



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 17, 2017 – 08:20 PM EST

PDB ID : 5H1C  
EMDB ID: : EMD-9567  
Title : Human RAD51 post-synaptic complexes  
Authors : Xu, J.; Zhao, L.; Xu, Y.; Zhao, W.; Sung, P.; Wang, H.W.  
Deposited on : 2016-10-08  
Resolution : 4.50 Å(reported)  
Based on PDB ID : 1SZP

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 1.7.1 (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) : rb-20028442

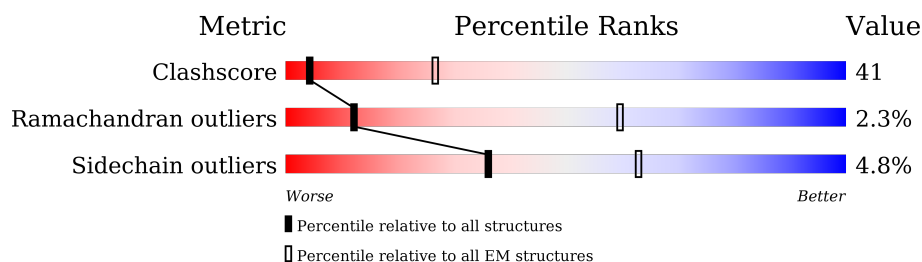
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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  $\geq 3$ , 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	339	
1	B	339	
1	C	339	
2	D	9	
3	E	9	

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
5	ANP	A	602	-	-	X	-
5	ANP	B	602	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7602 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 DNA repair protein RAD51 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	311	Total	C	N	O	S	0	0
			2379	1489	420	457	13		
1	B	311	Total	C	N	O	S	0	0
			2379	1489	420	457	13		
1	C	311	Total	C	N	O	S	0	0
			2379	1489	420	457	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	GLN	LYS	engineered mutation	UNP Q06609
B	313	GLN	LYS	engineered mutation	UNP Q06609
C	313	GLN	LYS	engineered mutation	UNP Q06609

- Molecule 2 is a DNA chain called DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	9	Total	C	N	O	P	0	0
			180	90	18	63	9		

- Molecule 3 is a DNA chain called DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	9	Total	C	N	O	P	0	0
			189	90	45	45	9		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

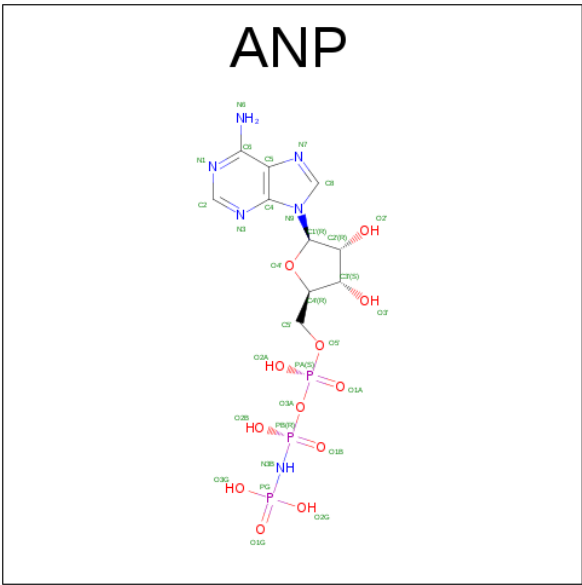
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Mg	0
			1	1	

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

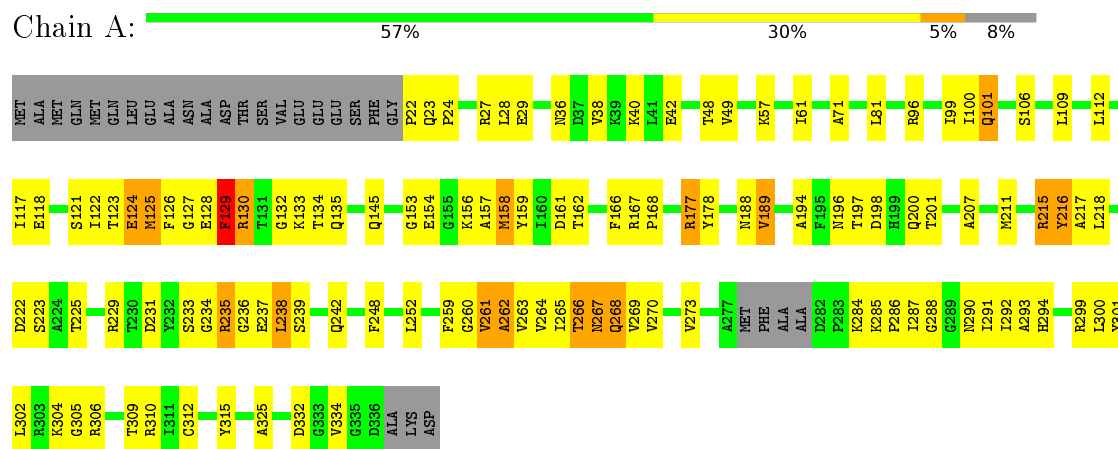


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	C	1	Total	C	N	O	P	0
			31	10	6	12	3	

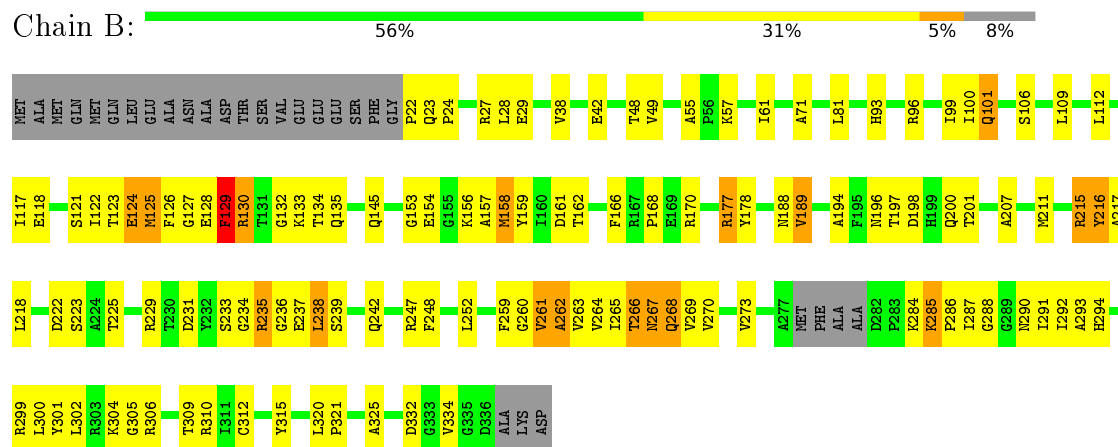
### 3 Residue-property plots

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.

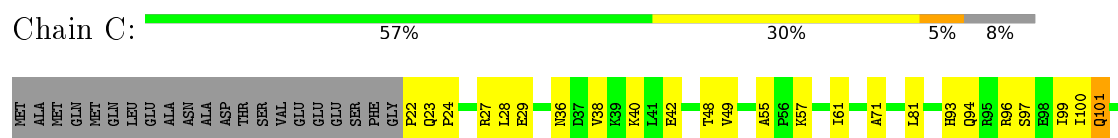
- Molecule 1: DNA repair protein RAD51 homolog 1

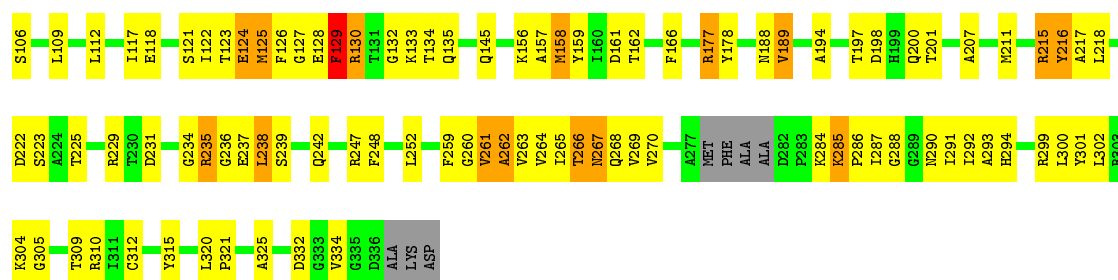


- Molecule 1: DNA repair protein RAD51 homolog 1



- Molecule 1: DNA repair protein RAD51 homolog 1





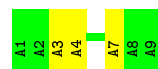
- Molecule 2: DNA (5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3')

Chain D:



- Molecule 3: DNA (5'-D(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*A)-3')

Chain E:



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	30194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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: 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	0.37	0/2413	0.52	0/3255
1	B	0.37	0/2413	0.52	0/3255
1	C	0.37	0/2413	0.52	0/3255
2	D	0.75	0/197	1.14	0/302
3	E	0.69	0/215	0.69	0/329
All	All	0.39	0/7651	0.55	0/10396

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	A	2379	0	2393	183	0
1	B	2379	0	2393	233	0
1	C	2379	0	2393	216	0
2	D	180	0	109	14	0
3	E	189	0	100	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	31	0	12	32	0
5	B	31	0	12	24	0
5	C	31	0	13	3	0
All	All	7602	0	7425	614	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 41.

