



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 07:30 AM EDT

PDB ID : 5KNE
EMDB ID: : EMD-8267
Title : CryoEM Reconstruction of Hsp104 Hexamer
Authors : Yokom, A.L.; Gates, S.N.; Jackrel, M.E.; Mack, K.L.; Su, M.; Shorter, J.;
Southworth, D.R.
Deposited on : unknown
Resolution : 5.64 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

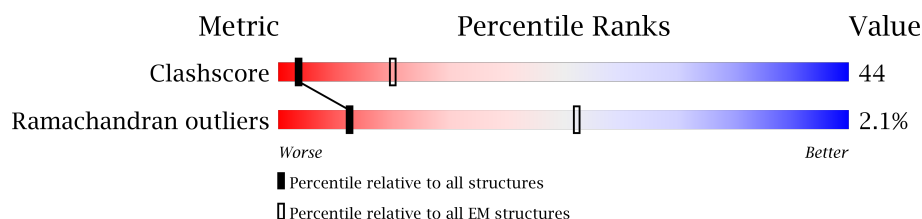
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.64 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	125131	1336
Ramachandran outliers	121729	1120

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	852	
1	B	852	
1	C	852	
1	D	852	
1	E	852	
1	F	852	

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
2	ANP	A	901	-	-	X	-
2	ANP	B	902	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ANP	E	901	-	-	X	-

2 Entry composition [i](#)

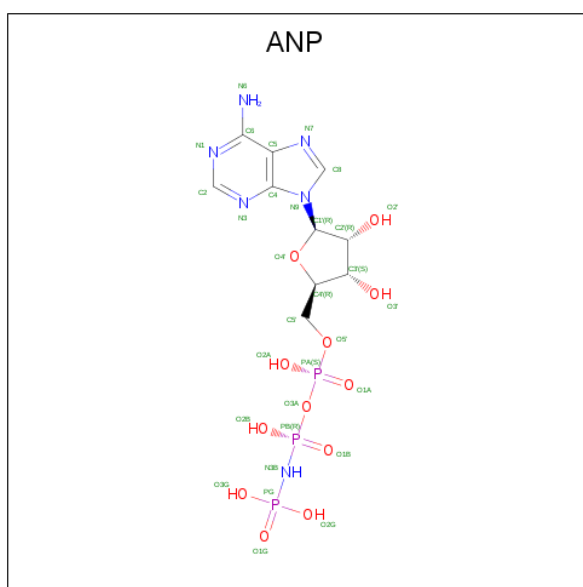
There are 2 unique types of molecules in this entry. The entry contains 16421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heat shock protein 104.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	553	Total	C	N	O	0	0
			2212	1106	553	553		
1	B	711	Total	C	N	O	0	0
			2844	1422	711	711		
1	C	769	Total	C	N	O	0	0
			3076	1538	769	769		
1	D	770	Total	C	N	O	0	0
			3080	1540	770	770		
1	E	610	Total	C	N	O	0	0
			2440	1220	610	610		
1	F	607	Total	C	N	O	0	0
			2428	1214	607	607		

