



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:20 PM GMT

PDB ID : 1SX3  
Title : GroEL14-(ATPgammaS)14  
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.  
Deposited on : 2004-03-30  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure 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/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

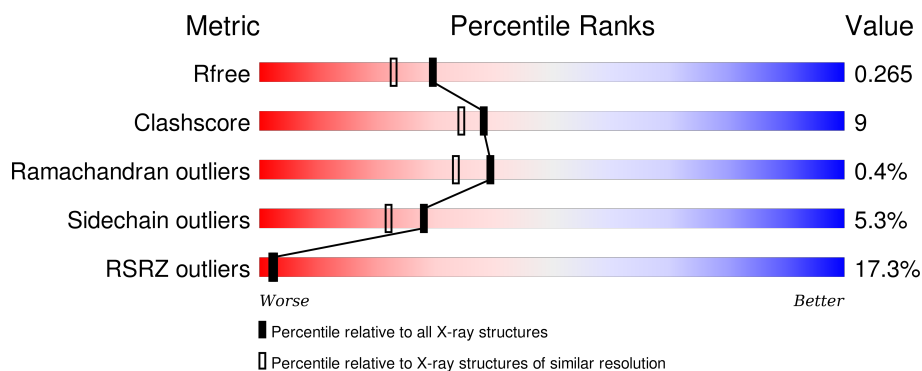
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	525	<div> <div>13%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	B	525	<div> <div>24%</div> <div>73%</div> <div>22%</div> <div>.</div> </div>
1	C	525	<div> <div>22%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	D	525	<div> <div>6%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	E	525	<div> <div>18%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	525	
1	G	525	
1	H	525	
1	I	525	
1	J	525	
1	K	525	
1	L	525	
1	M	525	
1	N	525	

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
3	K	D	1	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 55380 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	B	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	C	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	D	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	E	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	F	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	G	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	H	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	I	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	J	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	K	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	L	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	M	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	N	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	ENGINEERED	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	126	VAL	ALA	ENGINEERED	UNP P0A6F5
B	13	GLY	ARG	ENGINEERED	UNP P0A6F5
B	126	VAL	ALA	ENGINEERED	UNP P0A6F5
C	13	GLY	ARG	ENGINEERED	UNP P0A6F5
C	126	VAL	ALA	ENGINEERED	UNP P0A6F5
D	13	GLY	ARG	ENGINEERED	UNP P0A6F5
D	126	VAL	ALA	ENGINEERED	UNP P0A6F5
E	13	GLY	ARG	ENGINEERED	UNP P0A6F5
E	126	VAL	ALA	ENGINEERED	UNP P0A6F5
F	13	GLY	ARG	ENGINEERED	UNP P0A6F5
F	126	VAL	ALA	ENGINEERED	UNP P0A6F5
G	13	GLY	ARG	ENGINEERED	UNP P0A6F5
G	126	VAL	ALA	ENGINEERED	UNP P0A6F5
H	13	GLY	ARG	ENGINEERED	UNP P0A6F5
H	126	VAL	ALA	ENGINEERED	UNP P0A6F5
I	13	GLY	ARG	ENGINEERED	UNP P0A6F5
I	126	VAL	ALA	ENGINEERED	UNP P0A6F5
J	13	GLY	ARG	ENGINEERED	UNP P0A6F5
J	126	VAL	ALA	ENGINEERED	UNP P0A6F5
K	13	GLY	ARG	ENGINEERED	UNP P0A6F5
K	126	VAL	ALA	ENGINEERED	UNP P0A6F5
L	13	GLY	ARG	ENGINEERED	UNP P0A6F5
L	126	VAL	ALA	ENGINEERED	UNP P0A6F5
M	13	GLY	ARG	ENGINEERED	UNP P0A6F5
M	126	VAL	ALA	ENGINEERED	UNP P0A6F5
N	13	GLY	ARG	ENGINEERED	UNP P0A6F5
N	126	VAL	ALA	ENGINEERED	UNP P0A6F5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0
2	I	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	N	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0
2	M	1	Total 1	Mg 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

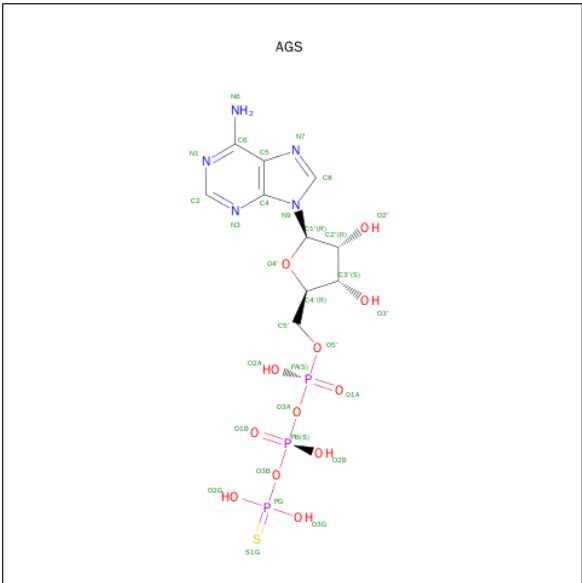
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	K 1	0	0
3	J	1	Total 1	K 1	0	0
3	D	2	Total 2	K 2	0	0
3	K	1	Total 1	K 1	0	0
3	E	2	Total 2	K 2	0	0
3	H	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0
3	I	1	Total 1	K 1	0	0
3	C	1	Total 1	K 1	0	0
3	A	1	Total 1	K 1	0	0
3	N	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		
3	M	1	Total	K	0	0
			1	1		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	I	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	J	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	K	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	L	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	M	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	N	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total 62	O 62	0	0
5	B	83	Total 83	O 83	0	0
5	C	57	Total 57	O 57	0	0
5	D	91	Total 91	O 91	0	0
5	E	92	Total 92	O 92	0	0
5	F	71	Total 71	O 71	0	0
5	G	83	Total 83	O 83	0	0
5	H	77	Total 77	O 77	0	0
5	I	60	Total 60	O 60	0	0
5	J	50	Total 50	O 50	0	0
5	K	47	Total 47	O 47	0	0
5	L	61	Total 61	O 61	0	0
5	M	53	Total 53	O 53	0	0