All (614) 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:C:158:MET:HE2	1:C:216:TYR:CD2	1.22	1.73
1:A:158:MET:HE2	1:A:216:TYR:CD2	1.20	1.65
1:B:158:MET:HE2	1:B:216:TYR:CD2	1.20	1.61
5:A:602:ANP:N6	1:B:321:PRO:CD	1.67	1.53
1:C:158:MET:CE	1:C:216:TYR:CD2	1.95	1.47
1:A:158:MET:CE	1:A:216:TYR:CD2	1.95	1.46
1:B:158:MET:CE	1:B:216:TYR:CD2	1.95	1.46
5:A:602:ANP:N1	1:B:321:PRO:CB	1.82	1.43
5:B:602:ANP:N1	1:C:321:PRO:CB	1.82	1.40
5:B:602:ANP:N1	1:C:321:PRO:HB3	1.28	1.40
5:A:602:ANP:N6	1:B:321:PRO:HD3	1.11	1.39
5:A:602:ANP:N1	1:B:321:PRO:HB3	1.27	1.38
1:C:127:GLY:O	1:C:269:VAL:CG2	1.72	1.36
1:C:126:PHE:CZ	1:C:286:PRO:HG3	1.58	1.36
1:A:127:GLY:O	1:A:269:VAL:CG2	1.72	1.36
1:C:130:ARG:NH1	1:C:304:LYS:NZ	1.73	1.36
1:B:130:ARG:NH1	1:B:304:LYS:NZ	1.73	1.35
1:B:126:PHE:CZ	1:B:286:PRO:HG3	1.58	1.35
5:A:602:ANP:C6	1:B:321:PRO:N	1.88	1.35
1:A:126:PHE:CZ	1:A:286:PRO:HG3	1.58	1.35
1:B:127:GLY:O	1:B:269:VAL:CG2	1.72	1.35
1:A:130:ARG:NH1	1:A:304:LYS:NZ	1.73	1.33
1:B:156:LYS:O	1:B:216:TYR:HD1	1.09	1.32
1:C:156:LYS:O	1:C:216:TYR:HD1	1.09	1.29
5:A:602:ANP:N1	1:B:321:PRO:CA	1.96	1.28
5:B:602:ANP:N1	1:C:321:PRO:CA	1.95	1.27
1:C:158:MET:HE2	1:C:216:TYR:CG	1.69	1.27
1:A:156:LYS:O	1:A:216:TYR:HD1	1.09	1.25
1:A:158:MET:HE2	1:A:216:TYR:CG	1.71	1.25
1:B:158:MET:HE2	1:B:216:TYR:CG	1.71	1.23

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PHE:CE2	1:B:286:PRO:HD3	1.72	1.23
1:C:126:PHE:CE2	1:C:286:PRO:HD3	1.72	1.22
1:A:126:PHE:CE2	1:A:286:PRO:HD3	1.72	1.22
5:A:602:ANP:N6	1:B:321:PRO:N	1.86	1.22
1:B:222:ASP:O	1:B:266:THR:HB	1.43	1.18
1:B:156:LYS:O	1:B:216:TYR:CD1	1.97	1.18
1:A:156:LYS:O	1:A:216:TYR:CD1	1.97	1.18
1:C:156:LYS:O	1:C:216:TYR:CD1	1.97	1.17
1:A:222:ASP:O	1:A:266:THR:HB	1.43	1.15
1:A:216:TYR:O	1:A:261:VAL:HG22	1.45	1.15
1:A:126:PHE:CZ	1:A:286:PRO:CG	2.29	1.15
1:B:126:PHE:CZ	1:B:286:PRO:CG	2.29	1.15
1:A:124:GLU:HB3	1:A:299:ARG:HD3	1.29	1.15
1:A:127:GLY:O	1:A:269:VAL:HG23	1.39	1.15
1:C:222:ASP:O	1:C:266:THR:HB	1.43	1.15
1:B:216:TYR:O	1:B:261:VAL:HG22	1.45	1.14
1:C:126:PHE:CZ	1:C:286:PRO:CG	2.29	1.14
1:A:156:LYS:C	1:A:216:TYR:HD1	1.49	1.14
1:C:156:LYS:C	1:C:216:TYR:HD1	1.49	1.14
1:A:130:ARG:NH1	1:A:304:LYS:HZ3	1.32	1.13
1:B:156:LYS:C	1:B:216:TYR:HD1	1.49	1.13
1:B:156:LYS:CB	1:B:216:TYR:CE1	2.31	1.13
1:B:124:GLU:HB3	1:B:299:ARG:HD3	1.29	1.13
5:B:602:ANP:C2	1:C:321:PRO:HA	1.79	1.13
1:A:236:GLY:HA2	1:A:237:GLU:HB2	1.30	1.13
1:B:130:ARG:NH1	1:B:304:LYS:HZ3	1.35	1.12
1:C:216:TYR:O	1:C:261:VAL:HG22	1.45	1.12
1:A:156:LYS:CB	1:A:216:TYR:CE1	2.31	1.12
1:C:156:LYS:CB	1:C:216:TYR:CE1	2.32	1.12
1:C:129:PHE:O	1:C:130:ARG:CG	1.97	1.12
1:B:236:GLY:HA2	1:B:237:GLU:HB2	1.30	1.12
1:B:127:GLY:O	1:B:269:VAL:HG23	1.39	1.11
5:A:602:ANP:C2	1:B:321:PRO:HA	1.80	1.11
1:A:129:PHE:O	1:A:130:ARG:CG	1.97	1.11
1:A:156:LYS:C	1:A:216:TYR:CD1	2.24	1.11
5:A:602:ANP:C6	1:B:321:PRO:CA	2.25	1.11
1:B:129:PHE:O	1:B:130:ARG:CG	1.97	1.10
1:B:156:LYS:C	1:B:216:TYR:CD1	2.24	1.10
5:B:602:ANP:C6	1:C:321:PRO:CA	2.25	1.10
1:C:156:LYS:C	1:C:216:TYR:CD1	2.24	1.10
1:C:127:GLY:O	1:C:269:VAL:HG23	1.39	1.09

