



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:00 PM GMT

PDB ID : 3Q9B  
Title : Crystal Structure of APAH complexed with M344  
Authors : Lombardi, P.M.; Christianson, D.W.  
Deposited on : 2011-01-07  
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

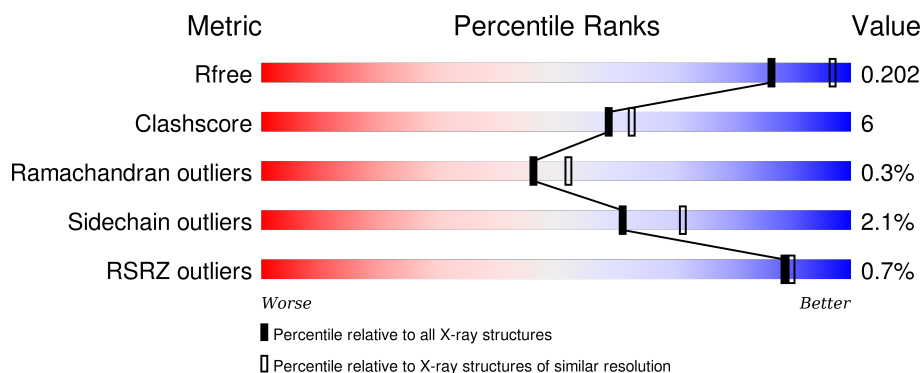
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 86%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">86%</span> </div> <div style="width: 13%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">13%</span> </div> </div>
1	B	341	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 84%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">84%</span> </div> <div style="width: 16%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">16%</span> </div> </div>
1	C	341	<div> <div style="width: 84%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">84%</span> </div> <div style="width: 15%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">15%</span> </div> </div>
1	D	341	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 81%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">81%</span> </div> <div style="width: 18%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">18%</span> </div> </div>
1	E	341	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 87%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">87%</span> </div> <div style="width: 12%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">12%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	341	
1	G	341	
1	H	341	
1	I	341	
1	J	341	
1	K	341	
1	L	341	

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	DMS	A	342	-	-	-	X
2	DMS	A	403	-	-	-	X
2	DMS	A	405	-	-	-	X
2	DMS	A	415	-	-	-	X
2	DMS	A	417	-	-	-	X
2	DMS	A	419	-	-	-	X
2	DMS	A	421	-	-	-	X
2	DMS	B	342	-	-	-	X
2	DMS	B	403	-	-	-	X
2	DMS	B	405	-	-	-	X
2	DMS	B	413	-	-	-	X
2	DMS	B	415	-	-	-	X
2	DMS	B	417	-	-	-	X
2	DMS	C	405	-	-	-	X
2	DMS	C	415	-	-	-	X
2	DMS	C	419	-	-	-	X
2	DMS	C	421	-	-	-	X
2	DMS	D	342	-	-	-	X
2	DMS	D	343	-	-	-	X
2	DMS	D	403	-	-	-	X
2	DMS	D	405	-	-	-	X
2	DMS	D	413	-	-	-	X
2	DMS	D	415	-	-	-	X
2	DMS	D	417	-	-	-	X
2	DMS	D	419	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	D	421	-	-	-	X
2	DMS	E	405	-	-	-	X
2	DMS	E	411	-	-	-	X
2	DMS	E	415	-	-	-	X
2	DMS	E	417	-	-	-	X
2	DMS	E	419	-	-	-	X
2	DMS	E	421	-	-	-	X
2	DMS	F	343	-	-	-	X
2	DMS	F	344	-	-	-	X
2	DMS	F	405	-	-	-	X
2	DMS	F	413	-	-	-	X
2	DMS	F	415	-	-	-	X
2	DMS	F	419	-	-	-	X
2	DMS	F	421	-	-	-	X
2	DMS	G	403	-	-	-	X
2	DMS	G	405	-	-	-	X
2	DMS	G	411	-	-	-	X
2	DMS	G	415	-	-	-	X
2	DMS	G	417	-	-	-	X
2	DMS	G	419	-	-	-	X
2	DMS	H	405	-	-	-	X
2	DMS	H	413	-	-	-	X
2	DMS	H	415	-	-	-	X
2	DMS	H	417	-	-	-	X
2	DMS	H	419	-	-	-	X
2	DMS	H	421	-	-	-	X
2	DMS	I	405	-	-	-	X
2	DMS	I	411	-	-	-	X
2	DMS	I	413	-	-	-	X
2	DMS	I	415	-	-	-	X
2	DMS	I	417	-	-	-	X
2	DMS	I	419	-	-	-	X
2	DMS	J	403	-	-	-	X
2	DMS	J	415	-	-	-	X
2	DMS	J	417	-	-	-	X
2	DMS	J	419	-	-	-	X
2	DMS	K	342	-	-	-	X
2	DMS	K	403	-	-	-	X
2	DMS	K	405	-	-	-	X
2	DMS	K	415	-	-	-	X
2	DMS	K	417	-	-	-	X
2	DMS	K	419	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	K	421	-	-	-	X
2	DMS	L	342	-	-	-	X
2	DMS	L	405	-	-	-	X
2	DMS	L	415	-	-	-	X
2	DMS	L	417	-	-	-	X
2	DMS	L	419	-	-	-	X
2	DMS	L	421	-	-	-	X
3	B3N	A	401	-	-	-	X
3	B3N	C	401	-	-	-	X
3	B3N	D	407	-	-	-	X
3	B3N	F	407	-	-	-	X
3	B3N	H	407	-	-	-	X
3	B3N	K	401	-	-	-	X
3	B3N	L	407	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33797 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Acetylpolysamine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	B	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	C	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	D	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	E	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	F	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	G	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	H	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	I	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	J	340	Total	C	N	O	S	0	0	0
			2563	1642	434	478	9			
1	K	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	L	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0

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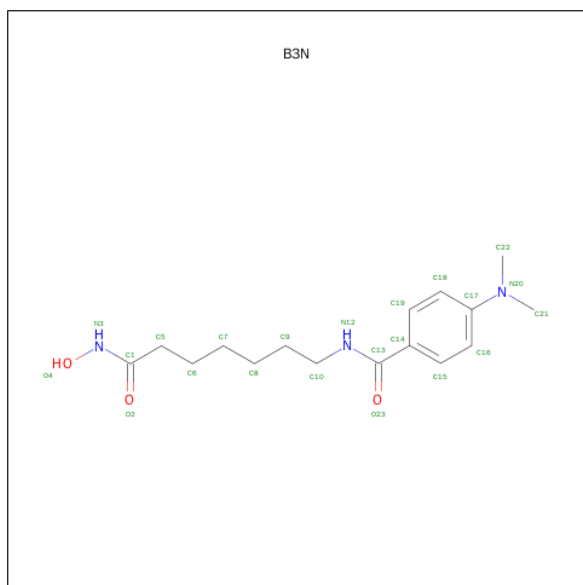
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	K	1	Total	C	O	S	0	0
			4	2	1	1		
2	K	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is 4-(DIMETHYLAMINO)-N-[7-(HYDROXYAMINO)-7-OXOHEPTYL]BENZAMIDE (three-letter code: B3N) (formula:  $C_{16}H_{25}N_3O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	16	3	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			22	16	3	3		
3	C	1	Total	C	N	O	0	0
			22	16	3	3		
3	D	1	Total	C	N	O	0	0
			22	16	3	3		
3	E	1	Total	C	N	O	0	0
			22	16	3	3		
3	F	1	Total	C	N	O	0	0
			22	16	3	3		
3	G	1	Total	C	N	O	0	0
			22	16	3	3		
3	H	1	Total	C	N	O	0	0
			22	16	3	3		
3	I	1	Total	C	N	O	0	0
			22	16	3	3		
3	J	1	Total	C	N	O	0	0
			22	16	3	3		
3	K	1	Total	C	N	O	0	0
			22	16	3	3		
3	L	1	Total	C	N	O	0	0
			22	16	3	3		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	K	0	0
			2	2		
4	J	2	Total	K	0	0
			2	2		
4	D	2	Total	K	0	0
			2	2		
4	K	2	Total	K	0	0
			2	2		
4	E	2	Total	K	0	0
			2	2		
4	H	2	Total	K	0	0
			2	2		
4	B	2	Total	K	0	0
			2	2		
4	I	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	K	0	0
			2	2		
4	A	2	Total	K	0	0
			2	2		
4	L	2	Total	K	0	0
			2	2		
4	F	2	Total	K	0	0
			2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Na	0	0
			1	1		
5	J	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		
5	K	1	Total	Na	0	0
			1	1		
5	E	1	Total	Na	0	0
			1	1		
5	H	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	I	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		
5	L	1	Total	Na	0	0
			1	1		
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total 1	Zn 1	0	0
6	D	1	Total 1	Zn 1	0	0
6	K	1	Total 1	Zn 1	0	0
6	E	1	Total 1	Zn 1	0	0
6	H	1	Total 1	Zn 1	0	0
6	B	1	Total 1	Zn 1	0	0
6	I	1	Total 1	Zn 1	0	0
6	C	1	Total 1	Zn 1	0	0
6	A	1	Total 1	Zn 1	0	0
6	L	1	Total 1	Zn 1	0	0
6	F	1	Total 1	Zn 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	184	Total 184	O 184	0	0
7	B	165	Total 165	O 165	0	0
7	C	192	Total 192	O 192	0	0
7	D	187	Total 187	O 187	0	0
7	E	181	Total 181	O 181	0	0
7	F	196	Total 196	O 196	0	0
7	G	184	Total 184	O 184	0	0
7	H	183	Total 183	O 183	0	0

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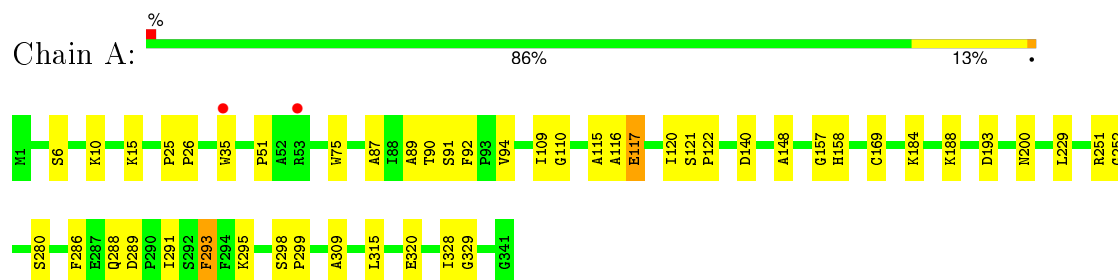
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	204	Total 204	O 204	0	0
7	J	174	Total 174	O 174	0	0
7	K	211	Total 211	O 211	0	0
7	L	182	Total 182	O 182	0	0



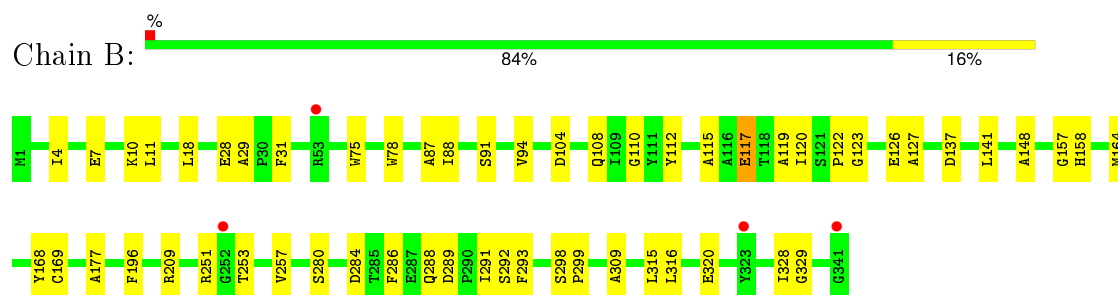
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

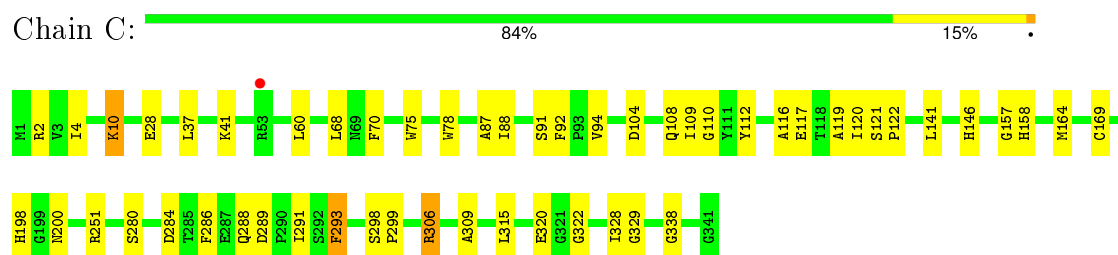
- Molecule 1: Acetylpolyamine amidohydrolase