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

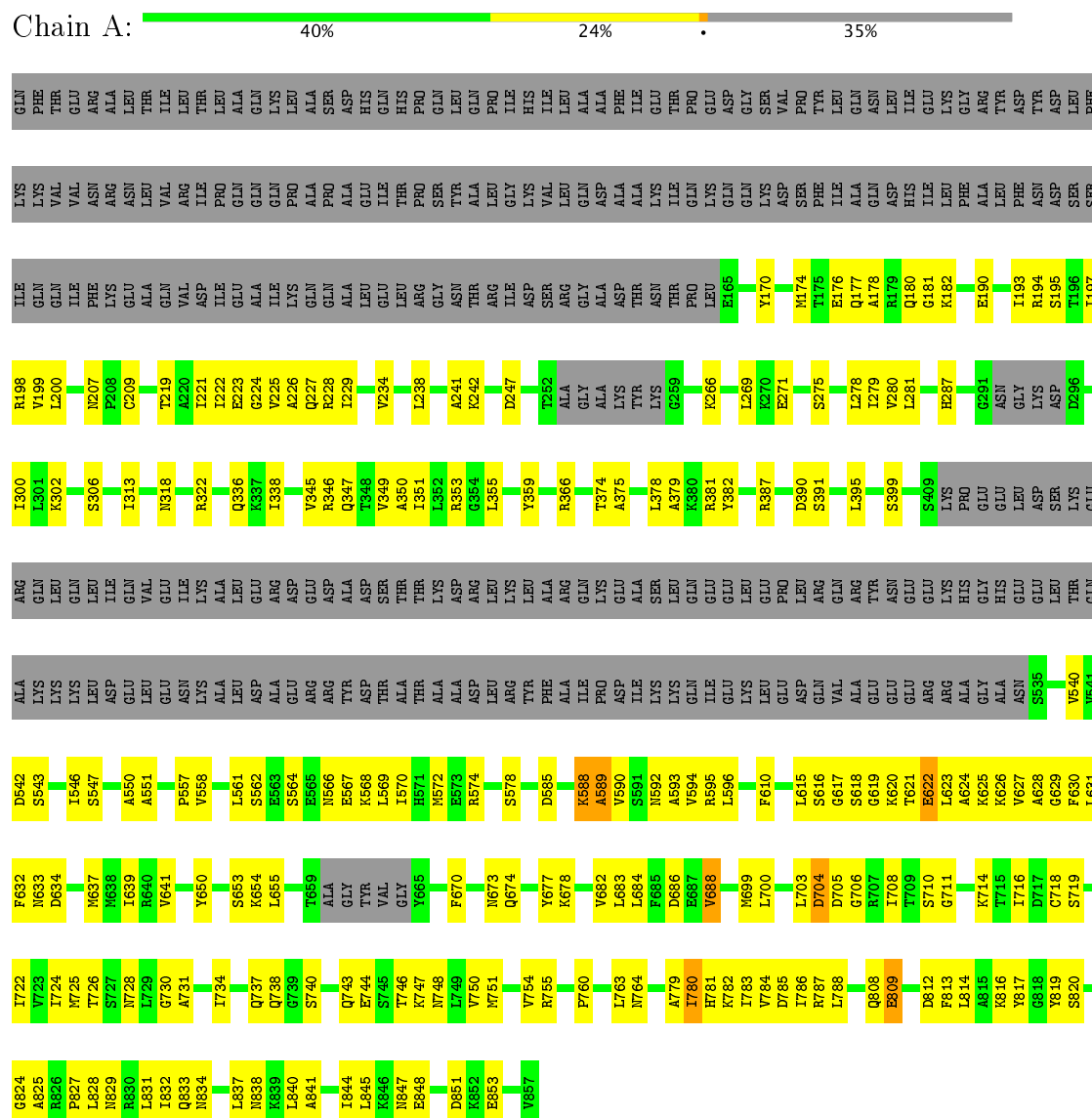


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0
2	B	1	Total 62	C 20	N 12	O 24	P 6	0
2	B	1	Total 62	C 20	N 12	O 24	P 6	0
2	C	1	Total 62	C 20	N 12	O 24	P 6	0
2	C	1	Total 62	C 20	N 12	O 24	P 6	0
2	D	1	Total 62	C 20	N 12	O 24	P 6	0
2	D	1	Total 62	C 20	N 12	O 24	P 6	0
2	E	1	Total 62	C 20	N 12	O 24	P 6	0
2	E	1	Total 62	C 20	N 12	O 24	P 6	0
2	F	1	Total 62	C 20	N 12	O 24	P 6	0
2	F	1	Total 62	C 20	N 12	O 24	P 6	0

