



# wwPDB X-ray Structure Validation Summary Report

Jul 23, 2014 – 11:08 AM EDT

PDB ID : 4V7N  
Title : Glycocyamine kinase, beta-beta homodimer from marine worm *Namalycastis* sp., with transition state analog Mg(II)-ADP-NO<sub>3</sub>-glycocyamine.  
Authors : Lim, K.; Pullalarevu, S.; Herzberg, O.  
Deposited on : 2009-12-15  
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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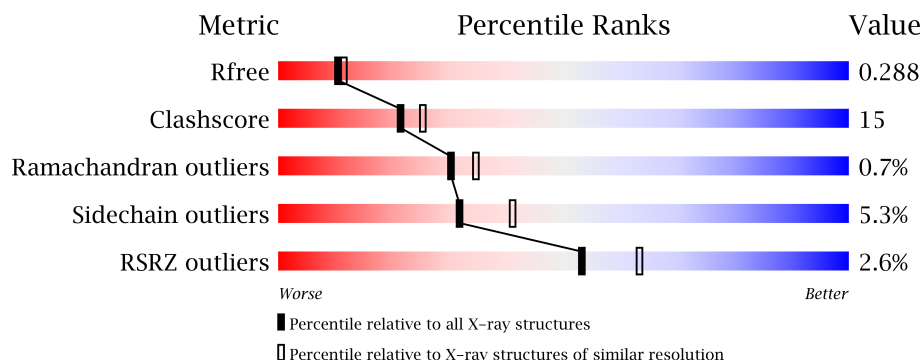
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23489
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	390	
1	AB	390	
1	AC	390	
1	AD	390	
1	AE	390	
1	AF	390	
1	AG	390	
1	AH	390	
1	AI	390	
1	AJ	390	
1	AK	390	
1	AL	390	
1	AM	390	
1	AN	390	

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Mol	Chain	Length	Quality of chain
1	AO	390	
1	AP	390	
1	AQ	390	
1	AR	390	
1	BA	390	
1	BB	390	
1	BC	390	
1	BD	390	
1	BE	390	
1	BF	390	
1	BG	390	
1	BH	390	
1	BI	390	
1	BJ	390	
1	BK	390	
1	BL	390	
1	BM	390	
1	BN	390	
1	BO	390	
1	BP	390	
1	BQ	390	
1	BR	390	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NMG	AE	401	-	X
2	NMG	AK	401	-	X
2	NMG	AN	401	-	X
2	NMG	AP	401	-	X
2	NMG	AQ	401	-	X
2	NMG	BB	401	-	X
2	NMG	BD	401	-	X
2	NMG	BE	401	-	X
2	NMG	BM	401	-	X
2	NMG	BN	401	-	X
2	NMG	BQ	401	-	X
4	MG	AA	503	-	X
4	MG	AB	403	-	X
4	MG	AC	403	-	X
4	MG	AD	403	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	MG	AE	403	-	X
4	MG	AF	403	-	X
4	MG	AG	403	-	X
4	MG	AI	403	-	X
4	MG	AK	403	-	X
4	MG	AM	403	-	X
4	MG	AP	403	-	X
4	MG	AQ	403	-	X
4	MG	AR	403	-	X
4	MG	BF	403	-	X
4	MG	BG	403	-	X
4	MG	BH	403	-	X
4	MG	BI	403	-	X
4	MG	BJ	403	-	X
4	MG	BK	403	-	X
4	MG	BL	403	-	X
4	MG	BM	403	-	X
4	MG	BN	403	-	X
4	MG	BO	403	-	X
4	MG	BP	403	-	X
4	MG	BQ	403	-	X
4	MG	BR	403	-	X
5	NO3	AA	504	X	-
5	NO3	AB	404	X	-
5	NO3	AC	404	X	X
5	NO3	AD	404	X	-
5	NO3	AE	404	X	-
5	NO3	AF	404	X	X
5	NO3	AG	404	X	-
5	NO3	AH	404	X	X
5	NO3	AI	404	X	X
5	NO3	AJ	404	X	-
5	NO3	AK	404	X	X
5	NO3	AL	404	X	X
5	NO3	AM	404	X	X
5	NO3	AN	404	X	X
5	NO3	AO	404	X	X
5	NO3	AP	404	X	X
5	NO3	AQ	404	X	X
5	NO3	AR	404	X	X
5	NO3	BA	504	X	X
5	NO3	BB	404	X	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	NO3	BC	404	X	X
5	NO3	BD	404	X	X
5	NO3	BE	404	X	-
5	NO3	BF	404	X	X
5	NO3	BG	404	X	X
5	NO3	BH	404	X	-
5	NO3	BI	404	X	-
5	NO3	BJ	404	X	-
5	NO3	BK	404	X	-
5	NO3	BL	404	X	X
5	NO3	BM	404	X	X
5	NO3	BN	404	X	-
5	NO3	BO	404	X	X
5	NO3	BP	404	X	-
5	NO3	BQ	404	X	-
5	NO3	BR	404	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 113311 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glycocyamine kinase beta chain.

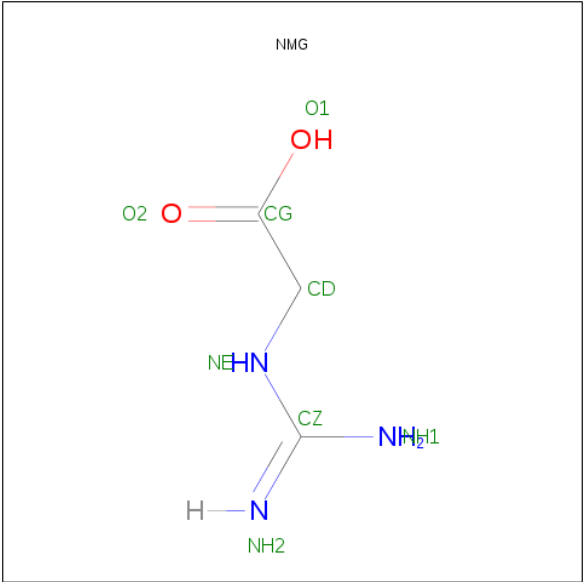
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	AB	387	Total	C	N	O	S	0	0	0
			3074	1939	543	571	21			
1	AC	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AD	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	AE	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AF	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	AG	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AH	384	Total	C	N	O	S	0	0	0
			3052	1925	539	567	21			
1	AI	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	AJ	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	AK	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AL	384	Total	C	N	O	S	0	0	0
			3052	1925	539	567	21			
1	AM	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	AN	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	AO	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	AP	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	AR	379	Total	C	N	O	S	0	0	0
			3005	1892	533	559	21			
1	BA	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BB	388	Total	C	N	O	S	0	0	0
			3080	1942	544	573	21			
1	BC	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BD	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	BE	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BF	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	BG	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BH	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	BI	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BJ	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	BK	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BL	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			
1	BM	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BN	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	BO	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	BP	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	BQ	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	BR	381	Total	C	N	O	S	0	0	0
			3021	1903	536	561	21			

- Molecule 2 is GUANIDINO ACETATE (three-letter code: NMG) (formula: C<sub>3</sub>H<sub>7</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AA	1	Total	C	N	O	0	0
			8	3	3	2		
2	AB	1	Total	C	N	O	0	0
			8	3	3	2		
2	AC	1	Total	C	N	O	0	0
			8	3	3	2		
2	AD	1	Total	C	N	O	0	0
			8	3	3	2		
2	AE	1	Total	C	N	O	0	0
			8	3	3	2		
2	AF	1	Total	C	N	O	0	0
			8	3	3	2		
2	AG	1	Total	C	N	O	0	0
			8	3	3	2		
2	AH	1	Total	C	N	O	0	0
			8	3	3	2		
2	AI	1	Total	C	N	O	0	0
			8	3	3	2		
2	AJ	1	Total	C	N	O	0	0
			8	3	3	2		
2	AK	1	Total	C	N	O	0	0
			8	3	3	2		
2	AL	1	Total	C	N	O	0	0
			8	3	3	2		
2	AM	1	Total	C	N	O	0	0
			8	3	3	2		
2	AN	1	Total	C	N	O	0	0
			8	3	3	2		

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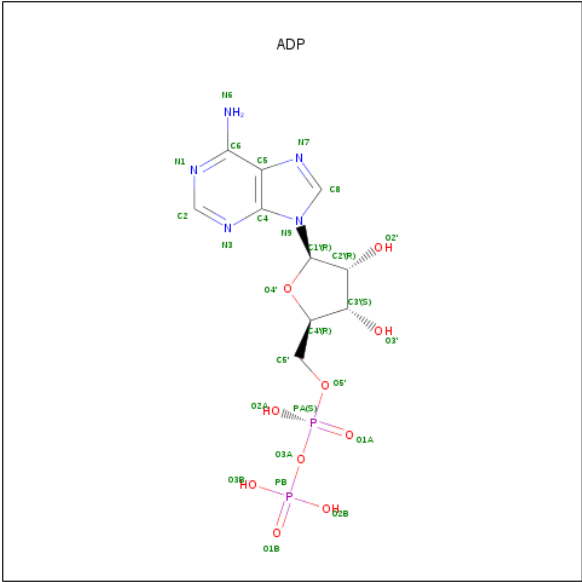
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AO	1	Total	C	N	O	0	0
			8	3	3	2		
2	AP	1	Total	C	N	O	0	0
			8	3	3	2		
2	AQ	1	Total	C	N	O	0	0
			8	3	3	2		
2	AR	1	Total	C	N	O	0	0
			8	3	3	2		
2	BA	1	Total	C	N	O	0	0
			8	3	3	2		
2	BB	1	Total	C	N	O	0	0
			8	3	3	2		
2	BC	1	Total	C	N	O	0	0
			8	3	3	2		
2	BD	1	Total	C	N	O	0	0
			8	3	3	2		
2	BE	1	Total	C	N	O	0	0
			8	3	3	2		
2	BF	1	Total	C	N	O	0	0
			8	3	3	2		
2	BG	1	Total	C	N	O	0	0
			8	3	3	2		
2	BH	1	Total	C	N	O	0	0
			8	3	3	2		
2	BI	1	Total	C	N	O	0	0
			8	3	3	2		
2	BJ	1	Total	C	N	O	0	0
			8	3	3	2		
2	BK	1	Total	C	N	O	0	0
			8	3	3	2		
2	BL	1	Total	C	N	O	0	0
			8	3	3	2		
2	BM	1	Total	C	N	O	0	0
			8	3	3	2		
2	BN	1	Total	C	N	O	0	0
			8	3	3	2		
2	BO	1	Total	C	N	O	0	0
			8	3	3	2		
2	BP	1	Total	C	N	O	0	0
			8	3	3	2		
2	BQ	1	Total	C	N	O	0	0
			8	3	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	BR	1	Total	C	N	O	0	0
			8	3	3	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AK	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	AL	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	AM	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	AN	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	AO	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	AP	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	AQ	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	AR	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BA	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BB	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BC	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BD	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BE	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BF	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BG	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BH	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BI	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BJ	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BK	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BL	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	BM	1	Total 27	C 10	N 5	O 10	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	BN	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BO	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BP	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BQ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	BR	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AP	1	Total	Mg	0	0
			1	1		
4	BA	1	Total	Mg	0	0
			1	1		
4	AK	1	Total	Mg	0	0
			1	1		
4	AB	1	Total	Mg	0	0
			1	1		
4	BL	1	Total	Mg	0	0
			1	1		
4	BE	1	Total	Mg	0	0
			1	1		
4	AN	1	Total	Mg	0	0
			1	1		
4	BP	1	Total	Mg	0	0
			1	1		
4	BI	1	Total	Mg	0	0
			1	1		
4	BB	1	Total	Mg	0	0
			1	1		
4	AJ	1	Total	Mg	0	0
			1	1		
4	AE	1	Total	Mg	0	0
			1	1		
4	BM	1	Total	Mg	0	0
			1	1		
4	BF	1	Total	Mg	0	0
			1	1		

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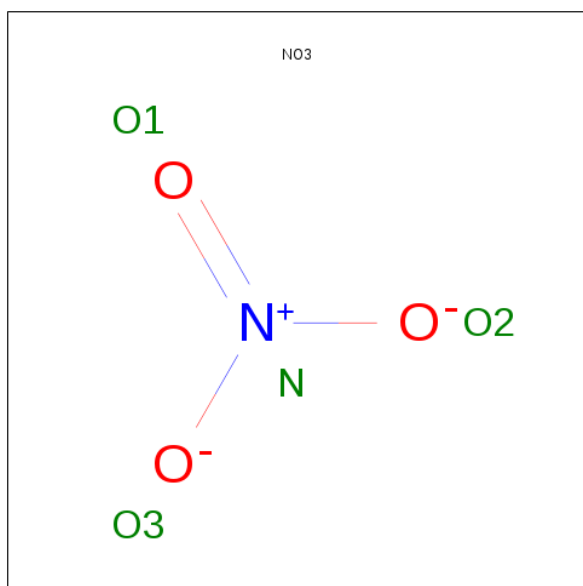
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AA	1	Total 1	Mg 1	0	0
4	BQ	1	Total 1	Mg 1	0	0
4	BJ	1	Total 1	Mg 1	0	0
4	AR	1	Total 1	Mg 1	0	0
4	BC	1	Total 1	Mg 1	0	0
4	AM	1	Total 1	Mg 1	0	0
4	AD	1	Total 1	Mg 1	0	0
4	BN	1	Total 1	Mg 1	0	0
4	BG	1	Total 1	Mg 1	0	0
4	AI	1	Total 1	Mg 1	0	0
4	BR	1	Total 1	Mg 1	0	0
4	BK	1	Total 1	Mg 1	0	0
4	AL	1	Total 1	Mg 1	0	0
4	AG	1	Total 1	Mg 1	0	0
4	BO	1	Total 1	Mg 1	0	0
4	AQ	1	Total 1	Mg 1	0	0
4	AH	1	Total 1	Mg 1	0	0
4	AC	1	Total 1	Mg 1	0	0
4	BD	1	Total 1	Mg 1	0	0
4	AO	1	Total 1	Mg 1	0	0
4	AF	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BH	1	Total	Mg	0	0
			1	1		