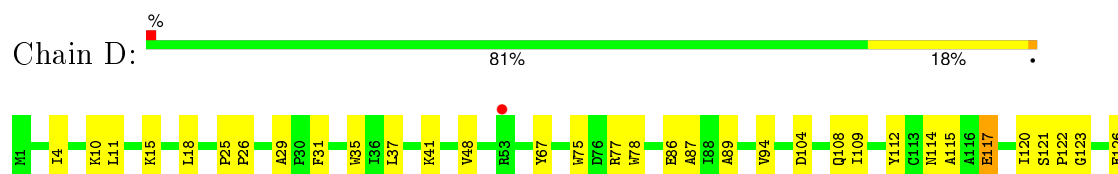
- Molecule 1: Acetylpolyamine amidohydrolase



- Molecule 1: Acetylpolyamine amidohydrolase

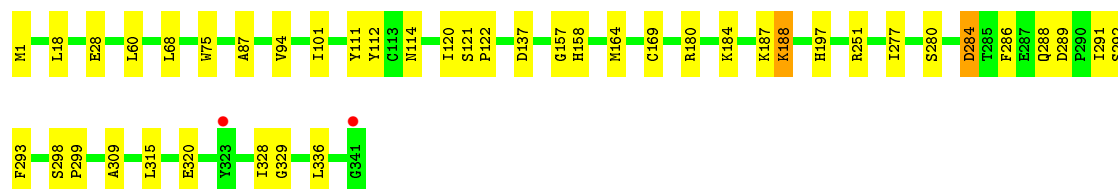
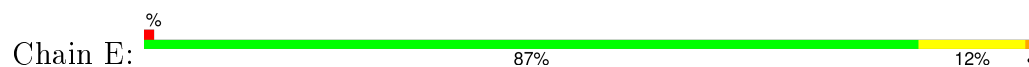


- Molecule 1: Acetylpolyamine amidohydrolase

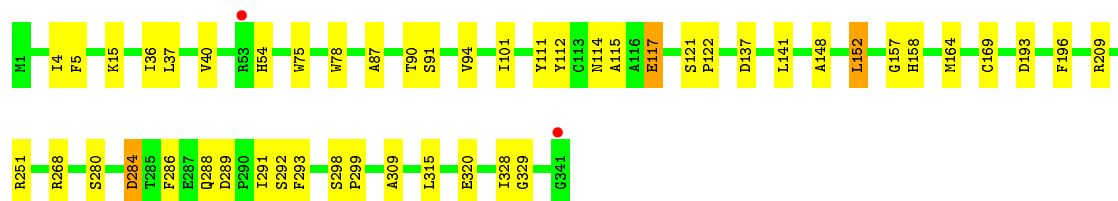
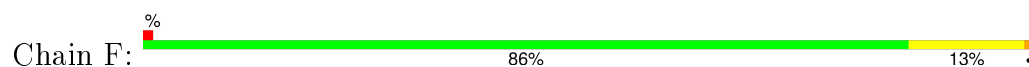




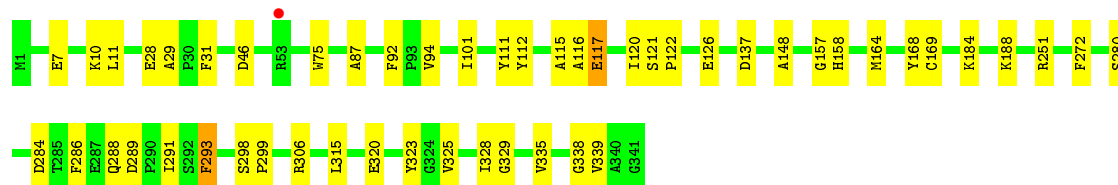
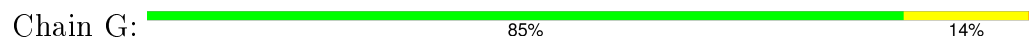
• Molecule 1: Acetylpolyamine amidohydrolase



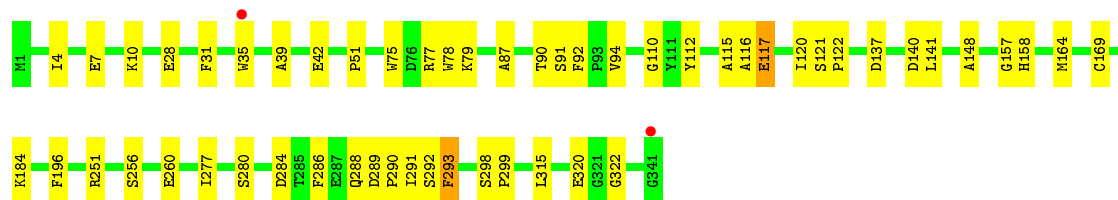
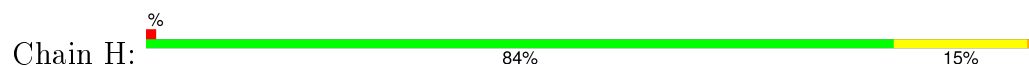
• Molecule 1: Acetylpolyamine amidohydrolase



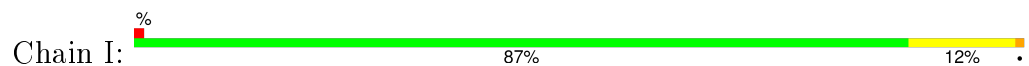
• Molecule 1: Acetylpolyamine amidohydrolase

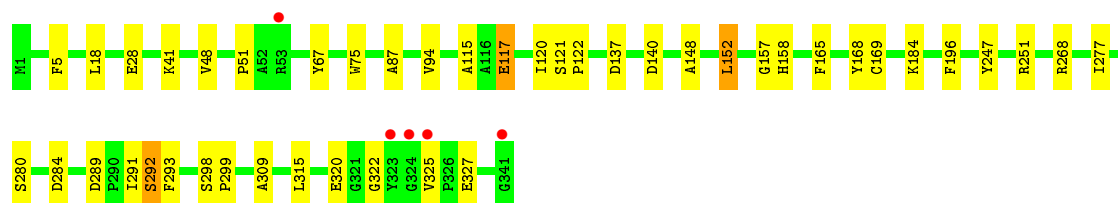


• Molecule 1: Acetylpolyamine amidohydrolase

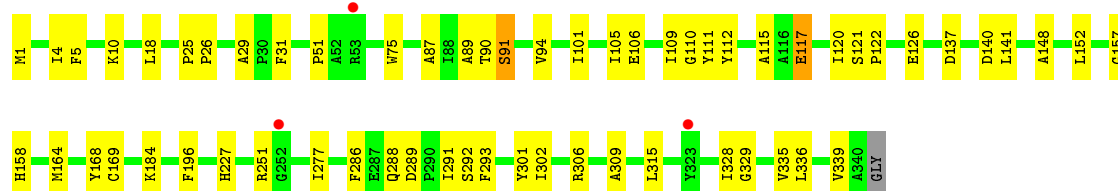
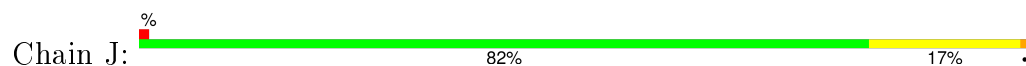


• Molecule 1: Acetylpolyamine amidohydrolase

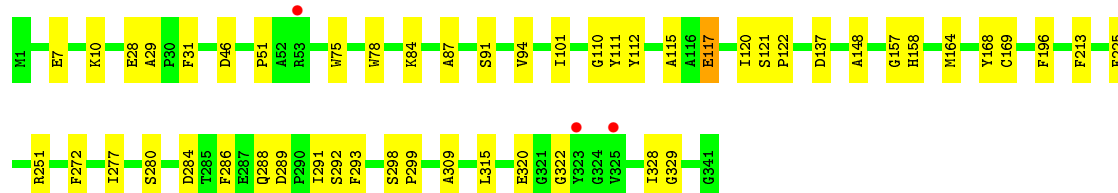
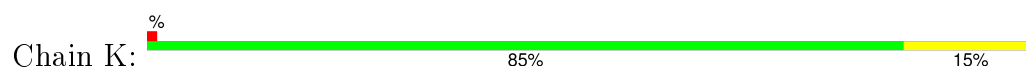




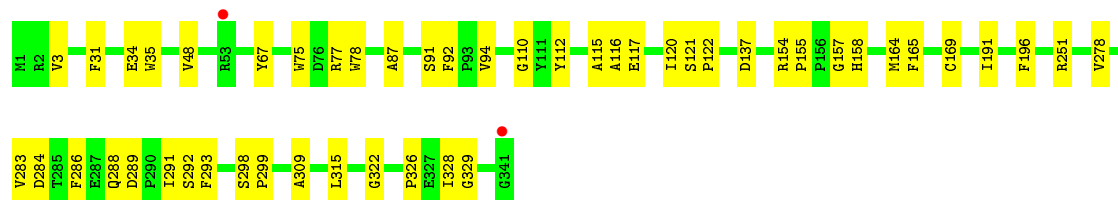
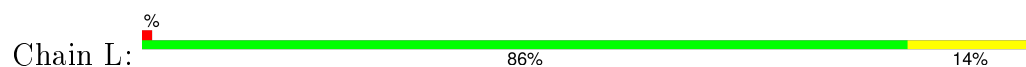
• Molecule 1: Acetylpolysamine amidohydrolase



• Molecule 1: Acetylpolysamine amidohydrolase



• Molecule 1: Acetylpolysamine amidohydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.66Å 119.73Å 119.53Å 98.09° 95.15° 115.33°	Depositor
Resolution (Å)	50.00 – 2.25 49.84 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.1 (50.00-2.25) 88.0 (49.84-2.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.25Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.171 , 0.202 0.172 , 0.202	Depositor DCC
$R_{free}$ test set	12853 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.6	EDS
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 270384 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	33797	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: B3N, NA, ZN, DMS, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/2636	0.58	0/3582
1	B	0.36	0/2636	0.56	0/3582
1	C	0.37	0/2636	0.59	0/3582
1	D	0.36	0/2636	0.58	0/3582
1	E	0.35	0/2636	0.56	0/3582
1	F	0.37	0/2636	0.58	0/3582
1	G	0.36	0/2636	0.56	0/3582
1	H	0.36	0/2636	0.56	0/3582
1	I	0.37	0/2636	0.57	0/3582
1	J	0.35	0/2631	0.56	0/3577
1	K	0.38	0/2636	0.59	0/3582
1	L	0.37	0/2636	0.56	0/3582
All	All	0.36	0/31627	0.57	0/42979

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	2568	0	2490	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2568	0	2491	29	0
1	C	2568	0	2490	30	0
1	D	2568	0	2490	41	0
1	E	2568	0	2490	28	0
1	F	2568	0	2490	32	0
1	G	2568	0	2491	26	0
1	H	2568	0	2490	32	0
1	I	2568	0	2491	25	0
1	J	2563	0	2488	34	0
1	K	2568	0	2491	30	0
1	L	2568	0	2490	29	0
2	A	40	0	60	0	0
2	B	36	0	54	0	0
2	C	24	0	36	0	0
2	D	44	0	66	0	0
2	E	40	0	60	0	0
2	F	44	0	66	0	0
2	G	40	0	60	0	0
2	H	32	0	48	0	0
2	I	32	0	48	0	0
2	J	28	0	42	0	0
2	K	40	0	60	0	0
2	L	32	0	48	0	0
3	A	22	0	24	0	0
3	B	22	0	24	0	0
3	C	22	0	24	0	0
3	D	22	0	24	0	0
3	E	22	0	24	0	0
3	F	22	0	24	0	0
3	G	22	0	24	0	0
3	H	22	0	24	1	0
3	I	22	0	24	0	0
3	J	22	0	24	1	0
3	K	22	0	24	1	0
3	L	22	0	24	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
7	A	184	0	0	1	0
7	B	165	0	0	2	0
7	C	192	0	0	2	0
7	D	187	0	0	5	0
7	E	181	0	0	1	0
7	F	196	0	0	2	0
7	G	184	0	0	1	0
7	H	183	0	0	1	0
7	I	204	0	0	0	0
7	J	174	0	0	1	0
7	K	211	0	0	0	0
7	L	182	0	0	1	0
All	All	33797	0	30818	361	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 6.