3 Residue-property plots [i](#)

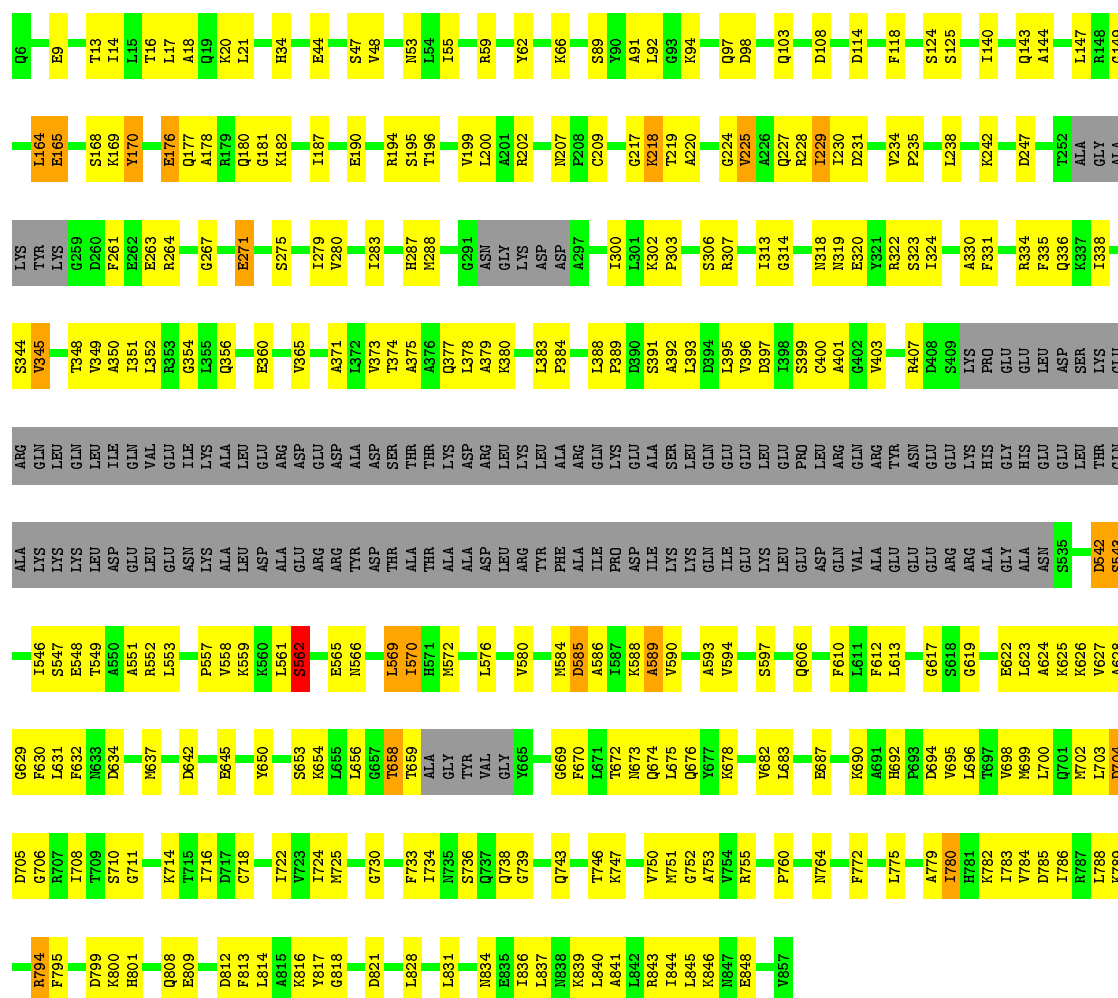
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Heat shock protein 104



