



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 06:09 PM BST

PDB ID : 3L2F
Title : Glycocyamine kinase, beta-beta homodimer from marine worm *Namalycastis* sp., with transition state analog Mg(II)-ADP-NO₃-glycocyamine.Part 1.
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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

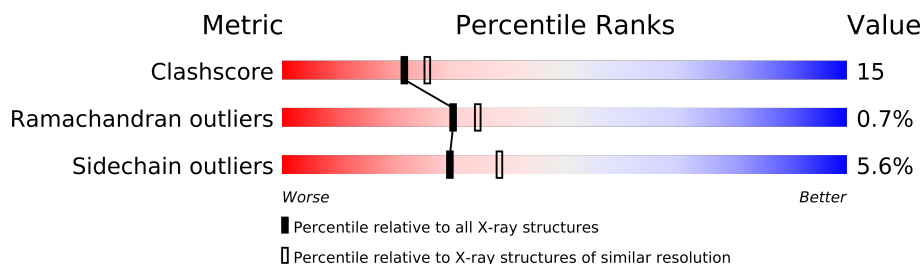
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	390	
1	B	390	
1	C	390	
1	D	390	
1	E	390	
1	F	390	
1	G	390	
1	H	390	
1	I	390	
1	J	390	
1	K	390	
1	L	390	
1	M	390	
1	N	390	
1	O	390	
1	P	390	
1	Q	390	

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Mol	Chain	Length	Quality of chain
1	R	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
5	NO3	A	801	X	-
5	NO3	B	802	X	-
5	NO3	C	803	X	-
5	NO3	D	804	X	-
5	NO3	E	805	X	-
5	NO3	F	806	X	-
5	NO3	G	807	X	-
5	NO3	H	808	X	-
5	NO3	I	809	X	-
5	NO3	J	810	X	-
5	NO3	K	811	X	-
5	NO3	L	812	X	-
5	NO3	M	813	X	-
5	NO3	N	814	X	-
5	NO3	O	815	X	-
5	NO3	P	816	X	-
5	NO3	Q	817	X	-
5	NO3	R	818	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 56675 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.

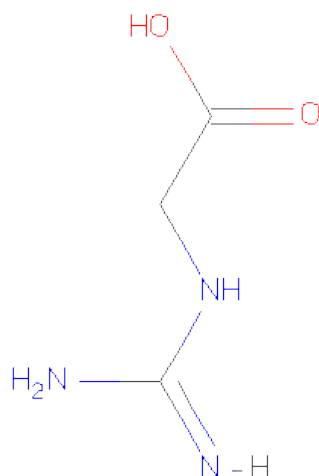
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	B	387	Total	C	N	O	S	0	0	0
			3074	1939	543	571	21			
1	C	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	D	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	E	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	F	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	G	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	H	384	Total	C	N	O	S	0	0	0
			3052	1925	539	567	21			
1	I	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	J	385	Total	C	N	O	S	0	0	0
			3061	1930	541	569	21			
1	K	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	L	384	Total	C	N	O	S	0	0	0
			3052	1925	539	567	21			
1	M	367	Total	C	N	O	S	0	0	0
			2910	1834	513	542	21			
1	N	382	Total	C	N	O	S	0	0	0
			3032	1912	537	562	21			
1	O	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	P	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	Q	366	Total	C	N	O	S	0	0	0
			2901	1828	511	541	21			
1	R	379	Total	C	N	O	S	0	0	0
			3005	1892	533	559	21			

- Molecule 2 is GUANIDINO ACETATE (three-letter code: NMG) (formula: $C_3H_7N_3O_2$).



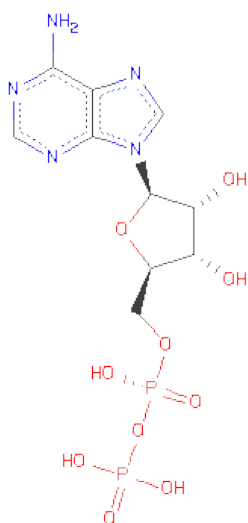
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	3	3	2		
2	B	1	Total	C	N	O	0	0
			8	3	3	2		
2	C	1	Total	C	N	O	0	0
			8	3	3	2		
2	D	1	Total	C	N	O	0	0
			8	3	3	2		
2	E	1	Total	C	N	O	0	0
			8	3	3	2		
2	F	1	Total	C	N	O	0	0
			8	3	3	2		
2	G	1	Total	C	N	O	0	0
			8	3	3	2		
2	H	1	Total	C	N	O	0	0
			8	3	3	2		
2	I	1	Total	C	N	O	0	0
			8	3	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	J	1	Total	C	N	O	0	0
			8	3	3	2		
2	K	1	Total	C	N	O	0	0
			8	3	3	2		
2	L	1	Total	C	N	O	0	0
			8	3	3	2		
2	M	1	Total	C	N	O	0	0
			8	3	3	2		
2	N	1	Total	C	N	O	0	0
			8	3	3	2		
2	O	1	Total	C	N	O	0	0
			8	3	3	2		
2	P	1	Total	C	N	O	0	0
			8	3	3	2		
2	Q	1	Total	C	N	O	0	0
			8	3	3	2		
2	R	1	Total	C	N	O	0	0
			8	3	3	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	M	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	N	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	O	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	P	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	Q	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	R	1	Total 27	C 10	N 5	O 10	P 2	0	0

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

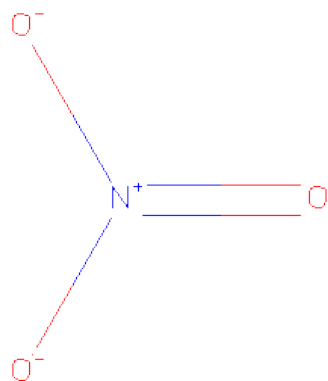
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	O	1	Total 1	Mg 1	0	0
4	R	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	D	1	Total	N	O	0	0
			4	1	3		
5	E	1	Total	N	O	0	0
			4	1	3		
5	F	1	Total	N	O	0	0
			4	1	3		
5	G	1	Total	N	O	0	0
			4	1	3		
5	H	1	Total	N	O	0	0
			4	1	3		
5	I	1	Total	N	O	0	0
			4	1	3		
5	J	1	Total	N	O	0	0
			4	1	3		
5	K	1	Total	N	O	0	0
			4	1	3		
5	L	1	Total	N	O	0	0
			4	1	3		
5	M	1	Total	N	O	0	0
			4	1	3		
5	N	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	O	1	Total	N	O	0	0
			4	1	3		
5	P	1	Total	N	O	0	0
			4	1	3		
5	Q	1	Total	N	O	0	0
			4	1	3		
5	R	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	138	Total	O	0	0
			138	138		
6	C	116	Total	O	0	0
			116	116		
6	D	149	Total	O	0	0
			149	149		
6	E	154	Total	O	0	0
			154	154		
6	F	116	Total	O	0	0
			116	116		
6	G	131	Total	O	0	0
			131	131		
6	H	88	Total	O	0	0
			88	88		
6	I	111	Total	O	0	0
			111	111		
6	J	136	Total	O	0	0
			136	136		
6	K	125	Total	O	0	0
			125	125		
6	L	157	Total	O	0	0
			157	157		
6	M	149	Total	O	0	0
			149	149		
6	N	116	Total	O	0	0
			116	116		
6	O	114	Total	O	0	0
			114	114		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	172	Total 172	O 172	0	0
6	Q	166	Total 166	O 166	0	0
6	R	167	Total 167	O 167	0	0