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLU:HB3	1:C:299:ARG:HD3	1.29	1.09
1:A:156:LYS:HB3	1:A:216:TYR:CE1	1.89	1.08
1:B:156:LYS:HB3	1:B:216:TYR:CE1	1.89	1.08
1:C:156:LYS:HB3	1:C:216:TYR:CE1	1.89	1.08
1:C:236:GLY:HA2	1:C:237:GLU:HB2	1.30	1.08
1:A:273:VAL:HG11	1:B:235:ARG:CD	1.83	1.07
1:C:129:PHE:O	1:C:130:ARG:HG3	1.54	1.07
1:A:129:PHE:O	1:A:130:ARG:HG3	1.54	1.06
1:C:134:THR:HG22	1:C:222:ASP:OD2	1.57	1.05
1:B:129:PHE:O	1:B:130:ARG:HG3	1.54	1.05
1:B:273:VAL:HG11	1:C:235:ARG:CD	1.86	1.05
1:A:134:THR:HG22	1:A:222:ASP:OD2	1.57	1.03
1:B:134:THR:HG22	1:B:222:ASP:OD2	1.57	1.03
1:A:127:GLY:O	1:A:269:VAL:HG21	1.58	1.02
1:C:130:ARG:NH1	1:C:304:LYS:HZ3	1.35	1.02
1:B:273:VAL:HG11	1:C:235:ARG:HD3	1.01	1.01
1:C:242:GLN:HG3	2:D:7:DT:P	2.00	1.00
1:C:127:GLY:O	1:C:269:VAL:HG21	1.58	1.00
1:C:130:ARG:HH12	1:C:304:LYS:NZ	1.57	1.00
1:A:134:THR:CG2	1:A:222:ASP:OD2	2.09	1.00
1:A:273:VAL:CG1	1:B:235:ARG:HD3	1.92	0.99
1:B:134:THR:CG2	1:B:222:ASP:OD2	2.09	0.99
1:C:158:MET:CE	1:C:216:TYR:HD2	1.67	0.99
1:C:134:THR:CG2	1:C:222:ASP:OD2	2.09	0.98
1:C:126:PHE:HZ	1:C:286:PRO:HG3	0.90	0.98
1:B:127:GLY:O	1:B:269:VAL:HG21	1.58	0.98
1:B:130:ARG:HH11	1:B:304:LYS:NZ	1.46	0.98
1:B:130:ARG:HH12	1:B:304:LYS:NZ	1.57	0.97
1:A:126:PHE:HZ	1:A:286:PRO:HG3	0.90	0.97
1:B:126:PHE:HZ	1:B:286:PRO:HG3	0.90	0.97
1:A:273:VAL:HG11	1:B:235:ARG:HD3	0.97	0.96
1:A:130:ARG:HH11	1:A:304:LYS:NZ	1.46	0.96
1:B:217:ALA:O	1:B:261:VAL:C	2.02	0.95
1:B:158:MET:CE	1:B:216:TYR:HD2	1.67	0.95
1:C:130:ARG:HH11	1:C:304:LYS:NZ	1.46	0.95
1:A:156:LYS:HB3	1:A:216:TYR:HE1	1.32	0.94
1:A:158:MET:CE	1:A:216:TYR:HD2	1.67	0.94
1:B:156:LYS:HB2	1:B:216:TYR:CE1	2.03	0.94
1:C:156:LYS:HB2	1:C:216:TYR:CE1	2.03	0.93
1:C:217:ALA:O	1:C:261:VAL:C	2.02	0.93
1:A:156:LYS:HB2	1:A:216:TYR:CE1	2.03	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:HB2	1:B:216:TYR:CD1	2.04	0.92
1:A:156:LYS:HB2	1:A:216:TYR:CD1	2.05	0.92
1:C:156:LYS:HB3	1:C:216:TYR:HE1	1.33	0.92
1:C:158:MET:HE1	1:C:216:TYR:CD2	2.03	0.92
1:C:242:GLN:CD	2:D:7:DT:OP2	2.08	0.91
1:C:156:LYS:HB2	1:C:216:TYR:CD1	2.04	0.91
1:B:124:GLU:CB	1:B:299:ARG:HD3	2.01	0.91
1:B:273:VAL:CG1	1:C:235:ARG:HD3	1.97	0.91
1:B:130:ARG:NH1	1:B:304:LYS:HZ2	1.48	0.91
1:B:156:LYS:HB3	1:B:216:TYR:HE1	1.32	0.90
1:C:126:PHE:CE2	1:C:286:PRO:CD	2.54	0.90
1:C:124:GLU:CB	1:C:299:ARG:HD3	2.01	0.90
1:A:130:ARG:HH12	1:A:304:LYS:NZ	1.57	0.90
1:A:126:PHE:CE2	1:A:286:PRO:CD	2.54	0.90
1:A:124:GLU:CB	1:A:299:ARG:HD3	2.01	0.90
1:A:158:MET:HE2	1:A:216:TYR:CE2	2.06	0.89
1:B:126:PHE:CE2	1:B:286:PRO:CD	2.54	0.89
5:B:602:ANP:C2	1:C:321:PRO:CA	2.45	0.89
1:B:158:MET:HE1	1:B:216:TYR:CD2	2.07	0.89
1:C:130:ARG:HH12	1:C:304:LYS:HZ3	1.15	0.88
1:A:158:MET:HE1	1:A:216:TYR:CD2	2.07	0.88
1:B:158:MET:HE2	1:B:216:TYR:CE2	2.06	0.87
5:A:602:ANP:C6	1:B:321:PRO:CD	2.44	0.87
1:A:222:ASP:O	1:A:266:THR:CB	2.23	0.86
1:B:218:LEU:HD13	1:B:262:ALA:HB3	1.57	0.86
5:B:602:ANP:C2	1:C:321:PRO:HB3	2.04	0.86
1:A:218:LEU:HD13	1:A:262:ALA:HB3	1.57	0.86
1:A:268:GLN:HG3	1:B:294:HIS:CG	2.10	0.86
1:C:129:PHE:O	1:C:130:ARG:HG2	1.75	0.86
1:A:130:ARG:HH11	1:A:304:LYS:HZ2	1.04	0.85
1:B:222:ASP:O	1:B:266:THR:CB	2.23	0.85
1:C:242:GLN:CG	2:D:7:DT:P	2.64	0.85
5:B:602:ANP:N1	1:C:321:PRO:HA	1.78	0.85
5:A:602:ANP:C2	1:B:321:PRO:HB3	2.04	0.85
1:C:222:ASP:O	1:C:266:THR:CB	2.23	0.85
1:C:218:LEU:HD13	1:C:262:ALA:HB3	1.57	0.84
1:A:129:PHE:O	1:A:130:ARG:HG2	1.75	0.84
1:B:129:PHE:O	1:B:130:ARG:HG2	1.75	0.84
5:A:602:ANP:C2	1:B:321:PRO:CA	2.47	0.84
1:B:268:GLN:HG3	1:C:294:HIS:CG	2.12	0.84
1:C:242:GLN:NE2	2:D:7:DT:OP1	2.10	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:O	1:A:261:VAL:C	2.02	0.84
1:A:156:LYS:CB	1:A:216:TYR:CD1	2.61	0.83
1:B:156:LYS:CB	1:B:216:TYR:CD1	2.61	0.83
1:B:158:MET:HE1	1:B:216:TYR:HD2	1.42	0.83
1:C:156:LYS:CB	1:C:216:TYR:CD1	2.61	0.83
5:A:602:ANP:C6	1:B:320:LEU:C	2.46	0.83
5:B:602:ANP:C2	1:C:321:PRO:CB	2.56	0.83
2:D:7:DT:OP1	2:D:7:DT:H4'	1.78	0.83
1:A:218:LEU:HD11	1:A:264:VAL:HG23	1.59	0.83
1:A:130:ARG:NH1	1:A:304:LYS:HZ2	1.52	0.83
1:B:218:LEU:HD11	1:B:264:VAL:HG23	1.59	0.83
5:A:602:ANP:C2	1:B:321:PRO:CB	2.57	0.83
1:A:158:MET:HE1	1:A:216:TYR:HD2	1.42	0.82
1:C:130:ARG:HH11	1:C:304:LYS:HZ2	1.00	0.82
1:C:236:GLY:CA	1:C:237:GLU:HB2	2.10	0.82
1:C:158:MET:HE1	1:C:216:TYR:HD2	1.39	0.82
1:C:218:LEU:HD11	1:C:264:VAL:HG23	1.59	0.82
1:C:130:ARG:NH1	1:C:304:LYS:HZ2	1.48	0.82
1:C:242:GLN:CD	2:D:7:DT:P	2.58	0.82
1:B:130:ARG:HH11	1:B:304:LYS:HZ2	1.00	0.82
1:B:236:GLY:CA	1:B:237:GLU:HB2	2.10	0.82
1:A:126:PHE:CZ	1:A:286:PRO:CD	2.64	0.81
1:B:126:PHE:CZ	1:B:286:PRO:CD	2.64	0.81
1:C:126:PHE:CZ	1:C:286:PRO:CD	2.64	0.81
1:C:158:MET:HE2	1:C:216:TYR:CE2	2.10	0.80
1:B:128:GLU:O	1:C:294:HIS:CE1	2.35	0.79
1:A:128:GLU:O	1:B:294:HIS:CE1	2.36	0.79
1:A:225:THR:HB	1:A:287:ILE:HD11	1.64	0.79
1:C:225:THR:HB	1:C:287:ILE:HD11	1.63	0.79
1:A:236:GLY:CA	1:A:237:GLU:HB2	2.10	0.79
1:C:242:GLN:OE1	2:D:7:DT:OP2	2.01	0.79
1:B:225:THR:HB	1:B:287:ILE:HD11	1.64	0.79
1:A:293:ALA:HA	1:A:299:ARG:HH22	1.50	0.77
1:C:57:LYS:HE3	1:C:61:ILE:HD11	1.65	0.77
1:B:128:GLU:O	1:B:129:PHE:HB3	1.85	0.77
1:B:57:LYS:HE3	1:B:61:ILE:HD11	1.65	0.76
1:A:130:ARG:HH12	1:A:304:LYS:HZ3	1.14	0.76
1:B:293:ALA:HA	1:B:299:ARG:HH22	1.50	0.76
1:C:128:GLU:O	1:C:129:PHE:HB3	1.85	0.76
1:C:293:ALA:HA	1:C:299:ARG:HH22	1.50	0.76
1:A:57:LYS:HE3	1:A:61:ILE:HD11	1.65	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PHE:HZ	1:B:286:PRO:CG	1.79	0.75
1:A:128:GLU:O	1:A:129:PHE:HB3	1.85	0.75
1:B:158:MET:CE	1:B:216:TYR:CG	2.50	0.75
1:B:126:PHE:CZ	1:B:286:PRO:HD3	2.21	0.75
5:B:602:ANP:C5	1:C:320:LEU:C	2.55	0.75
1:B:261:VAL:O	1:B:262:ALA:HB2	1.86	0.75
1:C:242:GLN:CG	2:D:7:DT:OP2	2.35	0.74
1:C:134:THR:HG21	1:C:222:ASP:OD2	1.88	0.74
1:C:261:VAL:O	1:C:262:ALA:HB2	1.86	0.73
1:A:261:VAL:O	1:A:262:ALA:HB2	1.86	0.73
5:A:602:ANP:C5	1:B:320:LEU:C	2.57	0.73
1:A:126:PHE:CZ	1:A:286:PRO:HD3	2.21	0.73
1:B:134:THR:HG21	1:B:222:ASP:OD2	1.88	0.73
