



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:07 PM BST

PDB ID : 2HIL
EMDB ID: : EMD-1236
Title : Structure of the Neisseria gonorrhoeae Type IV pilus filament from x-ray crystallography and electron cryomicroscopy
Authors : Craig, L.; Volkmann, N.; Egelman, E.H.; Tainer, J.A.
Deposited on : 2006-06-29
Resolution : 12.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

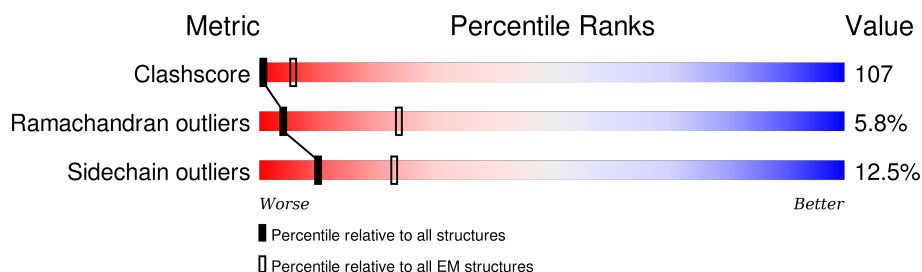
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.50 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.




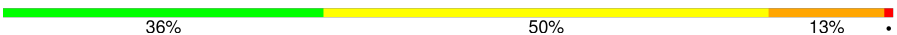

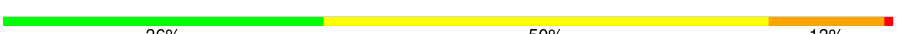
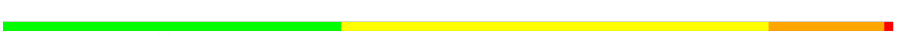

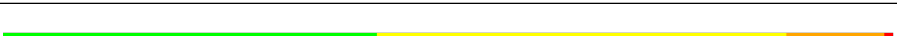
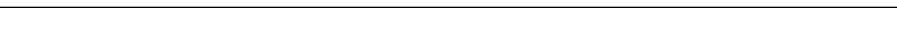
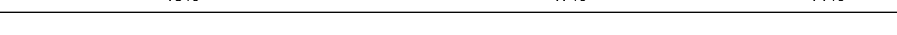
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	158	37% 49% 13% .
1	B	158	37% 49% 13% .
1	C	158	36% 50% 13% .
1	D	158	36% 50% 13% .
1	E	158	37% 49% 13% .
1	F	158	39% 48% 11% .
1	G	158	40% 47% 11% .
1	H	158	41% 46% 11% .
1	I	158	44% 44% 11% .

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Mol	Chain	Length	Quality of chain
1	J	158	 35% 51% 13%
1	K	158	 36% 50% 13%
1	L	158	 36% 50% 13%
1	M	158	 36% 50% 13%
1	N	158	 38% 48% 13%
1	O	158	 38% 49% 12%
1	P	158	 42% 46% 11%
1	Q	158	 40% 47% 11%
1	R	158	 40% 47% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MEA	A	1	-	-	X	-
1	MEA	B	1	-	-	X	-
1	MEA	C	1	-	-	X	-
1	MEA	D	1	-	-	X	-
1	MEA	E	1	-	-	X	-
1	MEA	F	1	-	-	X	-
1	MEA	G	1	-	-	X	-
1	MEA	H	1	-	-	X	-
1	MEA	J	1	-	-	X	-
1	MEA	K	1	-	-	X	-
1	MEA	L	1	-	-	X	-
1	MEA	M	1	-	-	X	-
1	MEA	N	1	-	-	X	-
1	MEA	O	1	-	-	X	-
1	MEA	P	1	-	-	X	-
1	MEA	Q	1	-	-	X	-
1	MEA	R	1	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22374 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 Fimbrial protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	B	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	C	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	D	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	E	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	F	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	G	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	H	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	I	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	J	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	K	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	L	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	M	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	N	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	O	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	P	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		
1	Q	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	158	Total	C	N	O	S	0	0
			1207	760	206	237	4		