All (361) 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:E:289:ASP:OD1	1:E:291:ILE:HG13	1.84	0.78
1:E:284:ASP:HB2	1:E:291:ILE:HD11	1.70	0.73
1:G:289:ASP:OD1	1:G:291:ILE:HG12	1.89	0.72
1:C:284:ASP:HB3	1:C:322:GLY:HA2	1.71	0.72
1:E:18:LEU:HD23	1:H:90:THR:HG22	1.74	0.69
1:L:157:GLY:HA2	1:L:169:CYS:HB3	1.73	0.69
1:C:251:ARG:HG3	7:C:2114:HOH:O	1.94	0.68
1:J:289:ASP:OD1	1:J:291:ILE:HG12	1.94	0.67
1:D:114:ASN:HD22	1:D:164:MET:HG3	1.60	0.67
1:F:157:GLY:HA2	1:F:169:CYS:HB3	1.77	0.66
1:K:157:GLY:HA2	1:K:169:CYS:HB3	1.76	0.66
1:K:284:ASP:HB3	1:K:322:GLY:HA2	1.78	0.66
1:K:7:GLU:O	1:K:10:LYS:HG2	1.95	0.66
1:B:157:GLY:HA2	1:B:169:CYS:HB3	1.78	0.65
1:D:157:GLY:HA2	1:D:169:CYS:HB3	1.77	0.65
1:G:306:ARG:HD2	1:G:338:GLY:O	1.96	0.65
1:H:51:PRO:HA	1:H:137:ASP:OD2	1.97	0.64
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.33	0.64
1:L:284:ASP:HB3	1:L:322:GLY:HA2	1.79	0.64
1:C:157:GLY:HA2	1:C:169:CYS:HB3	1.79	0.64
1:E:291:ILE:C	1:E:291:ILE:HD12	2.18	0.64
1:K:75:TRP:CE2	1:K:122:PRO:HG3	2.33	0.64
1:C:306:ARG:HG2	1:C:338:GLY:O	1.98	0.63
1:G:157:GLY:HA2	1:G:169:CYS:HB3	1.81	0.63
1:I:157:GLY:HA2	1:I:169:CYS:HB3	1.81	0.63
1:C:4:ILE:HD12	1:C:4:ILE:N	2.13	0.63
1:F:289:ASP:OD1	1:F:291:ILE:HG12	1.99	0.63
1:H:75:TRP:CE2	1:H:122:PRO:HG3	2.34	0.62
1:A:251:ARG:HG3	7:A:1782:HOH:O	1.99	0.62
1:H:284:ASP:HB3	1:H:322:GLY:HA2	1.80	0.62
1:J:157:GLY:HA2	1:J:169:CYS:HB3	1.81	0.62
1:D:289:ASP:OD1	1:D:291:ILE:HG12	2.01	0.61
1:C:37:LEU:HG	1:C:41:LYS:HE3	1.82	0.61
1:D:37:LEU:HG	1:D:41:LYS:HE3	1.81	0.61
1:E:180:ARG:O	1:E:184:LYS:HG2	2.01	0.60
1:D:41:LYS:HE2	1:D:48:VAL:HG21	1.83	0.60
1:A:35:TRP:HE3	1:A:35:TRP:HA	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASP:OD1	1:A:291:ILE:HG12	2.01	0.60
1:F:268:ARG:HD3	7:F:1554:HOH:O	2.01	0.60
1:H:157:GLY:HA2	1:H:169:CYS:HB3	1.84	0.59
1:H:35:TRP:HA	1:H:35:TRP:CE3	2.36	0.59
1:A:75:TRP:CE2	1:A:122:PRO:HG3	2.37	0.59
1:B:4:ILE:HD11	1:B:141:LEU:HD11	1.83	0.59
1:D:286:PHE:CE2	1:D:288:GLN:HB2	2.37	0.59
1:J:251:ARG:HA	1:J:293:PHE:CD2	2.38	0.59
1:D:75:TRP:CE2	1:D:122:PRO:HG3	2.37	0.59
1:A:157:GLY:HA2	1:A:169:CYS:HB3	1.84	0.58
1:L:115:ALA:HB1	1:L:117:GLU:OE1	2.03	0.58
1:H:115:ALA:HB1	1:H:117:GLU:OE1	2.03	0.58
1:J:140:ASP:OD1	1:J:184:LYS:HE3	2.04	0.58
1:G:87:ALA:HB3	1:G:120:ILE:HB	1.86	0.58
1:F:75:TRP:CE2	1:F:122:PRO:HG3	2.39	0.58
1:J:75:TRP:CE2	1:J:122:PRO:HG3	2.39	0.57
1:H:251:ARG:HA	1:H:293:PHE:CD2	2.39	0.57
1:F:280:SER:HB3	1:F:320:GLU:HG3	1.85	0.57
1:F:286:PHE:CE2	1:F:288:GLN:HB2	2.39	0.57
1:E:251:ARG:HA	1:E:293:PHE:CD2	2.39	0.57
1:J:51:PRO:HA	1:J:137:ASP:OD1	2.04	0.57
1:I:309:ALA:HA	1:I:315:LEU:HD11	1.87	0.57
1:C:286:PHE:CE2	1:C:288:GLN:HB2	2.40	0.57
1:K:84:LYS:NZ	1:K:84:LYS:HB2	2.20	0.57
1:I:87:ALA:HB3	1:I:120:ILE:HB	1.86	0.57
1:A:90:THR:HG22	1:I:18:LEU:HD23	1.87	0.56
1:B:328:ILE:HG23	1:B:329:GLY:N	2.21	0.56
1:G:7:GLU:O	1:G:10:LYS:HG2	2.05	0.56
1:G:75:TRP:CE2	1:G:122:PRO:HG3	2.41	0.56
1:J:309:ALA:HA	1:J:315:LEU:HD11	1.87	0.56
1:B:289:ASP:OD1	1:B:291:ILE:HG12	2.05	0.56
1:A:328:ILE:HG23	1:A:329:GLY:N	2.20	0.56
1:K:51:PRO:HA	1:K:137:ASP:OD1	2.06	0.56
1:E:157:GLY:HA2	1:E:169:CYS:HB3	1.88	0.55
1:A:309:ALA:HA	1:A:315:LEU:HD11	1.88	0.55
1:B:87:ALA:HB3	1:B:120:ILE:HB	1.87	0.55
1:H:35:TRP:HA	1:H:35:TRP:HE3	1.70	0.55
1:I:75:TRP:CE2	1:I:122:PRO:HG3	2.41	0.55
1:A:75:TRP:NE1	1:A:122:PRO:HG3	2.21	0.55
1:D:104:ASP:O	1:D:108:GLN:HG3	2.06	0.55
1:H:7:GLU:O	1:H:10:LYS:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ILE:HG23	1:C:329:GLY:N	2.22	0.55
1:B:280:SER:HB3	1:B:320:GLU:HG3	1.88	0.55
1:F:121:SER:HB2	1:F:122:PRO:CD	2.37	0.55
1:J:286:PHE:CE2	1:J:288:GLN:HB2	2.42	0.55
1:F:15:LYS:HA	1:F:15:LYS:HE2	1.88	0.54
1:L:251:ARG:HA	1:L:293:PHE:CD2	2.42	0.54
1:L:75:TRP:NE1	1:L:122:PRO:HG3	2.23	0.54
1:L:75:TRP:CE2	1:L:122:PRO:HG3	2.41	0.54
1:B:75:TRP:CE2	1:B:122:PRO:HG3	2.43	0.54
1:J:29:ALA:HB3	1:J:31:PHE:CE1	2.43	0.54
1:G:251:ARG:HA	1:G:293:PHE:CD2	2.43	0.54
1:D:87:ALA:HB3	1:D:120:ILE:HB	1.90	0.54
1:H:289:ASP:OD1	1:H:291:ILE:HG12	2.07	0.54
1:B:298:SER:HB2	1:B:299:PRO:HD3	1.90	0.54
1:K:298:SER:HB2	1:K:299:PRO:HD3	1.90	0.53
1:C:2:ARG:HD2	1:C:141:LEU:HD11	1.90	0.53
1:E:284:ASP:CB	1:E:291:ILE:HD11	2.38	0.53
1:E:87:ALA:HB3	1:E:120:ILE:HB	1.91	0.53
1:J:5:PHE:CD1	1:J:152:LEU:HD13	2.42	0.53
1:B:286:PHE:CE2	1:B:288:GLN:HB2	2.43	0.53
1:L:35:TRP:CZ3	1:L:326:PRO:HA	2.44	0.53
1:A:87:ALA:HB3	1:A:120:ILE:HB	1.91	0.53
1:C:280:SER:HB3	1:C:320:GLU:HG3	1.90	0.53
1:I:284:ASP:HB3	1:I:322:GLY:HA2	1.91	0.52
1:K:286:PHE:CE2	1:K:288:GLN:HB2	2.45	0.52
1:F:121:SER:HB2	1:F:122:PRO:HD2	1.92	0.52
1:K:289:ASP:OD1	1:K:291:ILE:HG12	2.09	0.52
1:G:101:ILE:HG12	1:G:111:TYR:CZ	2.45	0.52
1:E:291:ILE:HD12	1:E:292:SER:N	2.25	0.52
1:J:115:ALA:HB1	1:J:117:GLU:OE1	2.08	0.52
1:B:309:ALA:HA	1:B:315:LEU:HD11	1.90	0.52
1:B:148:ALA:HA	1:B:315:LEU:O	2.09	0.52
1:J:91:SER:O	1:J:110:GLY:HA3	2.10	0.52
1:D:18:LEU:HD23	1:J:90:THR:HG22	1.90	0.52
1:J:148:ALA:HA	1:J:315:LEU:O	2.10	0.52
1:D:146:HIS:HD2	7:D:435:HOH:O	1.93	0.52
1:E:101:ILE:HG12	1:E:111:TYR:CZ	2.44	0.52
1:J:4:ILE:HG22	1:J:51:PRO:HG3	1.92	0.51
1:A:15:LYS:HE2	1:A:15:LYS:HA	1.91	0.51
1:K:225:PHE:CD2	3:K:401:B3N:H81	2.45	0.51
1:K:280:SER:HB3	1:K:320:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:PHE:CG	1:I:292:SER:HB2	2.46	0.51
1:I:51:PRO:HA	1:I:137:ASP:OD2	2.10	0.51
1:C:298:SER:HB2	1:C:299:PRO:HD3	1.92	0.51
1:L:112:TYR:O	1:L:164:MET:HA	2.11	0.51
1:E:251:ARG:HG3	7:E:1995:HOH:O	2.10	0.50
1:L:3:VAL:HB	1:L:48:VAL:HG22	1.93	0.50
1:A:92:PHE:HZ	1:A:116:ALA:HB2	1.77	0.50
1:F:298:SER:HB2	1:F:299:PRO:HD3	1.93	0.50
1:F:209:ARG:HD2	7:F:1274:HOH:O	2.11	0.50
1:I:115:ALA:HB1	1:I:117:GLU:OE1	2.11	0.50
1:A:121:SER:HB2	1:A:122:PRO:CD	2.42	0.50
1:B:251:ARG:HA	1:B:293:PHE:CD2	2.46	0.50
1:L:87:ALA:HB3	1:L:120:ILE:HB	1.93	0.50
1:D:15:LYS:HG2	1:D:86:GLU:OE2	2.11	0.50
1:B:78:TRP:CE2	1:B:87:ALA:HA	2.47	0.50
1:G:298:SER:HB2	1:G:299:PRO:HD3	1.94	0.50
1:A:148:ALA:HA	1:A:315:LEU:O	2.11	0.49
1:C:75:TRP:CE2	1:C:122:PRO:HG3	2.47	0.49
1:G:280:SER:HB3	1:G:320:GLU:HG3	1.94	0.49
1:J:4:ILE:HD11	1:J:141:LEU:HD11	1.94	0.49
1:L:286:PHE:CE2	1:L:288:GLN:HB2	2.48	0.49
1:F:251:ARG:HA	1:F:293:PHE:CD2	2.47	0.49
1:F:148:ALA:HA	1:F:315:LEU:O	2.12	0.49
1:D:35:TRP:CE3	1:D:35:TRP:HA	2.47	0.49
1:F:115:ALA:HB1	1:F:117:GLU:OE1	2.12	0.49
1:I:251:ARG:HA	1:I:293:PHE:CD2	2.47	0.49
1:F:75:TRP:NE1	1:F:122:PRO:HG3	2.27	0.49
1:H:290:PRO:HB2	3:H:407:B3N:H212	1.94	0.49
1:A:115:ALA:HB1	1:A:117:GLU:OE1	2.13	0.49
1:L:92:PHE:HZ	1:L:116:ALA:HB2	1.77	0.49
1:I:5:PHE:CD1	1:I:152:LEU:HD13	2.48	0.49
1:D:309:ALA:HA	1:D:315:LEU:HD11	1.94	0.49
1:J:277:ILE:HB	1:J:315:LEU:HD23	1.94	0.49
1:B:18:LEU:HD23	1:F:90:THR:HG22	1.95	0.48
1:E:121:SER:HB2	1:E:122:PRO:CD	2.43	0.48
1:K:251:ARG:HA	1:K:293:PHE:CD2	2.48	0.48
1:B:29:ALA:HB3	1:B:31:PHE:CE1	2.49	0.48
1:C:92:PHE:HZ	1:C:116:ALA:HB2	1.78	0.48
1:G:251:ARG:HG3	7:G:2031:HOH:O	2.13	0.48
1:F:309:ALA:HA	1:F:315:LEU:HD11	1.96	0.48
1:H:78:TRP:CE2	1:H:87:ALA:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:SER:O	1:H:110:GLY:HA3	2.13	0.48
1:J:87:ALA:HB3	1:J:120:ILE:HB	1.95	0.48
1:H:298:SER:HB2	1:H:299:PRO:HD3	1.95	0.48
1:G:335:VAL:O	1:G:339:VAL:HG23	2.13	0.48
1:I:121:SER:HB2	1:I:122:PRO:CD	2.44	0.48
1:E:75:TRP:CE2	1:E:122:PRO:HG3	2.49	0.48
1:B:115:ALA:HB1	1:B:117:GLU:OE1	2.13	0.47
1:H:286:PHE:CE2	1:H:288:GLN:HB2	2.48	0.47
1:F:196:PHE:CD1	1:F:292:SER:HB2	2.49	0.47
1:L:196:PHE:CD1	1:L:292:SER:HB2	2.49	0.47
1:K:148:ALA:HA	1:K:315:LEU:O	2.14	0.47
1:K:91:SER:O	1:K:110:GLY:HA3	2.14	0.47
1:D:251:ARG:HA	1:D:293:PHE:CD2	2.49	0.47
1:I:148:ALA:HA	1:I:315:LEU:O	2.14	0.47
1:H:112:TYR:O	1:H:164:MET:HA	2.15	0.47
1:K:213:PHE:HB2	1:K:272:PHE:CD2	2.49	0.47
1:K:121:SER:HB2	1:K:122:PRO:CD	2.45	0.47
1:I:121:SER:HB2	1:I:122:PRO:HD2	1.97	0.47
1:A:91:SER:O	1:A:110:GLY:HA3	2.15	0.47
1:F:114:ASN:HD22	1:F:164:MET:HG3	1.80	0.47
1:C:112:TYR:O	1:C:164:MET:HA	2.15	0.47
1:E:280:SER:HB3	1:E:320:GLU:HG3	1.97	0.46
1:H:196:PHE:CD1	1:H:292:SER:HB2	2.50	0.46
1:I:298:SER:HB2	1:I:299:PRO:HD3	1.97	0.46
1:D:4:ILE:HD11	1:D:141:LEU:HD11	1.97	0.46
1:J:112:TYR:O	1:J:164:MET:HA	2.15	0.46
1:F:196:PHE:CG	1:F:292:SER:HB2	2.51	0.46
1:H:75:TRP:NE1	1:H:122:PRO:HG3	2.31	0.46
1:F:101:ILE:HG12	1:F:111:TYR:CZ	2.50	0.46
1:C:289:ASP:OD1	1:C:291:ILE:HG12	2.15	0.46
1:C:146:HIS:HD2	7:C:452:HOH:O	1.98	0.46