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AA	1	Total	N	O	0	0
			4	1	3		
5	AB	1	Total	N	O	0	0
			4	1	3		
5	AC	1	Total	N	O	0	0
			4	1	3		
5	AD	1	Total	N	O	0	0
			4	1	3		
5	AE	1	Total	N	O	0	0
			4	1	3		
5	AF	1	Total	N	O	0	0
			4	1	3		
5	AG	1	Total	N	O	0	0
			4	1	3		
5	AH	1	Total	N	O	0	0
			4	1	3		
5	AI	1	Total	N	O	0	0
			4	1	3		
5	AJ	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AK	1	Total	N	O	0	0
			4	1	3		
5	AL	1	Total	N	O	0	0
			4	1	3		
5	AM	1	Total	N	O	0	0
			4	1	3		
5	AN	1	Total	N	O	0	0
			4	1	3		
5	AO	1	Total	N	O	0	0
			4	1	3		
5	AP	1	Total	N	O	0	0
			4	1	3		
5	AQ	1	Total	N	O	0	0
			4	1	3		
5	AR	1	Total	N	O	0	0
			4	1	3		
5	BA	1	Total	N	O	0	0
			4	1	3		
5	BB	1	Total	N	O	0	0
			4	1	3		
5	BC	1	Total	N	O	0	0
			4	1	3		
5	BD	1	Total	N	O	0	0
			4	1	3		
5	BE	1	Total	N	O	0	0
			4	1	3		
5	BF	1	Total	N	O	0	0
			4	1	3		
5	BG	1	Total	N	O	0	0
			4	1	3		
5	BH	1	Total	N	O	0	0
			4	1	3		
5	BI	1	Total	N	O	0	0
			4	1	3		
5	BJ	1	Total	N	O	0	0
			4	1	3		
5	BK	1	Total	N	O	0	0
			4	1	3		
5	BL	1	Total	N	O	0	0
			4	1	3		
5	BM	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	BN	1	Total	N	O	0	0
			4	1	3		
5	BO	1	Total	N	O	0	0
			4	1	3		
5	BP	1	Total	N	O	0	0
			4	1	3		
5	BQ	1	Total	N	O	0	0
			4	1	3		
5	BR	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AA	106	Total	O	0	0
			106	106		
6	AB	138	Total	O	0	0
			138	138		
6	AC	116	Total	O	0	0
			116	116		
6	AD	149	Total	O	0	0
			149	149		
6	AE	154	Total	O	0	0
			154	154		
6	AF	117	Total	O	0	0
			117	117		
6	AG	131	Total	O	0	0
			131	131		
6	AH	88	Total	O	0	0
			88	88		
6	AI	111	Total	O	0	0
			111	111		
6	AJ	137	Total	O	0	0
			137	137		
6	AK	125	Total	O	0	0
			125	125		
6	AL	156	Total	O	0	0
			156	156		
6	AM	149	Total	O	0	0
			149	149		
6	AN	116	Total	O	0	0
			116	116		

*Continued on next page...*



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AO	113	Total 113	O 113	0	0
6	AP	172	Total 172	O 172	0	0
6	AQ	167	Total 167	O 167	0	0
6	AR	166	Total 166	O 166	0	0
6	BA	99	Total 99	O 99	0	0
6	BB	130	Total 130	O 130	0	0
6	BC	155	Total 155	O 155	0	0
6	BD	110	Total 110	O 110	0	0
6	BE	117	Total 117	O 117	0	0
6	BF	144	Total 144	O 144	0	0
6	BG	131	Total 131	O 131	0	0
6	BH	145	Total 145	O 145	0	0
6	BI	118	Total 118	O 118	0	0
6	BJ	145	Total 145	O 145	0	0
6	BK	127	Total 127	O 127	0	0
6	BL	90	Total 90	O 90	0	0
6	BM	141	Total 141	O 141	0	0
6	BN	116	Total 116	O 116	0	0
6	BO	173	Total 173	O 173	0	0
6	BP	151	Total 151	O 151	0	0
6	BQ	105	Total 105	O 105	0	0

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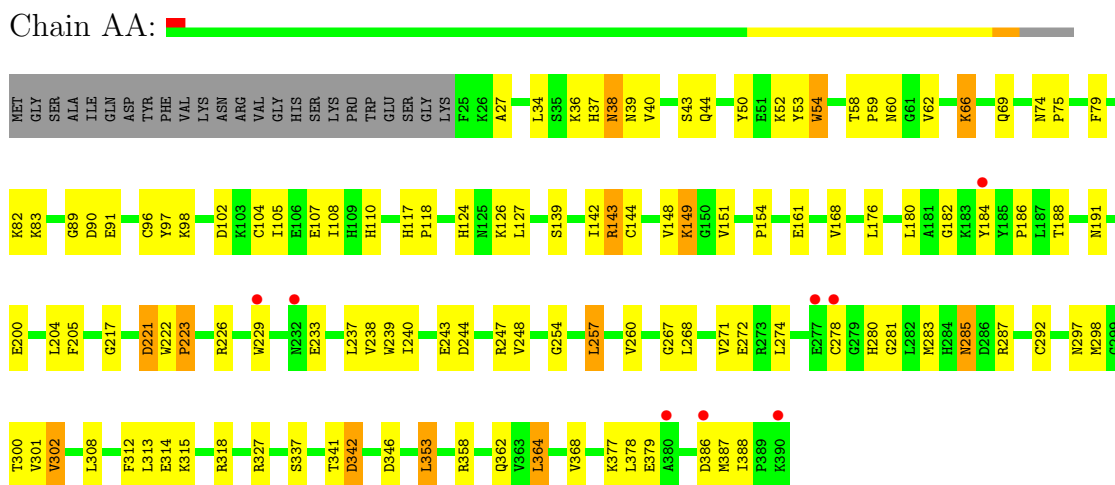
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	BR	166	Total 166	O 166	0	0

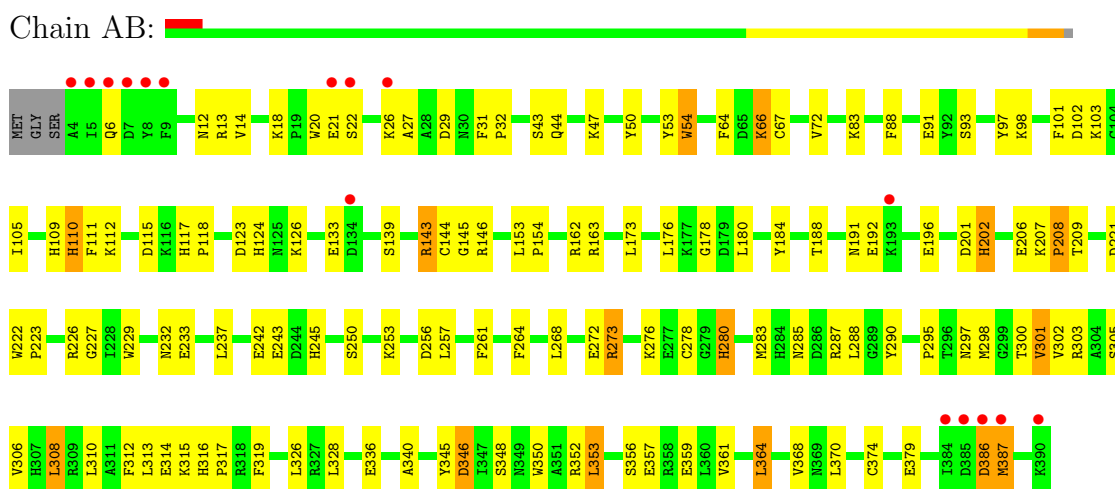
### 3 Residue-property plots

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 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.

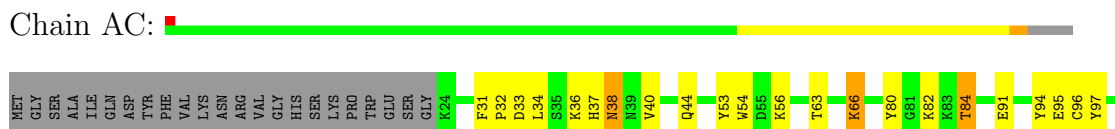
- Molecule 1: Glycocyamine kinase beta chain



- Molecule 1: Glycocyamine kinase beta chain



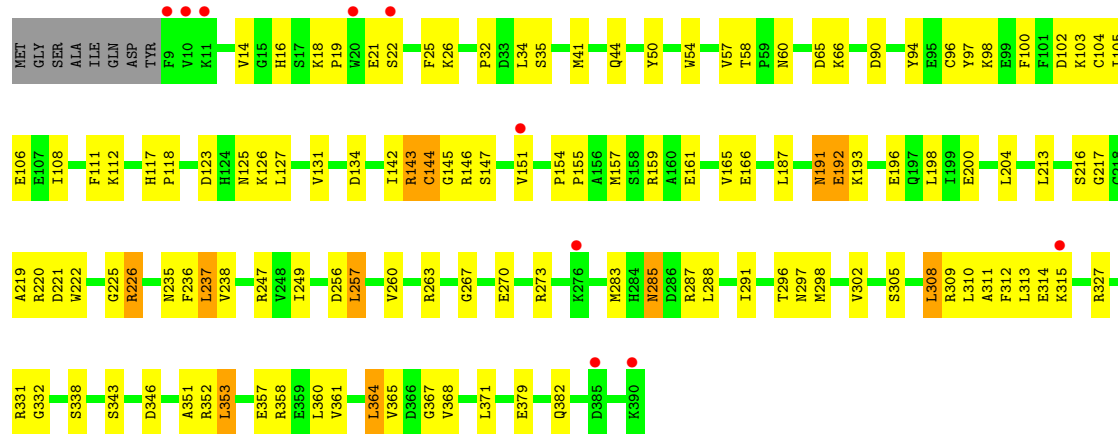
- Molecule 1: Glycocyamine kinase beta chain





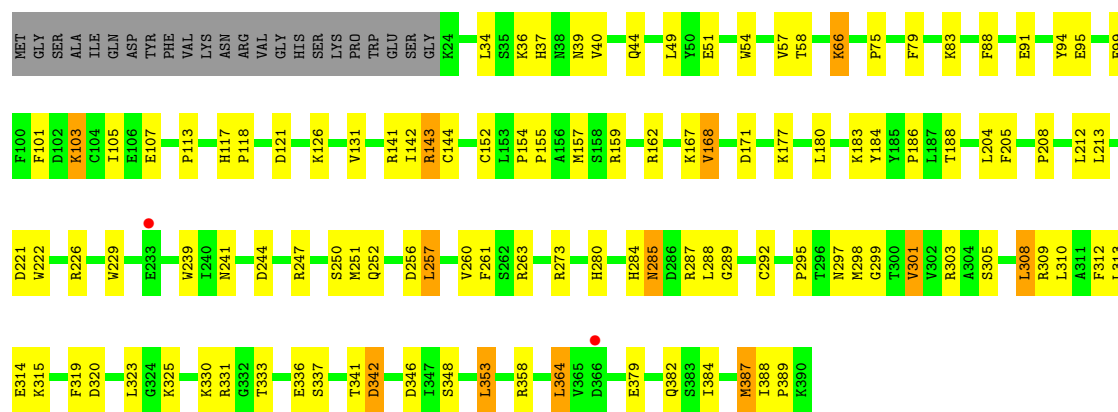
• Molecule 1: Glycocyamine kinase beta chain

Chain AD:



• Molecule 1: Glycocyamine kinase beta chain

Chain AE:

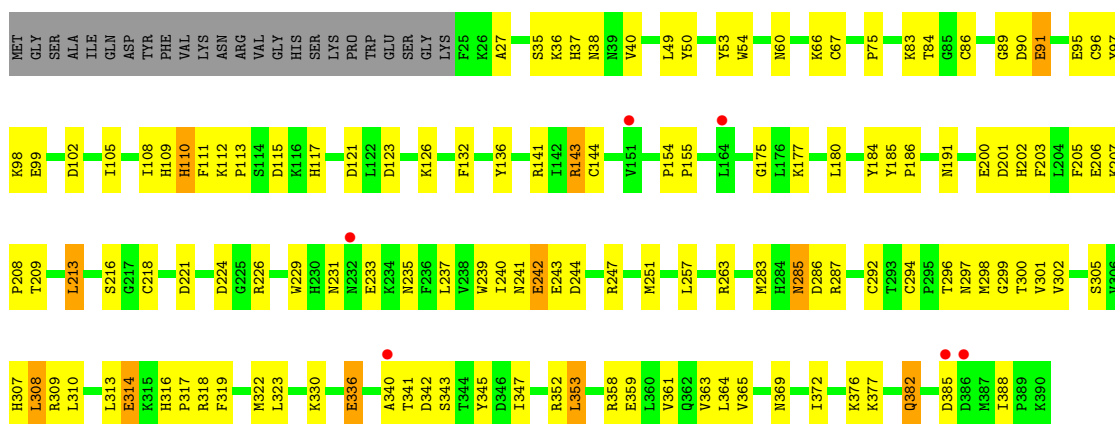


• Molecule 1: Glycocyamine kinase beta chain

Chain AF:

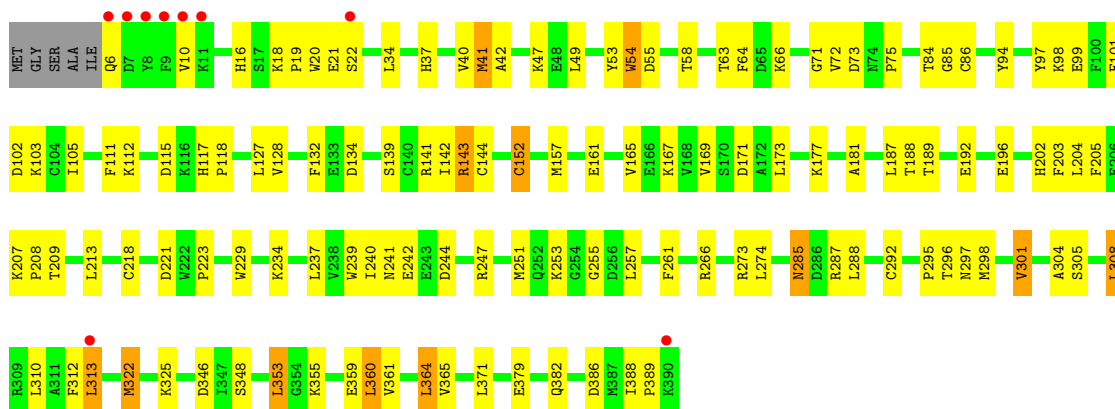






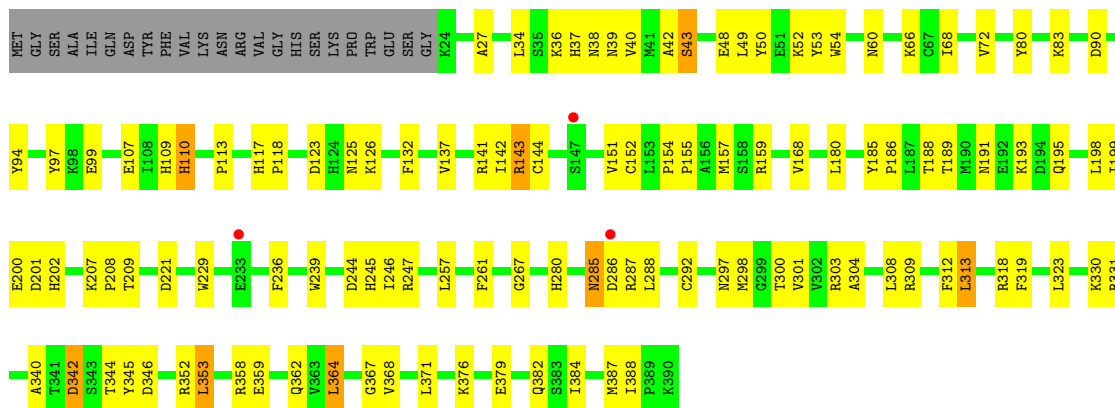
• Molecule 1: Glycocyamine kinase beta chain

Chain AJ:



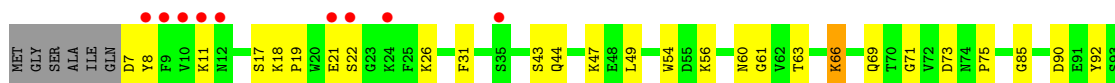
• Molecule 1: Glycocyamine kinase beta chain

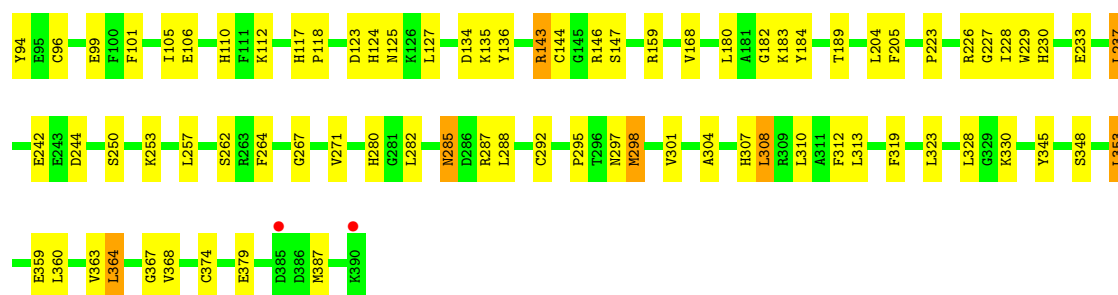
Chain AK:



• Molecule 1: Glycocyamine kinase beta chain

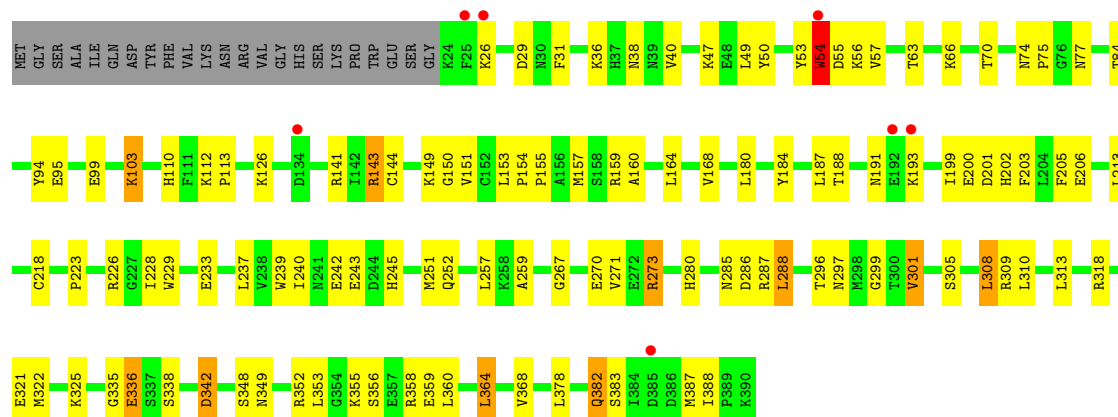
Chain AL:





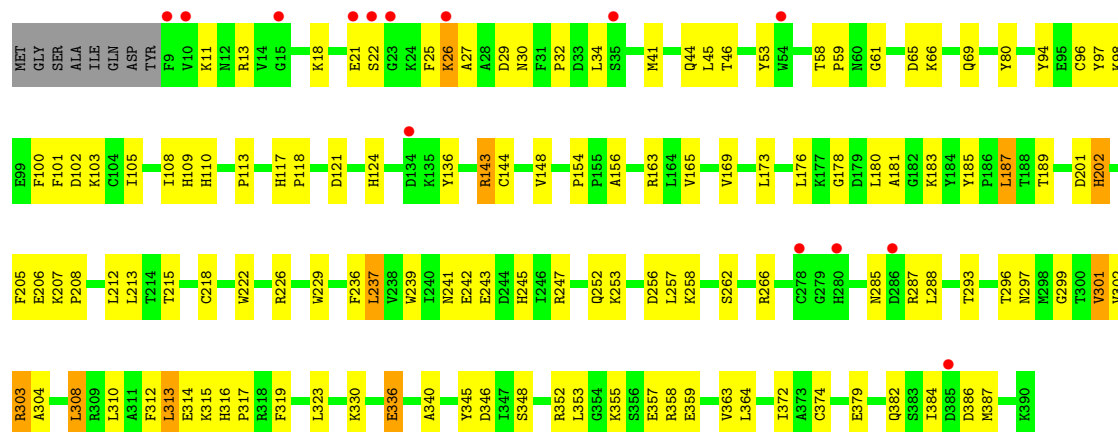
• Molecule 1: Glycocyamine kinase beta chain

Chain AM:



• Molecule 1: Glycocyamine kinase beta chain

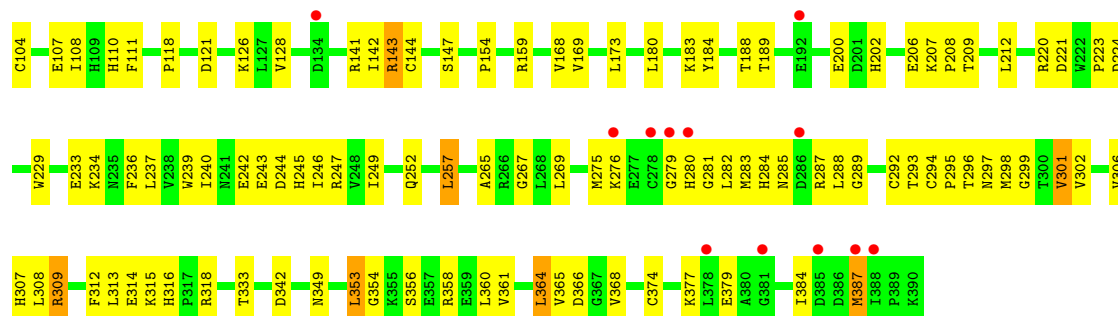
Chain AN:



• Molecule 1: Glycocyamine kinase beta chain

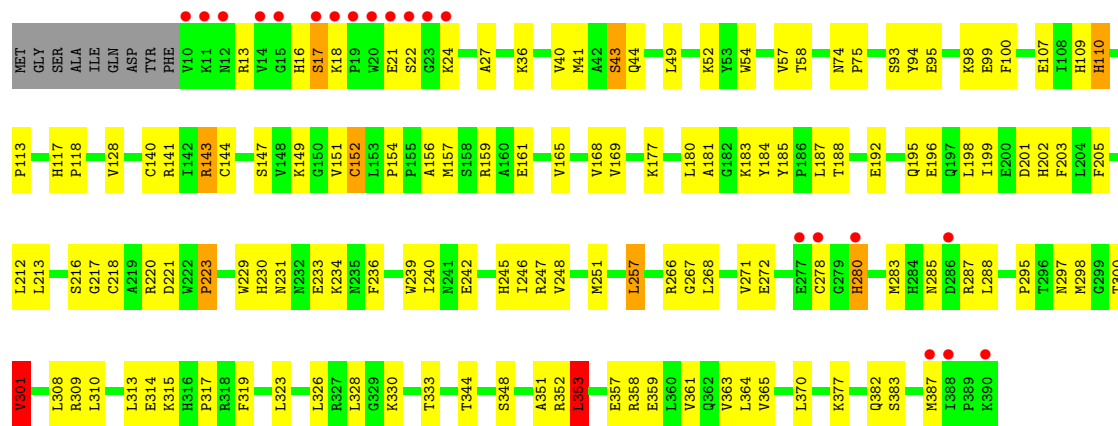
Chain AO:





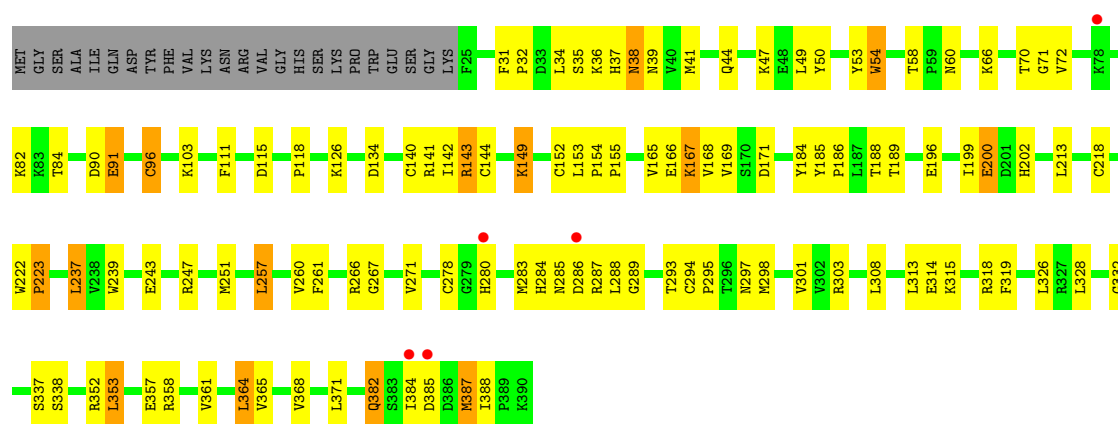
• Molecule 1: Glycocyamine kinase beta chain

Chain AP:



• Molecule 1: Glycocyamine kinase beta chain

Chain AQ:

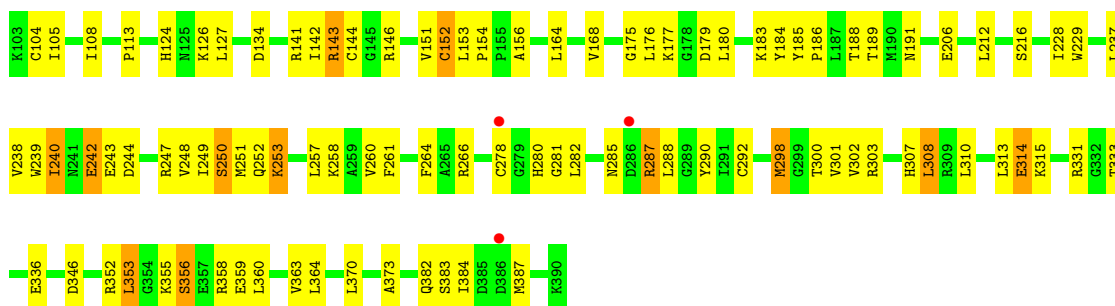


• Molecule 1: Glycocyamine kinase beta chain

Chain AR:

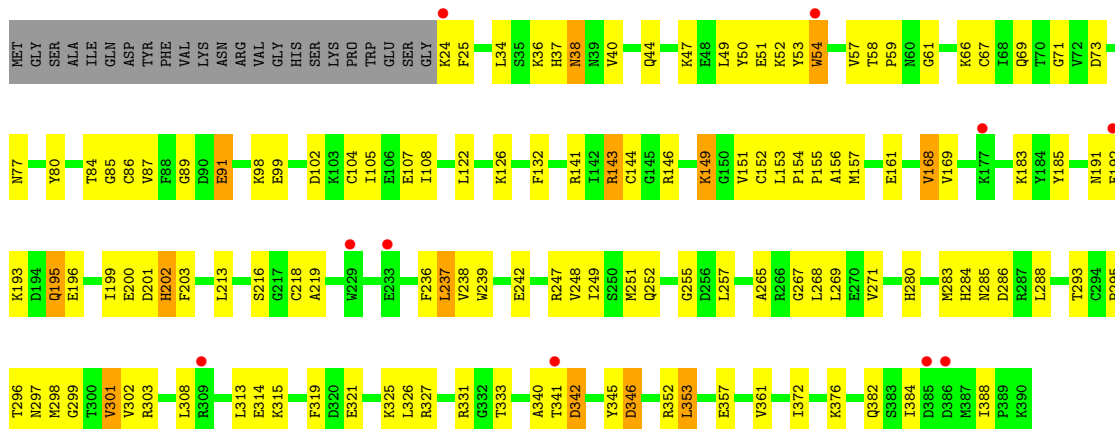






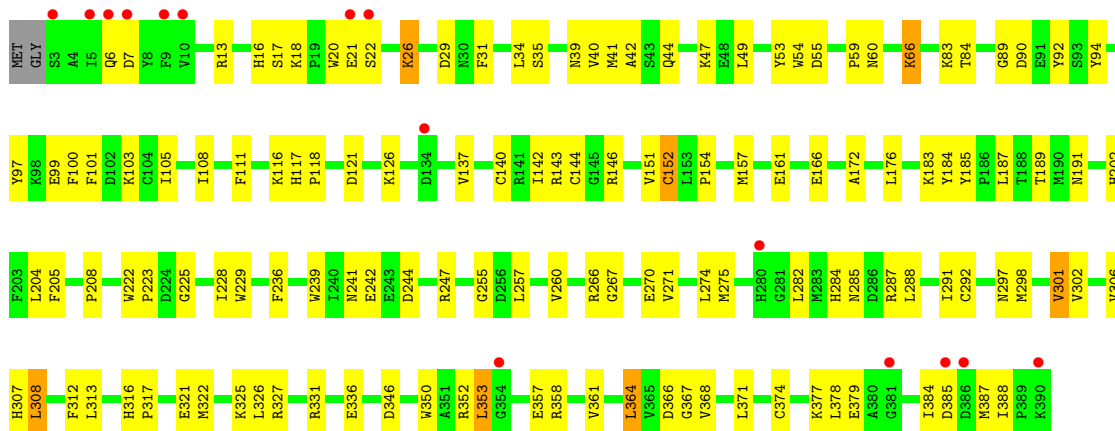
• Molecule 1: Glycocyamine kinase beta chain

Chain BA:



• Molecule 1: Glycocyamine kinase beta chain

Chain BB:

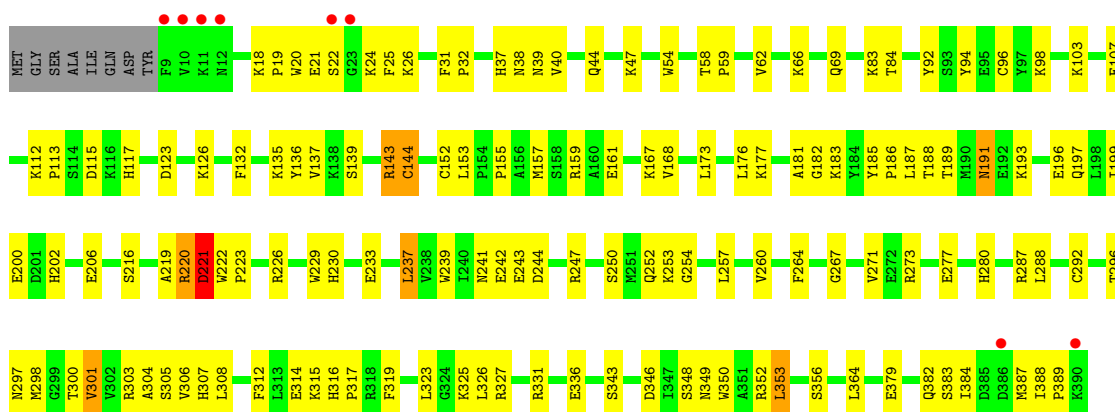


• Molecule 1: Glycocyamine kinase beta chain

Chain BC:

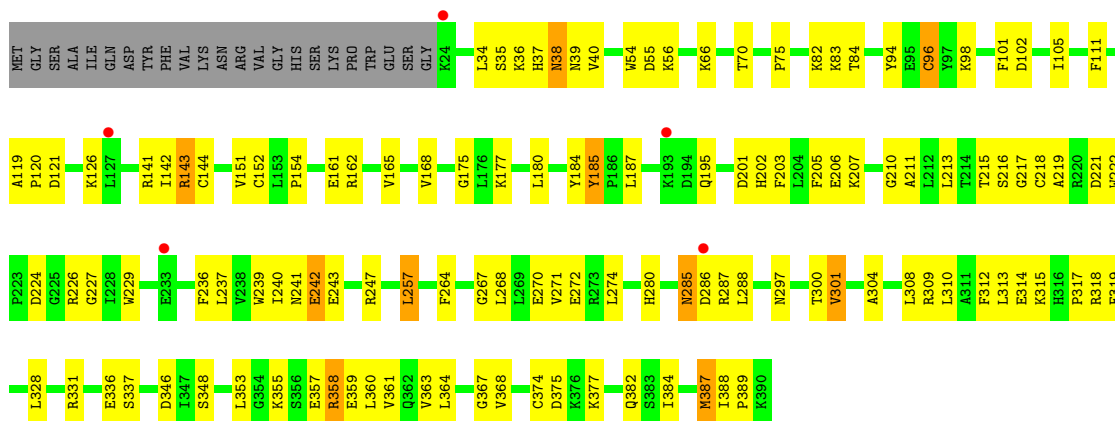






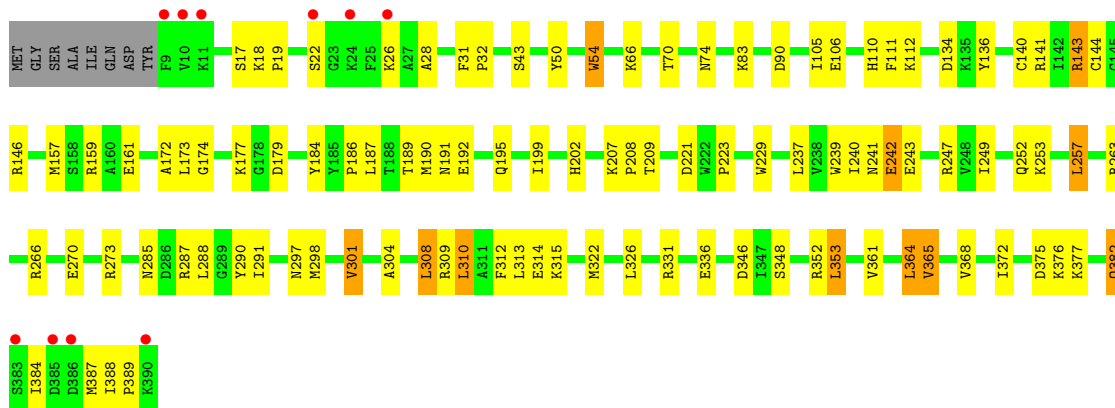
• Molecule 1: Glycocyamine kinase beta chain

Chain BG:



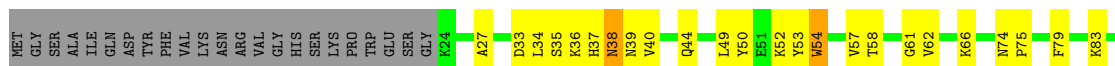
• Molecule 1: Glycocyamine kinase beta chain

Chain BH:

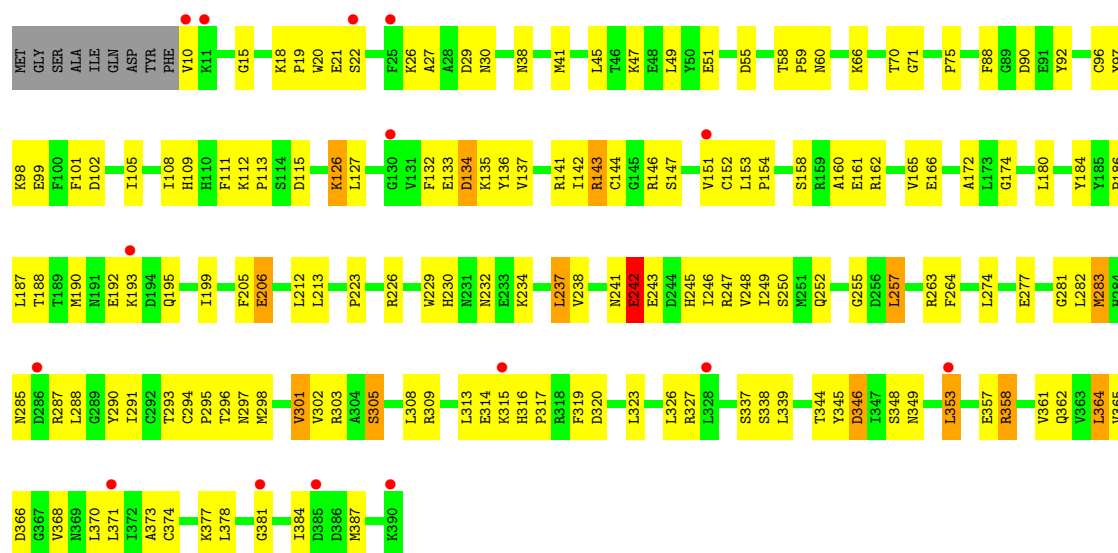


• Molecule 1: Glycocyamine kinase beta chain

Chain BI:

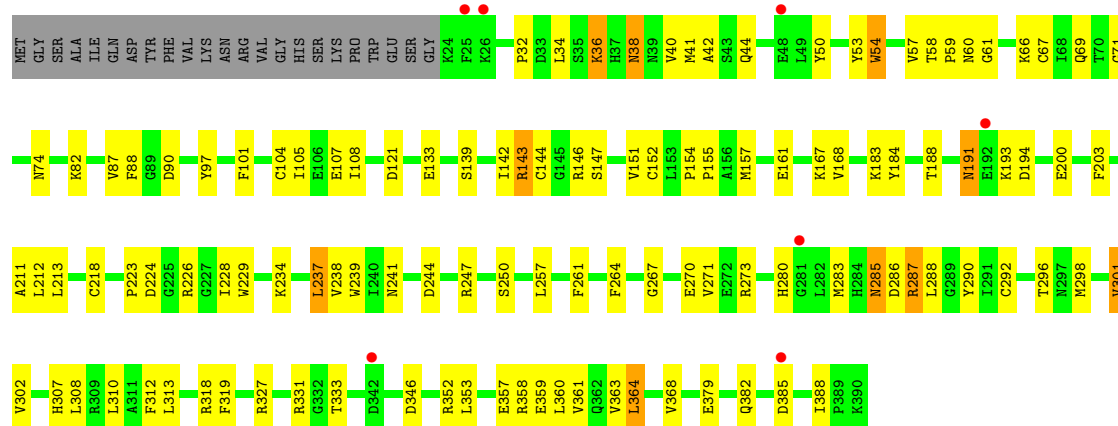






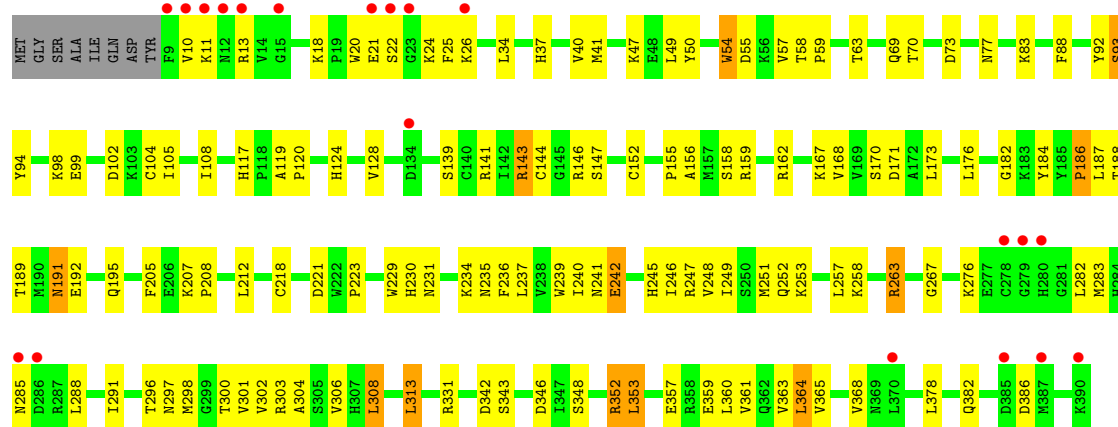
• Molecule 1: Glycocyamine kinase beta chain