5:A:602:ANP:N6	1:B:320:LEU:C	2.41	0.73
1:A:134:THR:HG21	1:A:222:ASP:OD2	1.88	0.72
1:B:126:PHE:HB3	1:B:301:TYR:HD1	1.55	0.72
1:A:259:PHE:O	1:A:261:VAL:HG23	1.90	0.72
5:A:602:ANP:N1	1:B:321:PRO:HA	1.78	0.72
1:C:158:MET:CE	1:C:216:TYR:CG	2.50	0.72
3:E:3:DA:H5'	3:E:4:DA:OP2	1.90	0.72
1:A:237:GLU:O	1:A:239:SER:N	2.22	0.72
1:C:259:PHE:O	1:C:261:VAL:HG23	1.90	0.72
1:A:216:TYR:O	1:A:261:VAL:CG2	2.34	0.71
1:B:216:TYR:O	1:B:261:VAL:CG2	2.34	0.71
1:C:242:GLN:HG3	2:D:6:DT:O3'	1.89	0.71
5:B:602:ANP:C6	1:C:320:LEU:C	2.44	0.71
5:A:602:ANP:O2B	5:A:602:ANP:O2A	2.08	0.71
1:B:237:GLU:O	1:B:239:SER:N	2.22	0.71
5:B:602:ANP:O2B	5:B:602:ANP:O2A	2.08	0.71
1:B:162:THR:HG22	1:B:194:ALA:HB3	1.73	0.71
1:B:96:ARG:HD3	1:B:99:ILE:HD13	1.73	0.71
1:C:216:TYR:O	1:C:261:VAL:CG2	2.34	0.70
1:B:156:LYS:C	1:B:216:TYR:CE1	2.65	0.70
5:C:401:ANP:O2A	5:C:401:ANP:O2B	2.08	0.70
1:B:259:PHE:O	1:B:261:VAL:HG23	1.90	0.70
1:C:126:PHE:HZ	1:C:286:PRO:CG	1.79	0.70
1:C:126:PHE:HB3	1:C:301:TYR:HD1	1.55	0.70
1:C:162:THR:HG22	1:C:194:ALA:HB3	1.73	0.70
1:C:96:ARG:HD3	1:C:99:ILE:HD13	1.73	0.70
1:A:162:THR:HG22	1:A:194:ALA:HB3	1.73	0.70
1:C:261:VAL:O	1:C:262:ALA:CB	2.39	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:HB3	1:A:301:TYR:HD1	1.55	0.70
1:A:126:PHE:HB2	1:A:300:LEU:O	1.92	0.70
1:A:156:LYS:C	1:A:216:TYR:CE1	2.65	0.70
1:C:126:PHE:HB2	1:C:301:TYR:HA	1.72	0.70
1:A:126:PHE:HB2	1:A:301:TYR:HA	1.72	0.70
1:B:126:PHE:HB2	1:B:301:TYR:HA	1.72	0.70
1:A:158:MET:CE	1:A:216:TYR:CG	2.50	0.69
1:C:156:LYS:C	1:C:216:TYR:CE1	2.65	0.69
1:C:162:THR:HG1	1:C:223:SER:HG	1.34	0.69
1:C:237:GLU:O	1:C:239:SER:N	2.22	0.69
1:A:233:SER:OG	1:B:247:ARG:NH2	2.25	0.69
1:B:126:PHE:HB2	1:B:300:LEU:O	1.92	0.69
1:C:126:PHE:CZ	1:C:286:PRO:HD3	2.21	0.69
5:B:602:ANP:O1B	5:B:602:ANP:O2G	2.11	0.69
1:A:96:ARG:HD3	1:A:99:ILE:HD13	1.73	0.69
1:B:130:ARG:HH12	1:B:304:LYS:HZ3	1.15	0.69
1:C:126:PHE:HB2	1:C:300:LEU:O	1.92	0.69
1:B:261:VAL:O	1:B:262:ALA:CB	2.39	0.69
5:A:602:ANP:O2G	5:A:602:ANP:O1B	2.11	0.68
1:A:268:GLN:CG	1:B:294:HIS:CG	2.76	0.68
5:C:401:ANP:O1B	5:C:401:ANP:O2G	2.11	0.68
5:B:602:ANP:C6	1:C:321:PRO:HA	2.15	0.68
1:A:270:VAL:O	1:A:284:LYS:O	2.12	0.68
1:B:22:PRO:HG3	1:B:215:ARG:HH22	1.58	0.68
1:C:133:LYS:HD2	1:C:266:THR:HG22	1.76	0.68
1:A:261:VAL:O	1:A:262:ALA:CB	2.39	0.67
1:C:22:PRO:HG3	1:C:215:ARG:HH22	1.58	0.67
1:A:22:PRO:HG3	1:A:215:ARG:HH22	1.58	0.67
5:A:602:ANP:C6	1:B:321:PRO:HA	2.14	0.67
1:C:270:VAL:O	1:C:284:LYS:O	2.11	0.67
1:B:268:GLN:CG	1:C:294:HIS:CG	2.77	0.67
1:C:242:GLN:HG3	2:D:7:DT:OP2	1.93	0.67
1:B:133:LYS:HD2	1:B:266:THR:HG22	1.76	0.66
1:B:270:VAL:O	1:B:284:LYS:O	2.11	0.66
1:C:235:ARG:NH2	3:E:4:DA:O4'	2.27	0.66
1:B:233:SER:OG	1:C:247:ARG:NH2	2.28	0.66
1:A:133:LYS:HD2	1:A:266:THR:HG22	1.76	0.65
1:A:218:LEU:HD13	1:A:262:ALA:CB	2.26	0.65
1:A:126:PHE:CE1	1:A:299:ARG:HD2	2.32	0.65
1:B:218:LEU:CD1	1:B:262:ALA:HB3	2.26	0.65
1:C:126:PHE:CE1	1:C:299:ARG:HD2	2.32	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PHE:CE1	1:B:299:ARG:HD2	2.32	0.65
1:C:218:LEU:CD1	1:C:262:ALA:HB3	2.26	0.65
1:C:242:GLN:HB3	1:C:291:ILE:HD12	1.78	0.64
1:B:126:PHE:HE2	1:B:286:PRO:HD3	1.55	0.64
1:C:218:LEU:HD13	1:C:262:ALA:CB	2.26	0.64
1:A:218:LEU:CD1	1:A:262:ALA:HB3	2.26	0.64
1:A:130:ARG:HD2	1:A:304:LYS:HD3	1.80	0.64
1:A:242:GLN:HB3	1:A:291:ILE:HD12	1.78	0.64
1:B:288:GLY:HA3	1:B:292:ILE:HD12	1.80	0.64
1:C:130:ARG:HD2	1:C:304:LYS:HD3	1.80	0.64
1:B:130:ARG:HD2	1:B:304:LYS:HD3	1.80	0.63
1:B:242:GLN:HB3	1:B:291:ILE:HD12	1.78	0.63
1:A:126:PHE:HE2	1:A:286:PRO:HD3	1.55	0.63
1:B:122:ILE:CG2	1:B:265:ILE:HD11	2.29	0.63
1:B:177:ARG:HD2	1:B:178:TYR:CZ	2.34	0.63
1:B:218:LEU:HD13	1:B:262:ALA:CB	2.26	0.63
1:C:293:ALA:HA	1:C:299:ARG:NH2	2.14	0.62
1:A:288:GLY:HA3	1:A:292:ILE:HD12	1.80	0.62
1:A:293:ALA:HA	1:A:299:ARG:NH2	2.14	0.62
1:C:177:ARG:HD2	1:C:178:TYR:CZ	2.34	0.62
1:B:112:LEU:HD11	1:B:325:ALA:HB3	1.79	0.62
1:C:122:ILE:CG2	1:C:265:ILE:HD11	2.29	0.62
1:A:156:LYS:CA	1:A:216:TYR:CD1	2.83	0.62
1:C:112:LEU:HD11	1:C:325:ALA:HB3	1.79	0.62
1:C:288:GLY:HA3	1:C:292:ILE:HD12	1.80	0.62
1:A:177:ARG:HD2	1:A:178:TYR:CZ	2.34	0.62
1:A:112:LEU:HD11	1:A:325:ALA:HB3	1.80	0.61
1:B:218:LEU:HD11	1:B:264:VAL:CG2	2.30	0.61
1:B:293:ALA:HA	1:B:299:ARG:NH2	2.14	0.61
1:B:156:LYS:CA	1:B:216:TYR:CD1	2.83	0.61
1:A:122:ILE:CG2	1:A:265:ILE:HD11	2.29	0.61
1:C:22:PRO:HG3	1:C:215:ARG:NH2	2.15	0.61
1:A:310:ARG:NH2	5:A:602:ANP:O2'	2.33	0.61
1:A:218:LEU:HD11	1:A:264:VAL:CG2	2.30	0.61
1:C:156:LYS:CA	1:C:216:TYR:CD1	2.83	0.61
1:A:122:ILE:HG23	1:A:265:ILE:HD11	1.83	0.61
1:B:310:ARG:NH2	5:B:602:ANP:O2'	2.33	0.61
1:B:122:ILE:HG23	1:B:265:ILE:HD11	1.83	0.61
1:C:122:ILE:HG23	1:C:265:ILE:HD11	1.83	0.61
5:B:602:ANP:C5	1:C:320:LEU:O	2.49	0.61
1:B:288:GLY:N	2:D:5:DT:OP1	2.32	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:HD3	1:C:178:TYR:CE1	2.37	0.60
1:A:177:ARG:HD3	1:A:178:TYR:CE1	2.36	0.60
1:B:177:ARG:HD3	1:B:178:TYR:CE1	2.36	0.60
1:B:22:PRO:HG3	1:B:215:ARG:NH2	2.16	0.60
1:A:124:GLU:HB3	1:A:299:ARG:CD	2.19	0.60
1:C:310:ARG:NH2	5:C:401:ANP:O2'	2.33	0.60
1:A:22:PRO:HG3	1:A:215:ARG:NH2	2.16	0.60
1:A:130:ARG:O	1:A:310:ARG:NH1	2.34	0.60
5:A:602:ANP:C5	1:B:320:LEU:O	2.50	0.59
1:C:126:PHE:HE2	1:C:286:PRO:HD3	1.55	0.59
1:A:126:PHE:CZ	1:A:299:ARG:NH1	2.70	0.59
1:B:130:ARG:O	1:B:310:ARG:NH1	2.34	0.59
1:A:177:ARG:CD	1:A:178:TYR:CZ	2.86	0.59
1:C:126:PHE:CZ	1:C:299:ARG:NH1	2.70	0.59
1:B:126:PHE:CZ	1:B:299:ARG:NH1	2.70	0.59
1:C:130:ARG:O	1:C:310:ARG:NH1	2.34	0.59
1:C:177:ARG:CD	1:C:178:TYR:CZ	2.86	0.59
5:A:602:ANP:C6	1:B:321:PRO:CB	2.67	0.59
1:A:126:PHE:HZ	1:A:286:PRO:CG	1.79	0.58
1:C:124:GLU:HB3	1:C:299:ARG:CD	2.19	0.58
1:B:177:ARG:CD	1:B:178:TYR:CZ	2.86	0.58
1:C:218:LEU:HD12	1:C:262:ALA:O	2.04	0.58
1:A:229:ARG:NH2	1:A:269:VAL:O	2.36	0.57
1:B:218:LEU:HD12	1:B:262:ALA:O	2.04	0.57
1:A:218:LEU:HD12	1:A:262:ALA:O	2.04	0.56
1:C:260:GLY:O	1:C:261:VAL:HB	2.05	0.56
1:B:267:ASN:OD1	1:B:267:ASN:N	2.38	0.56
1:C:218:LEU:HD11	1:C:264:VAL:CG2	2.31	0.56