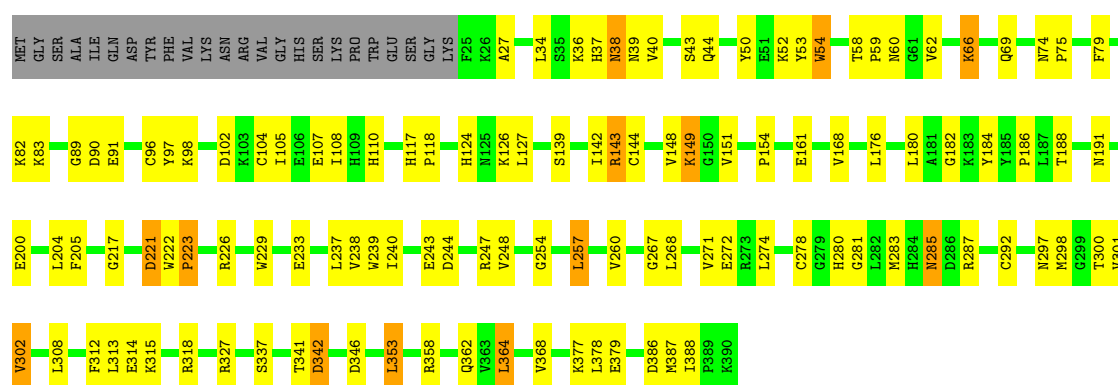
3 Residue-property plots

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.

Note EDS was not executed.

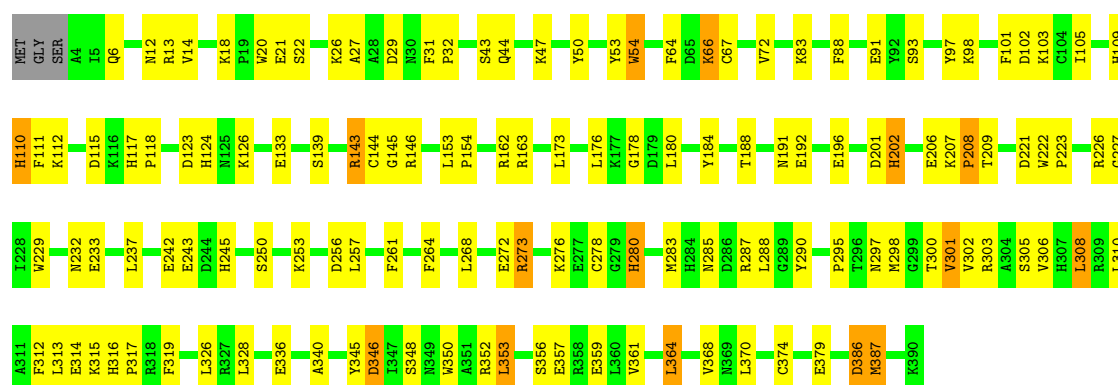
- Molecule 1: Glycocyamine kinase beta chain

Chain A:



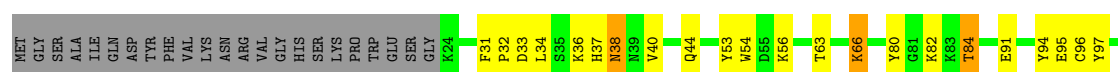
- Molecule 1: Glycocyamine kinase beta chain

Chain B:



- Molecule 1: Glycocyamine kinase beta chain

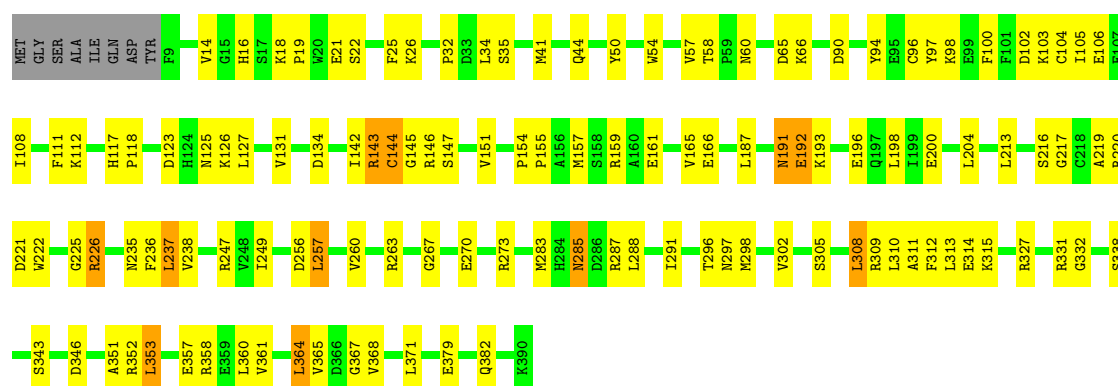
Chain C:





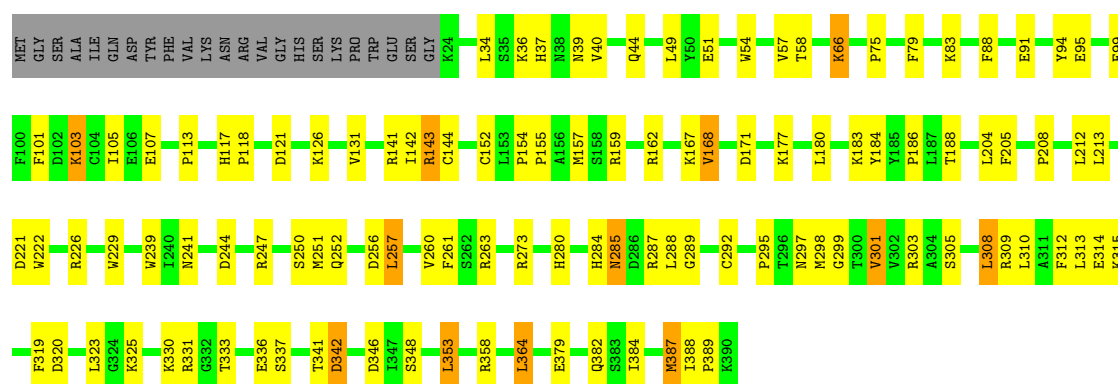
• Molecule 1: Glycocyamine kinase beta chain

Chain D:



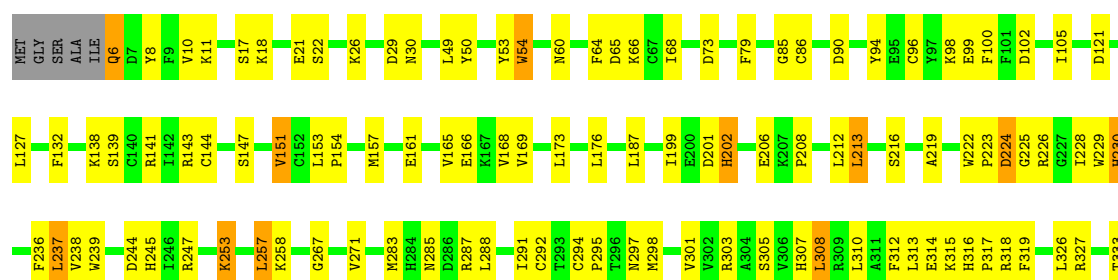
• Molecule 1: Glycocyamine kinase beta chain

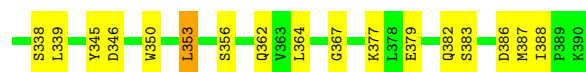
Chain E:



• Molecule 1: Glycocyamine kinase beta chain

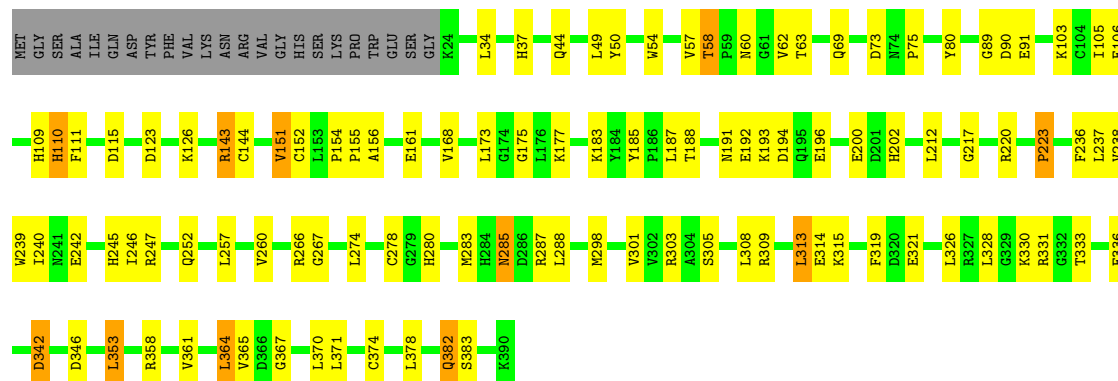
Chain F:





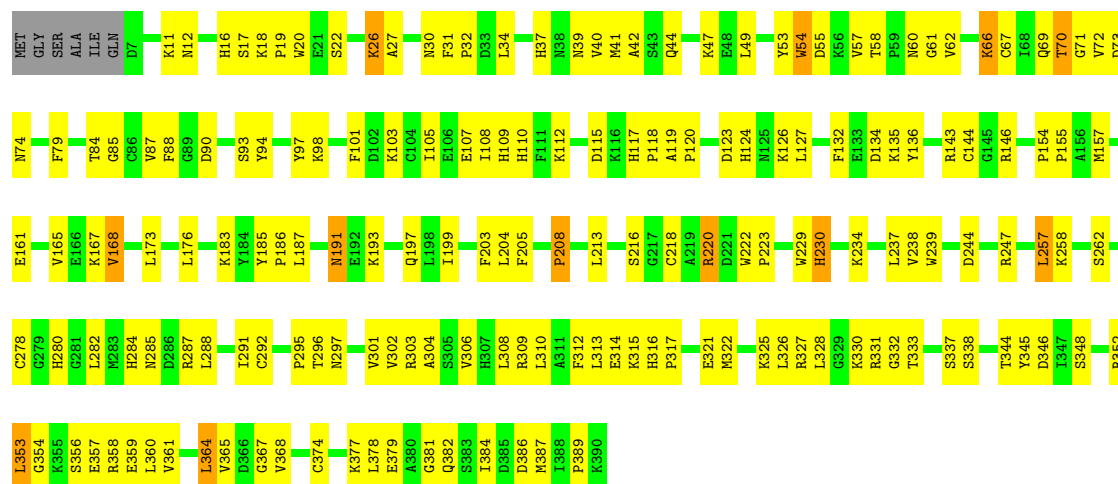
• Molecule 1: Glycocyamine kinase beta chain

Chain G:



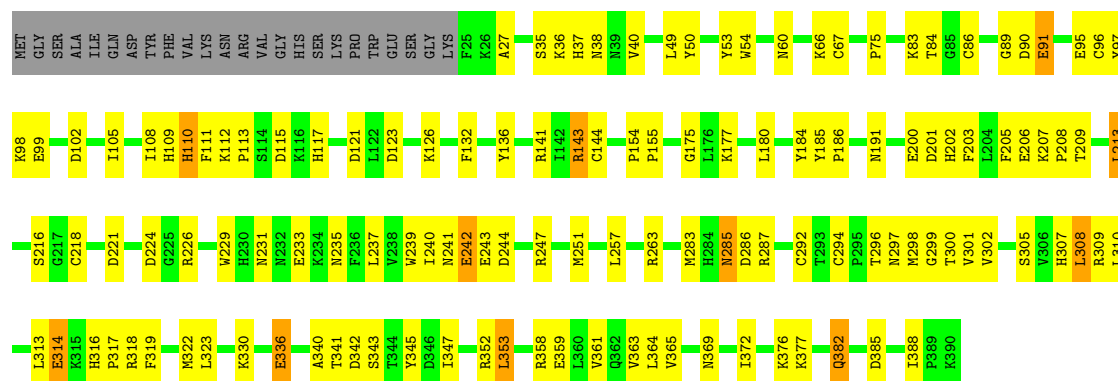
• Molecule 1: Glycocyamine kinase beta chain