Chain BM:



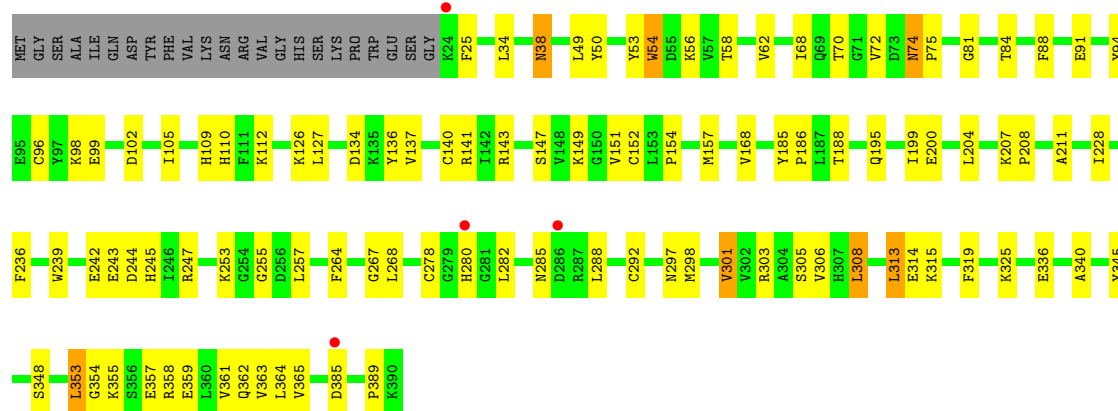
• Molecule 1: Glycocyamine kinase beta chain

Chain BN:



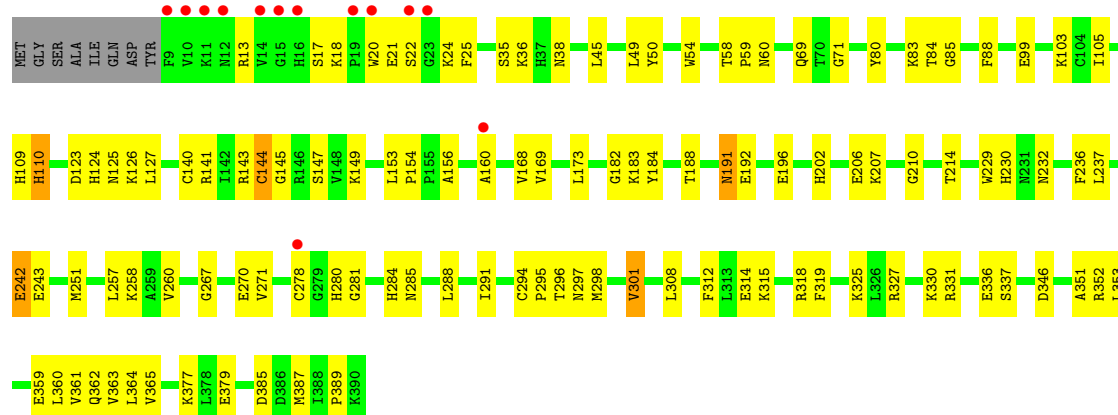
• Molecule 1: Glycocyamine kinase beta chain

Chain BO:



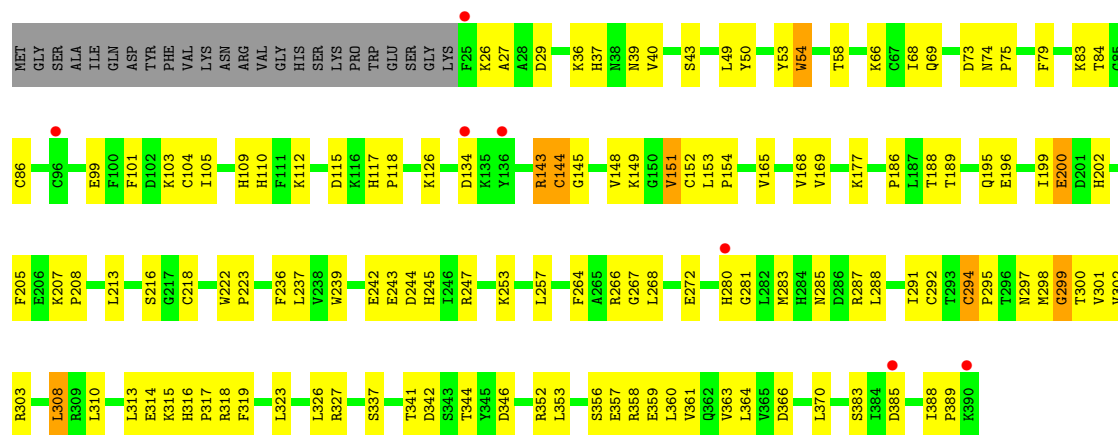
- Molecule 1: Glycocyamine kinase beta chain

Chain BP:



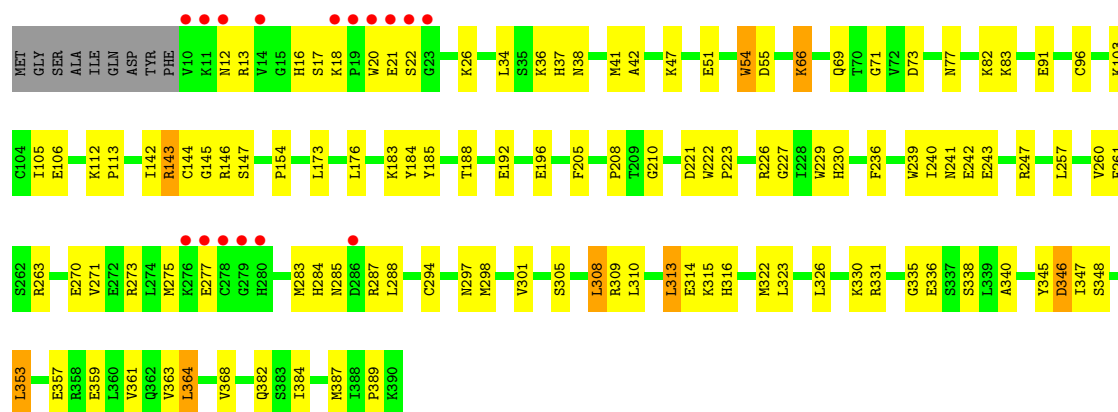
- Molecule 1: Glycocyamine kinase beta chain

Chain BQ:



- Molecule 1: Glycocyamine kinase beta chain

Chain BR:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	243.11Å 114.27Å 259.90Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 33.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 92.1 (33.05-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.29Å)	Xtriage
Refinement program	phenix	Depositor
R, $R_{free}$	0.197 , 0.263 0.230 , 0.288	Depositor DCC
$R_{free}$ test set	29369 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 22.7	EDS
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	38 of 610844 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	113311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6323e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMG, MG, ADP, NO3

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	AA	0.34	0/2963	0.51	0/3986
1	AB	0.37	0/3142	0.55	0/4227
1	AC	0.34	0/2972	0.53	0/3997
1	AD	0.38	0/3099	0.55	0/4168
1	AE	0.35	0/2972	0.52	0/3997
1	AF	0.37	0/3129	0.56	0/4209
1	AG	0.35	0/2972	0.53	1/3997 (0.0%)
1	AH	0.35	0/3120	0.53	0/4197
1	AI	0.34	0/2963	0.52	0/3986
1	AJ	0.37	0/3129	0.53	0/4209
1	AK	0.35	0/2972	0.52	0/3997
1	AL	0.38	0/3120	0.55	0/4197
1	AM	0.35	0/2972	0.54	0/3997
1	AN	0.37	0/3099	0.54	0/4168
1	AO	0.34	0/2963	0.53	0/3986
1	AP	0.39	0/3087	0.55	1/4152 (0.0%)
1	AQ	0.35	0/2963	0.53	0/3986
1	AR	0.38	0/3071	0.55	0/4131
1	BA	0.33	0/2972	0.51	0/3997
1	BB	0.36	0/3148	0.55	1/4235 (0.0%)
1	BC	0.34	0/2972	0.53	0/3997
1	BD	0.36	0/3129	0.54	0/4209
1	BE	0.34	0/2972	0.52	0/3997
1	BF	0.38	0/3099	0.56	0/4168
1	BG	0.35	0/2972	0.52	0/3997
1	BH	0.38	0/3099	0.55	0/4168
1	BI	0.36	0/2972	0.54	0/3997
1	BJ	0.37	0/3129	0.55	0/4209
1	BK	0.35	0/2972	0.54	0/3997
1	BL	0.36	0/3087	0.54	0/4152
1	BM	0.34	0/2972	0.53	0/3997
1	BN	0.35	0/3099	0.54	0/4168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BO	0.36	0/2972	0.54	0/3997
1	BP	0.37	0/3099	0.55	0/4168
1	BQ	0.34	0/2963	0.53	0/3986
1	BR	0.39	0/3087	0.57	1/4152 (0.0%)
All	All	0.36	0/109423	0.54	4/147178 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BB	308	LEU	CA-CB-CG	5.41	127.75	115.30
1	AP	353	LEU	CA-CB-CG	5.32	127.53	115.30
1	AG	364	LEU	CA-CB-CG	5.26	127.40	115.30
1	BR	353	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2901	0	2866	94	0
1	AB	3074	0	3034	107	0
1	AC	2910	0	2879	88	0
1	AD	3032	0	2997	81	0
1	AE	2910	0	2879	83	0
1	AF	3061	0	3018	96	0
1	AG	2910	0	2879	78	0
1	AH	3052	0	3010	141	0
1	AI	2901	0	2866	89	0
1	AJ	3061	0	3018	85	0
1	AK	2910	0	2879	89	0
1	AL	3052	0	3010	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AM	2910	0	2879	82	0
1	AN	3032	0	2997	96	0
1	AO	2901	0	2866	93	0
1	AP	3021	0	2988	108	0
1	AQ	2901	0	2866	85	0
1	AR	3005	0	2966	97	0
1	BA	2910	0	2879	93	0
1	BB	3080	0	3039	98	0
1	BC	2910	0	2879	90	0
1	BD	3061	0	3018	115	0
1	BE	2910	0	2879	102	0
1	BF	3032	0	2997	115	0
1	BG	2910	0	2879	90	0
1	BH	3032	0	2997	81	0
1	BI	2910	0	2879	107	0
1	BJ	3061	0	3018	78	0
1	BK	2910	0	2879	92	0
1	BL	3021	0	2988	119	0
1	BM	2910	0	2879	83	0
1	BN	3032	0	2997	101	0
1	BO	2910	0	2879	71	0
1	BP	3032	0	2997	77	0
1	BQ	2901	0	2866	95	0
1	BR	3021	0	2988	85	0
2	AA	8	0	5	0	0
2	AB	8	0	5	2	0
2	AC	8	0	5	0	0
2	AD	8	0	5	0	0
2	AE	8	0	5	1	0
2	AF	8	0	5	0	0
2	AG	8	0	5	2	0
2	AH	8	0	5	0	0
2	AI	8	0	5	1	0
2	AJ	8	0	5	0	0
2	AK	8	0	5	0	0
2	AL	8	0	5	0	0
2	AM	8	0	5	1	0
2	AN	8	0	5	1	0
2	AO	8	0	5	1	0
2	AP	8	0	5	0	0
2	AQ	8	0	5	0	0
2	AR	8	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BA	8	0	5	0	0
2	BB	8	0	5	1	0
2	BC	8	0	5	0	0
2	BD	8	0	5	1	0
2	BE	8	0	5	0	0
2	BF	8	0	5	0	0
2	BG	8	0	5	0	0
2	BH	8	0	5	1	0
2	BI	8	0	5	0	0
2	BJ	8	0	5	1	0
2	BK	8	0	5	0	0
2	BL	8	0	5	0	0
2	BM	8	0	5	0	0
2	BN	8	0	5	0	0
2	BO	8	0	5	2	0
2	BP	8	0	5	0	0
2	BQ	8	0	5	0	0
2	BR	8	0	5	1	0
3	AA	27	0	12	1	0
3	AB	27	0	12	2	0
3	AC	27	0	12	1	0
3	AD	27	0	12	0	0
3	AE	27	0	12	4	0
3	AF	27	0	12	7	0
3	AG	27	0	12	2	0
3	AH	27	0	12	3	0
3	AI	27	0	12	3	0
3	AJ	27	0	12	3	0
3	AK	27	0	12	5	0
3	AL	27	0	12	1	0
3	AM	27	0	12	2	0
3	AN	27	0	12	1	0
3	AO	27	0	12	4	0
3	AP	27	0	12	5	0
3	AQ	27	0	12	3	0
3	AR	27	0	12	2	0
3	BA	27	0	12	3	0
3	BB	27	0	12	4	0
3	BC	27	0	12	1	0
3	BD	27	0	12	3	0
3	BE	27	0	12	4	0
3	BF	27	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BG	27	0	12	3	0
3	BH	27	0	12	2	0
3	BI	27	0	12	2	0
3	BJ	27	0	12	2	0
3	BK	27	0	12	1	0
3	BL	27	0	12	2	0
3	BM	27	0	12	4	0
3	BN	27	0	12	3	0
3	BO	27	0	12	2	0
3	BP	27	0	12	2	0
3	BQ	27	0	12	3	0
3	BR	27	0	12	3	0
4	AA	1	0	0	0	0
4	AB	1	0	0	0	0
4	AC	1	0	0	0	0
4	AD	1	0	0	0	0
4	AE	1	0	0	0	0
4	AF	1	0	0	0	0
4	AG	1	0	0	0	0
4	AH	1	0	0	0	0
4	AI	1	0	0	0	0
4	AJ	1	0	0	0	0
4	AK	1	0	0	0	0
4	AL	1	0	0	0	0
4	AM	1	0	0	0	0
4	AN	1	0	0	0	0
4	AO	1	0	0	0	0
4	AP	1	0	0	0	0
4	AQ	1	0	0	0	0
4	AR	1	0	0	0	0
4	BA	1	0	0	0	0
4	BB	1	0	0	0	0
4	BC	1	0	0	0	0
4	BD	1	0	0	0	0
4	BE	1	0	0	0	0
4	BF	1	0	0	0	0
4	BG	1	0	0	0	0
4	BH	1	0	0	0	0
4	BI	1	0	0	0	0
4	BJ	1	0	0	0	0
4	BK	1	0	0	0	0
4	BL	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BM	1	0	0	0	0
4	BN	1	0	0	0	0
4	BO	1	0	0	0	0
4	BP	1	0	0	0	0
4	BQ	1	0	0	0	0
4	BR	1	0	0	0	0
5	AA	4	0	0	0	0
5	AB	4	0	0	0	0
5	AC	4	0	0	0	0
5	AD	4	0	0	1	0
5	AE	4	0	0	0	0
5	AF	4	0	0	0	0
5	AG	4	0	0	0	0
5	AH	4	0	0	0	0
5	AI	4	0	0	0	0
5	AJ	4	0	0	0	0
5	AK	4	0	0	0	0
5	AL	4	0	0	0	0
5	AM	4	0	0	0	0
5	AN	4	0	0	0	0
5	AO	4	0	0	1	0
5	AP	4	0	0	0	0
5	AQ	4	0	0	0	0
5	AR	4	0	0	1	0
5	BA	4	0	0	0	0
5	BB	4	0	0	1	0
5	BC	4	0	0	0	0
5	BD	4	0	0	1	0
5	BE	4	0	0	0	0
5	BF	4	0	0	0	0
5	BG	4	0	0	0	0
5	BH	4	0	0	1	0
5	BI	4	0	0	0	0
5	BJ	4	0	0	0	0
5	BK	4	0	0	1	0
5	BL	4	0	0	0	0
5	BM	4	0	0	0	0
5	BN	4	0	0	0	0
5	BO	4	0	0	0	0
5	BP	4	0	0	0	0
5	BQ	4	0	0	0	0
5	BR	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AA	106	0	0	6	0
6	AB	138	0	0	12	0
6	AC	116	0	0	5	0
6	AD	149	0	0	3	0
6	AE	154	0	0	6	0
6	AF	117	0	0	9	0
6	AG	131	0	0	4	0
6	AH	88	0	0	5	0
6	AI	111	0	0	3	0
6	AJ	137	0	0	5	0
6	AK	125	0	0	8	0
6	AL	156	0	0	5	0
6	AM	149	0	0	8	0
6	AN	116	0	0	7	0
6	AO	113	0	0	7	0
6	AP	172	0	0	14	0
6	AQ	167	0	0	10	0
6	AR	166	0	0	5	0
6	BA	99	0	0	2	0
6	BB	130	0	0	2	0
6	BC	155	0	0	4	0
6	BD	110	0	0	12	0
6	BE	117	0	0	7	0
6	BF	144	0	0	6	0
6	BG	131	0	0	5	0
6	BH	145	0	0	13	0
6	BI	118	0	0	9	0
6	BJ	145	0	0	7	0
6	BK	127	0	0	4	0
6	BL	90	0	0	6	0
6	BM	141	0	0	9	0
6	BN	116	0	0	6	0
6	BO	173	0	0	6	0
6	BP	151	0	0	9	0
6	BQ	105	0	0	13	0
6	BR	166	0	0	10	0
All	All	113311	0	106446	3296	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 3296 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AK:126:LYS:HB2	1:AK:358:ARG:HD2	1.38	1.04
1:AD:285:ASN:HB2	1:AD:291:ILE:HD11	1.40	1.02
1:BC:126:LYS:HB2	1:BC:358:ARG:HD2	1.39	1.02
1:BB:285:ASN:HD22	1:BB:288:LEU:H	1.06	1.00
1:AL:285:ASN:HD22	1:AL:288:LEU:H	1.03	0.99