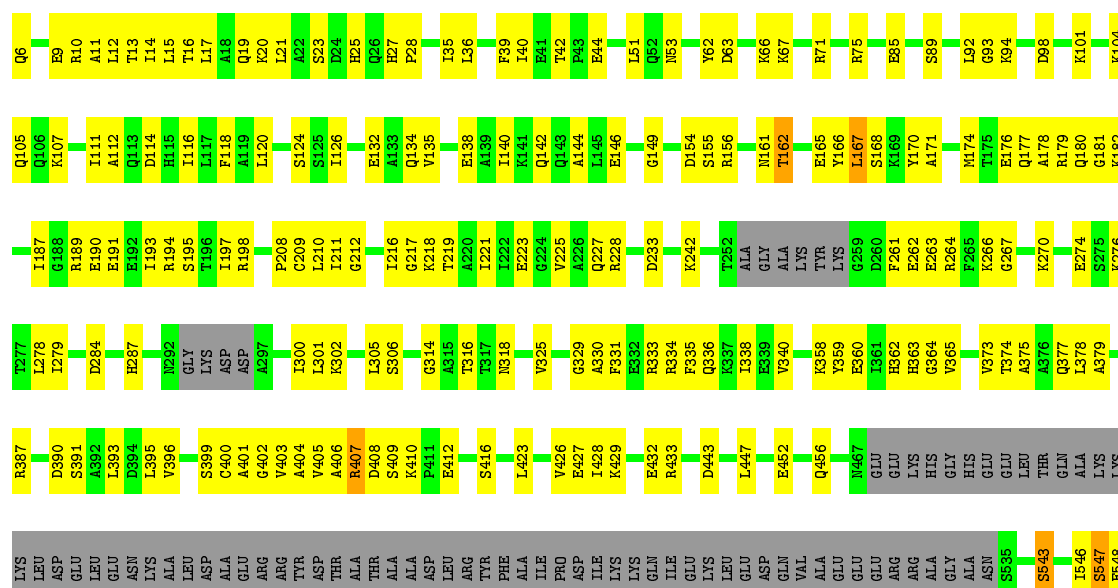
- Molecule 1: Heat shock protein 104





• Molecule 1: Heat shock protein 104

Chain C: 54% 35% 10%





Q797	D798	D799	D800	D801	D808	D811	D812	D813	D814	D815	D818	D819	D825	D828	D834	D838	D839	D840	D843	D844	D845	D846	D847	D848	D857
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	172043	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/2207	0.62	0/2750
1	B	0.47	1/2839 (0.0%)	0.73	5/3540 (0.1%)
1	C	0.42	0/3071	0.65	0/3830
1	D	0.41	1/3075 (0.0%)	0.64	4/3835 (0.1%)
1	E	0.39	0/2435	0.60	0/3035
1	F	0.27	0/2423	0.54	0/3020
All	All	0.40	2/16050 (0.0%)	0.64	9/20010 (0.0%)

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	A	0	6
1	B	0	13
1	C	0	11
1	D	0	3
1	E	0	4
1	F	0	4
All	All	0	41

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	659	THR	CA-C	-7.72	1.32	1.52
1	B	165	GLU	CA-C	-7.71	1.32	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	THR	N-CA-C	11.24	141.35	111.00
1	B	165	GLU	N-CA-C	-10.22	83.41	111.00
1	B	164	LEU	N-CA-C	-9.79	84.57	111.00
1	D	659	THR	CA-C-O	-9.11	100.97	120.10
1	D	658	THR	N-CA-C	-8.37	88.41	111.00

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	HIS	Peptide
1	A	588	LYS	Peptide
1	A	616	SER	Peptide
1	A	622	GLU	Peptide
1	A	704	ASP	Peptide

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	2212	0	600	136	0
1	B	2844	0	759	179	0
1	C	3076	0	815	193	0
1	D	3080	0	815	177	0
1	E	2440	0	655	133	0
1	F	2428	0	650	86	0
2	A	31	0	13	9	0
2	B	62	0	26	18	0
2	C	62	0	26	5	0
2	D	62	0	26	9	0
2	E	62	0	26	17	0
2	F	62	0	26	8	0
All	All	16421	0	4437	914	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 44.

