



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 03:26 AM GMT

PDB ID : 1MNF
Title : Domain motions in GroEL upon binding of an oligopeptide
Authors : Wang, J.; Chen, L.
Deposited on : 2002-09-05
Resolution : 3.00 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>

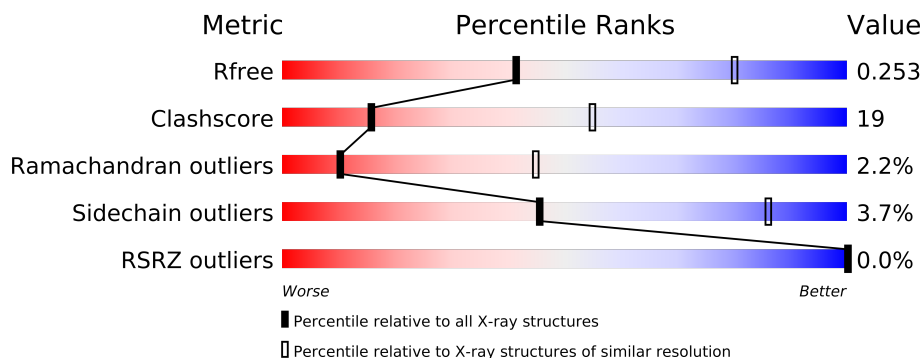
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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.



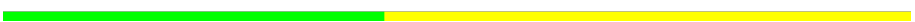




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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 ≥ 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	A	547	
1	B	547	
1	C	547	
1	D	547	
1	E	547	
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	

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Mol	Chain	Length	Quality of chain
2	1	12	
2	2	12	
2	O	12	
2	P	12	
2	Q	12	
2	R	12	
2	S	12	
2	T	12	
2	U	12	
2	V	12	
2	W	12	
2	X	12	
2	Y	12	
2	Z	12	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 55765 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	B	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	C	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	D	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	E	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	F	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	G	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	H	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	I	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	J	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	K	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	L	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	M	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			
1	N	525	Total	C	N	O	S	0	0	0
			3864	2403	667	774	20			

- Molecule 2 is a protein called 12-residue peptide substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	P	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	Q	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	R	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	S	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	T	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	U	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	V	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	W	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	X	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	Y	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	Z	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	1	12	Total 104	C 71	N 16	O 16	S 1	0	0	0
2	2	12	Total 104	C 71	N 16	O 16	S 1	0	0	0

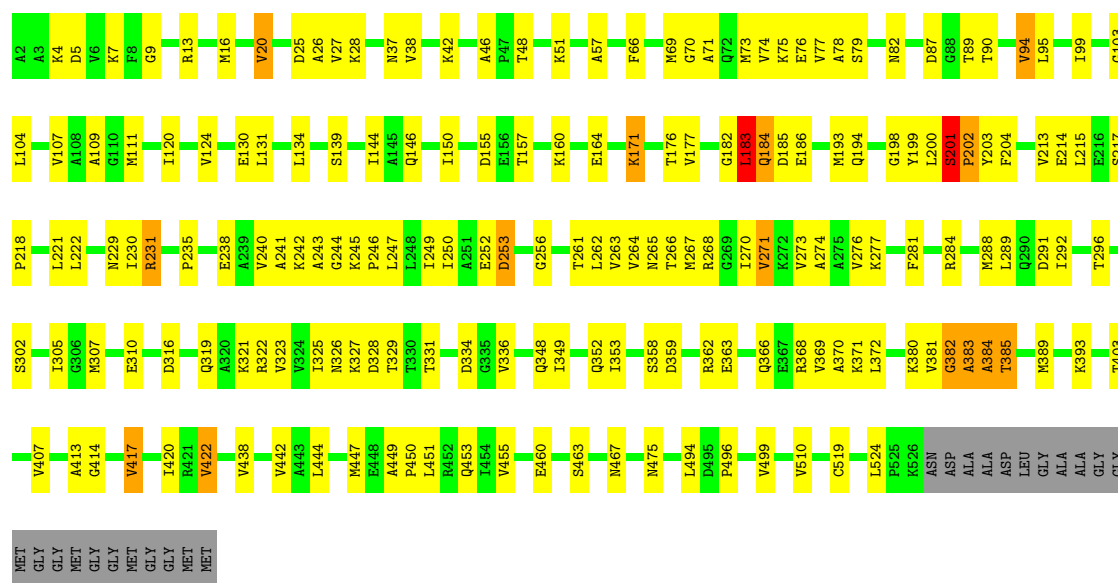
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	29	Total 29	O 29	0	0
3	C	12	Total 12	O 12	0	0
3	D	22	Total 22	O 22	0	0
3	E	19	Total 19	O 19	0	0
3	F	15	Total 15	O 15	0	0