1:H:39:ALA:HA	1:H:42:GLU:HG2	1.98	0.46
1:F:78:TRP:CE2	1:F:87:ALA:HA	2.51	0.46
1:E:309:ALA:HA	1:E:315:LEU:HD11	1.97	0.46
1:A:251:ARG:HA	1:A:293:PHE:CD2	2.50	0.46
1:C:78:TRP:CE2	1:C:87:ALA:HA	2.51	0.46
1:F:284:ASP:O	1:F:292:SER:HB3	2.16	0.46
1:L:298:SER:HB2	1:L:299:PRO:HD3	1.98	0.46
1:G:188:LYS:HD2	1:G:272:PHE:CZ	2.51	0.46
1:A:280:SER:HB3	1:A:320:GLU:HG3	1.98	0.46
1:G:115:ALA:HB1	1:G:117:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:SER:HB2	1:E:122:PRO:HD2	1.97	0.46
1:H:87:ALA:HB3	1:H:120:ILE:HB	1.99	0.45
1:J:328:ILE:HG23	1:J:329:GLY:N	2.31	0.45
1:G:121:SER:HB2	1:G:122:PRO:CD	2.47	0.45
1:E:114:ASN:HD22	1:E:164:MET:HG3	1.82	0.45
1:G:328:ILE:HG23	1:G:329:GLY:N	2.31	0.45
1:I:289:ASP:OD1	1:I:291:ILE:HG12	2.16	0.45
1:E:197:HIS:HE1	1:E:291:ILE:HD13	1.81	0.45
1:I:325:VAL:HB	1:I:327:GLU:OE2	2.16	0.45
1:I:140:ASP:OD1	1:I:184:LYS:HE3	2.16	0.45
1:K:328:ILE:HG23	1:K:329:GLY:N	2.31	0.45
1:K:196:PHE:CG	1:K:292:SER:HB2	2.50	0.45
1:D:115:ALA:HB1	1:D:117:GLU:OE1	2.16	0.45
1:L:121:SER:HB2	1:L:122:PRO:CD	2.47	0.45
1:L:283:VAL:HG21	1:L:328:ILE:HG13	1.98	0.45
1:G:286:PHE:CE2	1:G:288:GLN:HB2	2.52	0.45
1:L:92:PHE:CZ	1:L:116:ALA:HB2	2.52	0.45
1:G:29:ALA:HB3	1:G:31:PHE:CE1	2.52	0.45
1:D:328:ILE:HG23	1:D:329:GLY:N	2.31	0.45
1:A:298:SER:HB2	1:A:299:PRO:HD3	1.97	0.45
1:B:196:PHE:CG	1:B:292:SER:HB2	2.51	0.45
1:D:193:ASP:HA	1:D:280:SER:HB2	1.99	0.45
1:B:251:ARG:HG3	7:B:1754:HOH:O	2.16	0.45
1:E:112:TYR:O	1:E:164:MET:HA	2.16	0.45
1:L:328:ILE:HG23	1:L:329:GLY:N	2.32	0.45
1:E:1:MET:SD	1:E:336:LEU:HD22	2.57	0.45
1:K:87:ALA:HB3	1:K:120:ILE:HB	1.98	0.45
1:L:67:TYR:OH	1:L:165:PHE:HB3	2.17	0.45
1:A:121:SER:HB2	1:A:122:PRO:HD2	1.99	0.44
1:C:104:ASP:O	1:C:108:GLN:HG3	2.17	0.44
1:C:121:SER:HB2	1:C:122:PRO:CD	2.47	0.44
1:L:289:ASP:OD1	1:L:291:ILE:HG12	2.18	0.44
1:G:323:TYR:HD2	1:G:325:VAL:HG13	1.82	0.44
1:C:88:ILE:HG12	1:C:119:ALA:HB2	1.99	0.44
1:D:121:SER:HB2	1:D:122:PRO:HD2	1.99	0.44
1:H:280:SER:HB3	1:H:320:GLU:HG3	1.99	0.44
1:B:104:ASP:O	1:B:108:GLN:HG3	2.17	0.44
1:A:328:ILE:HG23	1:A:329:GLY:H	1.81	0.44
1:D:77:ARG:HD3	7:D:838:HOH:O	2.17	0.44
1:K:101:ILE:HG12	1:K:111:TYR:CZ	2.52	0.44
1:L:309:ALA:HA	1:L:315:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ALA:HB2	1:A:109:ILE:HG12	1.98	0.44
1:H:121:SER:HB2	1:H:122:PRO:CD	2.47	0.44
1:C:121:SER:HB2	1:C:122:PRO:HD2	1.99	0.44
1:D:11:LEU:HB2	1:D:127:ALA:HB2	1.99	0.44
1:D:306:ARG:HD2	1:G:299:PRO:HB2	1.98	0.44
1:K:309:ALA:HA	1:K:315:LEU:HD11	1.98	0.44
1:H:148:ALA:HA	1:H:315:LEU:O	2.18	0.44
1:B:91:SER:O	1:B:110:GLY:HA3	2.17	0.44
1:C:87:ALA:HB3	1:C:120:ILE:HB	1.99	0.44
1:C:198:HIS:CE1	1:C:200:ASN:HA	2.51	0.44
1:L:91:SER:O	1:L:110:GLY:HA3	2.18	0.44
1:E:328:ILE:HG23	1:E:329:GLY:N	2.33	0.44
1:D:89:ALA:HB2	1:D:109:ILE:HG12	1.98	0.43
1:I:280:SER:HB3	1:I:320:GLU:HG3	2.00	0.43
1:J:126:GLU:H	1:J:126:GLU:CD	2.21	0.43
1:L:154:ARG:HA	1:L:155:PRO:C	2.38	0.43
1:F:284:ASP:HB3	1:F:291:ILE:HD11	1.99	0.43
1:H:31:PHE:HD2	1:H:35:TRP:CD1	2.37	0.43
1:K:78:TRP:CE2	1:K:87:ALA:HA	2.53	0.43
1:D:78:TRP:CE2	1:D:87:ALA:HA	2.53	0.43
1:B:253:THR:HG23	1:B:257:VAL:HB	2.00	0.43
1:C:10:LYS:NZ	1:C:10:LYS:HB3	2.32	0.43
1:K:29:ALA:HB3	1:K:31:PHE:CD1	2.52	0.43
1:J:101:ILE:HG12	1:J:111:TYR:CZ	2.52	0.43
1:J:105:ILE:HG23	1:J:106:GLU:N	2.33	0.43
1:C:251:ARG:HA	1:C:293:PHE:CD2	2.54	0.43
1:L:117:GLU:HG3	3:L:407:B3N:H92	2.01	0.43
1:K:112:TYR:O	1:K:164:MET:HA	2.18	0.43
1:C:60:LEU:HD23	1:C:68:LEU:HD12	2.00	0.43
1:C:309:ALA:HA	1:C:315:LEU:HD11	2.00	0.43
1:E:298:SER:HB2	1:E:299:PRO:HD3	2.01	0.43
1:J:168:TYR:CE2	3:J:407:B3N:H71	2.52	0.43
1:E:197:HIS:CE1	1:E:291:ILE:HD13	2.54	0.43
1:D:299:PRO:HB2	1:G:306:ARG:HD3	2.00	0.43
1:F:112:TYR:O	1:F:164:MET:HA	2.18	0.43
1:D:269:ILE:O	1:D:272:PHE:HB3	2.18	0.43
1:J:196:PHE:CD1	1:J:292:SER:HB2	2.54	0.43
1:K:84:LYS:HZ2	1:K:84:LYS:HB2	1.83	0.43
1:J:335:VAL:O	1:J:339:VAL:HG23	2.18	0.43
1:K:75:TRP:CZ2	1:K:122:PRO:HG3	2.54	0.43
1:J:121:SER:HB2	1:J:122:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:277:ILE:HB	1:I:315:LEU:CD2	2.49	0.43
1:L:34:GLU:HG3	1:L:35:TRP:HD1	1.83	0.43
1:D:284:ASP:HB3	1:D:322:GLY:HA2	2.01	0.43
1:L:78:TRP:CE2	1:L:87:ALA:HA	2.55	0.42
1:K:277:ILE:HB	1:K:315:LEU:HD23	2.00	0.42
1:F:328:ILE:HG23	1:F:329:GLY:N	2.34	0.42
1:A:286:PHE:CE2	1:A:288:GLN:HB2	2.54	0.42
1:B:123:GLY:HA2	1:B:126:GLU:OE1	2.19	0.42
1:F:193:ASP:HA	1:F:280:SER:HB2	2.00	0.42
1:H:140:ASP:OD1	1:H:184:LYS:HE3	2.20	0.42
1:D:227:HIS:ND1	7:D:812:HOH:O	2.27	0.42
1:D:121:SER:HB2	1:D:122:PRO:CD	2.49	0.42
1:D:75:TRP:HZ3	1:D:86:GLU:HA	1.84	0.42
1:D:196:PHE:CD1	1:D:292:SER:HB2	2.54	0.42
1:L:31:PHE:O	1:L:34:GLU:HG2	2.20	0.42
1:K:115:ALA:HB1	1:K:117:GLU:OE1	2.18	0.42
1:L:77:ARG:HD3	7:L:416:HOH:O	2.18	0.42
1:G:11:LEU:HD13	1:G:126:GLU:HB3	2.02	0.42
1:J:227:HIS:ND1	7:J:818:HOH:O	2.36	0.42
1:I:196:PHE:CD2	1:I:292:SER:HB2	2.54	0.42
1:C:92:PHE:CZ	1:C:116:ALA:HB2	2.55	0.42
1:K:277:ILE:HB	1:K:315:LEU:CD2	2.50	0.42
1:I:41:LYS:HE3	1:I:48:VAL:HG21	2.02	0.42
1:F:37:LEU:O	1:F:40:VAL:HG22	2.20	0.42
1:E:60:LEU:HD23	1:E:68:LEU:HD12	2.01	0.42
1:J:277:ILE:HB	1:J:315:LEU:CD2	2.50	0.42
1:G:112:TYR:O	1:G:164:MET:HA	2.19	0.42
1:C:70:PHE:CZ	1:C:109:ILE:HA	2.54	0.42
1:A:92:PHE:CZ	1:A:116:ALA:HB2	2.54	0.42
1:H:77:ARG:HD3	7:H:364:HOH:O	2.19	0.42
1:I:277:ILE:HB	1:I:315:LEU:HD23	2.01	0.42
1:H:4:ILE:HD11	1:H:141:LEU:HD11	2.02	0.42
1:L:191:ILE:HG12	1:L:278:VAL:HB	2.02	0.42
1:A:252:GLY:O	1:A:295:LYS:HE2	2.20	0.42
1:G:92:PHE:HZ	1:G:116:ALA:HB2	1.84	0.42
1:G:148:ALA:HA	1:G:315:LEU:O	2.20	0.42
1:F:4:ILE:HD11	1:F:141:LEU:HD11	2.02	0.41
1:D:67:TYR:OH	1:D:165:PHE:HB3	2.19	0.41
1:J:301:TYR:O	1:J:335:VAL:HA	2.20	0.41
1:H:277:ILE:HB	1:H:315:LEU:HD23	2.01	0.41
1:F:36:ILE:O	1:F:40:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:HD2	7:B:1593:HOH:O	2.19	0.41
1:E:277:ILE:HB	1:E:315:LEU:CD2	2.50	0.41
1:D:209:ARG:HD2	7:D:1245:HOH:O	2.20	0.41
1:G:121:SER:HB2	1:G:122:PRO:HD2	2.01	0.41
1:F:54:HIS:NE2	1:F:137:ASP:OD1	2.47	0.41
1:B:112:TYR:O	1:B:164:MET:HA	2.20	0.41
1:D:25:PRO:HA	1:D:26:PRO:HD3	1.96	0.41
1:C:91:SER:O	1:C:110:GLY:HA3	2.20	0.41
1:I:67:TYR:OH	1:I:165:PHE:HB3	2.21	0.41
1:A:193:ASP:HA	1:A:280:SER:HB2	2.02	0.41
1:J:302:ILE:HG22	1:J:306:ARG:NH2	2.35	0.41
1:A:6:SER:HB2	1:A:51:PRO:HG3	2.02	0.41
1:H:92:PHE:HZ	1:H:116:ALA:HB2	1.86	0.41
1:J:89:ALA:HB2	1:J:109:ILE:HG12	2.02	0.41
1:B:7:GLU:O	1:B:10:LYS:HG2	2.20	0.41
1:E:187:LYS:C	1:E:188:LYS:HG2	2.41	0.41
1:D:112:TYR:O	1:D:164:MET:HA	2.21	0.41
1:B:328:ILE:CG2	1:B:329:GLY:N	2.83	0.41
1:E:286:PHE:CE2	1:E:288:GLN:HB2	2.56	0.41
1:D:29:ALA:HB3	1:D:31:PHE:CE1	2.56	0.41
1:J:25:PRO:HA	1:J:26:PRO:HD3	1.94	0.41
1:J:1:MET:SD	1:J:336:LEU:HD22	2.61	0.41
1:A:200:ASN:HB2	1:A:229:LEU:HD23	2.02	0.41
1:H:298:SER:N	1:H:299:PRO:CD	2.84	0.41
1:B:177:ALA:HB1	1:B:316:LEU:CD2	2.50	0.41
1:D:37:LEU:O	1:D:41:LYS:HG3	2.21	0.40
1:D:148:ALA:HA	1:D:315:LEU:O	2.20	0.40
1:H:256:SER:O	1:H:260:GLU:HG3	2.21	0.40
1:B:88:ILE:HG12	1:B:119:ALA:HB2	2.03	0.40
1:A:25:PRO:HA	1:A:26:PRO:HD3	2.00	0.40
1:K:298:SER:N	1:K:299:PRO:CD	2.84	0.40
1:D:123:GLY:HA2	1:D:126:GLU:OE1	2.20	0.40
1:D:251:ARG:HG3	7:D:2143:HOH:O	2.22	0.40
1:F:5:PHE:CD1	1:F:152:LEU:HD13	2.57	0.40
1:B:11:LEU:HB2	1:B:127:ALA:HB2	2.03	0.40
1:I:247:TYR:OH	1:I:268:ARG:HD2	2.21	0.40
1:A:140:ASP:OD1	1:A:184:LYS:HE3	2.21	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	46	52
1	B	339/341 (99%)	325 (96%)	13 (4%)	1 (0%)	46	52
1	C	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	46	52
1	D	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	46	52
1	E	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	46	52
1	F	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	46	52
1	G	339/341 (99%)	325 (96%)	13 (4%)	1 (0%)	46	52
1	H	339/341 (99%)	323 (95%)	15 (4%)	1 (0%)	46	52
1	I	339/341 (99%)	323 (95%)	15 (4%)	1 (0%)	46	52
1	J	338/341 (99%)	323 (96%)	14 (4%)	1 (0%)	46	52
1	K	339/341 (99%)	325 (96%)	13 (4%)	1 (0%)	46	52
1	L	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	46	52
All	All	4067/4092 (99%)	3904 (96%)	151 (4%)	12 (0%)	46	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	C	94	VAL
1	E	94	VAL
1	F	94	VAL
1	G	94	VAL
1	J	94	VAL
1	K	94	VAL
1	L	94	VAL
1	B	94	VAL
1	D	94	VAL
1	H	94	VAL
1	I	94	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 X-ray entries followed by that with respect to entries of similar resolution.