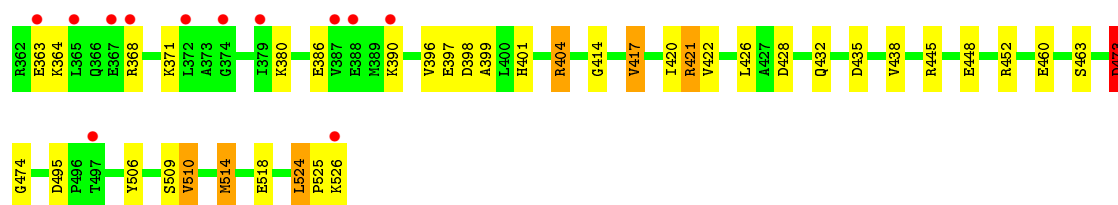
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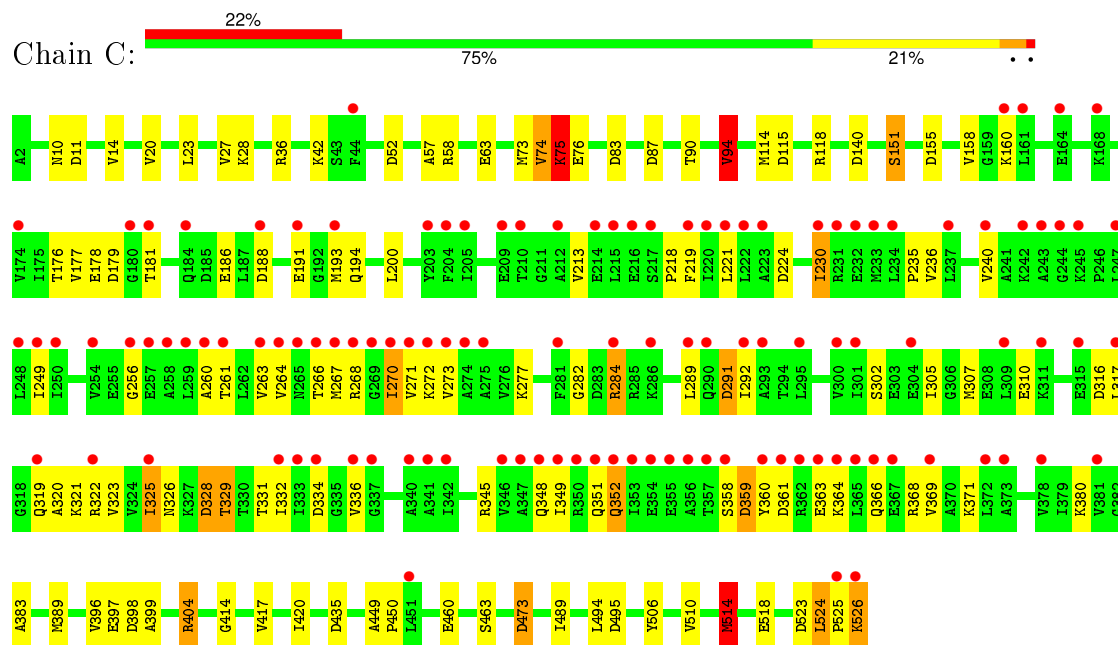
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	59	Total	O	0	0
			59	59		