1:C:109:LEU:HD23	1:C:112:LEU:HD12	1.88	0.56
1:A:260:GLY:O	1:A:261:VAL:HB	2.05	0.56
1:A:29:GLU:HG2	1:A:38:VAL:HG21	1.88	0.56
1:B:168:PRO:HB2	1:C:93:HIS:HD2	1.71	0.56
1:C:29:GLU:HG2	1:C:38:VAL:HG21	1.88	0.56
1:B:109:LEU:HD23	1:B:112:LEU:HD12	1.88	0.56
1:B:128:GLU:O	1:C:294:HIS:HE1	1.88	0.56
1:B:129:PHE:C	1:B:130:ARG:CG	2.74	0.56
1:C:124:GLU:CB	1:C:299:ARG:CD	2.82	0.55
1:C:242:GLN:CD	2:D:7:DT:OP1	2.44	0.55
1:A:267:ASN:N	1:A:267:ASN:OD1	2.38	0.55
1:A:109:LEU:HD23	1:A:112:LEU:HD12	1.88	0.55
1:C:229:ARG:NH2	1:C:269:VAL:O	2.36	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLY:O	1:B:261:VAL:HB	2.05	0.55
1:A:124:GLU:CB	1:A:299:ARG:CD	2.82	0.55
1:B:29:GLU:HG2	1:B:38:VAL:HG21	1.88	0.55
1:A:129:PHE:C	1:A:130:ARG:CG	2.74	0.54
1:B:229:ARG:NH2	1:B:269:VAL:O	2.36	0.54
1:A:198:ASP:O	1:A:201:THR:OG1	2.17	0.54
1:A:128:GLU:O	1:B:294:HIS:HE1	1.89	0.54
1:C:267:ASN:N	1:C:267:ASN:OD1	2.38	0.54
1:A:268:GLN:HG3	1:B:294:HIS:ND1	2.22	0.54
1:C:236:GLY:HA2	1:C:237:GLU:CB	2.18	0.54
1:C:158:MET:CE	1:C:216:TYR:CE2	2.82	0.54
1:C:177:ARG:CD	1:C:178:TYR:CE1	2.91	0.53
1:B:177:ARG:CD	1:B:178:TYR:CE1	2.91	0.53
1:B:268:GLN:HG3	1:C:294:HIS:ND1	2.23	0.53
1:A:168:PRO:HB2	1:B:93:HIS:HD2	1.73	0.53
1:B:126:PHE:CZ	1:B:286:PRO:CB	2.91	0.53
5:B:602:ANP:HN61	1:C:320:LEU:HA	1.72	0.53
1:A:126:PHE:CZ	1:A:286:PRO:CB	2.91	0.53
5:A:602:ANP:C5	1:B:321:PRO:N	2.65	0.53
1:A:236:GLY:HA2	1:A:237:GLU:CB	2.18	0.53
1:A:49:VAL:HG11	1:A:81:LEU:HD12	1.91	0.53
1:A:177:ARG:CD	1:A:178:TYR:CE1	2.91	0.53
1:A:28:LEU:HG	1:A:49:VAL:HG22	1.91	0.53
1:B:158:MET:CE	1:B:216:TYR:CB	2.87	0.53
1:C:158:MET:CE	1:C:216:TYR:CB	2.87	0.53
1:C:127:GLY:C	1:C:269:VAL:HG21	2.29	0.53
1:A:125:MET:HB2	1:A:266:THR:HG23	1.91	0.52
5:A:602:ANP:HN61	1:B:320:LEU:HA	1.75	0.52
1:B:161:ASP:OD1	1:B:162:THR:N	2.42	0.52
1:B:236:GLY:HA2	1:B:237:GLU:CB	2.18	0.52
1:A:161:ASP:OD1	1:A:162:THR:N	2.42	0.52
1:B:49:VAL:HG11	1:B:81:LEU:HD12	1.91	0.52
1:C:126:PHE:CZ	1:C:286:PRO:CB	2.91	0.52
1:C:235:ARG:O	1:C:235:ARG:NH2	2.43	0.52
1:A:158:MET:CE	1:A:216:TYR:CB	2.87	0.52
1:A:235:ARG:NH2	1:A:235:ARG:O	2.43	0.52
1:B:235:ARG:NH2	1:B:235:ARG:O	2.43	0.52
1:B:125:MET:HB2	1:B:266:THR:HG23	1.92	0.52
1:B:28:LEU:HG	1:B:49:VAL:HG22	1.91	0.52
1:C:121:SER:O	1:C:263:VAL:HG23	2.10	0.52
1:C:129:PHE:C	1:C:130:ARG:CG	2.74	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASP:OD1	1:C:162:THR:N	2.42	0.52
1:C:28:LEU:HG	1:C:49:VAL:HG22	1.91	0.52
1:C:49:VAL:HG11	1:C:81:LEU:HD12	1.91	0.52
1:A:158:MET:HE3	1:A:216:TYR:CB	2.39	0.52
1:B:121:SER:O	1:B:263:VAL:HG23	2.10	0.51
1:B:48:THR:HG21	1:B:259:PHE:HZ	1.75	0.51
1:C:48:THR:HG21	1:C:259:PHE:HZ	1.75	0.51
1:B:273:VAL:CG1	1:C:235:ARG:CD	2.73	0.51
1:C:125:MET:HB2	1:C:266:THR:HG23	1.91	0.51
1:A:121:SER:O	1:A:263:VAL:HG23	2.09	0.51
1:B:158:MET:HE3	1:B:216:TYR:CB	2.39	0.51
1:A:268:GLN:HG3	1:B:294:HIS:CD2	2.44	0.51
1:B:268:GLN:HG3	1:C:294:HIS:CD2	2.45	0.51
1:B:124:GLU:CB	1:B:299:ARG:CD	2.82	0.50
1:B:235:ARG:NH2	3:E:7:DA:O4'	2.44	0.50
1:A:269:VAL:HG11	1:A:284:LYS:HD2	1.94	0.50
1:B:198:ASP:O	1:B:201:THR:OG1	2.17	0.50
3:E:4:DA:OP1	3:E:4:DA:H4'	2.12	0.50
1:A:57:LYS:NZ	1:A:71:ALA:HB3	2.27	0.50
1:B:124:GLU:HB3	1:B:299:ARG:CD	2.19	0.50
1:A:304:LYS:HG2	1:A:305:GLY:O	2.12	0.50
1:B:235:ARG:HB3	1:B:238:LEU:HD13	1.94	0.50
1:B:269:VAL:HG11	1:B:284:LYS:HD2	1.94	0.50
1:A:48:THR:HG21	1:A:259:PHE:HZ	1.76	0.49
1:C:57:LYS:NZ	1:C:71:ALA:HB3	2.27	0.49
1:B:122:ILE:HA	1:B:263:VAL:HB	1.95	0.49
1:B:57:LYS:NZ	1:B:71:ALA:HB3	2.27	0.49
1:C:198:ASP:O	1:C:201:THR:OG1	2.17	0.49
1:B:222:ASP:HA	1:B:266:THR:OG1	2.13	0.49
1:B:304:LYS:HG2	1:B:305:GLY:O	2.12	0.49
1:C:269:VAL:HG11	1:C:284:LYS:HD2	1.94	0.49
1:C:304:LYS:HG2	1:C:305:GLY:O	2.12	0.49
1:A:157:ALA:O	1:A:189:VAL:HA	2.13	0.49
1:A:302:LEU:HD23	1:A:312:CYS:HA	1.94	0.49
1:B:302:LEU:HD23	1:B:312:CYS:HA	1.94	0.49
5:B:602:ANP:N6	1:C:320:LEU:HA	2.28	0.49
1:C:234:GLY:HA2	1:C:236:GLY:HA2	1.95	0.49
1:A:273:VAL:CG1	1:B:235:ARG:CD	2.69	0.49
1:C:133:LYS:HD2	1:C:266:THR:CG2	2.43	0.49
1:C:158:MET:HE3	1:C:216:TYR:CB	2.42	0.49
1:B:157:ALA:O	1:B:189:VAL:HA	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:HD23	1:C:312:CYS:HA	1.94	0.49
1:A:235:ARG:HB3	1:A:238:LEU:HD13	1.94	0.48
1:B:145:GLN:NE2	1:B:188:ASN:HB2	2.28	0.48
1:B:234:GLY:HA2	1:B:236:GLY:HA2	1.95	0.48
1:C:235:ARG:HB3	1:C:238:LEU:HD13	1.94	0.48
1:C:157:ALA:O	1:C:189:VAL:HA	2.13	0.48
1:A:122:ILE:HA	1:A:263:VAL:HB	1.95	0.48
1:C:145:GLN:NE2	1:C:188:ASN:HB2	2.28	0.48
1:C:222:ASP:HA	1:C:266:THR:OG1	2.13	0.48
2:D:5:DT:H2"	2:D:6:DT:H5"	1.95	0.48
1:A:145:GLN:NE2	1:A:188:ASN:HB2	2.28	0.48
1:A:306:ARG:O	1:A:309:THR:OG1	2.23	0.48
1:C:122:ILE:HA	1:C:263:VAL:HB	1.95	0.48
1:A:234:GLY:HA2	1:A:236:GLY:HA2	1.95	0.48
1:A:222:ASP:HA	1:A:266:THR:OG1	2.13	0.48
1:A:299:ARG:HB3	1:A:315:TYR:HB2	1.96	0.48
1:C:38:VAL:O	1:C:42:GLU:HG3	2.14	0.48
1:A:177:ARG:HG3	1:A:332:ASP:HB3	1.96	0.47
1:C:177:ARG:HG3	1:C:332:ASP:HB3	1.96	0.47
1:B:127:GLY:C	1:B:269:VAL:HG21	2.29	0.47
1:C:299:ARG:HB3	1:C:315:TYR:HB2	1.96	0.47
1:A:127:GLY:C	1:A:269:VAL:HG21	2.29	0.47
1:B:235:ARG:HA	1:B:236:GLY:HA3	1.70	0.47
1:B:299:ARG:HB3	1:B:315:TYR:HB2	1.96	0.47
1:B:158:MET:CE	1:B:216:TYR:CE2	2.82	0.47
1:C:236:GLY:C	1:C:237:GLU:OE1	2.53	0.47
1:B:162:THR:OG1	1:B:223:SER:OG	2.14	0.47
1:A:38:VAL:O	1:A:42:GLU:HG3	2.14	0.47
1:B:242:GLN:HG3	2:D:3:DT:H4'	1.97	0.47
1:B:306:ARG:O	1:B:309:THR:OG1	2.23	0.47
1:B:177:ARG:HG3	1:B:332:ASP:HB3	1.96	0.46
1:A:207:ALA:O	1:A:211:MET:HG2	2.16	0.46
1:B:236:GLY:C	1:B:237:GLU:OE1	2.53	0.46
1:A:236:GLY:C	1:A:237:GLU:OE1	2.53	0.46
1:B:38:VAL:O	1:B:42:GLU:HG3	2.14	0.46
1:C:122:ILE:CG2	1:C:265:ILE:CD1	2.94	0.46
5:A:602:ANP:N3	1:B:321:PRO:HA	2.26	0.46
1:B:122:ILE:CG2	1:B:265:ILE:CD1	2.94	0.46
1:B:207:ALA:O	1:B:211:MET:HG2	2.16	0.46
1:C:207:ALA:O	1:C:211:MET:HG2	2.16	0.46
5:B:602:ANP:N7	1:C:320:LEU:O	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLN:HA	1:B:118:GLU:HA	1.98	0.46
5:A:602:ANP:N7	1:B:320:LEU:O	2.49	0.46