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	253/253 (100%)	248 (98%)	5 (2%)	63	73
1	B	253/253 (100%)	247 (98%)	6 (2%)	57	67
1	C	253/253 (100%)	247 (98%)	6 (2%)	57	67
1	D	253/253 (100%)	247 (98%)	6 (2%)	57	67
1	E	253/253 (100%)	248 (98%)	5 (2%)	63	73
1	F	253/253 (100%)	248 (98%)	5 (2%)	63	73
1	G	253/253 (100%)	244 (96%)	9 (4%)	42	51
1	H	253/253 (100%)	248 (98%)	5 (2%)	63	73
1	I	253/253 (100%)	247 (98%)	6 (2%)	57	67
1	J	253/253 (100%)	248 (98%)	5 (2%)	63	73
1	K	253/253 (100%)	248 (98%)	5 (2%)	63	73
1	L	253/253 (100%)	251 (99%)	2 (1%)	86	92
All	All	3036/3036 (100%)	2971 (98%)	65 (2%)	61	71

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	117	GLU
1	A	158	HIS
1	A	188	LYS
1	A	293	PHE
1	B	28	GLU
1	B	117	GLU
1	B	137	ASP
1	B	158	HIS
1	B	168	TYR
1	B	284	ASP
1	C	10	LYS
1	C	28	GLU
1	C	117	GLU

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Mol	Chain	Res	Type
1	C	158	HIS
1	C	293	PHE
1	C	306	ARG
1	D	10	LYS
1	D	117	GLU
1	D	137	ASP
1	D	158	HIS
1	D	293	PHE
1	D	306	ARG
1	E	28	GLU
1	E	137	ASP
1	E	158	HIS
1	E	188	LYS
1	E	284	ASP
1	F	91	SER
1	F	117	GLU
1	F	152	LEU
1	F	158	HIS
1	F	284	ASP
1	G	28	GLU
1	G	46	ASP
1	G	117	GLU
1	G	137	ASP
1	G	158	HIS
1	G	168	TYR
1	G	184	LYS
1	G	284	ASP
1	G	293	PHE
1	H	28	GLU
1	H	79	LYS
1	H	117	GLU
1	H	158	HIS
1	H	293	PHE
1	I	28	GLU
1	I	117	GLU
1	I	152	LEU
1	I	158	HIS
1	I	168	TYR
1	I	292	SER
1	J	10	LYS
1	J	18	LEU
1	J	91	SER

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Mol	Chain	Res	Type
1	J	117	GLU
1	J	158	HIS
1	K	28	GLU
1	K	46	ASP
1	K	117	GLU
1	K	158	HIS
1	K	168	TYR
1	L	137	ASP
1	L	158	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	146	HIS
1	D	146	HIS
1	E	146	HIS
1	F	198	HIS
1	G	146	HIS
1	I	146	HIS
1	J	69	ASN
1	L	13	ASN
1	L	331	ASN