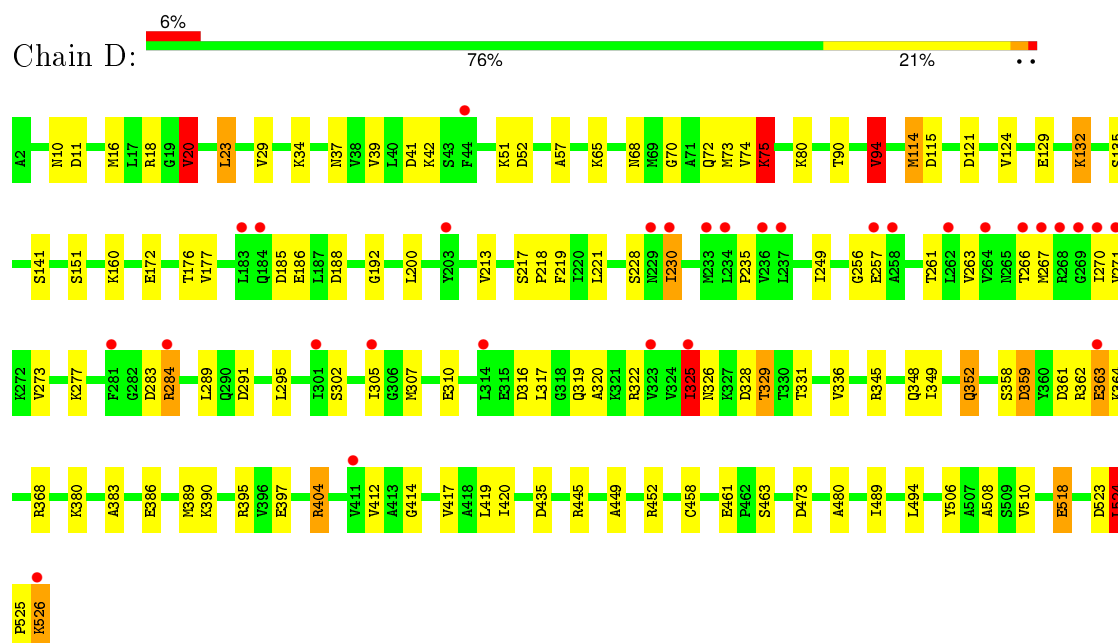




• Molecule 1: groEL protein

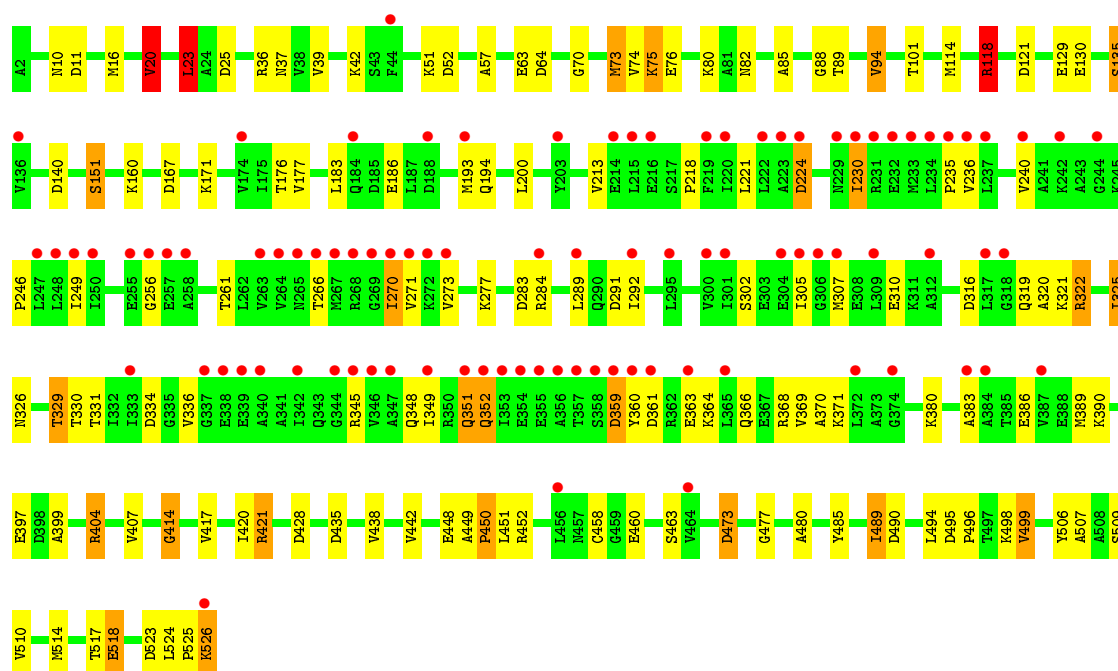


• Molecule 1: groEL protein

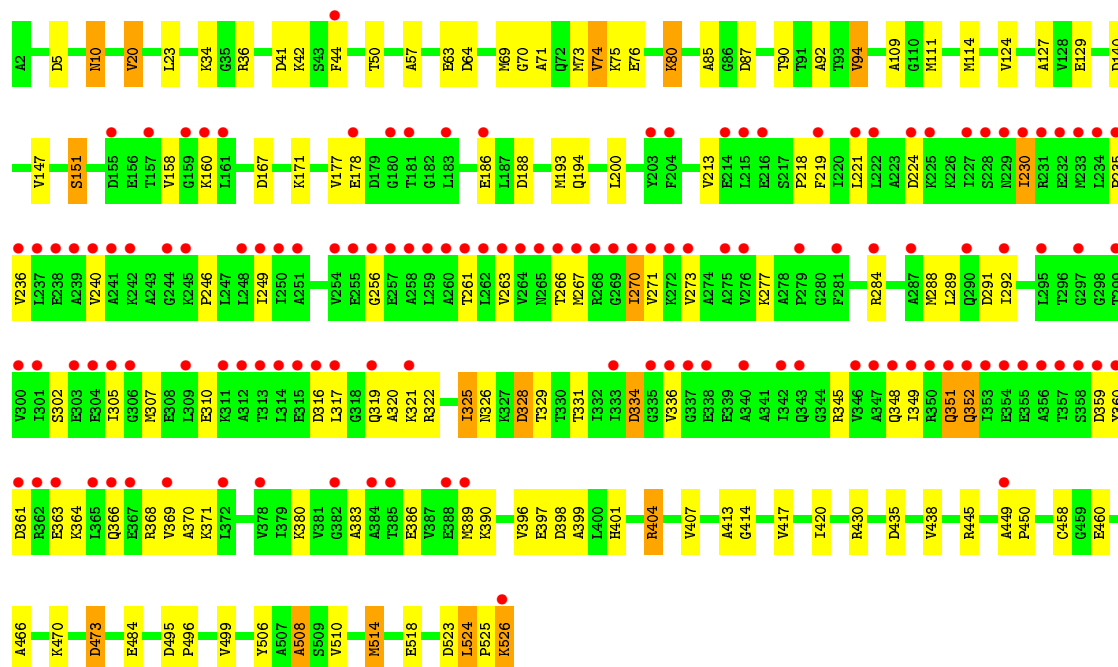


• Molecule 1: groEL protein

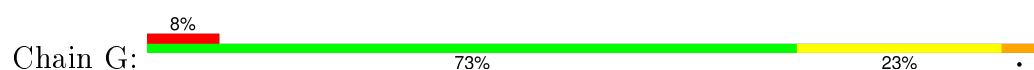


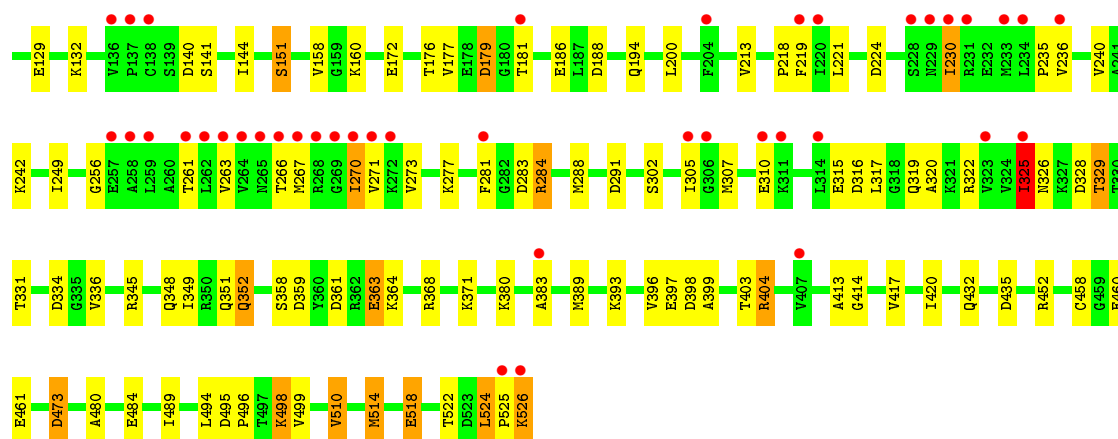