1:C:125:MET:CB	1:C:266:THR:HG23	2.46	0.45
1:A:101:GLN:HA	1:A:118:GLU:HA	1.98	0.45
1:A:122:ILE:CG2	1:A:265:ILE:CD1	2.94	0.45
1:B:125:MET:CB	1:B:266:THR:HG23	2.46	0.45
1:C:162:THR:HG21	1:C:200:GLN:HE21	1.81	0.45
5:A:602:ANP:C4	1:B:321:PRO:HA	2.46	0.45
1:A:125:MET:CB	1:A:266:THR:HG23	2.46	0.45
1:A:290:ASN:HB3	1:A:294:HIS:NE2	2.32	0.45
5:B:602:ANP:HN61	1:C:320:LEU:CA	2.29	0.45
5:B:602:ANP:N6	1:C:320:LEU:CA	2.79	0.45
5:B:602:ANP:C4	1:C:321:PRO:HA	2.46	0.45
1:A:177:ARG:HD2	1:A:178:TYR:CE2	2.52	0.45
1:C:23:GLN:HA	1:C:24:PRO:HD2	1.87	0.45
1:A:156:LYS:CA	1:A:216:TYR:CE1	2.99	0.45
1:A:159:TYR:CE2	1:A:161:ASP:HB2	2.52	0.44
1:B:177:ARG:HD2	1:B:178:TYR:CE2	2.52	0.44
1:C:101:GLN:HA	1:C:118:GLU:HA	1.98	0.44
1:C:177:ARG:HD2	1:C:178:TYR:CE2	2.52	0.44
1:B:196:ASN:ND2	1:C:55:ALA:O	2.50	0.44
1:A:235:ARG:HH21	1:A:235:ARG:CG	2.30	0.44
1:B:290:ASN:HB3	1:B:294:HIS:NE2	2.32	0.44
1:C:235:ARG:CG	1:C:235:ARG:HH21	2.31	0.44
1:B:159:TYR:CE2	1:B:161:ASP:HB2	2.52	0.44
1:C:290:ASN:HB3	1:C:294:HIS:NE2	2.32	0.44
1:A:124:GLU:OE1	1:A:299:ARG:NE	2.51	0.44
1:A:162:THR:HG21	1:A:200:GLN:HE21	1.81	0.44
1:B:133:LYS:HD2	1:B:266:THR:CG2	2.43	0.44
1:B:23:GLN:HA	1:B:24:PRO:HD2	1.87	0.44
1:C:124:GLU:OE2	1:C:267:ASN:ND2	2.46	0.44
1:C:159:TYR:CE2	1:C:161:ASP:HB2	2.52	0.44
1:C:124:GLU:OE1	1:C:299:ARG:NE	2.51	0.44
1:A:133:LYS:HD2	1:A:266:THR:CG2	2.43	0.44
1:B:145:GLN:HE21	1:B:188:ASN:HD22	1.66	0.44
1:B:162:THR:HG21	1:B:200:GLN:HE21	1.81	0.44
1:A:23:GLN:HA	1:A:24:PRO:HD2	1.87	0.44
1:C:145:GLN:HE21	1:C:188:ASN:HD22	1.66	0.44
1:A:145:GLN:HE21	1:A:188:ASN:HD22	1.66	0.44
1:A:197:THR:HG23	1:A:231:ASP:OD2	2.18	0.43
1:B:126:PHE:CE1	1:B:286:PRO:HB3	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLU:OE1	1:B:299:ARG:NE	2.51	0.43
1:B:124:GLU:OE2	1:B:267:ASN:ND2	2.46	0.43
1:C:126:PHE:CE1	1:C:286:PRO:HB3	2.54	0.43
5:A:602:ANP:N6	1:B:320:LEU:CA	2.82	0.43
1:B:197:THR:HG23	1:B:231:ASP:OD2	2.18	0.43
1:C:197:THR:HG23	1:C:231:ASP:OD2	2.19	0.43
1:A:48:THR:HG21	1:A:259:PHE:CZ	2.54	0.43
5:B:602:ANP:N3	1:C:321:PRO:HA	2.25	0.43
1:A:124:GLU:OE2	1:A:267:ASN:ND2	2.46	0.43
1:A:126:PHE:CE1	1:A:286:PRO:HB3	2.54	0.43
1:B:235:ARG:CG	1:B:235:ARG:HH21	2.30	0.43
1:A:132:GLY:O	1:A:135:GLN:HB3	2.19	0.43
1:B:248:PHE:CE2	1:B:252:LEU:HD11	2.54	0.43
1:A:167:ARG:HA	1:A:168:PRO:HD2	1.92	0.43
5:A:602:ANP:N6	1:B:320:LEU:HA	2.30	0.43
5:A:602:ANP:C5	1:B:321:PRO:HA	2.47	0.43
5:B:602:ANP:C5	1:C:321:PRO:HA	2.48	0.43
1:A:101:GLN:HA	1:A:117:ILE:O	2.19	0.43
1:C:101:GLN:HA	1:C:117:ILE:O	2.19	0.43
1:B:101:GLN:HA	1:B:117:ILE:O	2.19	0.42
1:B:132:GLY:O	1:B:135:GLN:HB3	2.19	0.42
1:B:309:THR:O	1:B:310:ARG:HD3	2.20	0.42
1:C:309:THR:O	1:C:310:ARG:HD3	2.20	0.42
1:A:268:GLN:OE1	1:B:294:HIS:HB3	2.19	0.42
5:A:602:ANP:HN61	1:B:320:LEU:CA	2.31	0.42
1:A:159:TYR:HE2	1:A:166:PHE:HB2	1.85	0.42
1:A:126:PHE:CB	1:A:301:TYR:HA	2.45	0.42
1:A:309:THR:O	1:A:310:ARG:HD3	2.20	0.42
1:C:248:PHE:CE2	1:C:252:LEU:HD11	2.54	0.42
1:A:218:LEU:HA	1:A:261:VAL:HG12	1.33	0.42
1:A:23:GLN:HG2	1:A:27:ARG:NH1	2.35	0.42
1:B:285:LYS:HA	1:B:286:PRO:HD2	1.87	0.42
1:B:57:LYS:HZ3	1:B:71:ALA:HB3	1.85	0.42
1:C:132:GLY:O	1:C:135:GLN:HB3	2.19	0.42
1:B:23:GLN:HG2	1:B:27:ARG:NH1	2.35	0.42
1:C:126:PHE:CB	1:C:301:TYR:HA	2.45	0.42
1:A:129:PHE:O	1:A:129:PHE:CD1	2.73	0.42
1:A:162:THR:OG1	1:A:223:SER:OG	2.14	0.42
1:C:218:LEU:HA	1:C:261:VAL:HG12	1.33	0.42
1:B:268:GLN:OE1	1:C:294:HIS:HB3	2.20	0.42
1:C:36:ASN:O	1:C:40:LYS:HG3	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:CE2	1:A:252:LEU:HD11	2.54	0.42
1:B:100:ILE:HD12	1:B:100:ILE:H	1.85	0.41
1:C:299:ARG:CG	1:C:315:TYR:HB2	2.50	0.41
1:B:129:PHE:CD1	1:B:129:PHE:O	2.73	0.41
1:C:129:PHE:O	1:C:129:PHE:CD1	2.73	0.41
1:C:125:MET:HB2	1:C:266:THR:CG2	2.50	0.41
1:C:94:GLN:O	1:C:97:SER:OG	2.26	0.41
1:A:100:ILE:HD12	1:A:100:ILE:H	1.85	0.41
1:B:48:THR:HG21	1:B:259:PHE:CZ	2.54	0.41
1:C:235:ARG:HA	1:C:236:GLY:HA3	1.70	0.41
1:A:153:GLY:O	1:A:154:GLU:HB2	2.21	0.41
1:A:299:ARG:CG	1:A:315:TYR:HB2	2.50	0.41
1:B:126:PHE:CB	1:B:301:TYR:HA	2.45	0.41
1:C:159:TYR:HE2	1:C:166:PHE:HB2	1.85	0.41
1:A:106:SER:HB3	1:A:334:VAL:HG12	2.02	0.41
1:A:288:GLY:HA3	1:A:292:ILE:CD1	2.49	0.41
1:A:36:ASN:O	1:A:40:LYS:HG3	2.20	0.41
1:B:170:ARG:HA	1:B:170:ARG:HD3	1.85	0.41
1:B:123:THR:O	1:B:265:ILE:HG13	2.21	0.41
1:A:123:THR:O	1:A:265:ILE:HG13	2.21	0.41
1:A:269:VAL:HG12	1:A:270:VAL:N	2.36	0.41
1:B:269:VAL:HG12	1:B:270:VAL:N	2.36	0.41
1:B:299:ARG:CG	1:B:315:TYR:HB2	2.50	0.41
1:C:299:ARG:HB3	1:C:315:TYR:O	2.21	0.41
1:B:288:GLY:HA3	1:B:292:ILE:CD1	2.49	0.41
1:C:269:VAL:HG12	1:C:270:VAL:N	2.36	0.41
1:C:48:THR:HG21	1:C:259:PHE:CZ	2.54	0.41
1:A:299:ARG:HB3	1:A:315:TYR:O	2.21	0.41
1:B:153:GLY:O	1:B:154:GLU:HB2	2.21	0.41
1:C:285:LYS:HA	1:C:286:PRO:HD2	1.87	0.41
1:A:125:MET:HB2	1:A:266:THR:CG2	2.50	0.41
1:B:126:PHE:HB3	1:B:301:TYR:CD1	2.46	0.41
1:C:100:ILE:HD12	1:C:100:ILE:H	1.85	0.41
1:C:236:GLY:CA	1:C:237:GLU:OE1	2.69	0.41
1:C:23:GLN:HG2	1:C:27:ARG:NH1	2.35	0.41
1:B:125:MET:HB2	1:B:266:THR:CG2	2.50	0.41
1:B:159:TYR:HE2	1:B:166:PHE:HB2	1.85	0.41
1:B:299:ARG:HB3	1:B:315:TYR:O	2.21	0.41
1:C:106:SER:HB3	1:C:334:VAL:HG12	2.02	0.41
1:C:57:LYS:HZ3	1:C:71:ALA:HB3	1.85	0.41
1:B:106:SER:HB3	1:B:334:VAL:HG12	2.02	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:ND2	1:B:55:ALA:O	2.52	0.40
1:B:236:GLY:CA	1:B:237:GLU:OE1	2.69	0.40
1:C:123:THR:O	1:C:265:ILE:HG13	2.21	0.40
1:C:235:ARG:HG3	1:C:235:ARG:NH2	2.36	0.40
1:B:125:MET:CG	1:B:266:THR:HG23	2.52	0.40
1:B:236:GLY:HA2	1:B:237:GLU:OE1	2.21	0.40
1:C:236:GLY:HA2	1:C:237:GLU:OE1	2.21	0.40
1:A:236:GLY:HA2	1:A:237:GLU:OE1	2.21	0.40
1:A:236:GLY:CA	1:A:237:GLU:OE1	2.69	0.40
1:B:156:LYS:CA	1:B:216:TYR:CE1	2.99	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	A	307/339 (91%)	285 (93%)	15 (5%)	7 (2%)	8	50
1	B	307/339 (91%)	285 (93%)	15 (5%)	7 (2%)	8	50
1	C	307/339 (91%)	285 (93%)	15 (5%)	7 (2%)	8	50
All	All	921/1017 (91%)	855 (93%)	45 (5%)	21 (2%)	12	50