Chain H:



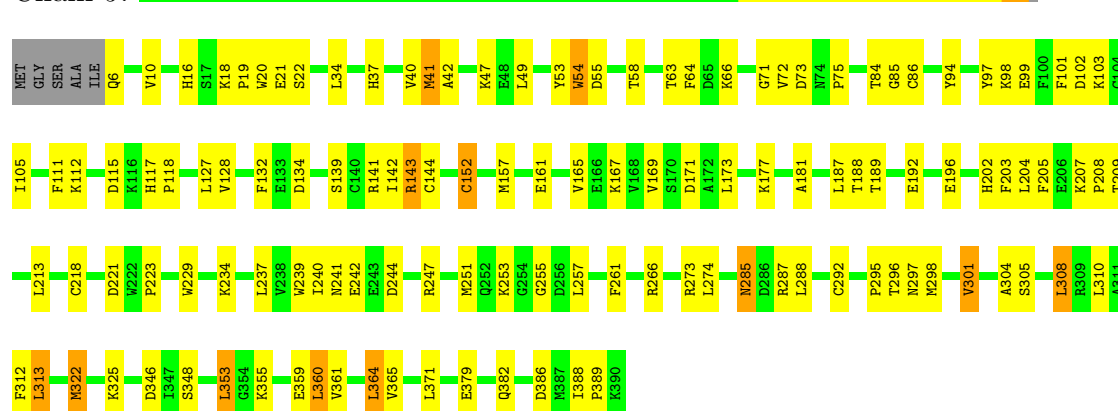
• Molecule 1: Glycocyamine kinase beta chain

Chain I:



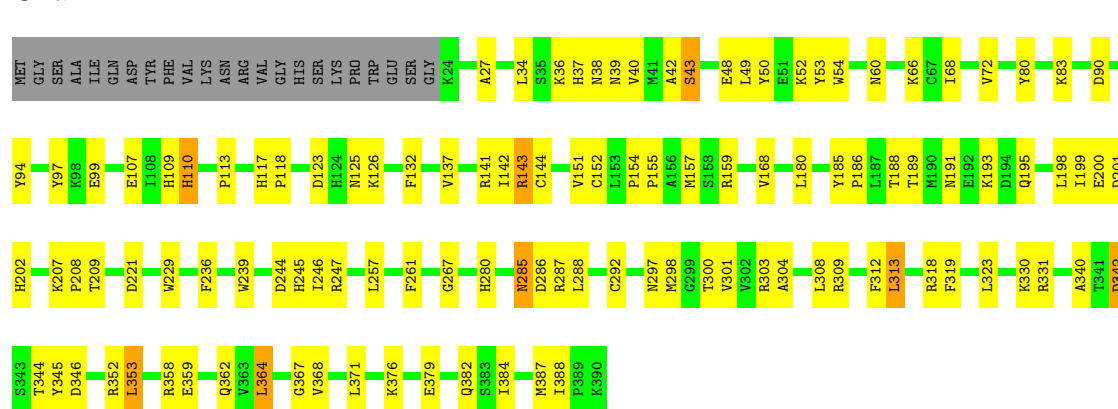
- Molecule 1: Glycocyamine kinase beta chain

Chain J:



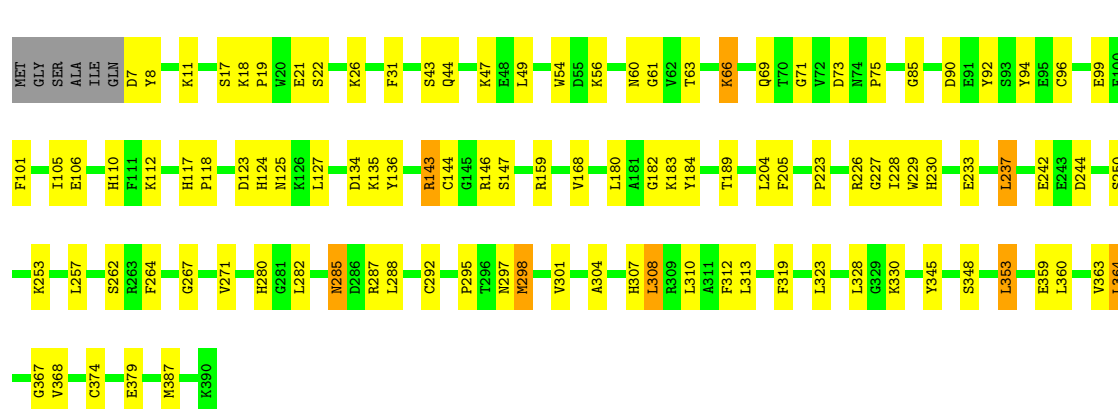
- Molecule 1: Glycocyamine kinase beta chain

Chain K:



- Molecule 1: Glycocyamine kinase beta chain

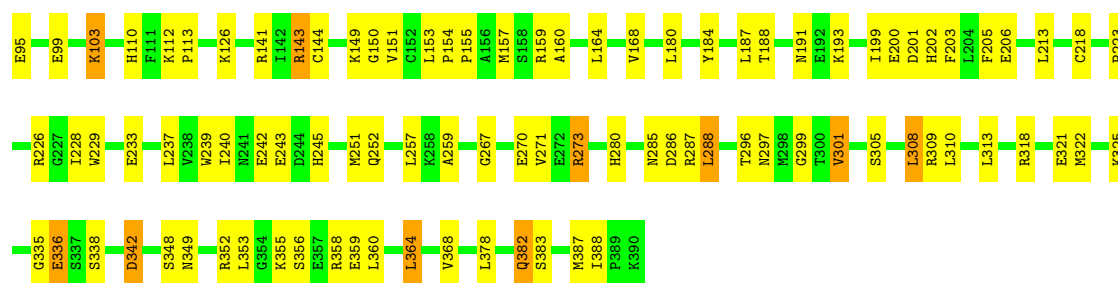
Chain L:



- Molecule 1: Glycocyamine kinase beta chain

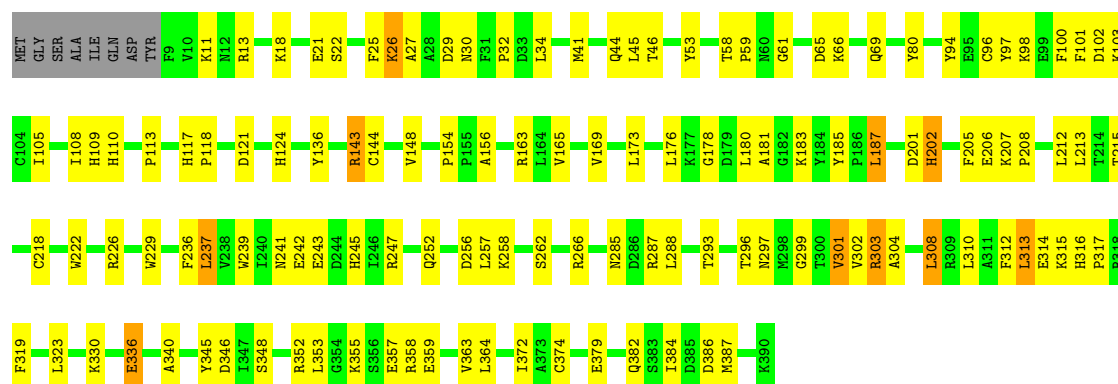
Chain M:





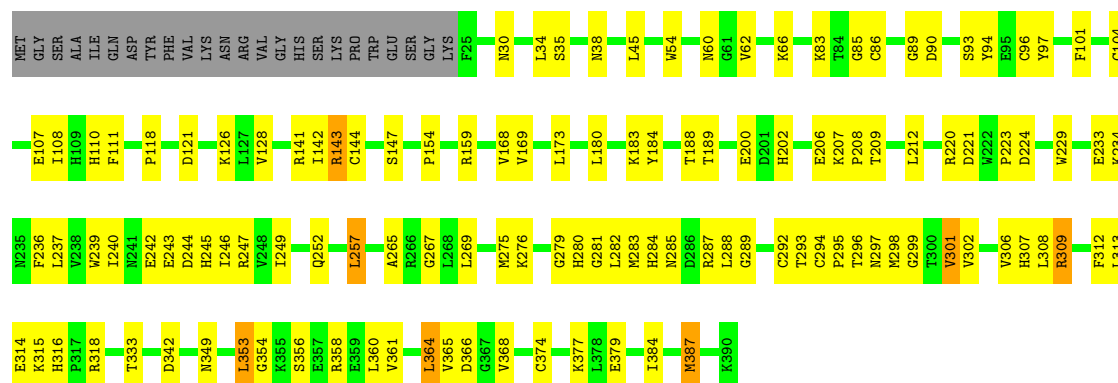
• Molecule 1: Glycocyamine kinase beta chain

Chain N:



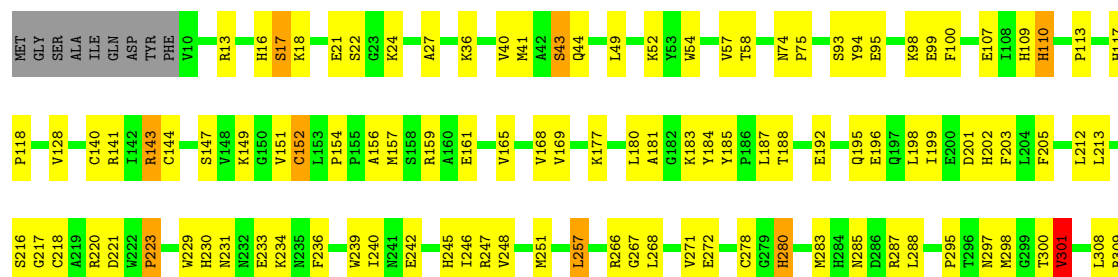
• Molecule 1: Glycocyamine kinase beta chain

Chain O:



• Molecule 1: Glycocyamine kinase beta chain

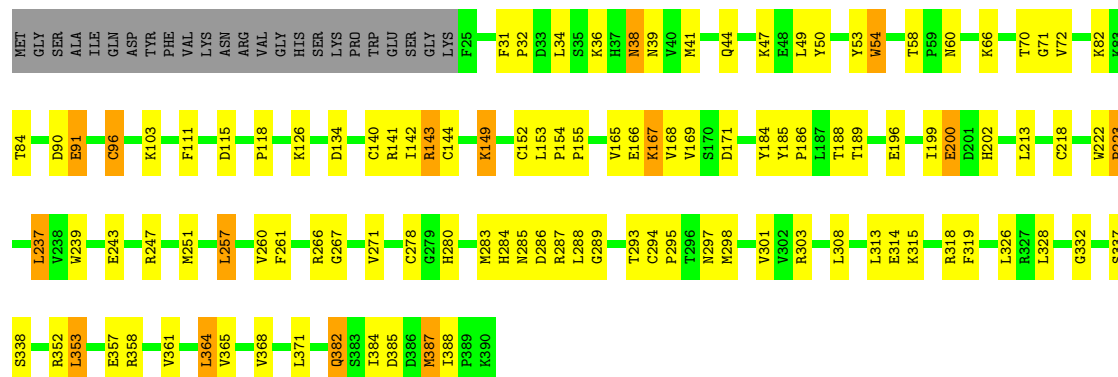
Chain P:





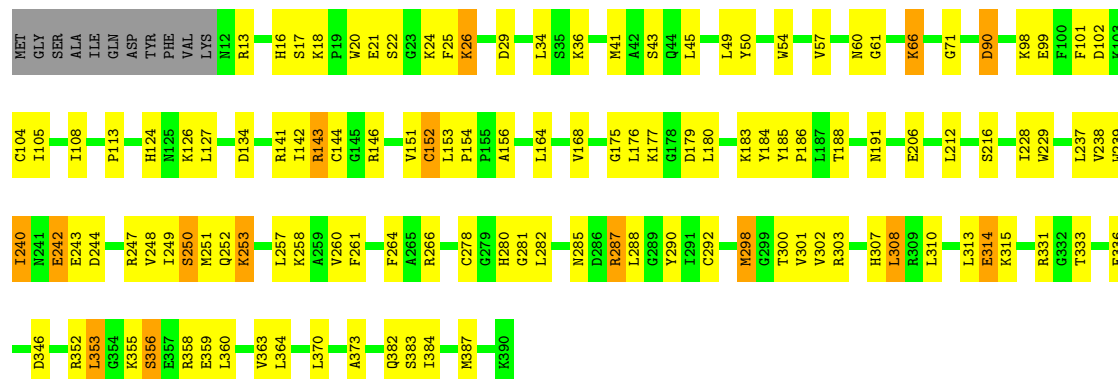
• Molecule 1: Glycocyamine kinase beta chain