- Molecule 1: groEL protein

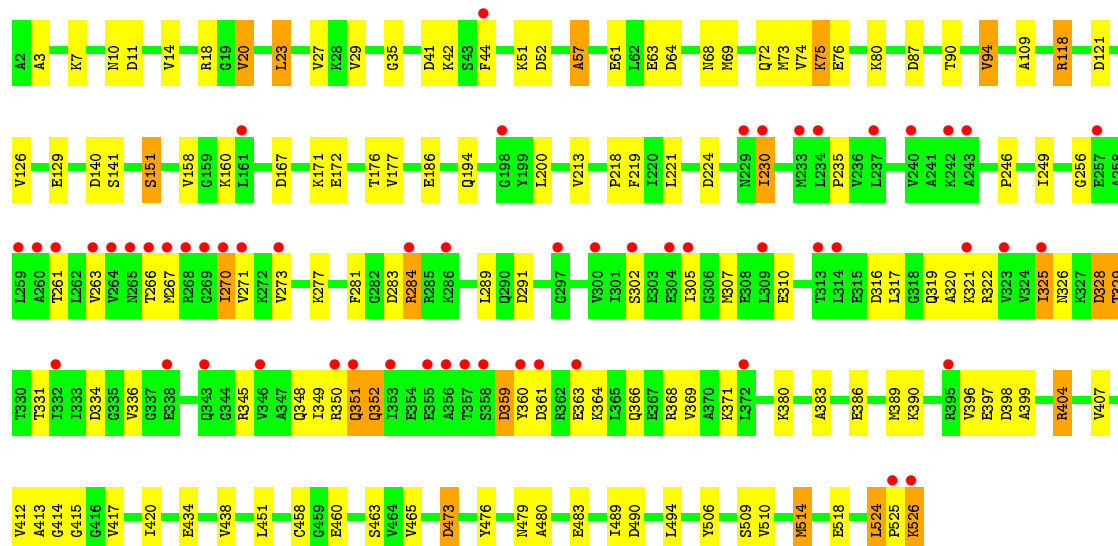


- Molecule 1: groEL protein

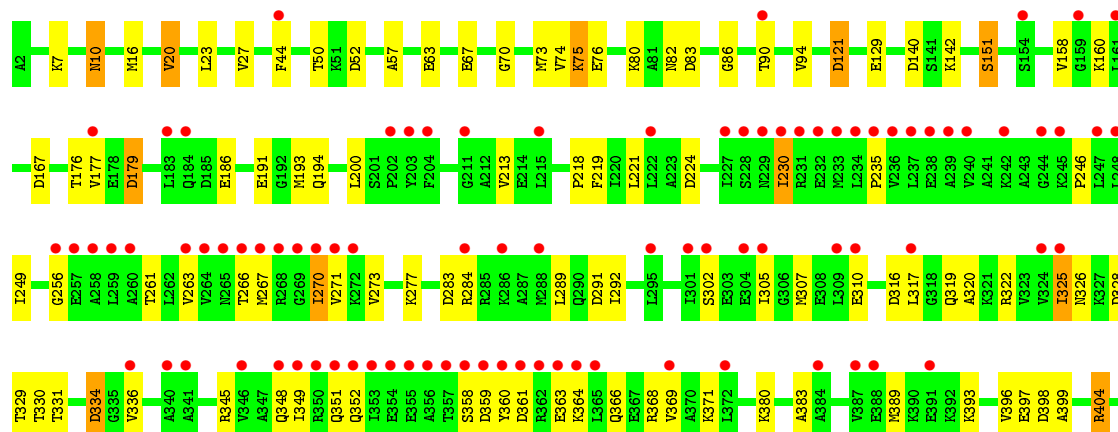
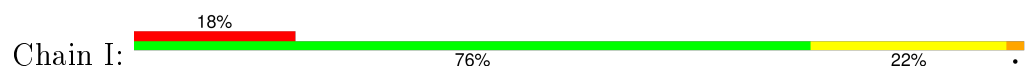




• Molecule 1: groEL protein

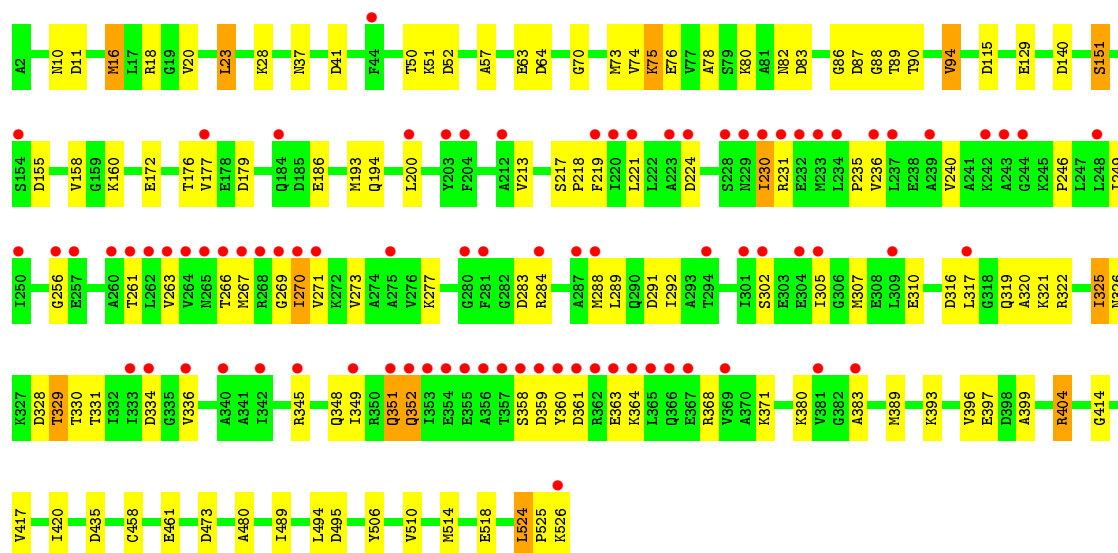
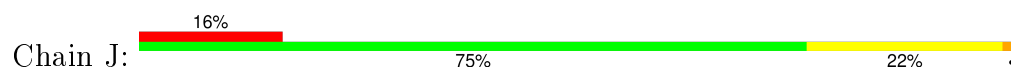