The worst 5 of 914 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:D:46:GLY:O	1:D:162:THR:CA	1.74	1.34
1:B:217:GLY:HA3	2:B:901:ANP:H8	1.32	1.10
1:D:672:THR:O	1:D:675:LEU:N	1.91	1.02
1:D:48:VAL:H	1:D:162:THR:H	1.01	0.97
1:B:699:MET:O	1:B:703:LEU:N	1.96	0.96

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	543/852 (64%)	455 (84%)	83 (15%)	5 (1%)	20	63
1	B	701/852 (82%)	565 (81%)	113 (16%)	23 (3%)	4	36
1	C	759/852 (89%)	615 (81%)	129 (17%)	15 (2%)	9	47
1	D	760/852 (89%)	603 (79%)	130 (17%)	27 (4%)	4	34
1	E	600/852 (70%)	498 (83%)	94 (16%)	8 (1%)	14	56
1	F	597/852 (70%)	485 (81%)	107 (18%)	5 (1%)	22	66
All	All	3960/5112 (78%)	3221 (81%)	656 (17%)	83 (2%)	12	45

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	164	LEU
1	B	165	GLU
1	B	169	LYS
1	B	170	TYR
1	B	658	THR

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

11 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
2	ANP	A	901	-	29,33,33	1.98	4 (13%)	28,52,52	1.52	4 (14%)
2	ANP	B	901	-	29,33,33	2.03	4 (13%)	28,52,52	1.18	3 (10%)
2	ANP	B	902	-	29,33,33	1.96	4 (13%)	28,52,52	1.35	2 (7%)
2	ANP	C	901	-	29,33,33	1.98	5 (17%)	28,52,52	1.37	2 (7%)
2	ANP	C	902	-	29,33,33	1.04	3 (10%)	28,52,52	1.47	5 (17%)
2	ANP	D	901	-	29,33,33	2.82	5 (17%)	28,52,52	1.14	2 (7%)
2	ANP	D	902	-	29,33,33	1.93	5 (17%)	28,52,52	1.46	1 (3%)
2	ANP	E	901	-	29,33,33	2.05	4 (13%)	28,52,52	1.60	2 (7%)
2	ANP	E	902	-	29,33,33	1.69	4 (13%)	28,52,52	1.20	2 (7%)
2	ANP	F	901	-	29,33,33	1.97	5 (17%)	28,52,52	1.22	2 (7%)
2	ANP	F	902	-	29,33,33	2.01	5 (17%)	28,52,52	1.18	2 (7%)

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	901	-	-	0/13/38/38	0/3/3/3
2	ANP	B	901	-	-	0/13/38/38	0/3/3/3
2	ANP	B	902	-	-	0/13/38/38	0/3/3/3
2	ANP	C	901	-	-	0/13/38/38	0/3/3/3
2	ANP	C	902	-	-	0/13/38/38	0/3/3/3
2	ANP	D	901	-	-	1/13/38/38	0/3/3/3
2	ANP	D	902	-	-	0/13/38/38	0/3/3/3
2	ANP	E	901	-	-	0/13/38/38	0/3/3/3
2	ANP	E	902	-	-	1/13/38/38	0/3/3/3
2	ANP	F	901	-	-	1/13/38/38	0/3/3/3
2	ANP	F	902	-	-	0/13/38/38	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	ANP	PB-O3A	-4.82	1.53	1.59
2	D	901	ANP	PB-O3A	-4.66	1.53	1.59
2	A	901	ANP	PB-O3A	-4.07	1.54	1.59
2	D	902	ANP	PB-O3A	-4.03	1.54	1.59
2	B	901	ANP	PB-O3A	-3.82	1.54	1.59

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	ANP	PA-O3A-PB	-6.45	109.60	132.38
2	D	902	ANP	PA-O3A-PB	-6.37	109.90	132.38
2	C	901	ANP	PA-O3A-PB	-5.89	111.59	132.38
2	B	902	ANP	PA-O3A-PB	-5.10	114.38	132.38
2	F	901	ANP	PA-O3A-PB	-4.72	115.72	132.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	901	ANP	O1B-PB-N3B-PG
2	D	901	ANP	O1B-PB-N3B-PG
2	E	902	ANP	O1G-PG-N3B-PB

There are no ring outliers.

10 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ANP	9	0
2	B	901	ANP	8	0
2	B	902	ANP	10	0
2	C	901	ANP	5	0
2	D	901	ANP	7	0
2	D	902	ANP	2	0
2	E	901	ANP	10	0
2	E	902	ANP	7	0
2	F	901	ANP	4	0
2	F	902	ANP	4	0

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.