Chain Q:



• Molecule 1: Glycocyamine kinase beta chain

Chain R:



4 Data and refinement statistics i

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	243.11Å 114.27Å 259.90Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.29Å)	Xtriage
Refinement program	phenix	Depositor
R, R_{free}	0.197 , 0.263	Depositor
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.184	Xtriage
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
Total number of atoms	56675	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities 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	A	0.34	0/2963	0.51	0/3986
1	B	0.37	0/3142	0.55	0/4227
1	C	0.34	0/2972	0.53	0/3997
1	D	0.38	0/3099	0.55	0/4168
1	E	0.35	0/2972	0.52	0/3997
1	F	0.37	0/3129	0.56	0/4209
1	G	0.35	0/2972	0.53	1/3997 (0.0%)
1	H	0.35	0/3120	0.53	0/4197
1	I	0.34	0/2963	0.52	0/3986
1	J	0.37	0/3129	0.53	0/4209
1	K	0.35	0/2972	0.52	0/3997
1	L	0.38	0/3120	0.55	0/4197
1	M	0.35	0/2972	0.54	0/3997
1	N	0.37	0/3099	0.54	0/4168
1	O	0.34	0/2963	0.53	0/3986
1	P	0.39	0/3087	0.55	1/4152 (0.0%)
1	Q	0.35	0/2963	0.53	0/3986
1	R	0.38	0/3071	0.55	0/4131
All	All	0.36	0/54708	0.54	2/73587 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	353	LEU	CA-CB-CG	5.32	127.53	115.30
1	G	364	LEU	CA-CB-CG	5.26	127.40	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	A	2901	0	2866	94	0
1	B	3074	0	3034	107	0
1	C	2910	0	2879	88	0
1	D	3032	0	2997	81	0
1	E	2910	0	2879	83	0
1	F	3061	0	3018	96	0
1	G	2910	0	2879	78	0
1	H	3052	0	3010	141	0
1	I	2901	0	2866	89	0
1	J	3061	0	3018	85	0
1	K	2910	0	2879	89	0
1	L	3052	0	3010	79	0
1	M	2910	0	2879	81	0
1	N	3032	0	2997	93	0
1	O	2901	0	2866	93	0
1	P	3021	0	2988	108	0
1	Q	2901	0	2866	80	0
1	R	3005	0	2966	92	0
2	A	8	0	5	0	0
2	B	8	0	5	2	0
2	C	8	0	5	0	0
2	D	8	0	5	0	0
2	E	8	0	5	1	0
2	F	8	0	5	0	0
2	G	8	0	5	2	0
2	H	8	0	5	0	0
2	I	8	0	5	1	0
2	J	8	0	5	0	0
2	K	8	0	5	0	0
2	L	8	0	5	0	0
2	M	8	0	5	1	0
2	N	8	0	5	1	0
2	O	8	0	5	1	0
2	P	8	0	5	0	0
2	Q	8	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	8	0	5	0	0
3	A	27	0	12	1	0
3	B	27	0	12	2	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
3	E	27	0	12	4	0
3	F	27	0	12	7	0
3	G	27	0	12	2	0
3	H	27	0	12	3	0
3	I	27	0	12	3	0
3	J	27	0	12	3	0
3	K	27	0	12	5	0
3	L	27	0	12	1	0
3	M	27	0	12	2	0
3	N	27	0	12	1	0
3	O	27	0	12	4	0
3	P	27	0	12	5	0
3	Q	27	0	12	3	0
3	R	27	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	1	0
5	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	4	0	0	0	0
5	G	4	0	0	0	0
5	H	4	0	0	0	0
5	I	4	0	0	0	0
5	J	4	0	0	0	0
5	K	4	0	0	0	0
5	L	4	0	0	0	0
5	M	4	0	0	0	0
5	N	4	0	0	0	0
5	O	4	0	0	1	0
5	P	4	0	0	0	0
5	Q	4	0	0	0	0
5	R	4	0	0	1	0
6	A	106	0	0	6	0
6	B	138	0	0	12	0
6	C	116	0	0	5	0
6	D	149	0	0	3	0
6	E	154	0	0	6	0
6	F	116	0	0	9	0
6	G	131	0	0	4	0
6	H	88	0	0	5	0
6	I	111	0	0	3	0
6	J	136	0	0	5	0
6	K	125	0	0	8	0
6	L	157	0	0	5	0
6	M	149	0	0	8	0
6	N	116	0	0	7	0
6	O	114	0	0	7	0
6	P	172	0	0	14	0
6	Q	166	0	0	9	0
6	R	167	0	0	5	0
All	All	56675	0	53203	1632	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 1632 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:126:LYS:HB2	1:K:358:ARG:HD2	1.38	1.04
1:D:285:ASN:HB2	1:D:291:ILE:HD11	1.40	1.02
1:L:285:ASN:HD22	1:L:288:LEU:H	1.03	0.99
1:O:285:ASN:HD22	1:O:288:LEU:H	1.10	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:377:LYS:HG3	1:F:387:MET:HE1	1.45	0.98

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	364/390 (93%)	335 (92%)	29 (8%)	0	100	100
1	B	385/390 (99%)	360 (94%)	21 (6%)	4 (1%)	22	23
1	C	365/390 (94%)	338 (93%)	26 (7%)	1 (0%)	50	60
1	D	380/390 (97%)	359 (94%)	21 (6%)	0	100	100
1	E	365/390 (94%)	344 (94%)	19 (5%)	2 (0%)	38	45
1	F	383/390 (98%)	361 (94%)	20 (5%)	2 (0%)	38	45
1	G	365/390 (94%)	338 (93%)	23 (6%)	4 (1%)	21	21
1	H	382/390 (98%)	337 (88%)	41 (11%)	4 (1%)	22	23
1	I	364/390 (93%)	340 (93%)	21 (6%)	3 (1%)	27	30
1	J	383/390 (98%)	352 (92%)	27 (7%)	4 (1%)	22	23
1	K	365/390 (94%)	347 (95%)	17 (5%)	1 (0%)	50	60
1	L	382/390 (98%)	362 (95%)	20 (5%)	0	100	100
1	M	365/390 (94%)	336 (92%)	24 (7%)	5 (1%)	16	15
1	N	380/390 (97%)	351 (92%)	26 (7%)	3 (1%)	27	30
1	O	364/390 (93%)	342 (94%)	18 (5%)	4 (1%)	21	21
1	P	379/390 (97%)	355 (94%)	21 (6%)	3 (1%)	27	30
1	Q	364/390 (93%)	342 (94%)	21 (6%)	1 (0%)	50	60
1	R	377/390 (97%)	351 (93%)	22 (6%)	4 (1%)	21	21
All	All	6712/7020 (96%)	6250 (93%)	417 (6%)	45 (1%)	30	34