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	AA	364/390 (93%)	335 (92%)	29 (8%)	0	100	100
1	AB	385/390 (99%)	360 (94%)	21 (6%)	4 (1%)	22	23
1	AC	365/390 (94%)	338 (93%)	26 (7%)	1 (0%)	50	60
1	AD	380/390 (97%)	359 (94%)	21 (6%)	0	100	100
1	AE	365/390 (94%)	344 (94%)	19 (5%)	2 (0%)	38	45
1	AF	383/390 (98%)	361 (94%)	20 (5%)	2 (0%)	38	45
1	AG	365/390 (94%)	338 (93%)	23 (6%)	4 (1%)	21	21
1	AH	382/390 (98%)	337 (88%)	41 (11%)	4 (1%)	22	23
1	AI	364/390 (93%)	340 (93%)	21 (6%)	3 (1%)	27	30
1	AJ	383/390 (98%)	352 (92%)	27 (7%)	4 (1%)	22	23
1	AK	365/390 (94%)	347 (95%)	17 (5%)	1 (0%)	50	60
1	AL	382/390 (98%)	362 (95%)	20 (5%)	0	100	100
1	AM	365/390 (94%)	336 (92%)	24 (7%)	5 (1%)	16	15
1	AN	380/390 (97%)	351 (92%)	26 (7%)	3 (1%)	27	30
1	AO	364/390 (93%)	342 (94%)	18 (5%)	4 (1%)	21	21
1	AP	379/390 (97%)	355 (94%)	21 (6%)	3 (1%)	27	30
1	AQ	364/390 (93%)	342 (94%)	21 (6%)	1 (0%)	50	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AR	377/390 (97%)	351 (93%)	22 (6%)	4 (1%)	21	21
1	BA	365/390 (94%)	337 (92%)	23 (6%)	5 (1%)	16	15
1	BB	386/390 (99%)	358 (93%)	24 (6%)	4 (1%)	22	23
1	BC	365/390 (94%)	341 (93%)	23 (6%)	1 (0%)	50	60
1	BD	383/390 (98%)	351 (92%)	29 (8%)	3 (1%)	27	30
1	BE	365/390 (94%)	337 (92%)	25 (7%)	3 (1%)	27	30
1	BF	380/390 (97%)	344 (90%)	33 (9%)	3 (1%)	27	30
1	BG	365/390 (94%)	334 (92%)	29 (8%)	2 (0%)	38	45
1	BH	380/390 (97%)	353 (93%)	23 (6%)	4 (1%)	21	21
1	BI	365/390 (94%)	342 (94%)	22 (6%)	1 (0%)	50	60
1	BJ	383/390 (98%)	355 (93%)	26 (7%)	2 (0%)	38	45
1	BK	365/390 (94%)	341 (93%)	23 (6%)	1 (0%)	50	60
1	BL	379/390 (97%)	331 (87%)	40 (11%)	8 (2%)	11	8
1	BM	365/390 (94%)	345 (94%)	19 (5%)	1 (0%)	50	60
1	BN	380/390 (97%)	349 (92%)	26 (7%)	5 (1%)	18	17
1	BO	365/390 (94%)	344 (94%)	19 (5%)	2 (0%)	38	45
1	BP	380/390 (97%)	348 (92%)	29 (8%)	3 (1%)	27	30
1	BQ	364/390 (93%)	342 (94%)	20 (6%)	2 (0%)	38	45
1	BR	379/390 (97%)	353 (93%)	24 (6%)	2 (0%)	38	45
All	All	13426/14040 (96%)	12455 (93%)	874 (6%)	97 (1%)	30	34

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AH	168	VAL
1	AM	54	TRP
1	AM	336	GLU
1	BG	242	GLU
1	BH	242	GLU

### 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	AA	315/335 (94%)	294 (93%)	21 (7%)	23	29
1	AB	333/335 (99%)	311 (93%)	22 (7%)	24	29
1	AC	316/335 (94%)	297 (94%)	19 (6%)	27	35
1	AD	329/335 (98%)	311 (94%)	18 (6%)	30	39
1	AE	316/335 (94%)	300 (95%)	16 (5%)	33	43
1	AF	332/335 (99%)	314 (95%)	18 (5%)	31	40
1	AG	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	AH	331/335 (99%)	312 (94%)	19 (6%)	29	37
1	AI	315/335 (94%)	296 (94%)	19 (6%)	27	35
1	AJ	332/335 (99%)	313 (94%)	19 (6%)	29	37
1	AK	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	AL	331/335 (99%)	315 (95%)	16 (5%)	35	46
1	AM	316/335 (94%)	296 (94%)	20 (6%)	25	32
1	AN	329/335 (98%)	313 (95%)	16 (5%)	35	45
1	AO	315/335 (94%)	300 (95%)	15 (5%)	35	46
1	AP	328/335 (98%)	314 (96%)	14 (4%)	40	52
1	AQ	315/335 (94%)	295 (94%)	20 (6%)	25	32
1	AR	326/335 (97%)	303 (93%)	23 (7%)	21	26
1	BA	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	BB	334/335 (100%)	317 (95%)	17 (5%)	33	43
1	BC	316/335 (94%)	303 (96%)	13 (4%)	41	55
1	BD	332/335 (99%)	313 (94%)	19 (6%)	29	37
1	BE	316/335 (94%)	299 (95%)	17 (5%)	31	40
1	BF	329/335 (98%)	311 (94%)	18 (6%)	30	39
1	BG	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	BH	329/335 (98%)	315 (96%)	14 (4%)	40	52
1	BI	316/335 (94%)	299 (95%)	17 (5%)	31	40
1	BJ	332/335 (99%)	315 (95%)	17 (5%)	33	43
1	BK	316/335 (94%)	299 (95%)	17 (5%)	31	40
1	BL	328/335 (98%)	310 (94%)	18 (6%)	30	39
1	BM	316/335 (94%)	300 (95%)	16 (5%)	33	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BN	329/335 (98%)	310 (94%)	19 (6%)	28	36
1	BO	316/335 (94%)	305 (96%)	11 (4%)	48	63
1	BP	329/335 (98%)	316 (96%)	13 (4%)	42	56
1	BQ	315/335 (94%)	296 (94%)	19 (6%)	27	35
1	BR	328/335 (98%)	311 (95%)	17 (5%)	32	42
All	All	11624/12060 (96%)	11007 (95%)	617 (5%)	32	41