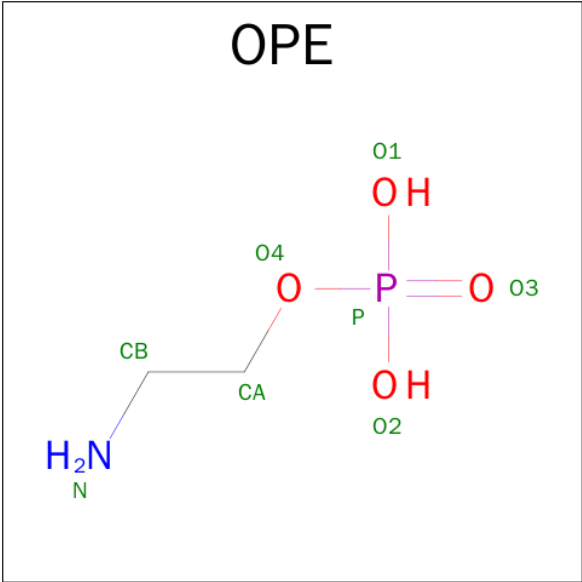
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	PRO	SEE REMARK 999	UNP P02974
A	71	THR	SER	SEE REMARK 999	UNP P02974
B	69	SER	PRO	SEE REMARK 999	UNP P02974
B	71	THR	SER	SEE REMARK 999	UNP P02974
C	69	SER	PRO	SEE REMARK 999	UNP P02974
C	71	THR	SER	SEE REMARK 999	UNP P02974
D	69	SER	PRO	SEE REMARK 999	UNP P02974
D	71	THR	SER	SEE REMARK 999	UNP P02974
E	69	SER	PRO	SEE REMARK 999	UNP P02974
E	71	THR	SER	SEE REMARK 999	UNP P02974
F	69	SER	PRO	SEE REMARK 999	UNP P02974
F	71	THR	SER	SEE REMARK 999	UNP P02974
G	69	SER	PRO	SEE REMARK 999	UNP P02974
G	71	THR	SER	SEE REMARK 999	UNP P02974
H	69	SER	PRO	SEE REMARK 999	UNP P02974
H	71	THR	SER	SEE REMARK 999	UNP P02974
I	69	SER	PRO	SEE REMARK 999	UNP P02974
I	71	THR	SER	SEE REMARK 999	UNP P02974
J	69	SER	PRO	SEE REMARK 999	UNP P02974
J	71	THR	SER	SEE REMARK 999	UNP P02974
K	69	SER	PRO	SEE REMARK 999	UNP P02974
K	71	THR	SER	SEE REMARK 999	UNP P02974
L	69	SER	PRO	SEE REMARK 999	UNP P02974
L	71	THR	SER	SEE REMARK 999	UNP P02974
M	69	SER	PRO	SEE REMARK 999	UNP P02974
M	71	THR	SER	SEE REMARK 999	UNP P02974
N	69	SER	PRO	SEE REMARK 999	UNP P02974
N	71	THR	SER	SEE REMARK 999	UNP P02974
O	69	SER	PRO	SEE REMARK 999	UNP P02974
O	71	THR	SER	SEE REMARK 999	UNP P02974
P	69	SER	PRO	SEE REMARK 999	UNP P02974
P	71	THR	SER	SEE REMARK 999	UNP P02974
Q	69	SER	PRO	SEE REMARK 999	UNP P02974
Q	71	THR	SER	SEE REMARK 999	UNP P02974
R	69	SER	PRO	SEE REMARK 999	UNP P02974
R	71	THR	SER	SEE REMARK 999	UNP P02974

- Molecule 2 is a polymer of unknown type called SUGAR (D-GALACTOSE).

Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total	C	N	O	0
			28	16	2	10	
2	B	2	Total	C	N	O	0
			28	16	2	10	
2	C	2	Total	C	N	O	0
			28	16	2	10	
2	D	2	Total	C	N	O	0
			28	16	2	10	
2	E	2	Total	C	N	O	0
			28	16	2	10	
2	F	2	Total	C	N	O	0
			28	16	2	10	
2	G	2	Total	C	N	O	0
			28	16	2	10	
2	H	2	Total	C	N	O	0
			28	16	2	10	
2	I	2	Total	C	N	O	0
			28	16	2	10	
2	J	2	Total	C	N	O	0
			28	16	2	10	
2	K	2	Total	C	N	O	0
			28	16	2	10	
2	L	2	Total	C	N	O	0
			28	16	2	10	
2	M	2	Total	C	N	O	0
			28	16	2	10	
2	N	2	Total	C	N	O	0
			28	16	2	10	
2	O	2	Total	C	N	O	0
			28	16	2	10	
2	P	2	Total	C	N	O	0
			28	16	2	10	
2	Q	2	Total	C	N	O	0
			28	16	2	10	
2	R	2	Total	C	N	O	0
			28	16	2	10	

- Molecule 3 is PHOSPHORIC ACID MONO-(2-AMINO-ETHYL) ESTER (three-letter code: OPE) (formula: C₂H₈NO₄P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	B	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	C	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	D	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	E	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	F	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	G	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	H	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	I	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	J	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	K	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	L	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	M	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	N	1	Total	C	N	O	P	0
			8	2	1	4	1	

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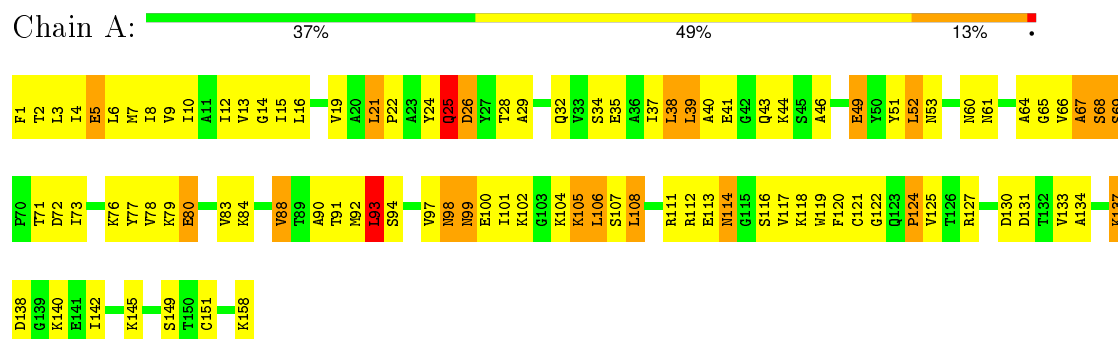
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Mol	Chain	Residues	Atoms					AltConf
3	O	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	P	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	Q	1	Total	C	N	O	P	0
			8	2	1	4	1	
3	R	1	Total	C	N	O	P	0
			8	2	1	4	1	