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	168	VAL
1	M	54	TRP
1	M	336	GLU
1	B	13	ARG
1	F	202	HIS

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	315/335 (94%)	294 (93%)	21 (7%)	23	29
1	B	333/335 (99%)	311 (93%)	22 (7%)	24	29
1	C	316/335 (94%)	297 (94%)	19 (6%)	27	35
1	D	329/335 (98%)	311 (94%)	18 (6%)	30	39
1	E	316/335 (94%)	300 (95%)	16 (5%)	33	43
1	F	332/335 (99%)	314 (95%)	18 (5%)	31	40
1	G	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	H	331/335 (99%)	312 (94%)	19 (6%)	29	37
1	I	315/335 (94%)	296 (94%)	19 (6%)	27	35
1	J	332/335 (99%)	313 (94%)	19 (6%)	29	37
1	K	316/335 (94%)	301 (95%)	15 (5%)	36	47
1	L	331/335 (99%)	315 (95%)	16 (5%)	35	46
1	M	316/335 (94%)	296 (94%)	20 (6%)	25	32
1	N	329/335 (98%)	313 (95%)	16 (5%)	35	45
1	O	315/335 (94%)	300 (95%)	15 (5%)	35	46
1	P	328/335 (98%)	314 (96%)	14 (4%)	40	52
1	Q	315/335 (94%)	295 (94%)	20 (6%)	25	32
1	R	326/335 (97%)	303 (93%)	23 (7%)	21	26
All	All	5811/6030 (96%)	5486 (94%)	325 (6%)	30	38