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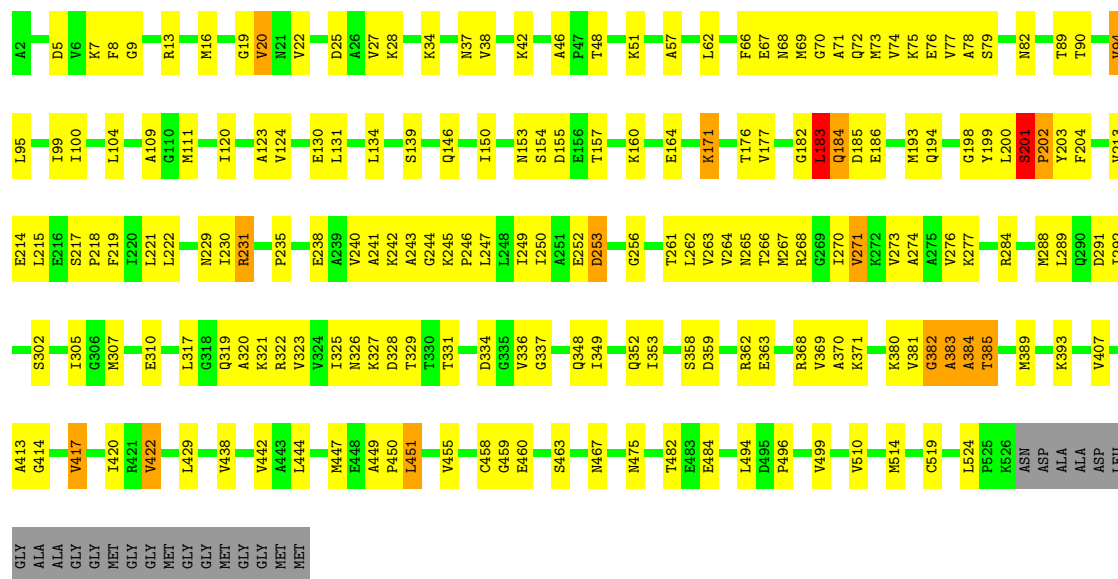
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	11	Total 11	O 11	0	0
3	H	13	Total 13	O 13	0	0
3	I	23	Total 23	O 23	0	0
3	J	10	Total 10	O 10	0	0
3	K	8	Total 8	O 8	0	0
3	L	10	Total 10	O 10	0	0
3	M	6	Total 6	O 6	0	0
3	N	15	Total 15	O 15	0	0



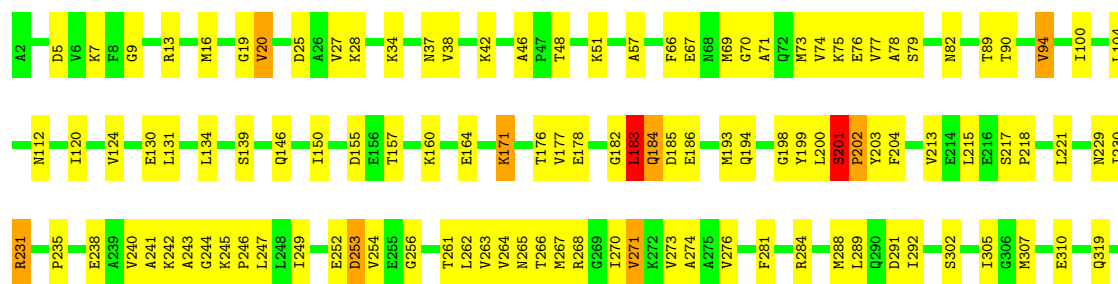
• Molecule 1: groEL protein

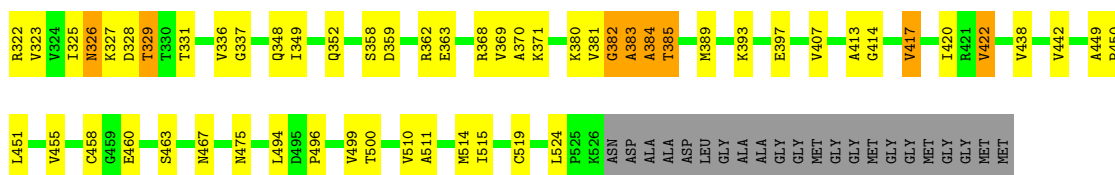
Chain D:



• Molecule 1: groEL protein

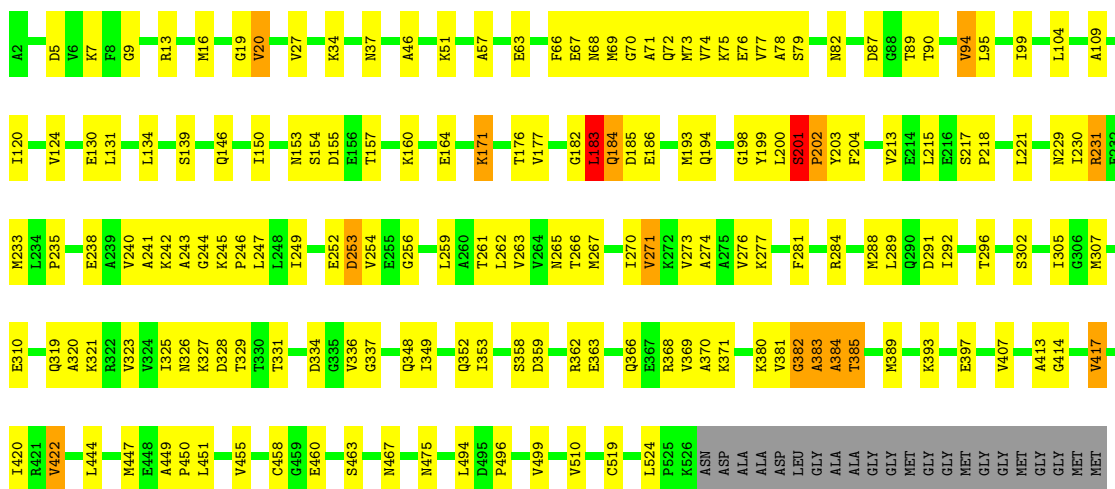
Chain E:





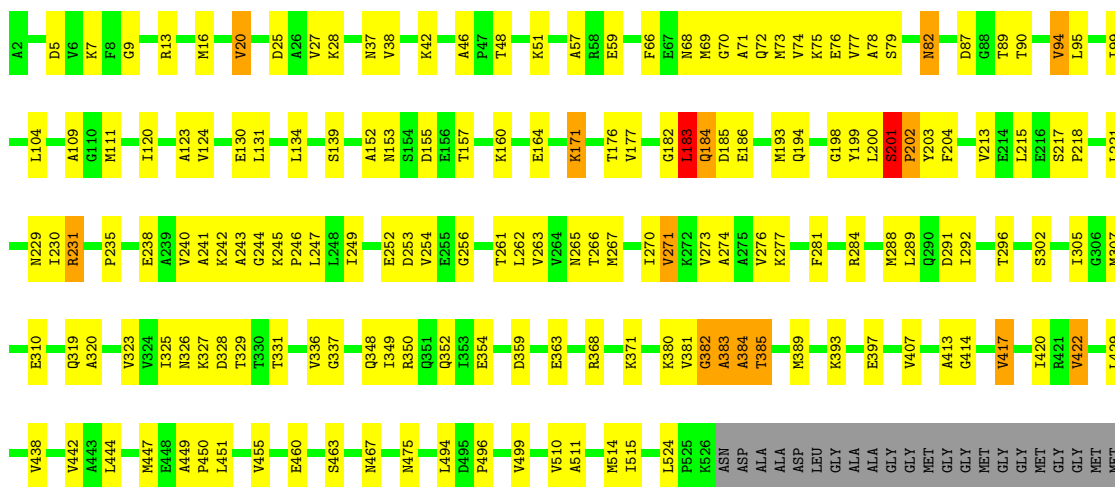
• Molecule 1: groEL protein

Chain F:



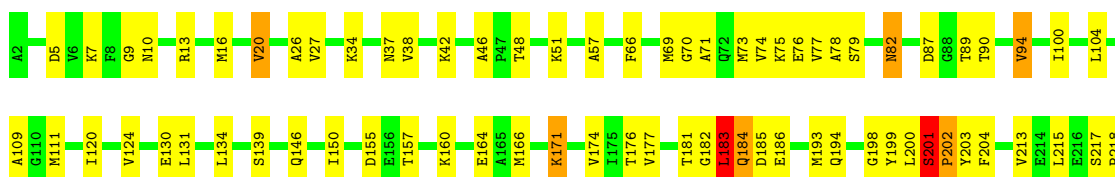
• Molecule 1: groEL protein

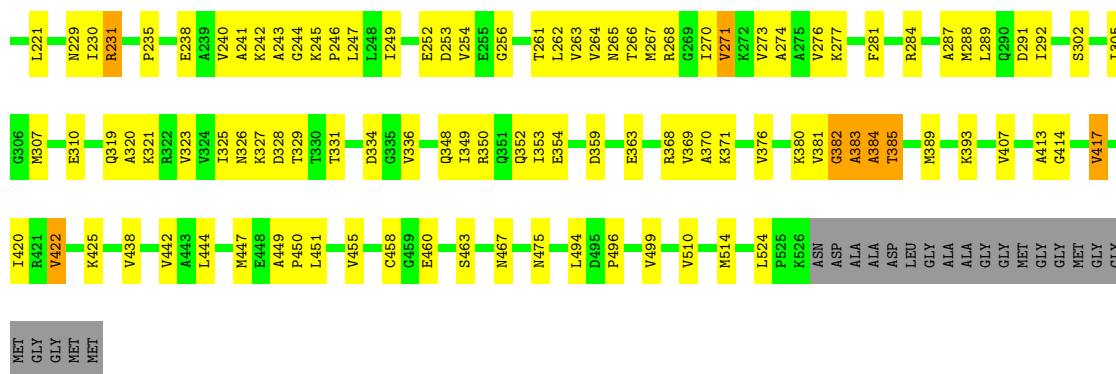
Chain G:



• Molecule 1: groEL protein

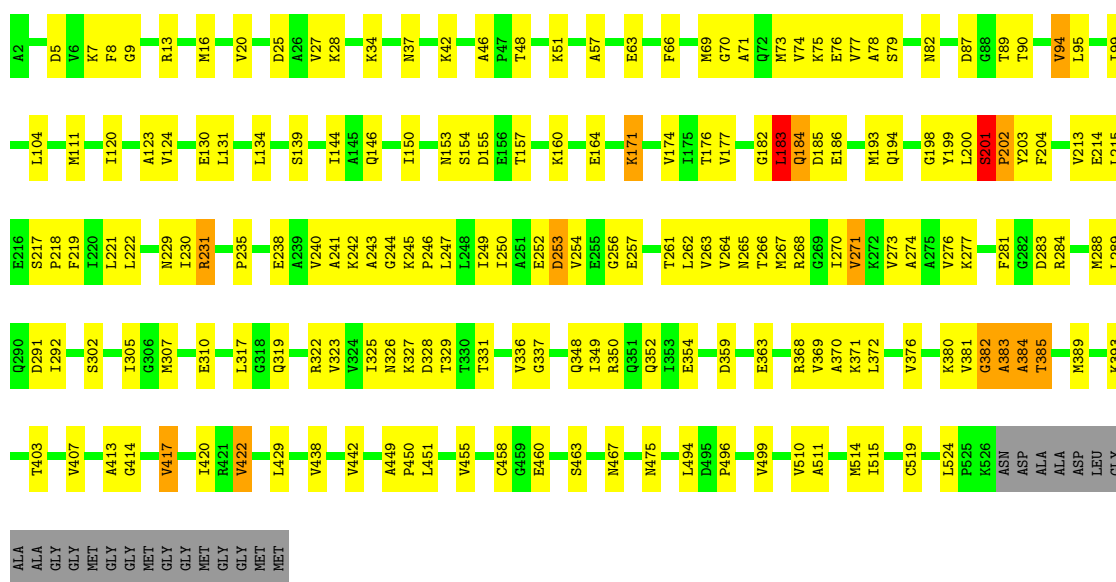
Chain H:





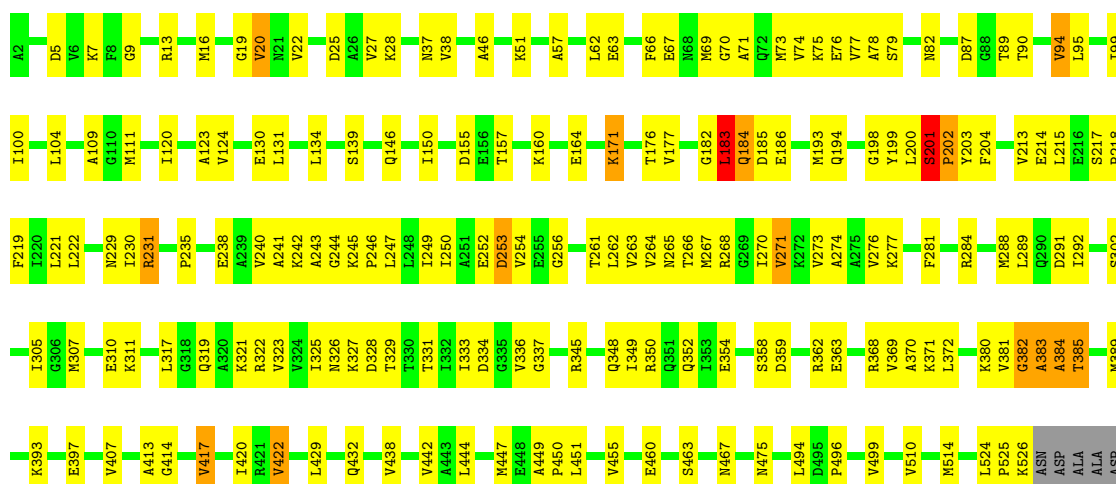
• Molecule 1: groEL protein

Chain I:



• Molecule 1: groEL protein

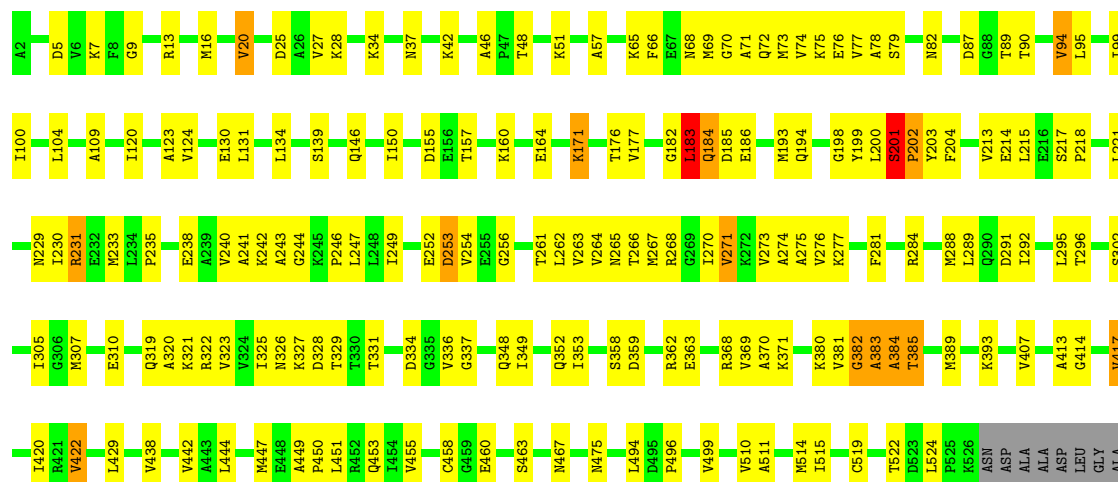
Chain J:



LEU
GLY
ALA
ALA
GLY
GLY
MET
GLY
GLY
MET
GLY
GLY
MET
GLY
MET
MET

• Molecule 1: groEL protein

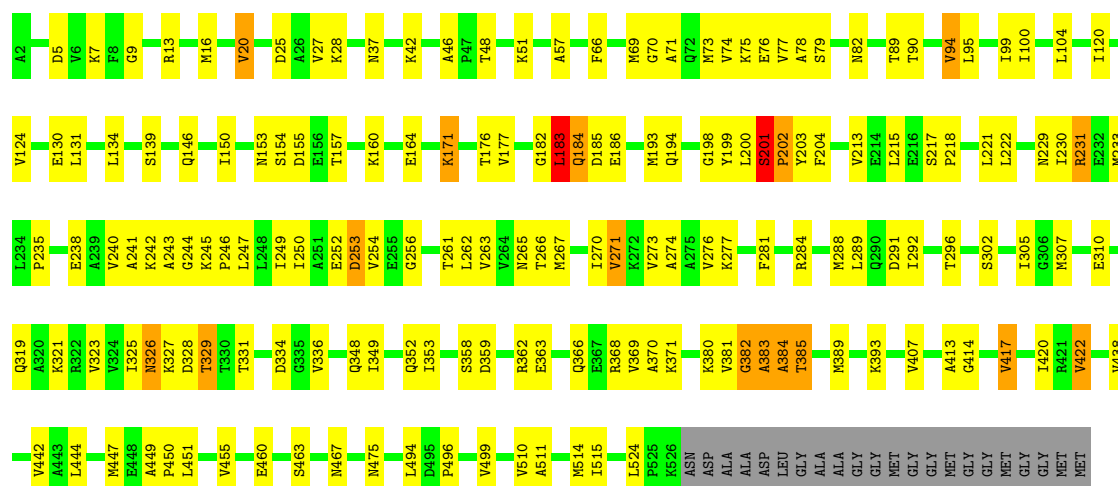
Chain K: 



ALA
GLY
GLY
MET
GLY
GLY
MET
GLY
GLY
MET
MET

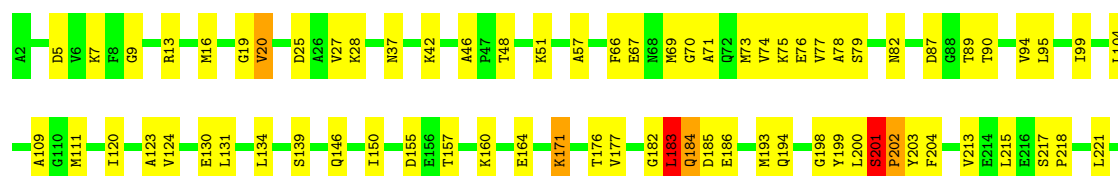
• Molecule 1: groEL protein

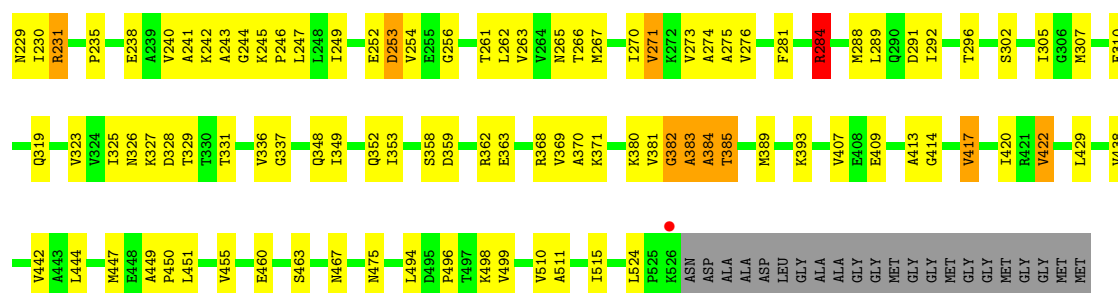
Chain L: 



