2	1.78	0.41
2:C:297:GLY:N	2:C:325:ILE:O	2.54	0.41
2:C:389:ASP:O	2:C:390:GLU:CB	2.68	0.41
3:A:123:GLU:HG2	3:A:123:GLU:H	1.74	0.41
4:G:613:GLY:O	4:E:605:LYS:HA	2.21	0.41
1:B:12:MET:HG3	1:B:109:MET:HB2	2.03	0.41
2:C:217:VAL:HA	2:C:243:GLN:O	2.20	0.41
1:B:156:LYS:HG2	2:C:202:TYR:CD2	2.56	0.40
2:C:170:LYS:O	2:C:225:PRO:HG3	2.21	0.40
2:C:182:GLU:HG2	2:C:183:TYR:H	1.86	0.40
3:A:82:LYS:O	3:A:90:MET:HG3	2.22	0.40
2:C:294:GLY:N	2:C:328:ASN:OD1	2.55	0.40
2:C:338:GLY:O	2:C:342:LYS:HG2	2.21	0.40
2:C:377:LYS:HD2	2:C:377:LYS:C	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	145/608 (24%)	138 (95%)	7 (5%)	0	100	100
2	C	239/617 (39%)	229 (96%)	10 (4%)	0	100	100
3	A	218/254 (86%)	204 (94%)	14 (6%)	0	100	100
4	E	46/618 (7%)	44 (96%)	2 (4%)	0	100	100
4	F	46/618 (7%)	42 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	47/618 (8%)	46 (98%)	1 (2%)	0	100	100
All	All	741/3333 (22%)	703 (95%)	38 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	125/533 (24%)	125 (100%)	0	100	100
2	C	215/541 (40%)	214 (100%)	1 (0%)	86	91
3	A	210/236 (89%)	209 (100%)	1 (0%)	86	91
4	E	37/524 (7%)	37 (100%)	0	100	100
4	F	37/524 (7%)	37 (100%)	0	100	100
4	G	38/524 (7%)	38 (100%)	0	100	100
All	All	662/2882 (23%)	660 (100%)	2 (0%)	90	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	359	LEU
3	A	222	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	ASN
2	C	143	GLN
2	C	283	ASN
2	C	374	GLN
3	A	120	GLN
4	E	582	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	F	595	GLN

### 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](#)

Of 1 ligands modelled in this entry, 1 is 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.