• Molecule 1: groEL protein

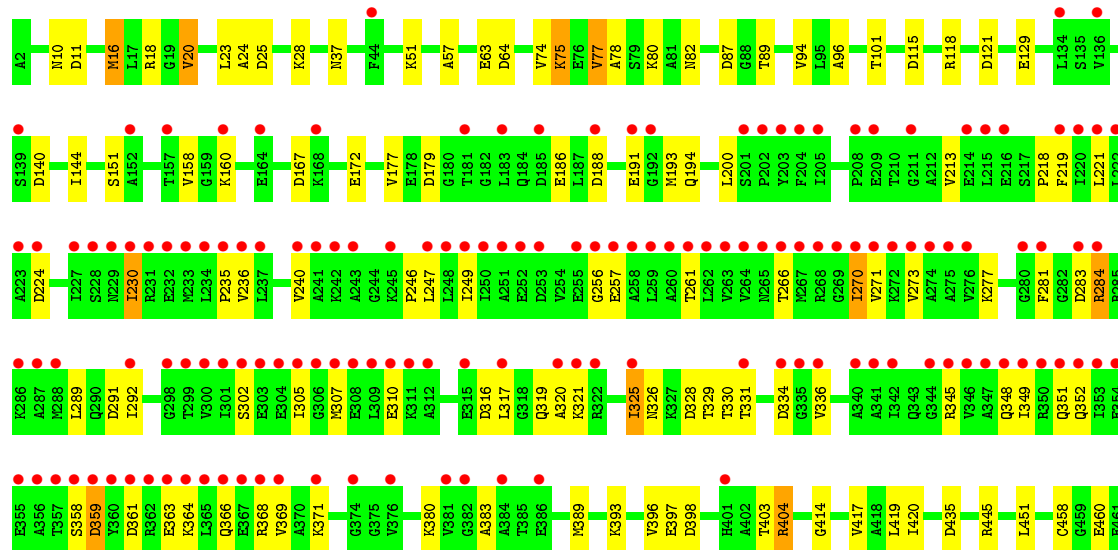
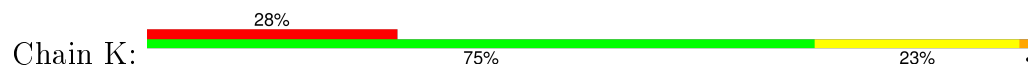




• Molecule 1: groEL protein

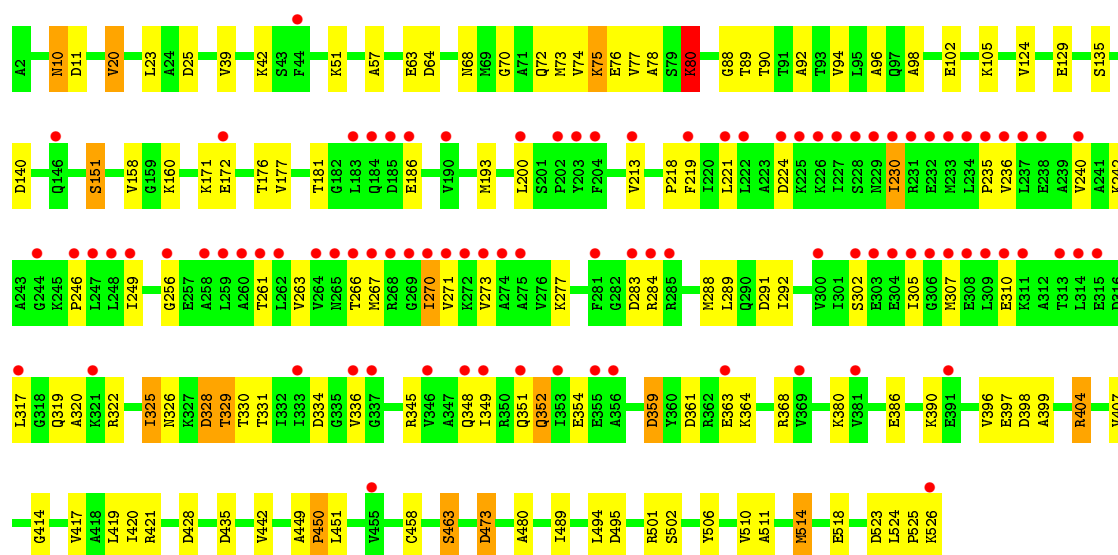


• Molecule 1: groEL protein

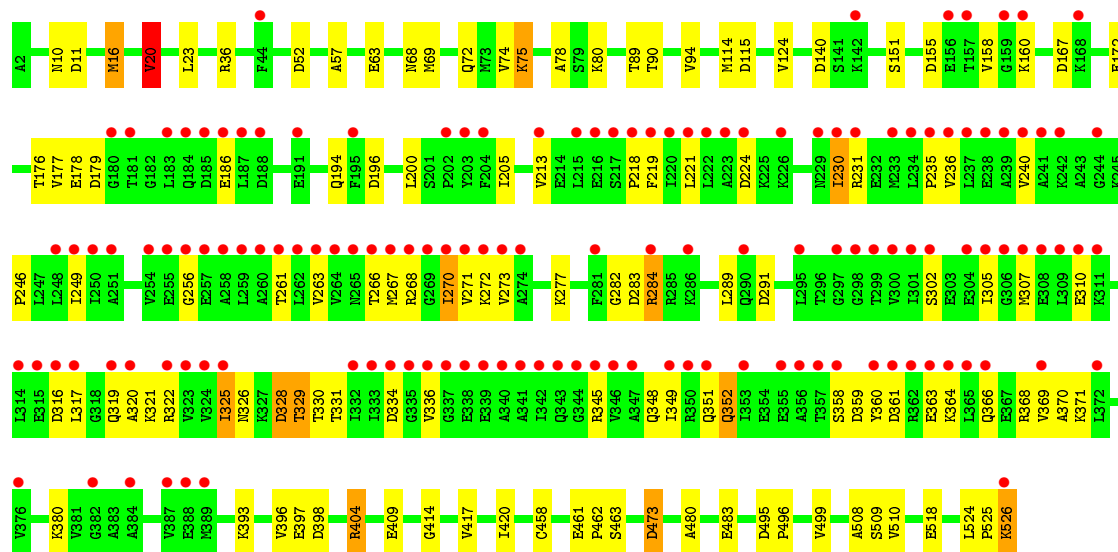
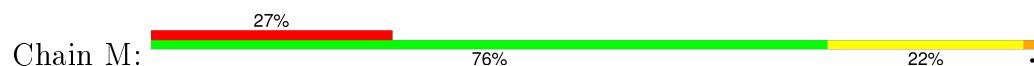