• Molecule 1: groEL protein

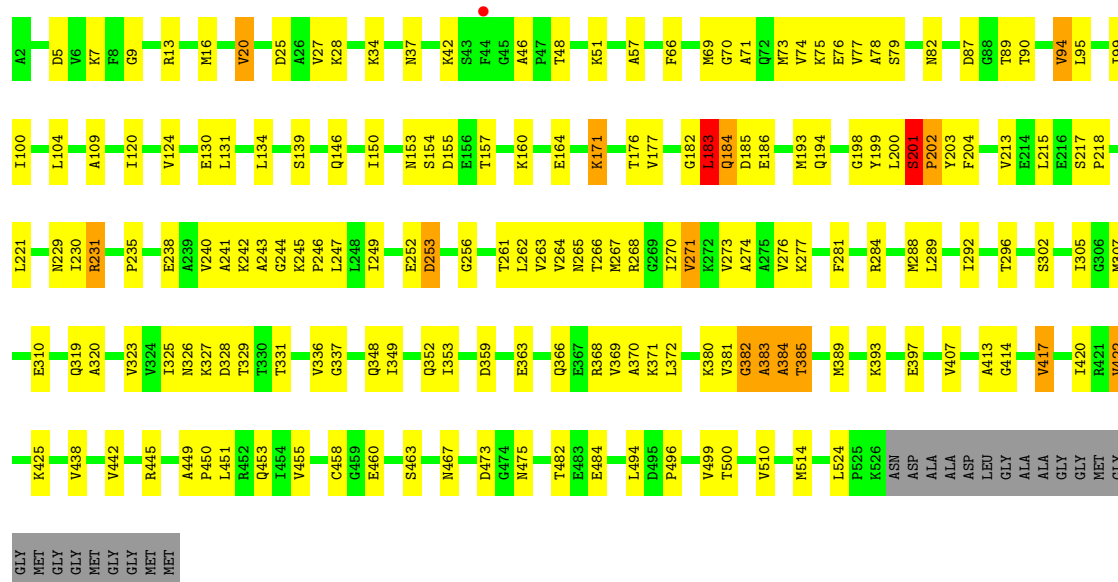
Chain M: 





- Molecule 1: groEL protein

Chain N:



- Molecule 2: 12-residue peptide substrate

Chain O:



- Molecule 2: 12-residue peptide substrate

Chain P:



- Molecule 2: 12-residue peptide substrate

Chain Q:



- Molecule 2: 12-residue peptide substrate

Chain R: 

S601	W602	M603	T604	T605	P606	W607	G608	F609	L610	H611	P612
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: 12-residue peptide substrate

Chain S: 

S601	W602	M603	T604	T605	P606	W607	G608	F609	L610	H611	P612
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: 12-residue peptide substrate

Chain T: 

S601	W602	M603	T604	T605	P606	W607	G608	F609	L610	H611	P612
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: 12-residue peptide substrate

Chain U: 

S601	W602	M603	T604	T605	P606	W607	G608	F609	L610	H611	P612
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: 12-residue peptide substrate

Chain V: 

S601	W602	M603	T604	T605	P606	W607	G608	F609	L610	H611	P612
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: 12-residue peptide substrate

Chain W: 

S601	W602	M603	T604	T605	P606	W607	G608	F609	L610	H611	P612
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: 12-residue peptide substrate

Chain X: 

S601	W602	M603	T604	T605	P606	W607	G608	F609	L610	H611	P612
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: 12-residue peptide substrate

Chain Y: 

S601	W602	M603	T604	T605	P606	W607	G608	F609	L610	H611	P612
------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: 12-residue peptide substrate

Chain Z: 



- Molecule 2: 12-residue peptide substrate

Chain 1: 



- Molecule 2: 12-residue peptide substrate

Chain 2: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.41 Å 260.69 Å 148.69 Å 90.00° 100.94° 90.00°	Depositor
Resolution (Å)	20.01 – 3.00 20.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.4 (20.01-3.00) 83.5 (20.01-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.84 (at 2.98 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.236 , 0.259 0.232 , 0.253	Depositor DCC
R_{free} test set	16677 reflections (9.95%)	DCC
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 12.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 167654 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	55765	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/3892	0.60	0/5254
1	B	0.39	0/3892	0.84	4/5254 (0.1%)
1	C	0.36	0/3892	0.60	0/5254
1	D	0.38	0/3892	0.60	0/5254
1	E	0.38	0/3892	0.60	0/5254
1	F	0.37	0/3892	0.59	0/5254
1	G	0.38	0/3892	0.59	0/5254
1	H	0.36	0/3892	0.60	0/5254
1	I	0.37	0/3892	0.60	0/5254
1	J	0.36	0/3892	0.59	0/5254
1	K	0.37	0/3892	0.60	0/5254
1	L	0.38	0/3892	0.59	0/5254
1	M	0.36	0/3892	0.66	3/5254 (0.1%)
1	N	0.37	0/3892	0.67	3/5254 (0.1%)
2	1	0.35	0/111	0.57	0/152
2	2	0.42	0/111	0.57	0/152
2	O	0.36	0/111	0.55	0/152
2	P	0.43	0/111	0.58	0/152
2	Q	0.43	0/111	0.56	0/152
2	R	0.37	0/111	0.55	0/152
2	S	0.38	0/111	0.57	0/152
2	T	0.34	0/111	0.57	0/152
2	U	0.42	0/111	0.56	0/152
2	V	0.37	0/111	0.58	0/152
2	W	0.38	0/111	0.55	0/152
2	X	0.40	0/111	0.55	0/152
2	Y	0.40	0/111	0.56	0/152
2	Z	0.33	0/111	0.57	0/152
All	All	0.37	0/56042	0.62	10/75684 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ARG	NE-CZ-NH1	-28.48	106.06	120.30
1	B	58	ARG	NE-CZ-NH2	26.84	133.72	120.30
1	N	368	ARG	NE-CZ-NH1	-15.03	112.78	120.30
1	B	58	ARG	CD-NE-CZ	14.68	144.15	123.60
1	N	368	ARG	NE-CZ-NH2	14.15	127.37	120.30