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	PHE
1	A	262	ALA
1	B	129	PHE
1	B	262	ALA
1	C	129	PHE
1	C	262	ALA
1	A	101	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	238	LEU
1	B	101	GLN
1	B	238	LEU
1	C	101	GLN
1	C	238	LEU
1	A	261	VAL
1	A	285	LYS
1	B	261	VAL
1	B	285	LYS
1	C	261	VAL
1	C	285	LYS
1	A	189	VAL
1	B	189	VAL
1	C	189	VAL

### 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	248/269 (92%)	236 (95%)	12 (5%)	31	69
1	B	248/269 (92%)	236 (95%)	12 (5%)	31	69
1	C	248/269 (92%)	236 (95%)	12 (5%)	31	69
All	All	744/807 (92%)	708 (95%)	36 (5%)	36	69

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	GLU
1	A	125	MET
1	A	129	PHE
1	A	130	ARG
1	A	158	MET
1	A	177	ARG
1	A	215	ARG
1	A	216	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	235	ARG
1	A	266	THR
1	A	267	ASN
1	A	268	GLN
1	B	124	GLU
1	B	125	MET
1	B	129	PHE
1	B	130	ARG
1	B	158	MET
1	B	177	ARG
1	B	215	ARG
1	B	216	TYR
1	B	235	ARG
1	B	266	THR
1	B	267	ASN
1	B	268	GLN
1	C	124	GLU
1	C	125	MET
1	C	129	PHE
1	C	130	ARG
1	C	158	MET
1	C	177	ARG
1	C	215	ARG
1	C	216	TYR
1	C	235	ARG
1	C	266	THR
1	C	267	ASN
1	C	268	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	188	ASN
1	A	200	GLN
1	A	313	GLN
1	B	93	HIS
1	B	138	HIS
1	B	188	ASN
1	B	200	GLN
1	B	294	HIS
1	B	313	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	93	HIS
1	C	138	HIS
1	C	188	ASN
1	C	200	GLN
1	C	268	GLN
1	C	294	HIS
1	C	313	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z  > 2$
5	ANP	A	602	4	29,33,33	1.26	4 (13%)	26,52,52	1.02	1 (3%)
5	ANP	B	602	4	29,33,33	1.26	4 (13%)	26,52,52	1.02	1 (3%)
5	ANP	C	401	4	29,33,33	1.26	4 (13%)	26,52,52	1.02	1 (3%)