• Molecule 1: groEL protein

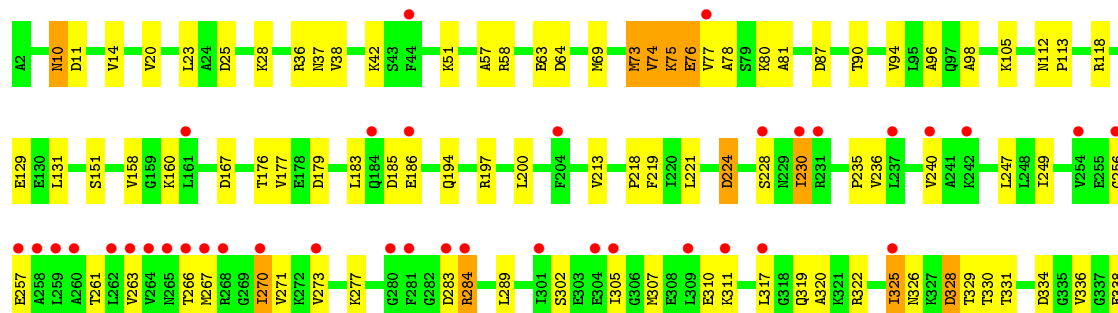


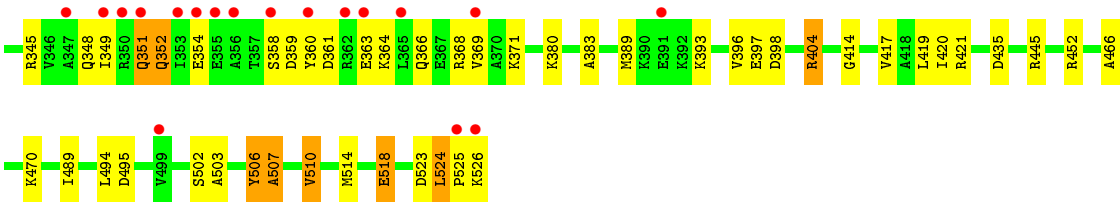


• Molecule 1: groEL protein



• Molecule 1: groEL protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.57Å 260.11Å 150.20Å 90.00° 101.14° 90.00°	Depositor
Resolution (Å)	39.84 – 2.00 39.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.84-2.00) 79.1 (39.89-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.245 , 0.265 0.246 , 0.265	Depositor DCC
$R_{free}$ test set	10672 reflections (1.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 645898 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	55380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, AGS, MG

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	1.09	12/3883 (0.3%)	1.03	21/5243 (0.4%)
1	B	1.27	27/3883 (0.7%)	1.11	25/5243 (0.5%)
1	C	1.02	10/3883 (0.3%)	0.99	22/5243 (0.4%)
1	D	1.28	18/3883 (0.5%)	1.13	25/5243 (0.5%)
1	E	1.31	32/3883 (0.8%)	1.19	37/5243 (0.7%)
1	F	1.10	18/3883 (0.5%)	1.04	21/5243 (0.4%)
1	G	1.26	25/3883 (0.6%)	1.09	21/5243 (0.4%)
1	H	1.25	32/3883 (0.8%)	1.09	24/5243 (0.5%)
1	I	1.11	9/3883 (0.2%)	1.02	19/5243 (0.4%)
1	J	1.08	11/3883 (0.3%)	1.08	21/5243 (0.4%)
1	K	1.03	10/3883 (0.3%)	1.00	18/5243 (0.3%)
1	L	1.15	19/3883 (0.5%)	1.07	22/5243 (0.4%)
1	M	1.03	10/3883 (0.3%)	1.08	18/5243 (0.3%)
1	N	1.15	16/3883 (0.4%)	1.09	26/5243 (0.5%)
All	All	1.16	249/54362 (0.5%)	1.07	320/73402 (0.4%)

The worst 5 of 249 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	510	VAL	CB-CG2	14.81	1.83	1.52
1	B	129	GLU	CD-OE2	13.14	1.40	1.25
1	B	510	VAL	CB-CG2	12.46	1.79	1.52
1	E	490	ASP	CB-CG	-11.51	1.27	1.51
1	B	129	GLU	CG-CD	11.47	1.69	1.51

The worst 5 of 320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	284	ARG	NE-CZ-NH2	21.49	131.04	120.30
1	M	284	ARG	NE-CZ-NH1	-20.20	110.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	231	ARG	NE-CZ-NH2	19.91	130.25	120.30
1	J	231	ARG	NE-CZ-NH1	-18.92	110.84	120.30
1	N	368	ARG	NE-CZ-NH2	16.05	128.32	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3979	74	1
1	B	3855	0	3979	76	0
1	C	3855	0	3979	71	0
1	D	3855	0	3979	75	0
1	E	3855	0	3979	68	0
1	F	3855	0	3979	77	0
1	G	3855	0	3979	82	2
1	H	3855	0	3979	68	1
1	I	3855	0	3979	64	1
1	J	3855	0	3979	66	0
1	K	3855	0	3979	67	0
1	L	3855	0	3979	75	1
1	M	3855	0	3979	77	0
1	N	3855	0	3979	70	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	31	0	12	3	0
4	B	31	0	12	4	0
4	C	31	0	12	2	0
4	D	31	0	12	4	0
4	E	31	0	12	3	0
4	F	31	0	11	3	0
4	G	31	0	12	4	0
4	H	31	0	12	4	0
4	I	31	0	12	4	0
4	J	31	0	12	5	0
4	K	31	0	12	2	0
4	L	31	0	12	3	0
4	M	31	0	12	3	0
4	N	31	0	12	5	0
5	A	62	0	0	3	0
5	B	83	0	0	5	0
5	C	57	0	0	3	0
5	D	91	0	0	6	0
5	E	92	0	0	4	0
5	F	71	0	0	1	0
5	G	83	0	0	8	0
5	H	77	0	0	4	0
5	I	60	0	0	3	0
5	J	50	0	0	1	0
5	K	47	0	0	3	0
5	L	61	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	53	0	0	3	0
5	N	59	0	0	2	0
All	All	55380	0	55873	997	5

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 9.

