wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:00 PM BST

PDB ID	:	4A6J
EMDB ID:	:	EMD-1980
Title	:	Structural model of ParM filament based on CryoEM map
Authors	:	Gayathri, P.; Fujii, T.; Moller-Jensen, J.; Van Den Ent, F.; Namba, K.; Lowe, J.
Deposited on	:	2011-11-04
Resolution	:	7.20 Å(reported)
Based on PDB ID	:	4A62

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

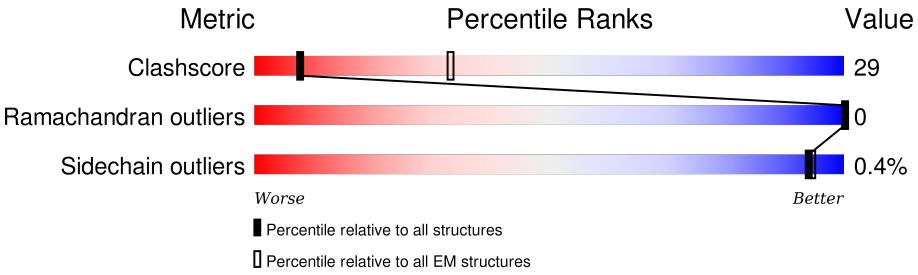
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.20 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	320	82% 18%
1	B	320	81% 18%
1	C	320	78% 22%
1	D	320	78% 22%
1	E	320	78% 22%
1	F	320	78% 22%
1	G	320	78% 22%
1	H	320	78% 22%
1	I	320	82% 18%

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Mol	Chain	Length	Quality of chain
1	J	320	

2 Entry composition

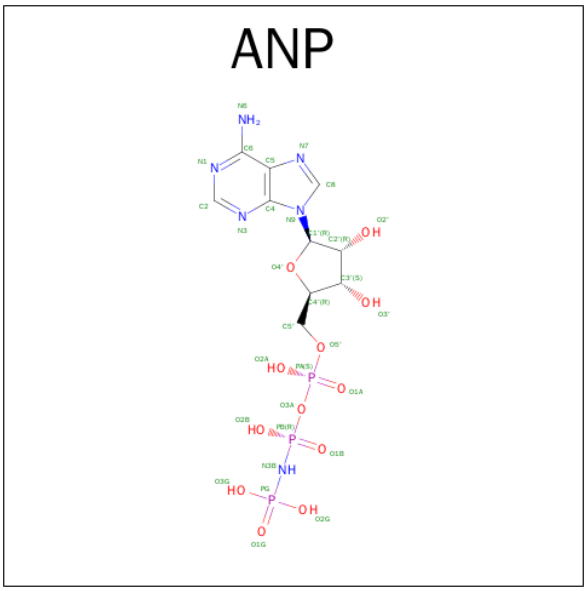
There are 3 unique types of molecules in this entry. The entry contains 25490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PLASMID SEGREGATION PROTEIN PARM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	B	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	C	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	D	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	E	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	F	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	G	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	H	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	I	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	J	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	E	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	G	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	H	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	J	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Mg	0
			1	1	
3	J	1	Total	Mg	0
			1	1	

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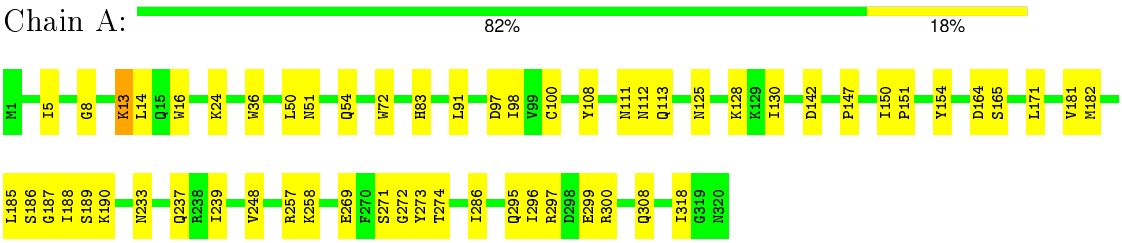
Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total Mg 1 1	0
3	E	1	Total Mg 1 1	0
3	H	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0
3	I	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0
3	A	1	Total Mg 1 1	0
3	F	1	Total Mg 1 1	0

3 Residue-property plots (i)

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.