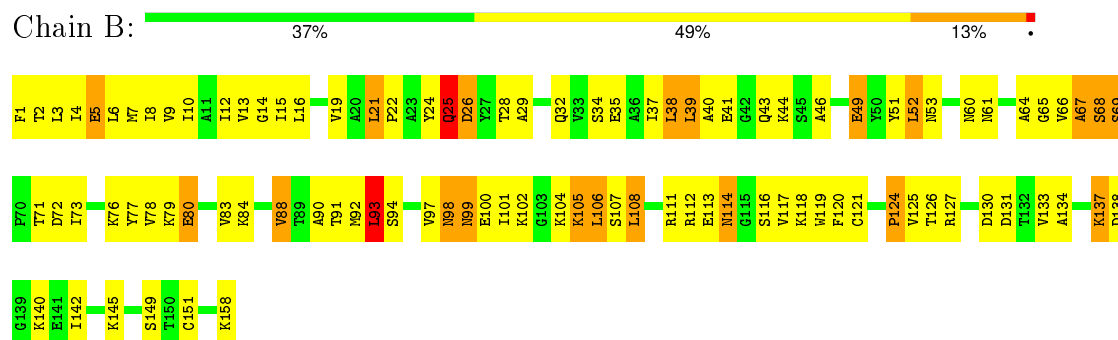
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