The worst 5 of 997 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:L:80:LYS:CD	1:L:80:LYS:CG	1.77	1.62
1:B:510:VAL:CG2	1:B:510:VAL:CB	1.79	1.61
4:A:1:AGS:S1G	4:A:1:AGS:PG	1.53	1.52
1:N:510:VAL:CG2	1:N:510:VAL:CB	1.83	1.51
4:J:1:AGS:S1G	4:J:1:AGS:PG	1.52	1.51

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:142:LYS:NZ	1:N:354:GLU:O[2_646]	1.85	0.35
1:G:315:GLU:OE2	1:N:338:GLU:OE1[1_554]	2.05	0.15
1:A:311:LYS:NZ	1:N:311:LYS:O[1_554]	2.09	0.11
1:H:350:ARG:NH1	1:L:354:GLU:OE1[1_455]	2.11	0.09
1:G:315:GLU:OE1	1:N:338:GLU:OE2[1_554]	2.14	0.06

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	523/525 (100%)	509 (97%)	12 (2%)	2 (0%)	39 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	523/525 (100%)	506 (97%)	15 (3%)	2 (0%)	39	33
1	C	523/525 (100%)	505 (97%)	16 (3%)	2 (0%)	39	33
1	D	523/525 (100%)	509 (97%)	13 (2%)	1 (0%)	52	48
1	E	523/525 (100%)	507 (97%)	14 (3%)	2 (0%)	39	33
1	F	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	39	33
1	G	523/525 (100%)	511 (98%)	10 (2%)	2 (0%)	39	33
1	H	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	39	33
1	I	523/525 (100%)	511 (98%)	10 (2%)	2 (0%)	39	33
1	J	523/525 (100%)	509 (97%)	12 (2%)	2 (0%)	39	33
1	K	523/525 (100%)	505 (97%)	15 (3%)	3 (1%)	30	22
1	L	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	39	33
1	M	523/525 (100%)	512 (98%)	9 (2%)	2 (0%)	39	33
1	N	523/525 (100%)	503 (96%)	18 (3%)	2 (0%)	39	33
All	All	7322/7350 (100%)	7111 (97%)	183 (2%)	28 (0%)	39	33

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	GLY
1	A	256	GLY
1	B	256	GLY
1	C	256	GLY
1	E	256	GLY

### 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	404/405 (100%)	383 (95%)	21 (5%)	29	23
1	B	404/405 (100%)	379 (94%)	25 (6%)	23	16
1	C	404/405 (100%)	381 (94%)	23 (6%)	25	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	404/405 (100%)	383 (95%)	21 (5%)	29	23
1	E	404/405 (100%)	382 (95%)	22 (5%)	27	21
1	F	404/405 (100%)	385 (95%)	19 (5%)	32	27
1	G	404/405 (100%)	381 (94%)	23 (6%)	25	19
1	H	404/405 (100%)	382 (95%)	22 (5%)	27	21
1	I	404/405 (100%)	387 (96%)	17 (4%)	36	31
1	J	404/405 (100%)	383 (95%)	21 (5%)	29	23
1	K	404/405 (100%)	384 (95%)	20 (5%)	30	24
1	L	404/405 (100%)	382 (95%)	22 (5%)	27	21
1	M	404/405 (100%)	384 (95%)	20 (5%)	30	24
1	N	404/405 (100%)	381 (94%)	23 (6%)	25	19
All	All	5656/5670 (100%)	5357 (95%)	299 (5%)	28	22

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	118	ARG
1	H	329	THR
1	N	10	ASN
1	G	188	ASP
1	G	514	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	326	ASN
1	H	453	GLN
1	M	475	ASN
1	G	351	GLN
1	H	265	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 30 are monoatomic - leaving 14 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$
4	AGS	A	1	3,2	24,33,33	4.11	5 (20%)	28,52,52	3.35	9 (32%)
4	AGS	B	1	3,2	24,33,33	4.23	4 (16%)	28,52,52	2.81	8 (28%)
4	AGS	C	1	3,2	24,33,33	4.32	4 (16%)	28,52,52	3.57	5 (17%)
4	AGS	D	561	3,2	24,33,33	4.75	7 (29%)	28,52,52	2.07	9 (32%)
4	AGS	E	1	3,2	24,33,33	4.84	5 (20%)	28,52,52	2.91	10 (35%)
4	AGS	F	1	3,2	24,33,33	4.37	4 (16%)	28,52,52	2.27	8 (28%)
4	AGS	G	1	3,2	24,33,33	4.99	6 (25%)	28,52,52	2.76	11 (39%)
4	AGS	H	1	3,2	24,33,33	4.40	6 (25%)	28,52,52	2.74	9 (32%)
4	AGS	I	1	3,2	24,33,33	4.45	4 (16%)	28,52,52	2.48	9 (32%)
4	AGS	J	1	3,2	24,33,33	4.17	3 (12%)	28,52,52	2.47	8 (28%)
4	AGS	K	1	3,2	24,33,33	4.43	6 (25%)	28,52,52	2.46	6 (21%)
4	AGS	L	1	3,2	24,33,33	4.49	5 (20%)	28,52,52	3.77	7 (25%)
4	AGS	M	1	3,2	24,33,33	4.30	4 (16%)	28,52,52	3.77	5 (17%)
4	AGS	N	1	3,2	24,33,33	4.82	5 (20%)	28,52,52	3.20	11 (39%)

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
4	AGS	A	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	B	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	C	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	D	561	3,2	-	0/15/38/38	0/3/3/3
4	AGS	E	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	F	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	G	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	H	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	I	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	J	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	K	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	L	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	M	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	N	1	3,2	-	0/15/38/38	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	AGS	PG-S1G	-23.10	1.45	1.90
4	E	1	AGS	PG-S1G	-22.39	1.47	1.90
4	N	1	AGS	PG-S1G	-22.37	1.47	1.90
4	D	561	AGS	PG-S1G	-21.48	1.48	1.90
4	L	1	AGS	PG-S1G	-21.03	1.49	1.90