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
5	ANP	A	602	4	-	0/13/38/38	0/3/3/3
5	ANP	B	602	4	-	0/13/38/38	0/3/3/3
5	ANP	C	401	4	-	0/13/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	ANP	PB-O3A	-2.90	1.55	1.59
5	B	602	ANP	PB-O3A	-2.87	1.55	1.59
5	A	602	ANP	PB-O3A	-2.86	1.55	1.59
5	C	401	ANP	PG-N3B	2.30	1.69	1.63
5	B	602	ANP	PG-N3B	2.33	1.69	1.63
5	A	602	ANP	PG-N3B	2.33	1.69	1.63
5	A	602	ANP	PB-O1B	3.08	1.49	1.46
5	B	602	ANP	PB-O1B	3.09	1.49	1.46
5	C	401	ANP	PB-O1B	3.17	1.49	1.46
5	C	401	ANP	PG-O1G	3.45	1.49	1.46
5	B	602	ANP	PG-O1G	3.46	1.49	1.46
5	A	602	ANP	PG-O1G	3.46	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	ANP	PA-O3A-PB	-3.95	118.37	132.71
5	B	602	ANP	PA-O3A-PB	-3.94	118.42	132.71
5	C	401	ANP	PA-O3A-PB	-3.93	118.45	132.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	ANP	32	0
5	B	602	ANP	24	0
5	C	401	ANP	3	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.