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	3864	0	3989	149	0
1	B	3864	0	3989	145	0
1	C	3864	0	3989	151	1
1	D	3864	0	3989	168	0
1	E	3864	0	3989	151	0
1	F	3864	0	3989	151	0
1	G	3864	0	3989	149	1
1	H	3864	0	3989	158	1
1	I	3864	0	3989	159	0
1	J	3864	0	3989	162	2
1	K	3864	0	3989	161	0
1	L	3864	0	3989	151	1
1	M	3864	0	3989	149	0
1	N	3864	0	3989	155	0
2	1	104	0	91	8	0
2	2	104	0	91	8	0
2	O	104	0	91	8	0
2	P	104	0	91	9	0
2	Q	104	0	91	10	0
2	R	104	0	91	11	0
2	S	104	0	91	9	0
2	T	104	0	91	9	0
2	U	104	0	91	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	104	0	91	9	0
2	W	104	0	91	9	0
2	X	104	0	91	8	0
2	Y	104	0	91	10	0
2	Z	104	0	91	6	0
3	A	20	0	0	2	0
3	B	29	0	0	4	0
3	C	12	0	0	0	0
3	D	22	0	0	0	0
3	E	19	0	0	0	0
3	F	15	0	0	0	0
3	G	11	0	0	0	0
3	H	13	0	0	2	0
3	I	23	0	0	1	0
3	J	10	0	0	3	0
3	K	8	0	0	0	0
3	L	10	0	0	1	0
3	M	6	0	0	0	0
3	N	15	0	0	3	0
All	All	55765	0	57120	2085	3

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 19.

The worst 5 of 2085 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:183:LEU:H	1:L:383:ALA:HB3	1.08	1.18
1:B:183:LEU:H	1:B:383:ALA:HB3	1.06	1.16
1:K:183:LEU:H	1:K:383:ALA:HB3	1.08	1.16
1:J:183:LEU:H	1:J:383:ALA:HB3	1.09	1.15
1:C:183:LEU:H	1:C:383:ALA:HB3	1.09	1.14

All (3) 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	Distance(Å)	Clash(Å)
1:G:354:GLU:OE1	1:J:432:GLN:O[2.655]	1.90	0.30
1:C:316:ASP:OD1	1:J:311:LYS:NZ[1.554]	2.13	0.07
1:H:166:MET:O	1:L:359:ASP:OD2[1.455]	2.13	0.07

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	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	10	43
1	B	523/547 (96%)	496 (95%)	15 (3%)	12 (2%)	10	43
1	C	523/547 (96%)	493 (94%)	18 (3%)	12 (2%)	10	43
1	D	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	10	43
1	E	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	10	43
1	F	523/547 (96%)	492 (94%)	19 (4%)	12 (2%)	10	43
1	G	523/547 (96%)	495 (95%)	17 (3%)	11 (2%)	11	47
1	H	523/547 (96%)	495 (95%)	17 (3%)	11 (2%)	11	47
1	I	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	10	43
1	J	523/547 (96%)	493 (94%)	18 (3%)	12 (2%)	10	43
1	K	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	10	43
1	L	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	10	43
1	M	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	10	43
1	N	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	10	43
2	1	10/12 (83%)	10 (100%)	0	0	100	100
2	2	10/12 (83%)	10 (100%)	0	0	100	100
2	O	10/12 (83%)	10 (100%)	0	0	100	100
2	P	10/12 (83%)	10 (100%)	0	0	100	100
2	Q	10/12 (83%)	10 (100%)	0	0	100	100
2	R	10/12 (83%)	10 (100%)	0	0	100	100
2	S	10/12 (83%)	10 (100%)	0	0	100	100
2	T	10/12 (83%)	10 (100%)	0	0	100	100
2	U	10/12 (83%)	10 (100%)	0	0	100	100
2	V	10/12 (83%)	10 (100%)	0	0	100	100
2	W	10/12 (83%)	10 (100%)	0	0	100	100
2	X	10/12 (83%)	10 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	10/12 (83%)	10 (100%)	0	0	100	100
2	Z	10/12 (83%)	10 (100%)	0	0	100	100
All	All	7462/7826 (95%)	7060 (95%)	236 (3%)	166 (2%)	10	45