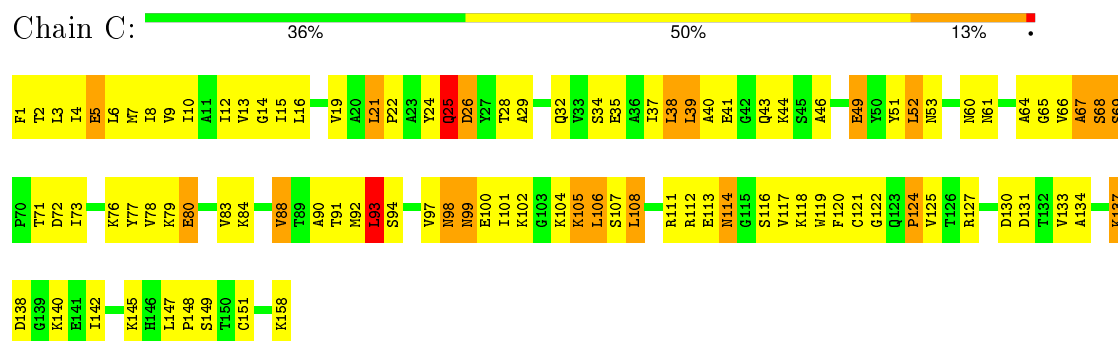
- Molecule 1: Fimbrial protein



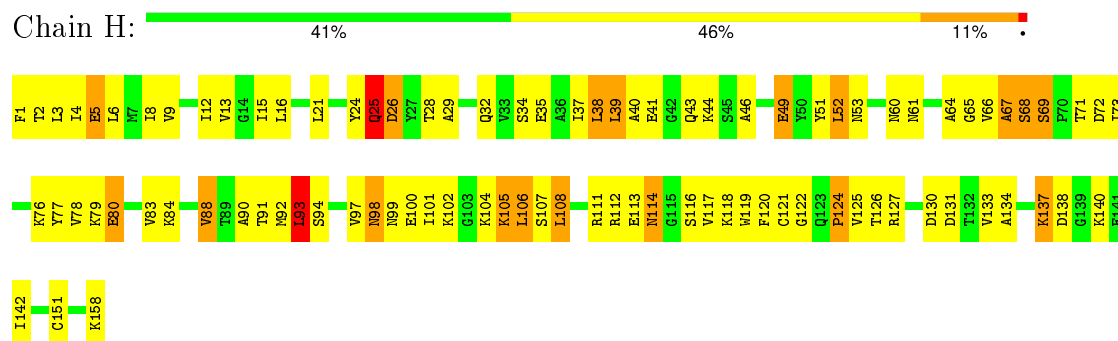
- Molecule 1: Fimbrial protein



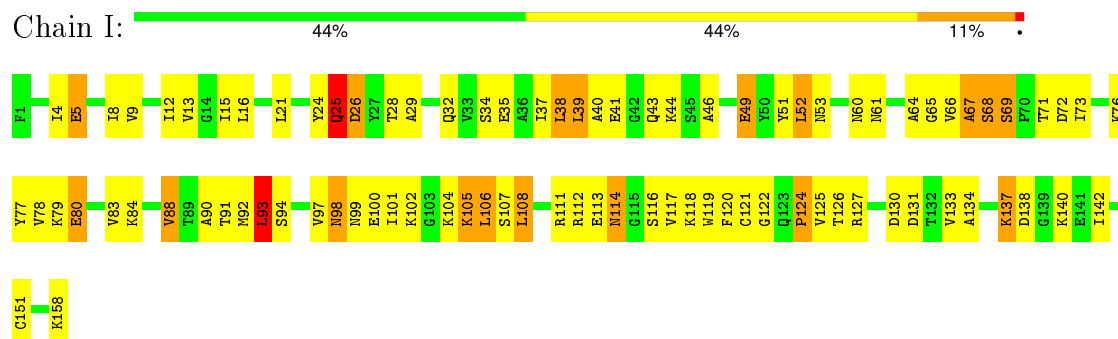
- Molecule 1: Fimbrial protein



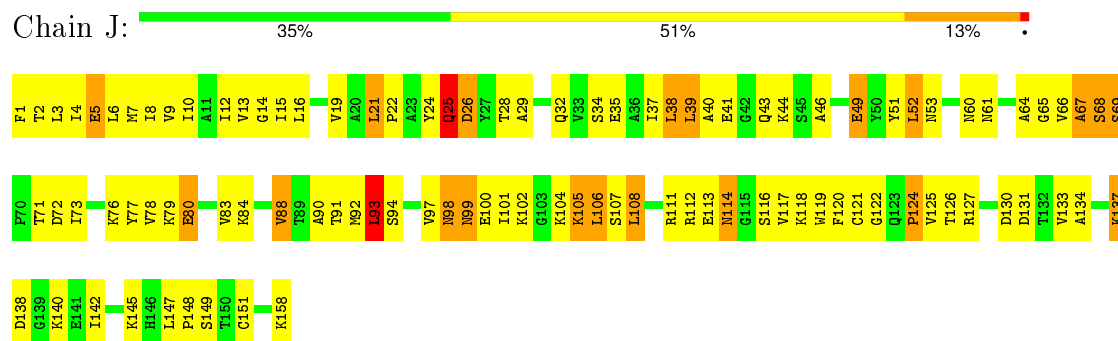
- Molecule 1: Fimbrial protein



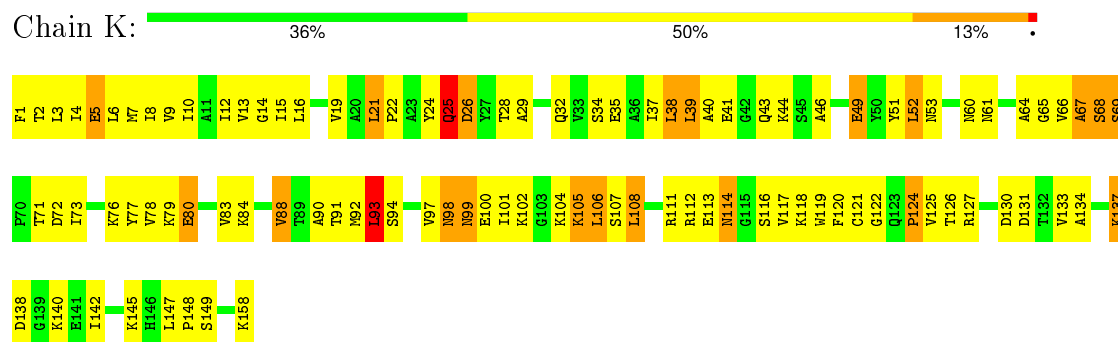
• Molecule 1: Fimbrial protein



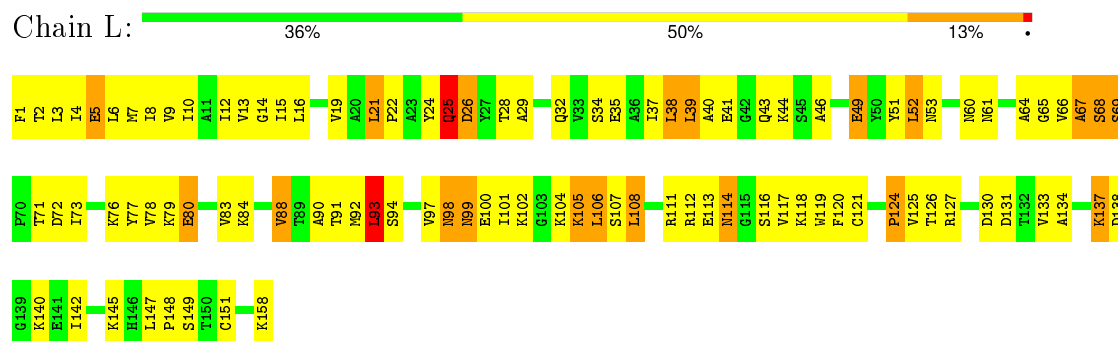
• Molecule 1: Fimbrial protein



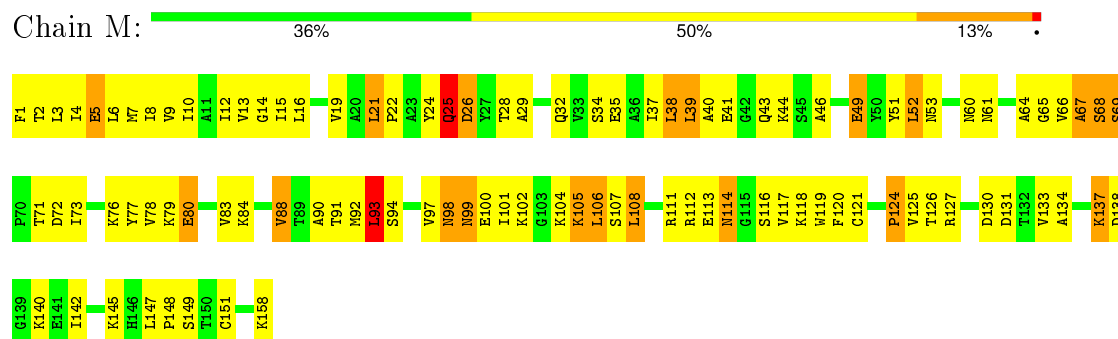
• Molecule 1: Fimbrial protein



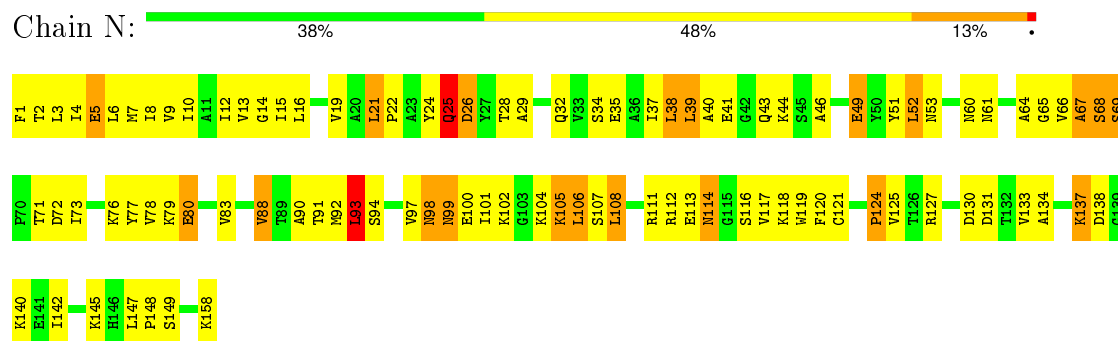
• Molecule 1: Fimbrial protein



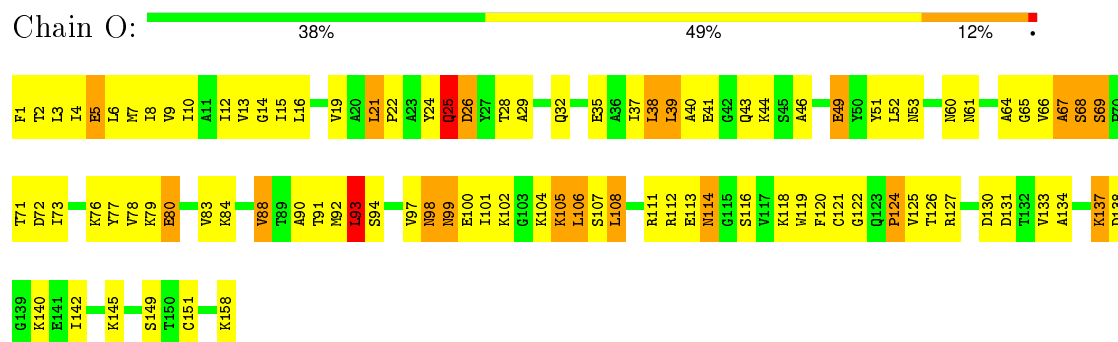
- Molecule 1: Fimbrial protein



- Molecule 1: Fimbrial protein



- Molecule 1: Fimbrial protein



- Molecule 1: Fimbrial protein

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Wiener filter	Depositor
Microscope	FEI/Philips CM200 FEG	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1000	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO163 film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, MEA, DT6, OPE

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	B	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	C	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	D	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	E	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	F	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	G	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	H	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	I	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	J	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	K	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	L	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	M	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	N	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	O	0.58	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	P	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	Q	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