5 of 617 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AP	364	LEU
1	BB	54	TRP
1	BP	110	HIS
1	AQ	143	ARG
1	AR	253	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
1	AO	382	GLN
1	BA	195	GLN
1	BP	280	HIS
1	AP	195	GLN
1	AQ	284	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 144 ligands modelled in this entry, 36 are monoatomic - leaving 108 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	NMG	AA	501	-	7,7,7	0.70	0	8,8,8	2.51	1 (12%)
3	ADP	AA	502	4	29,29,29	1.14	2 (6%)	45,45,45	1.92	6 (13%)
5	NO3	AA	504	4	3,3,3	3.24	3 (100%)	3,3,3	0.15	0
2	NMG	AB	401	-	7,7,7	0.79	0	8,8,8	3.07	2 (25%)
3	ADP	AB	402	4	29,29,29	1.14	2 (6%)	45,45,45	2.01	9 (20%)
5	NO3	AB	404	4	3,3,3	3.13	3 (100%)	3,3,3	0.21	0
2	NMG	AC	401	-	7,7,7	0.73	0	8,8,8	2.28	1 (12%)
3	ADP	AC	402	4	29,29,29	1.22	3 (10%)	45,45,45	1.94	7 (15%)
5	NO3	AC	404	4	3,3,3	3.31	3 (100%)	3,3,3	0.27	0
2	NMG	AD	401	-	7,7,7	0.68	0	8,8,8	2.06	2 (25%)
3	ADP	AD	402	4	29,29,29	1.24	3 (10%)	45,45,45	1.91	6 (13%)
5	NO3	AD	404	4	3,3,3	3.24	3 (100%)	3,3,3	0.18	0
2	NMG	AE	401	-	7,7,7	0.74	0	8,8,8	2.85	2 (25%)
3	ADP	AE	402	4	29,29,29	1.21	3 (10%)	45,45,45	1.96	6 (13%)
5	NO3	AE	404	4	3,3,3	3.33	3 (100%)	3,3,3	0.07	0
2	NMG	AF	401	-	7,7,7	0.98	0	8,8,8	2.53	2 (25%)
3	ADP	AF	402	4	29,29,29	1.19	2 (6%)	45,45,45	2.00	6 (13%)
5	NO3	AF	404	4	3,3,3	3.21	3 (100%)	3,3,3	0.24	0
2	NMG	AG	401	-	7,7,7	0.67	0	8,8,8	1.80	1 (12%)
3	ADP	AG	402	4	29,29,29	1.19	3 (10%)	45,45,45	1.97	10 (22%)
5	NO3	AG	404	4	3,3,3	3.38	3 (100%)	3,3,3	0.22	0
2	NMG	AH	401	-	7,7,7	0.70	0	8,8,8	2.20	1 (12%)
3	ADP	AH	402	4	29,29,29	1.14	2 (6%)	45,45,45	1.92	8 (17%)
5	NO3	AH	404	4	3,3,3	3.22	3 (100%)	3,3,3	0.14	0
2	NMG	AI	401	-	7,7,7	0.74	0	8,8,8	2.44	2 (25%)
3	ADP	AI	402	4	29,29,29	1.28	2 (6%)	45,45,45	1.87	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NO3	AI	404	4	3,3,3	3.36	3 (100%)	3,3,3	0.06	0
2	NMG	AJ	401	-	7,7,7	0.69	0	8,8,8	2.20	2 (25%)
3	ADP	AJ	402	4	29,29,29	1.22	2 (6%)	45,45,45	2.06	8 (17%)
5	NO3	AJ	404	4	3,3,3	3.28	3 (100%)	3,3,3	0.16	0
2	NMG	AK	401	-	7,7,7	0.69	0	8,8,8	1.52	1 (12%)
3	ADP	AK	402	4	29,29,29	1.16	3 (10%)	45,45,45	2.10	9 (20%)
5	NO3	AK	404	4	3,3,3	3.28	3 (100%)	3,3,3	0.19	0
2	NMG	AL	401	-	7,7,7	0.72	0	8,8,8	2.32	1 (12%)
3	ADP	AL	402	4	29,29,29	1.20	3 (10%)	45,45,45	1.86	9 (20%)
5	NO3	AL	404	4	3,3,3	3.26	3 (100%)	3,3,3	0.25	0
2	NMG	AM	401	-	7,7,7	0.84	0	8,8,8	2.15	1 (12%)
3	ADP	AM	402	4	29,29,29	1.23	2 (6%)	45,45,45	2.05	9 (20%)
5	NO3	AM	404	4	3,3,3	3.26	3 (100%)	3,3,3	0.18	0
2	NMG	AN	401	-	7,7,7	0.69	0	8,8,8	2.45	1 (12%)
3	ADP	AN	402	4	29,29,29	1.21	2 (6%)	45,45,45	2.01	7 (15%)
5	NO3	AN	404	4	3,3,3	3.34	3 (100%)	3,3,3	0.30	0
2	NMG	AO	401	-	7,7,7	0.73	0	8,8,8	1.94	1 (12%)
3	ADP	AO	402	4	29,29,29	1.11	2 (6%)	45,45,45	1.97	8 (17%)
5	NO3	AO	404	4	3,3,3	3.18	3 (100%)	3,3,3	0.19	0
2	NMG	AP	401	-	7,7,7	0.69	0	8,8,8	2.16	1 (12%)
3	ADP	AP	402	4	29,29,29	1.09	2 (6%)	45,45,45	2.13	9 (20%)
5	NO3	AP	404	4	3,3,3	3.18	3 (100%)	3,3,3	0.16	0
2	NMG	AQ	401	-	7,7,7	0.74	0	8,8,8	3.43	1 (12%)
3	ADP	AQ	402	4	29,29,29	1.15	2 (6%)	45,45,45	1.94	10 (22%)
5	NO3	AQ	404	4	3,3,3	3.30	3 (100%)	3,3,3	0.27	0
2	NMG	AR	401	-	7,7,7	0.69	0	8,8,8	3.18	1 (12%)
3	ADP	AR	402	4	29,29,29	1.11	2 (6%)	45,45,45	1.93	8 (17%)
5	NO3	AR	404	4	3,3,3	3.35	3 (100%)	3,3,3	0.23	0
2	NMG	BA	501	-	7,7,7	0.71	0	8,8,8	2.42	1 (12%)
3	ADP	BA	502	4	29,29,29	1.11	3 (10%)	45,45,45	1.98	8 (17%)
5	NO3	BA	504	4	3,3,3	3.24	3 (100%)	3,3,3	0.10	0
2	NMG	BB	401	-	7,7,7	0.74	0	8,8,8	3.34	2 (25%)
3	ADP	BB	402	4	29,29,29	1.13	2 (6%)	45,45,45	1.99	6 (13%)
5	NO3	BB	404	4	3,3,3	3.37	3 (100%)	3,3,3	0.13	0
2	NMG	BC	401	-	7,7,7	0.74	0	8,8,8	2.00	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	BC	402	4	29,29,29	1.11	2 (6%)	45,45,45	1.98	9 (20%)
5	NO3	BC	404	4	3,3,3	3.41	3 (100%)	3,3,3	0.27	0
2	NMG	BD	401	-	7,7,7	0.77	0	8,8,8	2.30	1 (12%)
3	ADP	BD	402	4	29,29,29	1.09	2 (6%)	45,45,45	1.99	6 (13%)
5	NO3	BD	404	4	3,3,3	3.22	3 (100%)	3,3,3	0.17	0
2	NMG	BE	401	-	7,7,7	0.73	0	8,8,8	2.25	1 (12%)
3	ADP	BE	402	4	29,29,29	1.22	3 (10%)	45,45,45	2.07	9 (20%)
5	NO3	BE	404	4	3,3,3	3.27	3 (100%)	3,3,3	0.23	0
2	NMG	BF	401	-	7,7,7	0.71	0	8,8,8	2.66	2 (25%)
3	ADP	BF	402	4	29,29,29	1.16	2 (6%)	45,45,45	2.11	11 (24%)
5	NO3	BF	404	4	3,3,3	3.40	3 (100%)	3,3,3	0.20	0
2	NMG	BG	401	-	7,7,7	0.75	0	8,8,8	1.77	2 (25%)
3	ADP	BG	402	4	29,29,29	1.18	3 (10%)	45,45,45	2.06	7 (15%)
5	NO3	BG	404	4	3,3,3	3.18	3 (100%)	3,3,3	0.16	0
2	NMG	BH	401	-	7,7,7	0.80	0	8,8,8	1.99	1 (12%)
3	ADP	BH	402	4	29,29,29	1.30	4 (13%)	45,45,45	1.83	6 (13%)
5	NO3	BH	404	4	3,3,3	3.32	3 (100%)	3,3,3	0.28	0
2	NMG	BI	401	-	7,7,7	0.80	0	8,8,8	2.80	2 (25%)
3	ADP	BI	402	4	29,29,29	1.18	2 (6%)	45,45,45	2.02	8 (17%)
5	NO3	BI	404	4	3,3,3	3.23	3 (100%)	3,3,3	0.09	0
2	NMG	BJ	401	-	7,7,7	0.73	0	8,8,8	2.50	2 (25%)
3	ADP	BJ	402	4	29,29,29	1.30	3 (10%)	45,45,45	1.95	9 (20%)
5	NO3	BJ	404	4	3,3,3	3.20	3 (100%)	3,3,3	0.23	0
2	NMG	BK	401	-	7,7,7	0.74	0	8,8,8	2.33	1 (12%)
3	ADP	BK	402	4	29,29,29	1.34	6 (20%)	45,45,45	1.89	9 (20%)
5	NO3	BK	404	4	3,3,3	3.23	3 (100%)	3,3,3	0.18	0
2	NMG	BL	401	-	7,7,7	0.75	0	8,8,8	2.27	1 (12%)
3	ADP	BL	402	4	29,29,29	1.22	2 (6%)	45,45,45	1.88	8 (17%)
5	NO3	BL	404	4	3,3,3	3.33	3 (100%)	3,3,3	0.10	0
2	NMG	BM	401	-	7,7,7	0.70	0	8,8,8	2.16	1 (12%)
3	ADP	BM	402	4	29,29,29	1.20	2 (6%)	45,45,45	2.02	9 (20%)
5	NO3	BM	404	4	3,3,3	3.25	3 (100%)	3,3,3	0.14	0
2	NMG	BN	401	-	7,7,7	0.75	0	8,8,8	2.09	1 (12%)
3	ADP	BN	402	4	29,29,29	1.20	3 (10%)	45,45,45	1.98	7 (15%)
5	NO3	BN	404	4	3,3,3	3.27	3 (100%)	3,3,3	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NMG	BO	401	-	7,7,7	0.62	0	8,8,8	2.63	2 (25%)
3	ADP	BO	402	4	29,29,29	1.20	2 (6%)	45,45,45	2.13	10 (22%)
5	NO3	BO	404	4	3,3,3	3.29	3 (100%)	3,3,3	0.21	0
2	NMG	BP	401	-	7,7,7	0.75	0	8,8,8	3.07	1 (12%)
3	ADP	BP	402	4	29,29,29	1.14	2 (6%)	45,45,45	2.20	10 (22%)
5	NO3	BP	404	-	3,3,3	3.36	3 (100%)	3,3,3	0.30	0
2	NMG	BQ	401	-	7,7,7	0.79	0	8,8,8	1.75	1 (12%)
3	ADP	BQ	402	4	29,29,29	1.16	2 (6%)	45,45,45	1.93	8 (17%)
5	NO3	BQ	404	4	3,3,3	3.27	3 (100%)	3,3,3	0.14	0
2	NMG	BR	401	-	7,7,7	0.85	0	8,8,8	2.90	1 (12%)
3	ADP	BR	402	4	29,29,29	1.23	4 (13%)	45,45,45	1.98	8 (17%)
5	NO3	BR	404	4	3,3,3	3.37	3 (100%)	3,3,3	0.12	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	NMG	AA	501	-	-	0/5/5/5	0/0/0/0
3	ADP	AA	502	4	-	0/16/32/32	0/3/3/3
5	NO3	AA	504	4	-	0/0/0/0	0/0/0/0
2	NMG	AB	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AB	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AB	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AC	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AC	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AC	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AD	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AD	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AD	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AE	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AE	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AE	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AF	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AF	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AF	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AG	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AG	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AG	404	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMG	AH	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AH	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AH	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AI	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AI	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AI	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AJ	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AJ	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AJ	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AK	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AK	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AK	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AL	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AL	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AL	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AM	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AM	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AM	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AN	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AN	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AN	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AO	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AO	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AO	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AP	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AP	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AP	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AQ	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AQ	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AQ	404	4	-	0/0/0/0	0/0/0/0
2	NMG	AR	401	-	-	0/5/5/5	0/0/0/0
3	ADP	AR	402	4	-	0/16/32/32	0/3/3/3
5	NO3	AR	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BA	501	-	-	0/5/5/5	0/0/0/0
3	ADP	BA	502	4	-	0/16/32/32	0/3/3/3
5	NO3	BA	504	4	-	0/0/0/0	0/0/0/0
2	NMG	BB	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BB	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BB	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BC	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BC	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BC	404	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMG	BD	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BD	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BD	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BE	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BE	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BE	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BF	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BF	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BF	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BG	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BG	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BG	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BH	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BH	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BH	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BI	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BI	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BI	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BJ	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BJ	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BJ	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BK	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BK	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BK	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BL	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BL	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BL	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BM	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BM	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BM	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BN	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BN	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BN	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BO	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BO	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BO	404	4	-	0/0/0/0	0/0/0/0
2	NMG	BP	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BP	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BP	404	-	-	0/0/0/0	0/0/0/0
2	NMG	BQ	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BQ	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BQ	404	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMG	BR	401	-	-	0/5/5/5	0/0/0/0
3	ADP	BR	402	4	-	0/16/32/32	0/3/3/3
5	NO3	BR	404	4	-	0/0/0/0	0/0/0/0

The worst 5 of 199 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AI	404	NO3	O1-N	4.10	1.41	1.24
5	BC	404	NO3	O1-N	4.07	1.41	1.24
5	AE	404	NO3	O1-N	4.06	1.41	1.24
5	BF	404	NO3	O1-N	4.05	1.41	1.24
5	BB	404	NO3	O1-N	4.05	1.41	1.24

The worst 5 of 339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AQ	401	NMG	CD-NE-CZ	9.39	130.02	122.14
2	BB	401	NMG	CD-NE-CZ	8.96	129.66	122.14
2	AR	401	NMG	CD-NE-CZ	8.67	129.42	122.14
2	BP	401	NMG	CD-NE-CZ	8.38	129.17	122.14
2	AB	401	NMG	CD-NE-CZ	8.12	128.96	122.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	AA	366/390 (93%)	0.45	8 (2%) 59 69	18, 30, 47, 54	0
1	AB	387/390 (99%)	0.37	16 (4%) 35 46	15, 25, 46, 57	0
1	AC	367/390 (94%)	0.39	2 (0%) 88 94	15, 29, 45, 54	0
1	AD	382/390 (97%)	0.32	10 (2%) 53 63	14, 25, 41, 58	0
1	AE	367/390 (94%)	0.29	2 (0%) 88 94	17, 25, 41, 55	0
1	AF	385/390 (98%)	0.39	11 (2%) 49 59	16, 27, 46, 59	0
1	AG	367/390 (94%)	0.34	6 (1%) 68 77	18, 27, 43, 54	0
1	AH	384/390 (98%)	0.59	20 (5%) 26 36	18, 30, 47, 61	0
1	AI	366/390 (93%)	0.35	6 (1%) 68 77	17, 28, 42, 51	0
1	AJ	385/390 (98%)	0.35	9 (2%) 57 67	16, 24, 43, 59	0
1	AK	367/390 (94%)	0.30	3 (0%) 83 90	17, 27, 43, 56	0
1	AL	384/390 (98%)	0.28	11 (2%) 49 59	14, 23, 41, 57	0
1	AM	367/390 (94%)	0.35	7 (1%) 64 73	17, 25, 40, 50	0
1	AN	382/390 (97%)	0.44	14 (3%) 39 50	16, 26, 43, 53	0
1	AO	366/390 (93%)	0.52	16 (4%) 33 43	18, 30, 45, 54	0
1	AP	381/390 (97%)	0.41	20 (5%) 26 36	15, 23, 39, 56	0
1	AQ	366/390 (93%)	0.27	5 (1%) 72 80	16, 25, 39, 51	0
1	AR	379/390 (97%)	0.31	11 (2%) 49 59	15, 23, 40, 50	0
1	BA	367/390 (94%)	0.48	10 (2%) 52 62	18, 30, 47, 54	0
1	BB	388/390 (99%)	0.35	15 (3%) 37 48	15, 25, 46, 58	0
1	BC	367/390 (94%)	0.29	4 (1%) 77 85	17, 26, 40, 52	0
1	BD	385/390 (98%)	0.42	12 (3%) 47 56	16, 27, 46, 59	0
1	BE	367/390 (94%)	0.36	9 (2%) 54 65	18, 29, 45, 53	0
1	BF	382/390 (97%)	0.26	8 (2%) 60 70	13, 24, 42, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	BG	367/390 (94%)	0.32	5 (1%) 72 80	16, 27, 42, 54	0
1	BH	382/390 (97%)	0.27	10 (2%) 53 63	15, 23, 41, 55	0
1	BI	367/390 (94%)	0.29	3 (0%) 83 90	17, 26, 41, 51	0
1	BJ	385/390 (98%)	0.32	12 (3%) 47 56	17, 25, 42, 61	0
1	BK	367/390 (94%)	0.32	6 (1%) 68 77	17, 26, 42, 50	0
1	BL	381/390 (97%)	0.59	15 (3%) 37 48	20, 31, 48, 59	0
1	BM	367/390 (94%)	0.36	7 (1%) 64 73	17, 26, 41, 51	0
1	BN	382/390 (97%)	0.51	20 (5%) 26 36	18, 27, 44, 52	0
1	BO	367/390 (94%)	0.26	4 (1%) 77 85	16, 25, 40, 51	0
1	BP	382/390 (97%)	0.36	13 (3%) 43 53	15, 24, 41, 50	0
1	BQ	366/390 (93%)	0.51	7 (1%) 64 73	19, 30, 44, 53	0
1	BR	381/390 (97%)	0.36	16 (4%) 35 45	15, 24, 40, 51	0
All	All	13498/14040 (96%)	0.37	353 (2%) 53 63	13, 26, 44, 61	0