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	AGS	N3-C2-N1	-18.39	114.81	128.89
4	L	1	AGS	N3-C2-N1	-17.31	115.64	128.89
4	C	1	AGS	N3-C2-N1	-17.14	115.77	128.89
4	A	1	AGS	N3-C2-N1	-14.84	117.53	128.89
4	N	1	AGS	N3-C2-N1	-11.94	119.75	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	AGS	3	0
4	B	1	AGS	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	AGS	2	0
4	D	561	AGS	4	0
4	E	1	AGS	3	0
4	F	1	AGS	3	0
4	G	1	AGS	4	0
4	H	1	AGS	4	0
4	I	1	AGS	4	0
4	J	1	AGS	5	0
4	K	1	AGS	2	0
4	L	1	AGS	3	0
4	M	1	AGS	3	0
4	N	1	AGS	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 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	525/525 (100%)	0.76	67 (12%)	5 5	10, 14, 16, 20	0
1	B	525/525 (100%)	1.42	126 (24%)	1 1	10, 14, 16, 20	0
1	C	525/525 (100%)	1.22	117 (22%)	1 1	10, 14, 16, 20	0
1	D	525/525 (100%)	0.58	30 (5%)	27 29	10, 14, 16, 20	0
1	E	525/525 (100%)	1.11	92 (17%)	2 2	9, 14, 16, 20	0
1	F	525/525 (100%)	1.37	129 (24%)	1 1	10, 14, 16, 20	0
1	G	525/525 (100%)	0.72	42 (8%)	15 16	10, 14, 16, 20	0
1	H	525/525 (100%)	0.73	56 (10%)	8 8	9, 14, 16, 20	0
1	I	525/525 (100%)	1.07	93 (17%)	2 2	9, 14, 16, 20	0
1	J	525/525 (100%)	1.00	83 (15%)	3 3	10, 14, 16, 20	0
1	K	525/525 (100%)	1.49	148 (28%)	1 1	10, 14, 16, 20	0
1	L	525/525 (100%)	0.96	91 (17%)	2 2	10, 14, 16, 20	0
1	M	525/525 (100%)	1.46	140 (26%)	1 1	10, 14, 16, 20	0
1	N	525/525 (100%)	0.75	56 (10%)	8 8	10, 14, 16, 20	0
All	All	7350/7350 (100%)	1.05	1270 (17%)	2 2	9, 14, 16, 20	0

The worst 5 of 1270 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	270	ILE	13.7
1	F	240	VAL	12.4
1	K	269	GLY	12.1
1	C	349	ILE	11.6
1	B	353	ILE	11.4

## 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
3	K	D	1	1/1	0.99	0.35	4.12	29,29,29,29	0
4	AGS	D	561	31/31	0.95	0.15	0.20	2,11,18,21	0
4	AGS	K	1	31/31	0.95	0.14	0.17	6,14,21,24	0
4	AGS	M	1	31/31	0.95	0.13	-0.10	5,12,18,21	0
4	AGS	A	1	31/31	0.97	0.13	-0.10	4,11,16,20	0
3	K	M	560	1/1	1.00	0.12	-0.18	14,14,14,14	0
4	AGS	C	1	31/31	0.96	0.14	-0.19	8,13,19,20	0
3	K	D	560	1/1	0.98	0.14	-0.29	16,16,16,16	0
4	AGS	G	1	31/31	0.96	0.14	-0.33	4,9,16,16	0
4	AGS	E	1	31/31	0.96	0.12	-0.36	2,11,19,20	0
4	AGS	L	1	31/31	0.94	0.13	-0.37	2,8,11,18	0
4	AGS	I	1	31/31	0.96	0.14	-0.47	5,12,16,20	0
4	AGS	N	1	31/31	0.96	0.12	-0.52	4,10,17,19	0
3	K	H	560	1/1	0.98	0.12	-0.57	15,15,15,15	0
4	AGS	F	1	31/31	0.96	0.13	-0.64	2,11,22,23	0
3	K	E	527	1/1	0.98	0.14	-0.91	31,31,31,31	0
4	AGS	H	1	31/31	0.96	0.12	-0.96	3,9,15,17	0
4	AGS	B	1	31/31	0.97	0.11	-1.20	8,13,21,24	0
3	K	L	560	1/1	0.99	0.12	-1.23	6,6,6,6	0
4	AGS	J	1	31/31	0.96	0.10	-1.30	2,7,14,15	0
3	K	I	560	1/1	0.99	0.14	-1.37	11,11,11,11	0
3	K	N	560	1/1	0.97	0.10	-1.56	11,11,11,11	0
3	K	B	560	1/1	0.97	0.12	-1.60	13,13,13,13	0
3	K	J	560	1/1	0.98	0.11	-1.66	11,11,11,11	0
3	K	G	560	1/1	0.98	0.13	-1.97	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	A	560	1/1	0.99	0.09	-2.37	13,13,13,13	0
3	K	F	560	1/1	0.99	0.09	-2.53	13,13,13,13	0
3	K	E	560	1/1	0.99	0.10	-2.76	11,11,11,11	0
3	K	K	560	1/1	0.99	0.09	-2.82	11,11,11,11	0
3	K	C	560	1/1	0.99	0.08	-3.20	19,19,19,19	0
2	MG	J	550	1/1	0.97	0.12	-	8,8,8,8	0
2	MG	L	550	1/1	0.88	0.12	-	9,9,9,9	0
2	MG	G	550	1/1	0.95	0.15	-	9,9,9,9	0
2	MG	I	550	1/1	0.96	0.15	-	9,9,9,9	0
2	MG	D	550	1/1	0.97	0.09	-	10,10,10,10	0
2	MG	E	550	1/1	0.98	0.08	-	6,6,6,6	0
2	MG	H	550	1/1	0.96	0.13	-	4,4,4,4	0
2	MG	F	550	1/1	0.96	0.15	-	7,7,7,7	0
2	MG	C	550	1/1	0.96	0.10	-	9,9,9,9	0
2	MG	B	550	1/1	0.92	0.12	-	8,8,8,8	0
2	MG	A	550	1/1	0.97	0.14	-	7,7,7,7	0
2	MG	N	550	1/1	0.90	0.14	-	7,7,7,7	0
2	MG	M	550	1/1	0.97	0.16	-	7,7,7,7	0
2	MG	K	550	1/1	0.96	0.08	-	7,7,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.