5 of 166 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	B	183	LEU
1	C	183	LEU
1	D	183	LEU
1	E	183	LEU

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	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	B	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	C	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	D	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	E	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	F	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	G	405/414 (98%)	389 (96%)	16 (4%)	42	84
1	H	405/414 (98%)	389 (96%)	16 (4%)	42	84
1	I	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	J	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	K	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	L	405/414 (98%)	390 (96%)	15 (4%)	45	86
1	M	405/414 (98%)	389 (96%)	16 (4%)	42	84
1	N	405/414 (98%)	390 (96%)	15 (4%)	45	86
2	1	11/11 (100%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	11/11 (100%)	11 (100%)	0	100	100
2	O	11/11 (100%)	11 (100%)	0	100	100
2	P	11/11 (100%)	11 (100%)	0	100	100
2	Q	11/11 (100%)	11 (100%)	0	100	100
2	R	11/11 (100%)	11 (100%)	0	100	100
2	S	11/11 (100%)	11 (100%)	0	100	100
2	T	11/11 (100%)	11 (100%)	0	100	100
2	U	11/11 (100%)	11 (100%)	0	100	100
2	V	11/11 (100%)	11 (100%)	0	100	100
2	W	11/11 (100%)	11 (100%)	0	100	100
2	X	11/11 (100%)	11 (100%)	0	100	100
2	Y	11/11 (100%)	11 (100%)	0	100	100
2	Z	11/11 (100%)	11 (100%)	0	100	100
All	All	5824/5950 (98%)	5611 (96%)	213 (4%)	45	86

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	183	LEU
1	H	417	VAL
1	M	422	VAL
1	G	289	LEU
1	H	82	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	265	ASN
1	H	453	GLN
1	M	475	ASN
1	G	319	GLN
1	H	37	ASN

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 ⓘ

There are no ligands in this entry.

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, 95th 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 ²)	Q<0.9
1	A	525/547 (95%)	-0.31	0	100	100	12, 36, 70, 88	0
1	B	525/547 (95%)	-0.30	0	100	100	12, 36, 70, 88	0
1	C	525/547 (95%)	-0.34	0	100	100	12, 36, 69, 88	0
1	D	525/547 (95%)	-0.32	0	100	100	12, 36, 69, 88	0
1	E	525/547 (95%)	-0.31	0	100	100	12, 36, 69, 88	0
1	F	525/547 (95%)	-0.32	0	100	100	13, 36, 69, 88	0
1	G	525/547 (95%)	-0.33	0	100	100	11, 35, 69, 88	0
1	H	525/547 (95%)	-0.31	0	100	100	12, 36, 71, 88	0
1	I	525/547 (95%)	-0.31	0	100	100	12, 36, 71, 88	0
1	J	525/547 (95%)	-0.33	0	100	100	13, 37, 69, 88	0
1	K	525/547 (95%)	-0.31	0	100	100	12, 36, 70, 88	0
1	L	525/547 (95%)	-0.32	0	100	100	12, 36, 69, 88	0
1	M	525/547 (95%)	-0.34	1 (0%)	93	54	12, 37, 70, 88	0
1	N	525/547 (95%)	-0.31	1 (0%)	93	54	12, 36, 70, 88	0
2	1	12/12 (100%)	-0.13	0	100	100	42, 55, 70, 74	0
2	2	12/12 (100%)	-0.11	0	100	100	43, 55, 71, 74	0
2	O	12/12 (100%)	-0.14	0	100	100	43, 55, 70, 74	0
2	P	12/12 (100%)	-0.16	0	100	100	42, 55, 70, 74	0
2	Q	12/12 (100%)	-0.17	0	100	100	43, 55, 70, 74	0
2	R	12/12 (100%)	0.00	0	100	100	43, 55, 70, 74	0
2	S	12/12 (100%)	0.01	0	100	100	43, 54, 70, 74	0
2	T	12/12 (100%)	-0.25	0	100	100	43, 54, 70, 74	0
2	U	12/12 (100%)	-0.09	0	100	100	43, 54, 70, 74	0
2	V	12/12 (100%)	-0.08	0	100	100	43, 54, 71, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
2	W	12/12 (100%)	-0.16	0	100	100	44, 55, 71, 74	0
2	X	12/12 (100%)	-0.14	0	100	100	43, 55, 70, 74	0
2	Y	12/12 (100%)	-0.05	0	100	100	44, 55, 70, 74	0
2	Z	12/12 (100%)	-0.15	0	100	100	43, 55, 70, 74	0
All	All	7518/7826 (96%)	-0.31	2 (0%)	100	100	11, 37, 71, 88	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	526	LYS	2.6
1	N	44	PHE	2.4

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.