### 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 167 ligands modelled in this entry, 47 are monoatomic - leaving 120 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	DMS	A	342	-	3,3,3	0.88	0	3,3,3	0.95	0
3	B3N	A	401	6	22,22,22	2.49	8 (36%)	26,27,27	0.81	0
2	DMS	A	403	-	3,3,3	0.82	0	3,3,3	0.99	0
2	DMS	A	405	-	3,3,3	0.83	0	3,3,3	0.92	0
2	DMS	A	411	-	3,3,3	0.86	0	3,3,3	0.92	0
2	DMS	A	413	-	3,3,3	0.84	0	3,3,3	0.95	0
2	DMS	A	415	-	3,3,3	0.87	0	3,3,3	0.95	0
2	DMS	A	417	-	3,3,3	0.85	0	3,3,3	0.96	0
2	DMS	A	419	-	3,3,3	0.85	0	3,3,3	0.95	0
2	DMS	A	421	-	3,3,3	0.86	0	3,3,3	0.96	0
2	DMS	A	423	-	3,3,3	0.87	0	3,3,3	0.94	0
2	DMS	B	342	-	3,3,3	0.84	0	3,3,3	0.95	0
2	DMS	B	403	-	3,3,3	0.81	0	3,3,3	0.93	0
2	DMS	B	405	-	3,3,3	0.85	0	3,3,3	0.91	0
3	B3N	B	407	6	22,22,22	2.53	9 (40%)	26,27,27	0.79	0
2	DMS	B	411	-	3,3,3	0.88	0	3,3,3	0.95	0
2	DMS	B	413	-	3,3,3	0.88	0	3,3,3	0.96	0
2	DMS	B	415	-	3,3,3	0.89	0	3,3,3	0.94	0
2	DMS	B	417	-	3,3,3	0.87	0	3,3,3	0.95	0
2	DMS	B	419	-	3,3,3	0.86	0	3,3,3	0.97	0
2	DMS	B	423	-	3,3,3	0.87	0	3,3,3	0.94	0
3	B3N	C	401	6	22,22,22	2.44	7 (31%)	26,27,27	1.00	1 (3%)
2	DMS	C	405	-	3,3,3	0.90	0	3,3,3	0.92	0
2	DMS	C	411	-	3,3,3	0.87	0	3,3,3	0.94	0
2	DMS	C	415	-	3,3,3	0.88	0	3,3,3	0.94	0
2	DMS	C	419	-	3,3,3	0.87	0	3,3,3	0.95	0
2	DMS	C	421	-	3,3,3	0.86	0	3,3,3	0.97	0
2	DMS	C	423	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	D	342	-	3,3,3	0.87	0	3,3,3	0.93	0
2	DMS	D	343	-	3,3,3	0.88	0	3,3,3	0.97	0
2	DMS	D	403	-	3,3,3	0.89	0	3,3,3	0.96	0
2	DMS	D	405	-	3,3,3	0.81	0	3,3,3	0.92	0
3	B3N	D	407	6	22,22,22	2.49	8 (36%)	26,27,27	0.82	0
2	DMS	D	411	-	3,3,3	0.89	0	3,3,3	0.94	0
2	DMS	D	413	-	3,3,3	0.87	0	3,3,3	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DMS	D	415	-	3,3,3	0.89	0	3,3,3	0.96	0
2	DMS	D	417	-	3,3,3	0.87	0	3,3,3	0.97	0
2	DMS	D	419	-	3,3,3	0.85	0	3,3,3	0.97	0
2	DMS	D	421	-	3,3,3	0.87	0	3,3,3	0.96	0
2	DMS	D	423	-	3,3,3	0.88	0	3,3,3	0.95	0
2	DMS	E	342	-	3,3,3	0.82	0	3,3,3	0.95	0
3	B3N	E	401	6	22,22,22	2.57	9 (40%)	26,27,27	0.79	0
2	DMS	E	403	-	3,3,3	0.84	0	3,3,3	0.95	0
2	DMS	E	405	-	3,3,3	0.85	0	3,3,3	0.91	0
2	DMS	E	411	-	3,3,3	0.89	0	3,3,3	0.94	0
2	DMS	E	413	-	3,3,3	0.86	0	3,3,3	0.97	0
2	DMS	E	415	-	3,3,3	0.87	0	3,3,3	0.96	0
2	DMS	E	417	-	3,3,3	0.87	0	3,3,3	0.96	0
2	DMS	E	419	-	3,3,3	0.87	0	3,3,3	0.95	0
2	DMS	E	421	-	3,3,3	0.84	0	3,3,3	0.94	0
2	DMS	E	423	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	F	342	-	3,3,3	0.90	0	3,3,3	0.95	0
2	DMS	F	343	-	3,3,3	0.85	0	3,3,3	0.96	0
2	DMS	F	344	-	3,3,3	0.86	0	3,3,3	0.94	0
2	DMS	F	405	-	3,3,3	0.86	0	3,3,3	0.92	0
3	B3N	F	407	6	22,22,22	2.41	7 (31%)	26,27,27	0.79	0
2	DMS	F	411	-	3,3,3	0.84	0	3,3,3	0.94	0
2	DMS	F	413	-	3,3,3	0.85	0	3,3,3	0.95	0
2	DMS	F	415	-	3,3,3	0.88	0	3,3,3	0.96	0
2	DMS	F	417	-	3,3,3	0.85	0	3,3,3	0.96	0
2	DMS	F	419	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	F	421	-	3,3,3	0.87	0	3,3,3	0.96	0
2	DMS	F	423	-	3,3,3	0.86	0	3,3,3	0.94	0
2	DMS	G	342	-	3,3,3	0.85	0	3,3,3	0.95	0
2	DMS	G	343	-	3,3,3	0.86	0	3,3,3	0.92	0
3	B3N	G	401	6	22,22,22	2.53	9 (40%)	26,27,27	0.83	0
2	DMS	G	403	-	3,3,3	0.84	0	3,3,3	0.94	0
2	DMS	G	405	-	3,3,3	0.84	0	3,3,3	0.93	0
2	DMS	G	411	-	3,3,3	0.88	0	3,3,3	0.93	0
2	DMS	G	413	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	G	415	-	3,3,3	0.88	0	3,3,3	0.96	0
2	DMS	G	417	-	3,3,3	0.89	0	3,3,3	0.93	0
2	DMS	G	419	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	G	423	-	3,3,3	0.89	0	3,3,3	0.95	0
2	DMS	H	405	-	3,3,3	0.85	0	3,3,3	0.92	0
3	B3N	H	407	6	22,22,22	2.58	9 (40%)	26,27,27	0.93	1 (3%)
2	DMS	H	411	-	3,3,3	0.88	0	3,3,3	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DMS	H	413	-	3,3,3	0.86	0	3,3,3	0.94	0
2	DMS	H	415	-	3,3,3	0.88	0	3,3,3	0.95	0
2	DMS	H	417	-	3,3,3	0.85	0	3,3,3	0.96	0
2	DMS	H	419	-	3,3,3	0.86	0	3,3,3	0.94	0
2	DMS	H	421	-	3,3,3	0.89	0	3,3,3	0.96	0
2	DMS	H	423	-	3,3,3	0.88	0	3,3,3	0.95	0
3	B3N	I	401	6	22,22,22	2.51	8 (36%)	26,27,27	0.84	0
2	DMS	I	405	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	I	411	-	3,3,3	0.88	0	3,3,3	0.95	0
2	DMS	I	413	-	3,3,3	0.88	0	3,3,3	0.91	0
2	DMS	I	415	-	3,3,3	0.88	0	3,3,3	0.98	0
2	DMS	I	417	-	3,3,3	0.87	0	3,3,3	0.96	0
2	DMS	I	419	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	I	421	-	3,3,3	0.88	0	3,3,3	0.98	0
2	DMS	I	423	-	3,3,3	0.88	0	3,3,3	0.95	0
2	DMS	J	403	-	3,3,3	0.85	0	3,3,3	0.95	0
2	DMS	J	405	-	3,3,3	0.88	0	3,3,3	0.94	0
3	B3N	J	407	6	22,22,22	2.57	8 (36%)	26,27,27	1.06	1 (3%)
2	DMS	J	413	-	3,3,3	0.86	0	3,3,3	0.96	0
2	DMS	J	415	-	3,3,3	0.86	0	3,3,3	0.98	0
2	DMS	J	417	-	3,3,3	0.87	0	3,3,3	0.95	0
2	DMS	J	419	-	3,3,3	0.86	0	3,3,3	0.96	0
2	DMS	J	423	-	3,3,3	0.87	0	3,3,3	0.95	0
2	DMS	K	342	-	3,3,3	0.84	0	3,3,3	0.94	0
3	B3N	K	401	6	22,22,22	2.59	8 (36%)	26,27,27	0.95	3 (11%)
2	DMS	K	403	-	3,3,3	0.85	0	3,3,3	0.97	0
2	DMS	K	405	-	3,3,3	0.85	0	3,3,3	0.95	0
2	DMS	K	411	-	3,3,3	0.87	0	3,3,3	0.94	0
2	DMS	K	413	-	3,3,3	0.91	0	3,3,3	0.96	0
2	DMS	K	415	-	3,3,3	0.88	0	3,3,3	0.96	0
2	DMS	K	417	-	3,3,3	0.85	0	3,3,3	0.95	0
2	DMS	K	419	-	3,3,3	0.89	0	3,3,3	0.93	0
2	DMS	K	421	-	3,3,3	0.87	0	3,3,3	0.96	0
2	DMS	K	423	-	3,3,3	0.87	0	3,3,3	0.94	0
2	DMS	L	342	-	3,3,3	0.87	0	3,3,3	0.97	0
2	DMS	L	405	-	3,3,3	0.88	0	3,3,3	0.93	0
3	B3N	L	407	6	22,22,22	2.47	7 (31%)	26,27,27	0.80	0
2	DMS	L	413	-	3,3,3	0.85	0	3,3,3	0.94	0
2	DMS	L	415	-	3,3,3	0.87	0	3,3,3	0.96	0
2	DMS	L	417	-	3,3,3	0.84	0	3,3,3	0.96	0
2	DMS	L	419	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	L	421	-	3,3,3	0.85	0	3,3,3	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DMS	L	423	-	3,3,3	0.87	0	3,3,3	0.96	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
2	DMS	A	342	-	-	0/0/0/0	0/0/0/0
3	B3N	A	401	6	-	0/20/20/20	0/1/1/1
2	DMS	A	403	-	-	0/0/0/0	0/0/0/0
2	DMS	A	405	-	-	0/0/0/0	0/0/0/0
2	DMS	A	411	-	-	0/0/0/0	0/0/0/0
2	DMS	A	413	-	-	0/0/0/0	0/0/0/0
2	DMS	A	415	-	-	0/0/0/0	0/0/0/0
2	DMS	A	417	-	-	0/0/0/0	0/0/0/0
2	DMS	A	419	-	-	0/0/0/0	0/0/0/0
2	DMS	A	421	-	-	0/0/0/0	0/0/0/0
2	DMS	A	423	-	-	0/0/0/0	0/0/0/0
2	DMS	B	342	-	-	0/0/0/0	0/0/0/0
2	DMS	B	403	-	-	0/0/0/0	0/0/0/0
2	DMS	B	405	-	-	0/0/0/0	0/0/0/0
3	B3N	B	407	6	-	0/20/20/20	0/1/1/1
2	DMS	B	411	-	-	0/0/0/0	0/0/0/0
2	DMS	B	413	-	-	0/0/0/0	0/0/0/0
2	DMS	B	415	-	-	0/0/0/0	0/0/0/0
2	DMS	B	417	-	-	0/0/0/0	0/0/0/0
2	DMS	B	419	-	-	0/0/0/0	0/0/0/0
2	DMS	B	423	-	-	0/0/0/0	0/0/0/0
3	B3N	C	401	6	-	0/20/20/20	0/1/1/1
2	DMS	C	405	-	-	0/0/0/0	0/0/0/0
2	DMS	C	411	-	-	0/0/0/0	0/0/0/0
2	DMS	C	415	-	-	0/0/0/0	0/0/0/0
2	DMS	C	419	-	-	0/0/0/0	0/0/0/0
2	DMS	C	421	-	-	0/0/0/0	0/0/0/0
2	DMS	C	423	-	-	0/0/0/0	0/0/0/0
2	DMS	D	342	-	-	0/0/0/0	0/0/0/0
2	DMS	D	343	-	-	0/0/0/0	0/0/0/0
2	DMS	D	403	-	-	0/0/0/0	0/0/0/0
2	DMS	D	405	-	-	0/0/0/0	0/0/0/0
3	B3N	D	407	6	-	0/20/20/20	0/1/1/1
2	DMS	D	411	-	-	0/0/0/0	0/0/0/0
2	DMS	D	413	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DMS	D	415	-	-	0/0/0/0	0/0/0/0
2	DMS	D	417	-	-	0/0/0/0	0/0/0/0
2	DMS	D	419	-	-	0/0/0/0	0/0/0/0
2	DMS	D	421	-	-	0/0/0/0	0/0/0/0
2	DMS	D	423	-	-	0/0/0/0	0/0/0/0
2	DMS	E	342	-	-	0/0/0/0	0/0/0/0
3	B3N	E	401	6	-	0/20/20/20	0/1/1/1
2	DMS	E	403	-	-	0/0/0/0	0/0/0/0
2	DMS	E	405	-	-	0/0/0/0	0/0/0/0
2	DMS	E	411	-	-	0/0/0/0	0/0/0/0
2	DMS	E	413	-	-	0/0/0/0	0/0/0/0
2	DMS	E	415	-	-	0/0/0/0	0/0/0/0
2	DMS	E	417	-	-	0/0/0/0	0/0/0/0
2	DMS	E	419	-	-	0/0/0/0	0/0/0/0
2	DMS	E	421	-	-	0/0/0/0	0/0/0/0
2	DMS	E	423	-	-	0/0/0/0	0/0/0/0
2	DMS	F	342	-	-	0/0/0/0	0/0/0/0
2	DMS	F	343	-	-	0/0/0/0	0/0/0/0
2	DMS	F	344	-	-	0/0/0/0	0/0/0/0
2	DMS	F	405	-	-	0/0/0/0	0/0/0/0
3	B3N	F	407	6	-	0/20/20/20	0/1/1/1
2	DMS	F	411	-	-	0/0/0/0	0/0/0/0
2	DMS	F	413	-	-	0/0/0/0	0/0/0/0
2	DMS	F	415	-	-	0/0/0/0	0/0/0/0
2	DMS	F	417	-	-	0/0/0/0	0/0/0/0
2	DMS	F	419	-	-	0/0/0/0	0/0/0/0
2	DMS	F	421	-	-	0/0/0/0	0/0/0/0
2	DMS	F	423	-	-	0/0/0/0	0/0/0/0
2	DMS	G	342	-	-	0/0/0/0	0/0/0/0
2	DMS	G	343	-	-	0/0/0/0	0/0/0/0
3	B3N	G	401	6	-	0/20/20/20	0/1/1/1
2	DMS	G	403	-	-	0/0/0/0	0/0/0/0
2	DMS	G	405	-	-	0/0/0/0	0/0/0/0
2	DMS	G	411	-	-	0/0/0/0	0/0/0/0
2	DMS	G	413	-	-	0/0/0/0	0/0/0/0
2	DMS	G	415	-	-	0/0/0/0	0/0/0/0
2	DMS	G	417	-	-	0/0/0/0	0/0/0/0
2	DMS	G	419	-	-	0/0/0/0	0/0/0/0
2	DMS	G	423	-	-	0/0/0/0	0/0/0/0
2	DMS	H	405	-	-	0/0/0/0	0/0/0/0
3	B3N	H	407	6	-	0/20/20/20	0/1/1/1
2	DMS	H	411	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DMS	H	413	-	-	0/0/0/0	0/0/0/0
2	DMS	H	415	-	-	0/0/0/0	0/0/0/0
2	DMS	H	417	-	-	0/0/0/0	0/0/0/0
2	DMS	H	419	-	-	0/0/0/0	0/0/0/0
2	DMS	H	421	-	-	0/0/0/0	0/0/0/0
2	DMS	H	423	-	-	0/0/0/0	0/0/0/0
3	B3N	I	401	6	-	0/20/20/20	0/1/1/1
2	DMS	I	405	-	-	0/0/0/0	0/0/0/0
2	DMS	I	411	-	-	0/0/0/0	0/0/0/0
2	DMS	I	413	-	-	0/0/0/0	0/0/0/0
2	DMS	I	415	-	-	0/0/0/0	0/0/0/0
2	DMS	I	417	-	-	0/0/0/0	0/0/0/0
2	DMS	I	419	-	-	0/0/0/0	0/0/0/0
2	DMS	I	421	-	-	0/0/0/0	0/0/0/0
2	DMS	I	423	-	-	0/0/0/0	0/0/0/0
2	DMS	J	403	-	-	0/0/0/0	0/0/0/0
2	DMS	J	405	-	-	0/0/0/0	0/0/0/0
3	B3N	J	407	6	-	0/20/20/20	0/1/1/1
2	DMS	J	413	-	-	0/0/0/0	0/0/0/0
2	DMS	J	415	-	-	0/0/0/0	0/0/0/0
2	DMS	J	417	-	-	0/0/0/0	0/0/0/0
2	DMS	J	419	-	-	0/0/0/0	0/0/0/0
2	DMS	J	423	-	-	0/0/0/0	0/0/0/0
2	DMS	K	342	-	-	0/0/0/0	0/0/0/0
3	B3N	K	401	6	-	0/20/20/20	0/1/1/1
2	DMS	K	403	-	-	0/0/0/0	0/0/0/0
2	DMS	K	405	-	-	0/0/0/0	0/0/0/0
2	DMS	K	411	-	-	0/0/0/0	0/0/0/0
2	DMS	K	413	-	-	0/0/0/0	0/0/0/0
2	DMS	K	415	-	-	0/0/0/0	0/0/0/0
2	DMS	K	417	-	-	0/0/0/0	0/0/0/0
2	DMS	K	419	-	-	0/0/0/0	0/0/0/0
2	DMS	K	421	-	-	0/0/0/0	0/0/0/0
2	DMS	K	423	-	-	0/0/0/0	0/0/0/0
2	DMS	L	342	-	-	0/0/0/0	0/0/0/0
2	DMS	L	405	-	-	0/0/0/0	0/0/0/0
3	B3N	L	407	6	-	0/20/20/20	0/1/1/1
2	DMS	L	413	-	-	0/0/0/0	0/0/0/0
2	DMS	L	415	-	-	0/0/0/0	0/0/0/0
2	DMS	L	417	-	-	0/0/0/0	0/0/0/0
2	DMS	L	419	-	-	0/0/0/0	0/0/0/0
2	DMS	L	421	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DMS	L	423	-	-	0/0/0/0	0/0/0/0