1	R	0.59	1/1215 (0.1%)	0.66	1/1647 (0.1%)
All	All	0.59	18/21870 (0.1%)	0.66	18/29646 (0.1%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	26	ASP	N-CA	15.11	1.76	1.46
1	R	26	ASP	N-CA	15.11	1.76	1.46
1	Q	26	ASP	N-CA	15.10	1.76	1.46
1	D	26	ASP	N-CA	15.10	1.76	1.46
1	F	26	ASP	N-CA	15.09	1.76	1.46

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	25	GLN	C-N-CA	-7.58	102.74	121.70
1	O	25	GLN	C-N-CA	-7.58	102.75	121.70
1	P	25	GLN	C-N-CA	-7.58	102.75	121.70
1	M	25	GLN	C-N-CA	-7.58	102.76	121.70
1	Q	25	GLN	C-N-CA	-7.58	102.76	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A	1207	0	1199	497	0
1	B	1207	0	1199	495	0
1	C	1207	0	1199	490	0
1	D	1207	0	1199	491	0
1	E	1207	0	1199	497	0
1	F	1207	0	1201	409	0
1	G	1207	0	1201	379	0
1	H	1207	0	1201	380	0
1	I	1207	0	1202	293	0
1	J	1207	0	1199	492	0
1	K	1207	0	1199	496	0
1	L	1207	0	1199	501	0
1	M	1207	0	1199	497	0
1	N	1207	0	1199	493	0
1	O	1207	0	1203	415	0
1	P	1207	0	1203	377	0
1	Q	1207	0	1203	377	0
1	R	1207	0	1203	296	0
2	A	28	0	25	1	0
2	B	28	0	25	1	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
2	E	28	0	25	1	0
2	F	28	0	25	1	0
2	G	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	28	0	25	1	0
2	I	28	0	25	1	0
2	J	28	0	25	1	0
2	K	28	0	25	1	0
2	L	28	0	25	1	0
2	M	28	0	25	1	0
2	N	28	0	25	1	0
2	O	28	0	25	1	0
2	P	28	0	25	1	0
2	Q	28	0	25	1	0
2	R	28	0	25	1	0
3	A	8	0	6	0	0
3	B	8	0	6	0	0
3	C	8	0	6	0	0
3	D	8	0	6	0	0
3	E	8	0	6	0	0
3	F	8	0	6	0	0
3	G	8	0	6	0	0
3	H	8	0	6	0	0
3	I	8	0	6	0	0
3	J	8	0	6	0	0
3	K	8	0	6	0	0
3	L	8	0	6	0	0
3	M	8	0	6	0	0
3	N	8	0	6	0	0
3	O	8	0	6	0	0
3	P	8	0	6	0	0
3	Q	8	0	6	0	0
3	R	8	0	6	0	0
All	All	22374	0	22165	4771	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 107.