The worst 5 of 353 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BJ	7	ASP	8.9
1	AN	21	GLU	8.4
1	BJ	6	GLN	7.5
1	BR	22	SER	7.4
1	BP	22	SER	7.4

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	BR	403	1/1	0.49	19.26	37,37,37,37	0
4	MG	AQ	403	1/1	0.24	12.00	15,15,15,15	0
4	MG	AE	403	1/1	0.33	11.79	15,15,15,15	0
5	NO3	AK	404	4/4	0.24	11.06	24,25,27,28	0
4	MG	AC	403	1/1	0.21	8.42	16,16,16,16	0
5	NO3	BL	404	4/4	0.33	8.38	25,31,33,33	0
4	MG	BN	403	1/1	0.34	8.00	22,22,22,22	0
5	NO3	AO	404	4/4	0.28	7.66	23,25,28,36	0
4	MG	AK	403	1/1	0.26	7.37	12,12,12,12	0
2	NMG	AP	401	8/8	0.27	7.16	19,22,24,25	0
5	NO3	AN	404	4/4	0.33	7.08	22,24,25,26	0
5	NO3	AC	404	4/4	0.23	6.66	22,24,26,27	0
4	MG	BG	403	1/1	0.29	6.62	20,20,20,20	0
5	NO3	AF	404	4/4	0.30	6.50	21,22,25,26	0
4	MG	BO	403	1/1	0.23	6.46	10,10,10,10	0
4	MG	AP	403	1/1	0.24	6.29	25,25,25,25	0
5	NO3	BF	404	4/4	0.29	6.25	18,21,22,25	0
2	NMG	BD	401	8/8	0.24	6.03	20,23,24,24	0
4	MG	BH	403	1/1	0.33	5.90	19,19,19,19	0
4	MG	BK	403	1/1	0.20	5.73	11,11,11,11	0
4	MG	AM	403	1/1	0.17	5.23	13,13,13,13	0
5	NO3	BG	404	4/4	0.23	4.77	21,22,25,27	0
4	MG	AG	403	1/1	0.20	4.63	18,18,18,18	0
4	MG	AD	403	1/1	0.24	4.54	13,13,13,13	0
2	NMG	AQ	401	8/8	0.20	4.48	16,20,21,25	0
5	NO3	AP	404	4/4	0.25	4.44	20,21,24,27	0
4	MG	BM	403	1/1	0.20	4.32	9,9,9,9	0
5	NO3	AL	404	4/4	0.28	4.26	20,21,22,22	0
5	NO3	AR	404	4/4	0.23	4.22	21,22,27,29	0
4	MG	AR	403	1/1	0.22	4.14	11,11,11,11	0
4	MG	AB	403	1/1	0.24	4.11	11,11,11,11	0
4	MG	BQ	403	1/1	0.21	4.09	12,12,12,12	0
4	MG	AF	403	1/1	0.24	4.06	12,12,12,12	0
2	NMG	AN	401	8/8	0.25	4.02	21,24,31,31	0
5	NO3	AI	404	4/4	0.20	3.88	22,25,28,28	0
5	NO3	BA	504	4/4	0.23	3.70	25,27,28,31	0
4	MG	BL	403	1/1	0.21	3.61	18,18,18,18	0
4	MG	BJ	403	1/1	0.21	3.56	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NO3	BD	404	4/4	0.21	3.55	21,23,23,27	0
2	NMG	BB	401	8/8	0.22	3.55	14,20,22,23	0
2	NMG	AE	401	8/8	0.22	3.49	18,21,23,25	0
5	NO3	AQ	404	4/4	0.21	3.46	18,22,22,22	0
5	NO3	BR	404	4/4	0.21	3.24	14,19,22,22	0
4	MG	BI	403	1/1	0.20	3.04	10,10,10,10	0
4	MG	AA	503	1/1	0.21	2.92	16,16,16,16	0
5	NO3	AM	404	4/4	0.18	2.91	22,25,26,28	0
4	MG	BP	403	1/1	0.20	2.85	8,8,8,8	0
5	NO3	BO	404	4/4	0.18	2.83	23,23,23,28	0
5	NO3	BM	404	4/4	0.19	2.64	21,22,24,24	0
5	NO3	AH	404	4/4	0.21	2.39	21,23,25,26	0
2	NMG	BN	401	8/8	0.22	2.35	21,22,25,26	0
5	NO3	BB	404	4/4	0.18	2.32	20,21,24,24	0
4	MG	BF	403	1/1	0.21	2.29	11,11,11,11	0
2	NMG	BE	401	8/8	0.21	2.26	25,28,29,31	0
2	NMG	BQ	401	8/8	0.23	2.23	25,28,33,33	0
5	NO3	BC	404	4/4	0.20	2.19	16,21,24,24	0
2	NMG	BM	401	8/8	0.22	2.18	22,24,25,26	0
4	MG	AI	403	1/1	0.17	2.16	15,15,15,15	0
2	NMG	AK	401	8/8	0.18	2.11	20,24,25,29	0
2	NMG	AR	401	8/8	0.18	1.92	18,21,24,24	0
4	MG	BB	403	1/1	0.18	1.90	18,18,18,18	0
5	NO3	BQ	404	4/4	0.18	1.87	25,26,26,27	0
2	NMG	AA	501	8/8	0.20	1.76	20,23,25,25	0
2	NMG	AH	401	8/8	0.20	1.50	21,23,30,34	0
2	NMG	BK	401	8/8	0.16	1.50	21,25,26,29	0
5	NO3	AJ	404	4/4	0.20	1.47	18,24,27,27	0
4	MG	BA	503	1/1	0.20	1.47	13,13,13,13	0
4	MG	AO	403	1/1	0.19	1.44	18,18,18,18	0
4	MG	BC	403	1/1	0.19	1.37	11,11,11,11	0
2	NMG	BG	401	8/8	0.19	1.33	20,23,25,25	0
4	MG	BD	403	1/1	0.16	1.25	21,21,21,21	0
2	NMG	BI	401	8/8	0.18	1.21	23,26,27,27	0
4	MG	AJ	403	1/1	0.17	1.18	10,10,10,10	0
2	NMG	AJ	401	8/8	0.17	1.09	19,24,26,30	0
2	NMG	AO	401	8/8	0.19	1.07	22,27,32,32	0
3	ADP	AF	402	27/27	0.17	1.03	21,27,30,35	0
5	NO3	AB	404	4/4	0.17	0.93	16,17,23,23	0
2	NMG	AC	401	8/8	0.18	0.93	22,24,26,27	0
2	NMG	BL	401	8/8	0.19	0.91	28,32,34,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NMG	BC	401	8/8	0.17	0.88	16,22,25,25	0
5	NO3	AE	404	4/4	0.17	0.88	21,23,23,25	0
3	ADP	AO	402	27/27	0.17	0.80	19,24,28,31	0
2	NMG	AG	401	8/8	0.15	0.79	16,21,22,25	0
4	MG	AL	403	1/1	0.17	0.71	22,22,22,22	0
2	NMG	BH	401	8/8	0.16	0.71	18,22,24,24	0
5	NO3	BN	404	4/4	0.18	0.67	23,24,24,26	0
3	ADP	AI	402	27/27	0.16	0.64	18,24,29,33	0
5	NO3	BK	404	4/4	0.15	0.60	21,21,22,24	0
4	MG	AN	403	1/1	0.17	0.52	13,13,13,13	0
5	NO3	BJ	404	4/4	0.16	0.51	22,24,25,29	0
4	MG	AH	403	1/1	0.16	0.49	16,16,16,16	0
3	ADP	AP	402	27/27	0.15	0.47	17,21,26,30	0
3	ADP	AQ	402	27/27	0.15	0.47	14,18,22,23	0
3	ADP	BG	402	27/27	0.15	0.41	21,27,29,30	0
3	ADP	AK	402	27/27	0.14	0.40	17,22,24,26	0
3	ADP	BB	402	27/27	0.15	0.35	18,21,23,26	0
5	NO3	AD	404	4/4	0.15	0.33	24,29,29,30	0
3	ADP	BQ	402	27/27	0.15	0.31	16,22,28,29	0
5	NO3	BI	404	4/4	0.14	0.30	19,20,25,25	0
2	NMG	BO	401	8/8	0.16	0.26	21,26,28,29	0
5	NO3	BH	404	4/4	0.17	0.25	20,21,22,23	0
2	NMG	AL	401	8/8	0.15	0.24	17,19,21,22	0
4	MG	BE	403	1/1	0.16	0.23	14,14,14,14	0
3	ADP	BP	402	27/27	0.15	0.21	14,18,21,21	0
3	ADP	AM	402	27/27	0.14	0.16	17,20,24,25	0
2	NMG	BF	401	8/8	0.15	0.15	16,19,24,24	0
3	ADP	BD	402	27/27	0.15	0.14	19,25,28,31	0
3	ADP	BC	402	27/27	0.15	0.13	13,20,22,24	0
2	NMG	AM	401	8/8	0.14	0.13	17,20,21,24	0
2	NMG	AF	401	8/8	0.15	0.10	17,22,26,27	0
2	NMG	BR	401	8/8	0.13	0.10	15,17,22,23	0
3	ADP	BA	502	27/27	0.16	0.10	21,25,29,32	0
3	ADP	AG	402	27/27	0.14	0.09	17,21,25,27	0
3	ADP	BO	402	27/27	0.15	0.09	12,18,21,25	0
3	ADP	BK	402	27/27	0.14	0.08	12,19,23,25	0
3	ADP	BF	402	27/27	0.15	0.02	13,18,22,24	0
3	ADP	AJ	402	27/27	0.15	0.01	15,18,22,25	0
3	ADP	AA	502	27/27	0.15	0.00	23,28,31,35	0
3	ADP	AH	402	27/27	0.15	-0.02	20,26,30,37	0
3	ADP	AE	402	27/27	0.15	-0.04	18,21,23,28	0
3	ADP	BL	402	27/27	0.15	-0.08	23,29,34,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NMG	AI	401	8/8	0.13	-0.18	18,22,24,27	0
3	ADP	AR	402	27/27	0.13	-0.23	11,19,21,24	0
2	NMG	AD	401	8/8	0.14	-0.27	18,24,26,26	0
3	ADP	BI	402	27/27	0.14	-0.27	16,21,25,27	0
3	ADP	AN	402	27/27	0.14	-0.33	13,20,23,23	0
3	ADP	BE	402	27/27	0.14	-0.35	19,25,29,31	0
3	ADP	AD	402	27/27	0.14	-0.46	16,21,24,27	0
3	ADP	BH	402	27/27	0.13	-0.47	14,17,21,23	0
2	NMG	AB	401	8/8	0.13	-0.50	16,23,28,28	0
3	ADP	BR	402	27/27	0.13	-0.61	13,17,21,23	0
5	NO3	BP	404	4/4	0.13	-0.63	18,20,22,24	0
3	ADP	BJ	402	27/27	0.13	-0.70	12,18,20,21	0
3	ADP	AL	402	27/27	0.13	-0.71	14,18,21,23	0
2	NMG	BP	401	8/8	0.12	-0.80	15,17,20,24	0
3	ADP	AC	402	27/27	0.13	-0.82	24,27,32,33	0
2	NMG	BJ	401	8/8	0.12	-0.84	25,26,28,29	0
2	NMG	BA	501	8/8	0.14	-0.91	21,26,27,28	0
3	ADP	BN	402	27/27	0.13	-0.91	10,20,23,26	0
3	ADP	BM	402	27/27	0.12	-1.18	13,20,23,26	0
5	NO3	BE	404	4/4	0.13	-1.29	24,25,26,29	0
3	ADP	AB	402	27/27	0.12	-1.40	14,18,21,22	0
5	NO3	AA	504	4/4	0.11	-2.05	25,26,27,28	0
5	NO3	AG	404	4/4	0.11	-2.27	19,21,25,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.