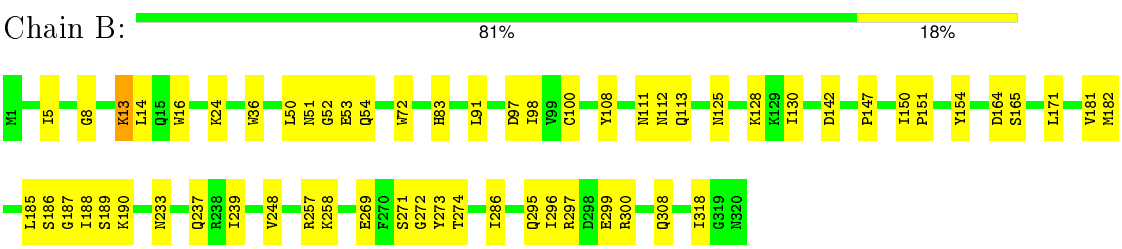
- Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain A:



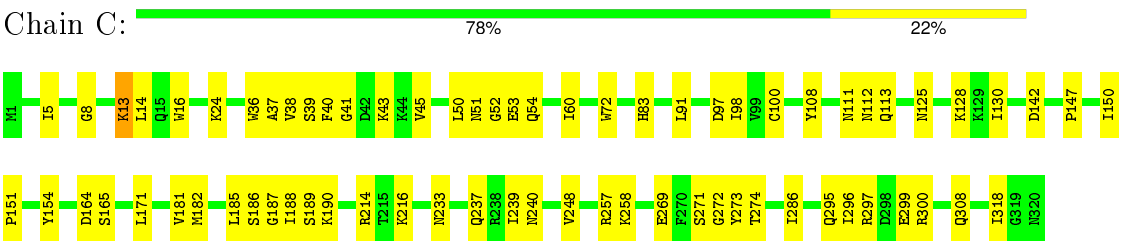
- Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain B:



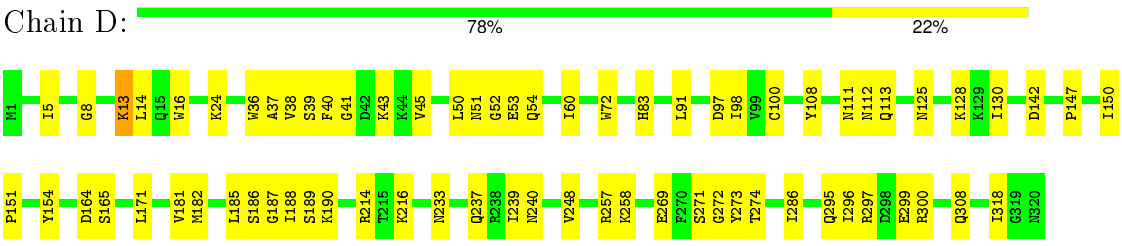
- Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain C:



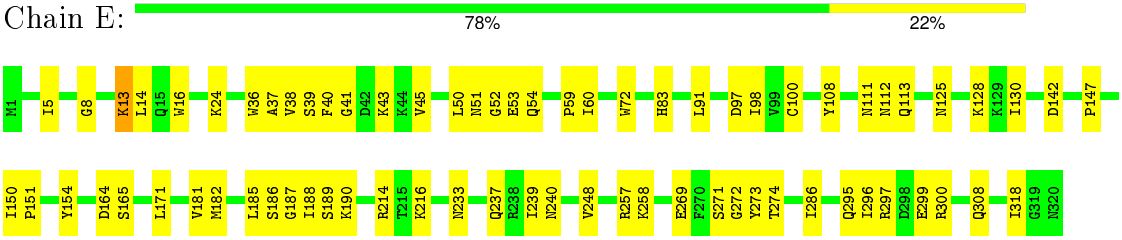
- Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain D:



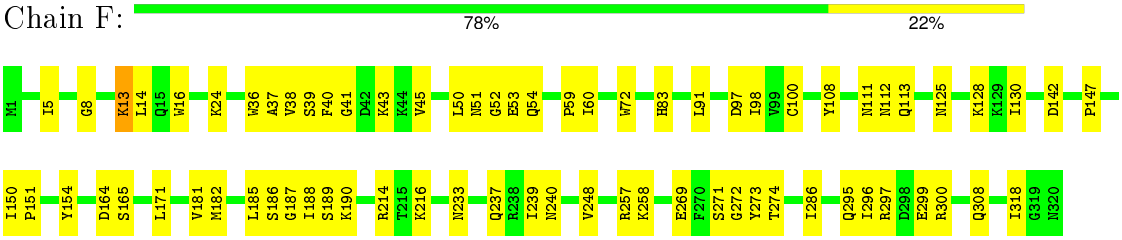
- Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain E:



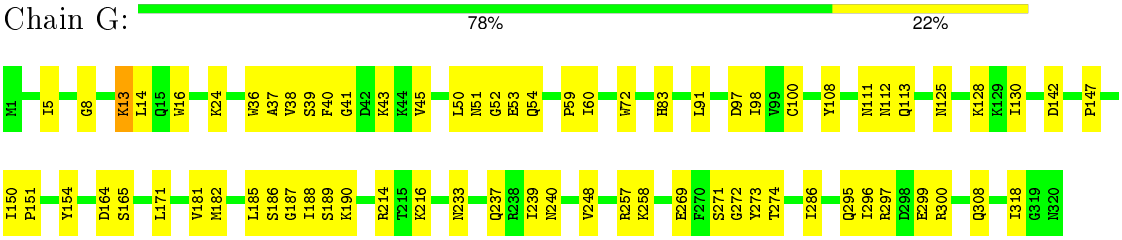
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain F:



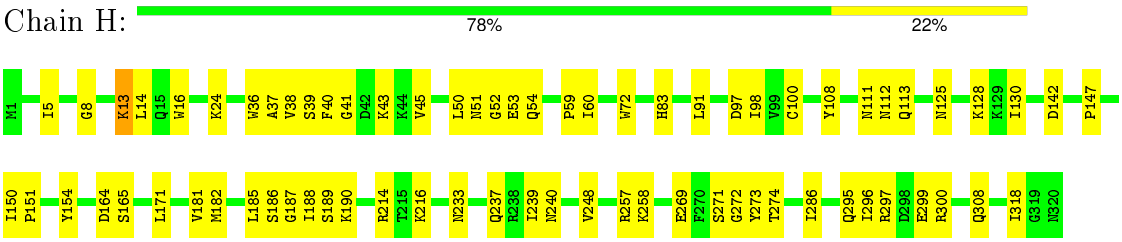
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain G:



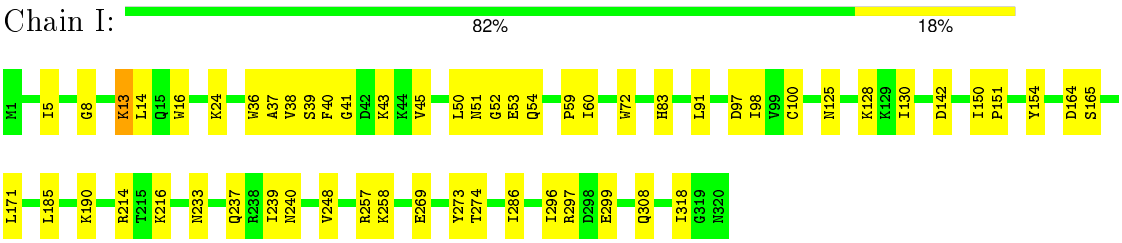
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain H:



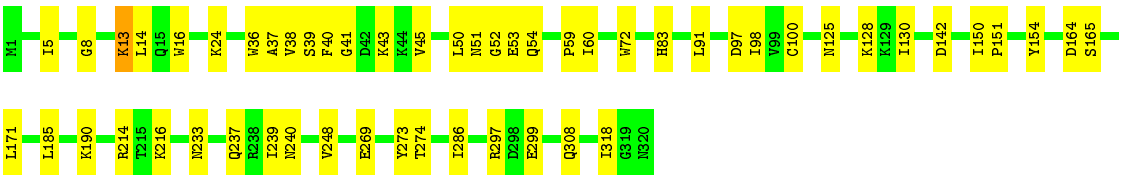
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain I:



• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

Chain J:


M1
T5
G8
K13
L14
Q15
W16
K24
W36
A37
V38
S39
F40
G41
D42
K43
K44
V45
L50
N51
G52
E53
Q54
P59
I60
W72
H83
L91
D97
I98
V99
C100
N125
K128
K129
I130
D142
I150
P151
Y154
D164
S165
L171
L185
K190
R214
T215
K216
N233
Q237
R238
I239
N240
V248
E269
Y273
T274
I286
R297
D298
E299
Q308
I318
G319
N320

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3 EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	50000	Depositor
Image detector	TEMCAM-F415MP	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	0.36	0/2561	0.51	0/3467
1	B	0.36	0/2561	0.51	0/3467
1	C	0.36	0/2561	0.51	0/3467
1	D	0.36	0/2561	0.51	0/3467
1	E	0.36	0/2561	0.51	0/3467
1	F	0.36	0/2561	0.51	0/3467
1	G	0.36	0/2561	0.51	0/3467
1	H	0.36	0/2561	0.51	0/3467
1	I	0.36	0/2561	0.51	0/3467
1	J	0.36	0/2561	0.51	0/3467
All	All	0.36	0/25610	0.51	0/34670

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

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	2517	0	2505	178	0
1	B	2517	0	2505	193	0
1	C	2517	0	2502	332	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2517	0	2502	334	0
1	E	2517	0	2502	333	0
1	F	2517	0	2502	336	0
1	G	2517	0	2502	332	0
1	H	2517	0	2502	336	0
1	I	2517	0	2503	192	0
1	J	2517	0	2503	179	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
2	E	31	0	13	0	0
2	F	31	0	13	0	0
2	G	31	0	13	0	0
2	H	31	0	13	0	0
2	I	31	0	13	0	0
2	J	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	25490	0	25158	1488	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 29.