The worst 5 of 4771 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:K:8:ILE:HD11	1:L:1:MEA:CE2	1.24	1.68
1:E:1:MEA:CE2	1:F:8:ILE:HD11	1.24	1.66
1:Q:8:ILE:HD11	1:R:1:MEA:CE2	1.24	1.64
1:C:1:MEA:CE2	1:D:8:ILE:HD11	1.24	1.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MEA:CE2	1:C:8:ILE:HD11	1.24	1.62

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	A	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	B	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	C	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	D	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	E	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	F	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	G	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	H	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	I	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	J	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	K	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	L	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	M	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	N	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	O	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	P	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	Q	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
1	R	156/158 (99%)	138 (88%)	9 (6%)	9 (6%)	2	27
All	All	2808/2844 (99%)	2484 (88%)	162 (6%)	162 (6%)	4	27

5 of 162 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	LEU
1	A	98	ASN
1	B	93	LEU
1	B	98	ASN
1	C	93	LEU

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	A	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	B	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	C	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	D	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	E	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	F	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	G	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	H	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	I	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	J	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	K	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	L	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	M	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	N	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	O	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	P	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	Q	128/129 (99%)	112 (88%)	16 (12%)	6	30
1	R	128/129 (99%)	112 (88%)	16 (12%)	6	30
All	All	2304/2322 (99%)	2016 (88%)	288 (12%)	10	30

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	25	GLN
1	K	21	LEU
1	Q	105	LYS
1	I	52	LEU
1	J	25	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	98	ASN
1	K	98	ASN
1	Q	146	HIS
1	I	146	HIS
1	J	98	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MEA	A	1	1	9,11,13	0.58	0	11,13,16	0.67	1 (9%)
1	MEA	B	1	1	9,11,13	0.58	0	11,13,16	0.67	1 (9%)
1	MEA	C	1	1	9,11,13	0.58	0	11,13,16	0.67	1 (9%)
1	MEA	D	1	1	9,11,13	0.59	0	11,13,16	0.67	1 (9%)
1	MEA	E	1	1	9,11,13	0.59	0	11,13,16	0.67	1 (9%)
1	MEA	F	1	1	9,11,13	0.59	0	11,13,16	0.67	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MEA	G	1	1	9,11,13	0.59	0	11,13,16	0.67	1 (9%)
1	MEA	H	1	1	9,11,13	0.59	0	11,13,16	0.67	1 (9%)
1	MEA	I	1	1	9,11,13	0.59	0	11,13,16	0.67	1 (9%)
1	MEA	J	1	1	9,11,13	0.58	0	11,13,16	0.67	1 (9%)
1	MEA	K	1	1	9,11,13	0.58	0	11,13,16	0.67	1 (9%)
1	MEA	L	1	1	9,11,13	0.59	0	11,13,16	0.67	1 (9%)
1	MEA	M	1	1	9,11,13	0.59	0	11,13,16	0.67	1 (9%)
1	MEA	N	1	1	9,11,13	0.60	0	11,13,16	0.67	1 (9%)
1	MEA	O	1	1	9,11,13	0.60	0	11,13,16	0.68	1 (9%)
1	MEA	P	1	1	9,11,13	0.59	0	11,13,16	0.68	1 (9%)
1	MEA	Q	1	1	9,11,13	0.60	0	11,13,16	0.68	1 (9%)
1	MEA	R	1	1	9,11,13	0.59	0	11,13,16	0.68	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEA	A	1	1	-	0/4/6/10	0/1/1/1
1	MEA	B	1	1	-	0/4/6/10	0/1/1/1
1	MEA	C	1	1	-	0/4/6/10	0/1/1/1
1	MEA	D	1	1	-	0/4/6/10	0/1/1/1
1	MEA	E	1	1	-	0/4/6/10	0/1/1/1
1	MEA	F	1	1	-	0/4/6/10	0/1/1/1
1	MEA	G	1	1	-	0/4/6/10	0/1/1/1
1	MEA	H	1	1	-	0/4/6/10	0/1/1/1
1	MEA	I	1	1	-	0/4/6/10	0/1/1/1
1	MEA	J	1	1	-	0/4/6/10	0/1/1/1
1	MEA	K	1	1	-	0/4/6/10	0/1/1/1
1	MEA	L	1	1	-	0/4/6/10	0/1/1/1
1	MEA	M	1	1	-	0/4/6/10	0/1/1/1
1	MEA	N	1	1	-	0/4/6/10	0/1/1/1
1	MEA	O	1	1	-	0/4/6/10	0/1/1/1
1	MEA	P	1	1	-	0/4/6/10	0/1/1/1
1	MEA	Q	1	1	-	0/4/6/10	0/1/1/1
1	MEA	R	1	1	-	0/4/6/10	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	1	MEA	O-C-CA	-2.16	119.92	125.72
1	F	1	MEA	O-C-CA	-2.16	119.93	125.72
1	B	1	MEA	O-C-CA	-2.16	119.93	125.72
1	R	1	MEA	O-C-CA	-2.16	119.93	125.72
1	A	1	MEA	O-C-CA	-2.16	119.93	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	MEA	17	0
1	B	1	MEA	17	0
1	C	1	MEA	15	0
1	D	1	MEA	17	0
1	E	1	MEA	15	0
1	F	1	MEA	17	0
1	G	1	MEA	16	0
1	H	1	MEA	17	0
1	J	1	MEA	16	0
1	K	1	MEA	15	0
1	L	1	MEA	17	0
1	M	1	MEA	17	0
1	N	1	MEA	16	0
1	O	1	MEA	17	0
1	P	1	MEA	17	0
1	Q	1	MEA	16	0
1	R	1	MEA	17	0