5 of 325 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	386	ASP
1	J	346	ASP
1	Q	382	GLN
1	I	110	HIS
1	I	364	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	316	HIS
1	K	38	ASN
1	Q	280	HIS
1	I	195	GLN
1	J	124	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 72 ligands modelled in this entry, 18 are monoatomic - leaving 54 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	A	501	-	7,7,7	0.68	0	8,8,8	1.74	1 (12%)
3	ADP	A	601	4	29,29,29	1.11	2 (6%)	45,45,45	1.69	6 (13%)
5	NO3	A	801	4	3,3,3	3.23	3 (100%)	3,3,3	0.13	0
2	NMG	B	502	-	7,7,7	0.77	0	8,8,8	2.14	2 (25%)
3	ADP	B	602	4	29,29,29	1.12	2 (6%)	45,45,45	1.92	9 (20%)
5	NO3	B	802	4	3,3,3	3.11	3 (100%)	3,3,3	0.18	0
2	NMG	C	503	-	7,7,7	0.72	0	8,8,8	1.63	1 (12%)
3	ADP	C	603	4	29,29,29	1.19	2 (6%)	45,45,45	1.70	6 (13%)
5	NO3	C	803	4	3,3,3	3.29	3 (100%)	3,3,3	0.25	0
2	NMG	D	504	-	7,7,7	0.66	0	8,8,8	1.57	2 (25%)
3	ADP	D	604	4	29,29,29	1.20	2 (6%)	45,45,45	1.68	6 (13%)
5	NO3	D	804	4	3,3,3	3.22	3 (100%)	3,3,3	0.15	0
2	NMG	E	505	-	7,7,7	0.72	0	8,8,8	1.98	2 (25%)
3	ADP	E	605	4	29,29,29	1.16	3 (10%)	45,45,45	1.68	5 (11%)
5	NO3	E	805	4	3,3,3	3.32	3 (100%)	3,3,3	0.06	0
2	NMG	F	506	-	7,7,7	0.96	0	8,8,8	1.79	1 (12%)
3	ADP	F	606	4	29,29,29	1.16	2 (6%)	45,45,45	1.77	7 (15%)
5	NO3	F	806	4	3,3,3	3.20	3 (100%)	3,3,3	0.21	0
2	NMG	G	507	-	7,7,7	0.65	0	8,8,8	1.42	1 (12%)
3	ADP	G	607	4	29,29,29	1.16	2 (6%)	45,45,45	1.93	9 (20%)
5	NO3	G	807	4	3,3,3	3.36	3 (100%)	3,3,3	0.22	0
2	NMG	H	508	-	7,7,7	0.68	0	8,8,8	1.59	1 (12%)
3	ADP	H	608	4	29,29,29	1.11	2 (6%)	45,45,45	1.64	7 (15%)
5	NO3	H	808	4	3,3,3	3.20	3 (100%)	3,3,3	0.11	0
2	NMG	I	509	-	7,7,7	0.72	0	8,8,8	1.74	1 (12%)
3	ADP	I	609	4	29,29,29	1.26	2 (6%)	45,45,45	1.76	8 (17%)
5	NO3	I	809	4	3,3,3	3.34	3 (100%)	3,3,3	0.05	0
2	NMG	J	510	-	7,7,7	0.67	0	8,8,8	1.64	2 (25%)
3	ADP	J	610	4	29,29,29	1.20	2 (6%)	45,45,45	1.88	8 (17%)
5	NO3	J	810	4	3,3,3	3.27	3 (100%)	3,3,3	0.14	0
2	NMG	K	511	-	7,7,7	0.67	0	8,8,8	1.22	1 (12%)
3	ADP	K	611	4	29,29,29	1.12	2 (6%)	45,45,45	1.95	9 (20%)
5	NO3	K	811	4	3,3,3	3.26	3 (100%)	3,3,3	0.17	0
2	NMG	L	512	-	7,7,7	0.71	0	8,8,8	1.70	1 (12%)
3	ADP	L	612	4	29,29,29	1.17	2 (6%)	45,45,45	1.63	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NO3	L	812	4	3,3,3	3.24	3 (100%)	3,3,3	0.24	0
2	NMG	M	513	-	7,7,7	0.82	0	8,8,8	1.56	1 (12%)
3	ADP	M	613	4	29,29,29	1.21	2 (6%)	45,45,45	1.89	10 (22%)
5	NO3	M	813	4	3,3,3	3.25	3 (100%)	3,3,3	0.16	0
2	NMG	N	514	-	7,7,7	0.68	0	8,8,8	1.71	1 (12%)
3	ADP	N	614	4	29,29,29	1.18	2 (6%)	45,45,45	1.87	8 (17%)
5	NO3	N	814	4	3,3,3	3.32	3 (100%)	3,3,3	0.27	0
2	NMG	O	515	-	7,7,7	0.71	0	8,8,8	1.45	1 (12%)
3	ADP	O	615	4	29,29,29	1.09	2 (6%)	45,45,45	1.71	6 (13%)
5	NO3	O	815	4	3,3,3	3.16	3 (100%)	3,3,3	0.16	0
2	NMG	P	516	-	7,7,7	0.67	0	8,8,8	1.59	1 (12%)
3	ADP	P	616	4	29,29,29	1.06	2 (6%)	45,45,45	1.91	8 (17%)
5	NO3	P	816	4	3,3,3	3.16	3 (100%)	3,3,3	0.13	0
2	NMG	Q	517	-	7,7,7	0.72	0	8,8,8	2.29	1 (12%)
3	ADP	Q	617	4	29,29,29	1.13	2 (6%)	45,45,45	1.89	9 (20%)
5	NO3	Q	817	4	3,3,3	3.28	3 (100%)	3,3,3	0.25	0
2	NMG	R	518	-	7,7,7	0.68	0	8,8,8	2.13	1 (12%)
3	ADP	R	618	4	29,29,29	1.09	2 (6%)	45,45,45	1.73	8 (17%)
5	NO3	R	818	4	3,3,3	3.33	3 (100%)	3,3,3	0.22	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	A	501	-	-	0/5/5/5	0/0/0/0
3	ADP	A	601	4	-	0/16/32/32	0/1/3/3
5	NO3	A	801	4	-	0/0/0/0	0/0/0/0
2	NMG	B	502	-	-	0/5/5/5	0/0/0/0
3	ADP	B	602	4	-	0/16/32/32	0/1/3/3
5	NO3	B	802	4	-	0/0/0/0	0/0/0/0
2	NMG	C	503	-	-	0/5/5/5	0/0/0/0
3	ADP	C	603	4	-	0/16/32/32	0/1/3/3
5	NO3	C	803	4	-	0/0/0/0	0/0/0/0
2	NMG	D	504	-	-	0/5/5/5	0/0/0/0
3	ADP	D	604	4	-	0/16/32/32	0/1/3/3
5	NO3	D	804	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMG	E	505	-	-	0/5/5/5	0/0/0/0
3	ADP	E	605	4	-	0/16/32/32	0/1/3/3
5	NO3	E	805	4	-	0/0/0/0	0/0/0/0
2	NMG	F	506	-	-	0/5/5/5	0/0/0/0
3	ADP	F	606	4	-	0/16/32/32	0/1/3/3
5	NO3	F	806	4	-	0/0/0/0	0/0/0/0
2	NMG	G	507	-	-	0/5/5/5	0/0/0/0
3	ADP	G	607	4	-	0/16/32/32	0/1/3/3
5	NO3	G	807	4	-	0/0/0/0	0/0/0/0
2	NMG	H	508	-	-	0/5/5/5	0/0/0/0
3	ADP	H	608	4	-	0/16/32/32	0/1/3/3
5	NO3	H	808	4	-	0/0/0/0	0/0/0/0
2	NMG	I	509	-	-	0/5/5/5	0/0/0/0
3	ADP	I	609	4	-	0/16/32/32	0/1/3/3
5	NO3	I	809	4	-	0/0/0/0	0/0/0/0
2	NMG	J	510	-	-	0/5/5/5	0/0/0/0
3	ADP	J	610	4	-	0/16/32/32	0/1/3/3
5	NO3	J	810	4	-	0/0/0/0	0/0/0/0
2	NMG	K	511	-	-	0/5/5/5	0/0/0/0
3	ADP	K	611	4	-	0/16/32/32	0/1/3/3
5	NO3	K	811	4	-	0/0/0/0	0/0/0/0
2	NMG	L	512	-	-	0/5/5/5	0/0/0/0
3	ADP	L	612	4	-	0/16/32/32	0/1/3/3
5	NO3	L	812	4	-	0/0/0/0	0/0/0/0
2	NMG	M	513	-	-	0/5/5/5	0/0/0/0
3	ADP	M	613	4	-	0/16/32/32	0/1/3/3
5	NO3	M	813	4	-	0/0/0/0	0/0/0/0
2	NMG	N	514	-	-	0/5/5/5	0/0/0/0
3	ADP	N	614	4	-	0/16/32/32	0/1/3/3
5	NO3	N	814	4	-	0/0/0/0	0/0/0/0
2	NMG	O	515	-	-	0/5/5/5	0/0/0/0
3	ADP	O	615	4	-	0/16/32/32	0/1/3/3
5	NO3	O	815	4	-	0/0/0/0	0/0/0/0
2	NMG	P	516	-	-	0/5/5/5	0/0/0/0
3	ADP	P	616	4	-	0/16/32/32	0/1/3/3
5	NO3	P	816	4	-	0/0/0/0	0/0/0/0
2	NMG	Q	517	-	-	0/5/5/5	0/0/0/0
3	ADP	Q	617	4	-	0/16/32/32	0/1/3/3
5	NO3	Q	817	4	-	0/0/0/0	0/0/0/0
2	NMG	R	518	-	-	0/5/5/5	0/0/0/0
3	ADP	R	618	4	-	0/16/32/32	0/1/3/3
5	NO3	R	818	4	-	0/0/0/0	0/0/0/0

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	809	NO3	O1-N	4.08	1.41	1.24
5	E	805	NO3	O1-N	4.04	1.41	1.24
5	G	807	NO3	O1-N	4.02	1.41	1.24
5	R	818	NO3	O1-N	4.02	1.41	1.24
5	L	812	NO3	O1-N	3.90	1.40	1.24

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	616	ADP	N3-C2-N1	-7.99	122.03	128.71
3	K	611	ADP	N3-C2-N1	-7.81	122.18	128.71
3	J	610	ADP	N3-C2-N1	-6.99	122.86	128.71
3	B	602	ADP	N3-C2-N1	-6.96	122.89	128.71
3	M	613	ADP	N3-C2-N1	-6.80	123.02	128.71

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.