The worst 5 of 1488 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:A:147:PRO:CG	1:C:40:PHE:CE1	1.84	1.60
1:C:147:PRO:CG	1:E:40:PHE:CE1	1.83	1.60
1:E:147:PRO:CG	1:G:40:PHE:CE1	1.82	1.59
1:F:147:PRO:CG	1:H:40:PHE:CE1	1.83	1.58
1:G:147:PRO:CG	1:I:40:PHE:CE1	1.83	1.57

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	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	B	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	C	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	D	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	E	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	F	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	G	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	H	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	I	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	J	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
All	All	3190/3200 (100%)	3060 (96%)	130 (4%)	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 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	284/284 (100%)	283 (100%)	1 (0%)	93	96
1	B	284/284 (100%)	283 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	284/284 (100%)	283 (100%)	1 (0%)	93	96
1	D	284/284 (100%)	283 (100%)	1 (0%)	93	96
1	E	284/284 (100%)	283 (100%)	1 (0%)	93	96
1	F	284/284 (100%)	283 (100%)	1 (0%)	93	96
1	G	284/284 (100%)	283 (100%)	1 (0%)	93	96
1	H	284/284 (100%)	283 (100%)	1 (0%)	93	96
1	I	284/284 (100%)	283 (100%)	1 (0%)	93	96
1	J	284/284 (100%)	283 (100%)	1 (0%)	93	96
All	All	2840/2840 (100%)	2830 (100%)	10 (0%)	94	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	13	LYS
1	F	13	LYS
1	H	13	LYS
1	D	13	LYS
1	G	13	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	83	HIS
1	E	113	GLN
1	H	83	HIS
1	D	83	HIS
1	D	113	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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	ANP	A	500	3	29,33,33	2.01	9 (31%)	26,52,52	2.04	4 (15%)
2	ANP	B	500	3	29,33,33	2.02	9 (31%)	26,52,52	2.04	4 (15%)
2	ANP	C	500	3	29,33,33	2.03	9 (31%)	26,52,52	2.03	4 (15%)
2	ANP	D	500	3	29,33,33	2.02	9 (31%)	26,52,52	2.04	4 (15%)
2	ANP	E	500	3	29,33,33	2.04	9 (31%)	26,52,52	2.05	4 (15%)
2	ANP	F	500	3	29,33,33	2.00	9 (31%)	26,52,52	2.06	4 (15%)
2	ANP	G	500	3	29,33,33	2.02	9 (31%)	26,52,52	2.05	4 (15%)
2	ANP	H	500	3	29,33,33	2.00	9 (31%)	26,52,52	2.06	4 (15%)
2	ANP	I	500	3	29,33,33	2.03	9 (31%)	26,52,52	2.03	4 (15%)
2	ANP	J	500	3	29,33,33	2.00	9 (31%)	26,52,52	2.04	4 (15%)

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	ANP	A	500	3	-	0/13/38/38	0/3/3/3
2	ANP	B	500	3	-	0/13/38/38	0/3/3/3
2	ANP	C	500	3	-	0/13/38/38	0/3/3/3
2	ANP	D	500	3	-	0/13/38/38	0/3/3/3
2	ANP	E	500	3	-	0/13/38/38	0/3/3/3
2	ANP	F	500	3	-	0/13/38/38	0/3/3/3
2	ANP	G	500	3	-	0/13/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	H	500	3	-	0/13/38/38	0/3/3/3
2	ANP	I	500	3	-	0/13/38/38	0/3/3/3
2	ANP	J	500	3	-	0/13/38/38	0/3/3/3

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	ANP	PG-O2G	-2.20	1.50	1.56
2	H	500	ANP	PG-O2G	-2.17	1.50	1.56
2	F	500	ANP	PG-O2G	-2.17	1.50	1.56
2	B	500	ANP	PG-O2G	-2.16	1.51	1.56
2	J	500	ANP	PG-O2G	-2.16	1.51	1.56

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	500	ANP	N3-C2-N1	-7.82	122.73	128.87
2	F	500	ANP	N3-C2-N1	-7.75	122.78	128.87
2	G	500	ANP	N3-C2-N1	-7.72	122.81	128.87
2	B	500	ANP	N3-C2-N1	-7.71	122.81	128.87
2	J	500	ANP	N3-C2-N1	-7.71	122.81	128.87

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.