5.5 Carbohydrates

36 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is

the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLA	A	160	2	11,11,12	0.38	0	15,15,17	0.74	0
2	DT6	A	161	1,2	17,17,18	0.59	0	16,23,25	0.75	1 (6%)
2	GLA	B	160	2	11,11,12	0.38	0	15,15,17	0.73	0
2	DT6	B	161	1,2	17,17,18	0.59	0	16,23,25	0.74	1 (6%)
2	GLA	C	160	2	11,11,12	0.38	0	15,15,17	0.74	0
2	DT6	C	161	1,2	17,17,18	0.60	0	16,23,25	0.75	1 (6%)
2	GLA	D	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	D	161	1,2	17,17,18	0.59	0	16,23,25	0.74	1 (6%)
2	GLA	E	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	E	161	1,2	17,17,18	0.59	0	16,23,25	0.74	1 (6%)
2	GLA	F	160	2	11,11,12	0.36	0	15,15,17	0.74	0
2	DT6	F	161	1,2	17,17,18	0.59	0	16,23,25	0.74	1 (6%)
2	GLA	G	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	G	161	1,2	17,17,18	0.60	0	16,23,25	0.74	1 (6%)
2	GLA	H	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	H	161	1,2	17,17,18	0.60	0	16,23,25	0.74	1 (6%)
2	GLA	I	160	2	11,11,12	0.36	0	15,15,17	0.73	0
2	DT6	I	161	1,2	17,17,18	0.60	0	16,23,25	0.74	1 (6%)
2	GLA	J	160	2	11,11,12	0.38	0	15,15,17	0.74	0
2	DT6	J	161	1,2	17,17,18	0.60	0	16,23,25	0.75	1 (6%)
2	GLA	K	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	K	161	1,2	17,17,18	0.60	0	16,23,25	0.75	1 (6%)
2	GLA	L	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	L	161	1,2	17,17,18	0.61	0	16,23,25	0.76	1 (6%)
2	GLA	M	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	M	161	1,2	17,17,18	0.61	0	16,23,25	0.75	1 (6%)
2	GLA	N	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	N	161	1,2	17,17,18	0.60	0	16,23,25	0.75	1 (6%)
2	GLA	O	160	2	11,11,12	0.37	0	15,15,17	0.74	0
2	DT6	O	161	1,2	17,17,18	0.61	0	16,23,25	0.74	1 (6%)
2	GLA	P	160	2	11,11,12	0.37	0	15,15,17	0.75	0
2	DT6	P	161	1,2	17,17,18	0.60	0	16,23,25	0.74	1 (6%)
2	GLA	Q	160	2	11,11,12	0.36	0	15,15,17	0.75	0
2	DT6	Q	161	1,2	17,17,18	0.61	0	16,23,25	0.73	1 (6%)
2	GLA	R	160	2	11,11,12	0.36	0	15,15,17	0.74	0
2	DT6	R	161	1,2	17,17,18	0.62	0	16,23,25	0.73	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	A	160	2	-	0/2/19/22	0/1/1/1
2	DT6	A	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	B	160	2	-	0/2/19/22	0/1/1/1
2	DT6	B	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	C	160	2	-	0/2/19/22	0/1/1/1
2	DT6	C	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	D	160	2	-	0/2/19/22	0/1/1/1
2	DT6	D	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	E	160	2	-	0/2/19/22	0/1/1/1
2	DT6	E	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	F	160	2	-	0/2/19/22	0/1/1/1
2	DT6	F	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	G	160	2	-	0/2/19/22	0/1/1/1
2	DT6	G	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	H	160	2	-	0/2/19/22	0/1/1/1
2	DT6	H	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	I	160	2	-	0/2/19/22	0/1/1/1
2	DT6	I	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	J	160	2	-	0/2/19/22	0/1/1/1
2	DT6	J	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	K	160	2	-	0/2/19/22	0/1/1/1
2	DT6	K	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	L	160	2	-	0/2/19/22	0/1/1/1
2	DT6	L	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	M	160	2	-	0/2/19/22	0/1/1/1
2	DT6	M	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	N	160	2	-	0/2/19/22	0/1/1/1
2	DT6	N	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	O	160	2	-	0/2/19/22	0/1/1/1
2	DT6	O	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	P	160	2	-	0/2/19/22	0/1/1/1
2	DT6	P	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	Q	160	2	-	0/2/19/22	0/1/1/1
2	DT6	Q	161	1,2	-	0/10/27/30	0/1/1/1
2	GLA	R	160	2	-	0/2/19/22	0/1/1/1
2	DT6	R	161	1,2	-	0/10/27/30	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	L	161	DT6	C2-N2-C7	-2.42	119.96	123.11
2	J	161	DT6	C2-N2-C7	-2.40	119.98	123.11
2	M	161	DT6	C2-N2-C7	-2.39	120.00	123.11
2	N	161	DT6	C2-N2-C7	-2.39	120.00	123.11
2	K	161	DT6	C2-N2-C7	-2.38	120.01	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