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	407	B3N	O4-N3	-9.00	1.23	1.39
3	C	401	B3N	O4-N3	-8.99	1.23	1.39
3	L	407	B3N	O4-N3	-8.98	1.23	1.39
3	A	401	B3N	O4-N3	-8.98	1.23	1.39
3	B	407	B3N	O4-N3	-8.98	1.23	1.39
3	H	407	B3N	O4-N3	-8.98	1.23	1.39
3	D	407	B3N	O4-N3	-8.97	1.23	1.39
3	G	401	B3N	O4-N3	-8.97	1.23	1.39
3	I	401	B3N	O4-N3	-8.97	1.23	1.39
3	E	401	B3N	O4-N3	-8.95	1.23	1.39
3	K	401	B3N	O4-N3	-8.95	1.23	1.39
3	J	407	B3N	O4-N3	-8.95	1.23	1.39
3	H	407	B3N	C1-N3	2.05	1.34	1.32
3	F	407	B3N	C19-C18	2.07	1.42	1.38
3	B	407	B3N	C1-N3	2.10	1.34	1.32
3	A	401	B3N	C15-C14	2.11	1.42	1.39
3	B	407	B3N	C15-C14	2.11	1.42	1.39
3	I	401	B3N	C15-C14	2.14	1.42	1.39
3	E	401	B3N	C15-C14	2.17	1.43	1.39
3	G	401	B3N	C1-N3	2.24	1.34	1.32
3	G	401	B3N	C15-C14	2.28	1.43	1.39
3	C	401	B3N	C16-C15	2.28	1.42	1.38
3	F	407	B3N	C16-C15	2.31	1.42	1.38
3	C	401	B3N	C18-C17	2.34	1.43	1.39
3	H	407	B3N	C15-C14	2.34	1.43	1.39
3	J	407	B3N	C15-C14	2.35	1.43	1.39
3	D	407	B3N	C15-C14	2.37	1.43	1.39
3	L	407	B3N	C16-C15	2.38	1.43	1.38
3	A	401	B3N	C19-C18	2.45	1.43	1.38
3	K	401	B3N	C15-C14	2.45	1.43	1.39
3	D	407	B3N	C19-C18	2.46	1.43	1.38
3	C	401	B3N	C19-C18	2.46	1.43	1.38
3	A	401	B3N	C16-C15	2.47	1.43	1.38
3	I	401	B3N	C16-C15	2.47	1.43	1.38
3	F	407	B3N	C16-C17	2.50	1.44	1.39
3	E	401	B3N	C1-N3	2.52	1.35	1.32
3	C	401	B3N	C16-C17	2.52	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	401	B3N	C16-C17	2.53	1.44	1.39
3	F	407	B3N	C19-C14	2.57	1.43	1.39
3	B	407	B3N	C19-C18	2.57	1.43	1.38
3	G	401	B3N	C16-C15	2.57	1.43	1.38
3	A	401	B3N	C18-C17	2.57	1.44	1.39
3	E	401	B3N	C16-C17	2.58	1.44	1.39
3	D	407	B3N	C16-C15	2.59	1.43	1.38
3	L	407	B3N	C16-C17	2.59	1.44	1.39
3	C	401	B3N	C19-C14	2.59	1.43	1.39
3	F	407	B3N	C18-C17	2.63	1.44	1.39
3	A	401	B3N	C16-C17	2.64	1.44	1.39
3	L	407	B3N	C19-C18	2.65	1.43	1.38
3	J	407	B3N	C16-C15	2.66	1.43	1.38
3	G	401	B3N	C16-C17	2.67	1.44	1.39
3	B	407	B3N	C16-C17	2.68	1.44	1.39
3	D	407	B3N	C19-C14	2.69	1.43	1.39
3	I	401	B3N	C19-C18	2.69	1.43	1.38
3	K	401	B3N	C16-C15	2.69	1.43	1.38
3	D	407	B3N	C16-C17	2.70	1.44	1.39
3	G	401	B3N	C19-C14	2.71	1.43	1.39
3	J	407	B3N	C16-C17	2.71	1.44	1.39
3	G	401	B3N	C19-C18	2.71	1.43	1.38
3	A	401	B3N	C19-C14	2.73	1.44	1.39
3	J	407	B3N	C19-C18	2.75	1.43	1.38
3	B	407	B3N	C18-C17	2.77	1.44	1.39
3	L	407	B3N	C19-C14	2.77	1.44	1.39
3	E	401	B3N	C19-C14	2.78	1.44	1.39
3	E	401	B3N	C19-C18	2.79	1.43	1.38
3	D	407	B3N	C18-C17	2.79	1.44	1.39
3	H	407	B3N	C16-C15	2.80	1.43	1.38
3	E	401	B3N	C16-C15	2.81	1.43	1.38
3	L	407	B3N	C18-C17	2.82	1.44	1.39
3	B	407	B3N	C16-C15	2.84	1.43	1.38
3	K	401	B3N	C16-C17	2.84	1.44	1.39
3	B	407	B3N	C19-C14	2.85	1.44	1.39
3	I	401	B3N	C19-C14	2.86	1.44	1.39
3	E	401	B3N	C18-C17	2.88	1.44	1.39
3	G	401	B3N	C18-C17	2.88	1.44	1.39
3	H	407	B3N	C19-C14	2.88	1.44	1.39
3	H	407	B3N	C19-C18	2.91	1.44	1.38
3	J	407	B3N	C18-C17	2.93	1.45	1.39
3	F	407	B3N	C17-N20	2.93	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	407	B3N	C17-N20	2.99	1.44	1.37
3	H	407	B3N	C17-N20	3.02	1.44	1.37
3	L	407	B3N	C17-N20	3.04	1.44	1.37
3	I	401	B3N	C18-C17	3.04	1.45	1.39
3	K	401	B3N	C19-C18	3.05	1.44	1.38
3	H	407	B3N	C16-C17	3.06	1.45	1.39
3	I	401	B3N	C17-N20	3.09	1.45	1.37
3	J	407	B3N	C19-C14	3.14	1.44	1.39
3	G	401	B3N	C17-N20	3.15	1.45	1.37
3	K	401	B3N	C19-C14	3.16	1.44	1.39
3	H	407	B3N	C18-C17	3.18	1.45	1.39
3	B	407	B3N	C17-N20	3.19	1.45	1.37
3	A	401	B3N	C17-N20	3.26	1.45	1.37
3	K	401	B3N	C18-C17	3.26	1.45	1.39
3	J	407	B3N	C17-N20	3.34	1.45	1.37
3	E	401	B3N	C17-N20	3.35	1.45	1.37
3	C	401	B3N	C17-N20	3.37	1.45	1.37
3	K	401	B3N	C17-N20	3.41	1.45	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	407	B3N	C6-C5-C1	-3.74	103.34	113.24
3	C	401	B3N	C6-C5-C1	-3.19	104.81	113.24
3	H	407	B3N	O2-C1-N3	-2.76	120.28	123.53
3	K	401	B3N	C6-C5-C1	-2.11	107.66	113.24
3	K	401	B3N	O2-C1-N3	-2.11	121.04	123.53
3	K	401	B3N	C10-N12-C13	2.07	126.78	122.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	407	B3N	1	0
3	J	407	B3N	1	0
3	K	401	B3N	1	0
3	L	407	B3N	1	0

## 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	341/341 (100%)	-0.60	2 (0%) 90 91	10, 19, 31, 48	0
1	B	341/341 (100%)	-0.49	4 (1%) 81 83	12, 23, 37, 53	0
1	C	341/341 (100%)	-0.57	1 (0%) 94 95	10, 20, 32, 49	0
1	D	341/341 (100%)	-0.57	2 (0%) 90 91	11, 21, 31, 48	0
1	E	341/341 (100%)	-0.56	2 (0%) 90 91	11, 23, 37, 51	0
1	F	341/341 (100%)	-0.59	2 (0%) 90 91	11, 20, 31, 46	0
1	G	341/341 (100%)	-0.59	1 (0%) 94 95	12, 23, 38, 50	0
1	H	341/341 (100%)	-0.46	2 (0%) 90 91	10, 22, 33, 47	0
1	I	341/341 (100%)	-0.58	5 (1%) 76 79	10, 20, 33, 48	0
1	J	340/341 (99%)	-0.53	3 (0%) 85 87	12, 23, 39, 53	0
1	K	341/341 (100%)	-0.61	3 (0%) 85 87	10, 20, 32, 48	0
1	L	341/341 (100%)	-0.46	2 (0%) 90 91	12, 21, 33, 46	0
All	All	4091/4092 (99%)	-0.55	29 (0%) 89 90	10, 21, 35, 53	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	341	GLY	4.9
1	H	341	GLY	4.7
1	C	53	ARG	4.3
1	B	323	TYR	4.1
1	B	53	ARG	3.8
1	L	341	GLY	3.7
1	I	323	TYR	3.5
1	J	323	TYR	3.5
1	K	323	TYR	3.2
1	D	53	ARG	3.2
1	H	35	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	325	VAL	3.0
1	I	325	VAL	2.7
1	G	53	ARG	2.6
1	I	324	GLY	2.6
1	K	53	ARG	2.6
1	J	53	ARG	2.5
1	B	341	GLY	2.5
1	A	35	TRP	2.4
1	I	341	GLY	2.3
1	J	252	GLY	2.2
1	I	53	ARG	2.2
1	E	323	TYR	2.1
1	B	252	GLY	2.1
1	E	341	GLY	2.1
1	L	53	ARG	2.1
1	A	53	ARG	2.1
1	F	53	ARG	2.1
1	D	341	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	DMS	E	421	4/4	0.91	0.21	12.40	67,67,68,69	0
2	DMS	C	421	4/4	0.95	0.18	11.20	59,60,60,60	0
2	DMS	E	415	4/4	0.91	0.26	10.71	69,70,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DMS	G	417	4/4	0.85	0.22	10.51	66,67,67,68	0
2	DMS	K	405	4/4	0.98	0.18	10.09	48,48,49,49	0
2	DMS	I	415	4/4	0.88	0.25	9.69	61,61,62,62	0
2	DMS	L	417	4/4	0.93	0.19	8.83	76,76,76,76	0
2	DMS	L	415	4/4	0.94	0.24	8.59	61,61,62,62	0
2	DMS	D	417	4/4	0.85	0.22	8.50	63,65,65,65	0
2	DMS	A	415	4/4	0.90	0.32	8.45	62,63,63,63	0
2	DMS	B	415	4/4	0.87	0.28	8.27	70,72,72,72	0
2	DMS	E	417	4/4	0.85	0.24	7.47	63,64,64,65	0
2	DMS	K	417	4/4	0.91	0.20	7.40	66,66,66,66	0
2	DMS	J	415	4/4	0.88	0.28	7.24	58,58,60,60	0
2	DMS	D	413	4/4	0.94	0.19	6.96	60,60,60,60	0
2	DMS	H	421	4/4	0.94	0.15	6.53	59,60,60,60	0
2	DMS	K	419	4/4	0.87	0.21	6.39	72,72,73,73	0
2	DMS	A	342	4/4	0.98	0.18	6.15	43,44,45,45	0
2	DMS	I	413	4/4	0.98	0.12	6.09	38,39,39,40	0
2	DMS	D	343	4/4	0.94	0.16	6.07	62,63,64,64	0
2	DMS	G	405	4/4	0.98	0.17	6.06	44,45,45,46	0
2	DMS	K	415	4/4	0.92	0.21	5.91	59,60,60,60	0
2	DMS	H	405	4/4	0.98	0.14	5.87	43,44,44,44	0
2	DMS	I	419	4/4	0.92	0.16	5.82	63,63,63,64	0
2	DMS	F	343	4/4	0.94	0.19	5.74	58,58,58,59	0
2	DMS	J	417	4/4	0.89	0.18	5.60	65,65,65,66	0
2	DMS	B	342	4/4	0.98	0.16	5.59	44,45,45,46	0
2	DMS	G	415	4/4	0.91	0.21	5.55	65,66,66,66	0
2	DMS	L	405	4/4	0.96	0.16	5.49	45,46,46,46	0
2	DMS	D	415	4/4	0.90	0.22	5.37	65,66,66,66	0
2	DMS	H	415	4/4	0.92	0.24	5.26	60,61,61,62	0
2	DMS	C	415	4/4	0.90	0.27	5.05	64,65,65,65	0
2	DMS	F	415	4/4	0.89	0.23	4.74	59,60,61,61	0
2	DMS	A	405	4/4	0.98	0.12	4.72	37,37,38,38	0
2	DMS	A	403	4/4	0.97	0.16	4.59	42,43,43,44	0
2	DMS	J	403	4/4	0.97	0.17	4.56	43,45,46,46	0
2	DMS	L	421	4/4	0.94	0.16	4.49	61,61,62,62	0
2	DMS	K	421	4/4	0.95	0.13	4.39	57,58,59,59	0
2	DMS	H	413	4/4	0.99	0.11	4.33	43,43,45,45	0
2	DMS	C	405	4/4	0.98	0.12	4.22	39,40,40,41	0
2	DMS	I	417	4/4	0.91	0.20	4.19	66,66,67,67	0
2	DMS	F	344	4/4	0.97	0.20	4.10	59,60,60,61	0
2	DMS	D	405	4/4	0.98	0.14	4.09	39,39,40,41	0
2	DMS	L	342	4/4	0.92	0.15	4.07	57,58,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DMS	A	419	4/4	0.95	0.17	3.98	61,61,62,62	0
2	DMS	B	405	4/4	0.98	0.19	3.94	43,44,44,45	0
3	B3N	D	407	22/22	0.94	0.17	3.93	29,33,36,37	0
2	DMS	A	421	4/4	0.94	0.17	3.92	60,61,61,61	0
3	B3N	F	407	22/22	0.91	0.15	3.72	29,36,38,39	0
2	DMS	F	421	4/4	0.92	0.19	3.65	60,60,61,61	0
2	DMS	A	417	4/4	0.95	0.16	3.59	63,63,64,64	0
2	DMS	K	342	4/4	0.97	0.17	3.56	50,51,51,52	0
2	DMS	E	405	4/4	0.98	0.22	3.46	46,46,46,46	0
2	DMS	B	413	4/4	0.93	0.19	3.44	65,65,66,67	0
2	DMS	B	403	4/4	0.97	0.15	3.36	48,49,50,50	0
2	DMS	L	419	4/4	0.92	0.22	3.32	69,69,69,69	0
2	DMS	F	405	4/4	0.98	0.11	3.29	39,40,40,40	0
2	DMS	H	417	4/4	0.95	0.15	3.19	67,67,67,67	0
3	B3N	L	407	22/22	0.95	0.14	3.11	29,39,41,42	0
2	DMS	C	419	4/4	0.96	0.19	3.08	61,62,62,63	0
2	DMS	D	342	4/4	0.96	0.13	3.07	36,36,36,37	0
2	DMS	D	403	4/4	0.96	0.16	2.92	46,47,47,49	0
2	DMS	G	419	4/4	0.95	0.15	2.81	69,70,70,71	0
2	DMS	E	419	4/4	0.96	0.21	2.79	72,72,72,73	0
2	DMS	B	417	4/4	0.93	0.15	2.78	70,70,71,71	0
3	B3N	H	407	22/22	0.93	0.15	2.75	29,36,38,38	0
3	B3N	A	401	22/22	0.95	0.14	2.71	29,35,39,39	0
2	DMS	G	403	4/4	0.97	0.15	2.70	54,55,55,55	0
2	DMS	D	421	4/4	0.96	0.13	2.69	58,58,58,59	0
2	DMS	G	411	4/4	0.95	0.13	2.68	33,34,34,35	0
2	DMS	K	403	4/4	0.96	0.17	2.65	41,41,42,42	0
2	DMS	E	411	4/4	0.95	0.14	2.56	43,44,44,44	0
2	DMS	H	419	4/4	0.96	0.21	2.51	70,70,70,70	0
2	DMS	D	419	4/4	0.95	0.19	2.38	67,67,68,68	0
2	DMS	F	413	4/4	0.94	0.14	2.35	45,46,47,48	0
2	DMS	J	419	4/4	0.92	0.12	2.35	66,67,68,68	0
2	DMS	I	411	4/4	0.97	0.13	2.16	38,39,40,40	0
2	DMS	I	405	4/4	0.98	0.16	2.14	41,41,41,42	0
3	B3N	C	401	22/22	0.92	0.15	2.11	29,33,37,37	0
2	DMS	F	419	4/4	0.90	0.13	2.02	65,65,66,66	0
3	B3N	K	401	22/22	0.82	0.23	2.01	29,43,46,59	0
2	DMS	E	403	4/4	0.98	0.12	1.99	46,47,47,47	0
2	DMS	F	411	4/4	0.97	0.14	1.94	41,41,42,42	0
2	DMS	F	342	4/4	0.95	0.13	1.88	42,43,44,45	0
3	B3N	G	401	22/22	0.90	0.18	1.84	29,42,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DMS	J	405	4/4	0.98	0.11	1.83	38,40,40,41	0
2	DMS	G	342	4/4	0.98	0.14	1.82	52,52,52,52	0
2	DMS	F	417	4/4	0.97	0.13	1.76	63,63,63,63	0
2	DMS	B	423	4/4	0.87	0.33	1.65	76,77,77,78	0
2	DMS	A	423	4/4	0.90	0.23	1.57	67,68,68,69	0
2	DMS	G	343	4/4	0.96	0.11	1.56	42,42,43,43	0
2	DMS	C	423	4/4	0.90	0.32	1.49	72,73,73,73	0
2	DMS	H	411	4/4	0.97	0.12	1.44	34,35,35,36	0
2	DMS	B	419	4/4	0.95	0.13	1.36	66,66,66,67	0
3	B3N	E	401	22/22	0.89	0.17	1.34	29,43,49,49	0
3	B3N	I	401	22/22	0.85	0.21	1.27	29,48,52,54	0
2	DMS	F	423	4/4	0.83	0.22	1.20	72,73,73,73	0
2	DMS	D	411	4/4	0.97	0.11	1.15	34,35,35,35	0
2	DMS	J	423	4/4	0.96	0.21	1.10	68,68,68,69	0
2	DMS	A	411	4/4	0.97	0.12	0.94	38,38,38,41	0
2	DMS	H	423	4/4	0.88	0.18	0.83	70,71,71,72	0
2	DMS	D	423	4/4	0.91	0.21	0.82	70,71,71,71	0
3	B3N	B	407	22/22	0.90	0.17	0.79	29,45,46,47	0
3	B3N	J	407	22/22	0.88	0.17	0.77	29,47,49,49	0
2	DMS	G	423	4/4	0.93	0.19	0.77	69,69,69,70	0
2	DMS	I	423	4/4	0.94	0.17	0.75	60,61,61,61	0
2	DMS	G	413	4/4	0.97	0.12	0.65	53,53,54,54	0
2	DMS	E	413	4/4	0.97	0.11	0.60	46,47,48,48	0
2	DMS	J	413	4/4	0.97	0.09	0.53	45,46,47,47	0
2	DMS	I	421	4/4	0.95	0.10	0.52	59,59,59,60	0
2	DMS	K	411	4/4	0.97	0.10	0.45	32,33,33,34	0
2	DMS	K	423	4/4	0.96	0.16	0.43	62,62,63,63	0
2	DMS	K	413	4/4	0.96	0.10	0.39	40,42,42,43	0
2	DMS	L	423	4/4	0.93	0.15	0.35	72,73,73,73	0
4	K	K	346	1/1	0.91	0.16	0.33	40,40,40,40	1
2	DMS	E	342	4/4	0.97	0.10	0.32	47,47,47,48	0
2	DMS	C	411	4/4	0.98	0.11	0.29	37,39,40,40	0
2	DMS	E	423	4/4	0.95	0.13	0.27	69,69,69,70	0
4	K	C	345	1/1	0.89	0.12	0.22	35,35,35,35	1
2	DMS	B	411	4/4	0.96	0.13	0.21	40,40,40,41	0
4	K	L	346	1/1	0.90	0.13	0.10	44,44,44,44	1
4	K	A	346	1/1	0.89	0.11	0.00	39,39,39,39	1
2	DMS	A	413	4/4	0.97	0.09	-0.17	43,45,45,46	0
4	K	H	345	1/1	0.96	0.12	-0.22	47,47,47,47	1
4	K	D	347	1/1	0.94	0.11	-0.36	35,35,35,35	1
4	K	J	345	1/1	0.81	0.15	-0.40	48,48,48,48	1
4	K	F	345	1/1	0.99	0.07	-0.49	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	A	343	1/1	0.98	0.07	-0.97	11,11,11,11	0
4	K	F	348	1/1	0.94	0.07	-1.00	41,41,41,41	1
4	K	B	346	1/1	0.93	0.10	-1.17	42,42,42,42	1
5	NA	B	344	1/1	0.99	0.07	-1.18	25,25,25,25	0
4	K	K	343	1/1	0.99	0.07	-1.23	13,13,13,13	0
6	ZN	I	344	1/1	0.98	0.05	-1.26	31,31,31,31	0
4	K	G	347	1/1	0.87	0.08	-1.28	47,47,47,47	1
4	K	B	343	1/1	1.00	0.06	-1.33	19,19,19,19	0
6	ZN	G	346	1/1	0.98	0.05	-1.39	29,29,29,29	0
4	K	E	346	1/1	0.93	0.07	-1.39	45,45,45,45	1
6	ZN	D	346	1/1	1.00	0.08	-1.40	22,22,22,22	0
6	ZN	K	345	1/1	0.98	0.03	-1.47	31,31,31,31	0
6	ZN	C	344	1/1	1.00	0.07	-1.69	22,22,22,22	0
5	NA	F	346	1/1	0.99	0.07	-1.69	17,17,17,17	0
5	NA	H	343	1/1	0.99	0.06	-1.73	20,20,20,20	0
5	NA	I	343	1/1	0.97	0.06	-1.76	20,20,20,20	0
4	K	G	344	1/1	1.00	0.07	-1.77	16,16,16,16	0
2	DMS	L	413	4/4	0.99	0.07	-1.87	42,42,42,43	0
4	K	J	342	1/1	1.00	0.06	-1.89	18,18,18,18	0
5	NA	L	344	1/1	0.99	0.07	-1.90	20,20,20,20	0
4	K	C	342	1/1	0.99	0.05	-1.92	15,15,15,15	0
6	ZN	J	344	1/1	0.98	0.04	-1.96	30,30,30,30	0
5	NA	K	344	1/1	0.97	0.06	-2.02	17,17,17,17	0
5	NA	E	344	1/1	0.98	0.05	-2.03	20,20,20,20	0
5	NA	G	345	1/1	0.93	0.06	-2.07	20,20,20,20	0
6	ZN	B	345	1/1	0.99	0.04	-2.11	29,29,29,29	0
4	K	H	342	1/1	0.99	0.05	-2.15	15,15,15,15	0
4	K	E	343	1/1	1.00	0.07	-2.50	16,16,16,16	0
4	K	D	344	1/1	0.99	0.06	-2.62	16,16,16,16	0
4	K	I	342	1/1	0.99	0.06	-2.74	16,16,16,16	0
6	ZN	L	345	1/1	0.99	0.04	-2.77	21,21,21,21	0
5	NA	C	343	1/1	1.00	0.05	-2.87	17,17,17,17	0
6	ZN	H	344	1/1	0.99	0.03	-3.35	21,21,21,21	0
5	NA	D	345	1/1	0.97	0.06	-3.37	20,20,20,20	0
4	K	L	343	1/1	0.99	0.04	-3.41	15,15,15,15	0
6	ZN	A	345	1/1	1.00	0.05	-4.44	21,21,21,21	0
5	NA	J	343	1/1	0.99	0.04	-4.44	13,13,13,13	0
6	ZN	F	347	1/1	1.00	0.03	-7.05	21,21,21,21	0
5	NA	A	344	1/1	0.97	0.03	-8.23	13,13,13,13	0
6	ZN	E	345	1/1	0.99	0.04	-9.61	26,26,26,26	0

## 6.5 Other polymers

There are no such residues in this entry.