36 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	160	GLA	1	0
2	A	161	DT6	1	0
2	B	160	GLA	1	0
2	B	161	DT6	1	0
2	C	160	GLA	1	0
2	C	161	DT6	1	0
2	D	160	GLA	1	0
2	D	161	DT6	1	0
2	E	160	GLA	1	0
2	E	161	DT6	1	0
2	F	160	GLA	1	0
2	F	161	DT6	1	0
2	G	160	GLA	1	0
2	G	161	DT6	1	0
2	H	160	GLA	1	0
2	H	161	DT6	1	0
2	I	160	GLA	1	0
2	I	161	DT6	1	0
2	J	160	GLA	1	0
2	J	161	DT6	1	0
2	K	160	GLA	1	0
2	K	161	DT6	1	0
2	L	160	GLA	1	0
2	L	161	DT6	1	0
2	M	160	GLA	1	0
2	M	161	DT6	1	0
2	N	160	GLA	1	0
2	N	161	DT6	1	0
2	O	160	GLA	1	0
2	O	161	DT6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	160	GLA	1	0
2	P	161	DT6	1	0
2	Q	160	GLA	1	0
2	Q	161	DT6	1	0
2	R	160	GLA	1	0
2	R	161	DT6	1	0

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OPE	A	824	1	6,7,7	0.90	0	6,9,9	1.06	0
3	OPE	B	824	1	6,7,7	0.89	0	6,9,9	1.05	0
3	OPE	C	824	1	6,7,7	0.89	0	6,9,9	1.05	0
3	OPE	D	824	1	6,7,7	0.89	0	6,9,9	1.06	0
3	OPE	E	824	1	6,7,7	0.89	0	6,9,9	1.06	0
3	OPE	F	824	1	6,7,7	0.88	0	6,9,9	1.05	0
3	OPE	G	824	1	6,7,7	0.88	0	6,9,9	1.04	0
3	OPE	H	824	1	6,7,7	0.88	0	6,9,9	1.05	0
3	OPE	I	824	1	6,7,7	0.87	0	6,9,9	1.04	0
3	OPE	J	824	1	6,7,7	0.89	0	6,9,9	1.05	0
3	OPE	K	824	1	6,7,7	0.90	0	6,9,9	1.06	0
3	OPE	L	824	1	6,7,7	0.90	0	6,9,9	1.06	0
3	OPE	M	824	1	6,7,7	0.91	0	6,9,9	1.07	0
3	OPE	N	824	1	6,7,7	0.90	0	6,9,9	1.06	0
3	OPE	O	824	1	6,7,7	0.90	0	6,9,9	1.06	0
3	OPE	P	824	1	6,7,7	0.90	0	6,9,9	1.06	0
3	OPE	Q	824	1	6,7,7	0.90	0	6,9,9	1.07	0
3	OPE	R	824	1	6,7,7	0.90	0	6,9,9	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OPE	A	824	1	-	0/5/5/5	0/0/0/0
3	OPE	B	824	1	-	0/5/5/5	0/0/0/0
3	OPE	C	824	1	-	0/5/5/5	0/0/0/0
3	OPE	D	824	1	-	0/5/5/5	0/0/0/0
3	OPE	E	824	1	-	0/5/5/5	0/0/0/0
3	OPE	F	824	1	-	0/5/5/5	0/0/0/0
3	OPE	G	824	1	-	0/5/5/5	0/0/0/0
3	OPE	H	824	1	-	0/5/5/5	0/0/0/0
3	OPE	I	824	1	-	0/5/5/5	0/0/0/0
3	OPE	J	824	1	-	0/5/5/5	0/0/0/0
3	OPE	K	824	1	-	0/5/5/5	0/0/0/0
3	OPE	L	824	1	-	0/5/5/5	0/0/0/0
3	OPE	M	824	1	-	0/5/5/5	0/0/0/0
3	OPE	N	824	1	-	0/5/5/5	0/0/0/0
3	OPE	O	824	1	-	0/5/5/5	0/0/0/0
3	OPE	P	824	1	-	0/5/5/5	0/0/0/0
3	OPE	Q	824	1	-	0/5/5/5	0/0/0/0
3	OPE	R	824	1	-	0/5/5/5	0/0/0/0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.