



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:43 pm GMT

PDB ID : 1MNF
Title : Domain motions in GroEL upon binding of an oligopeptide
Authors : Wang, J.; Chen, L.
Deposited on : 2003-12-02
Resolution : 3.00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	trunk28620

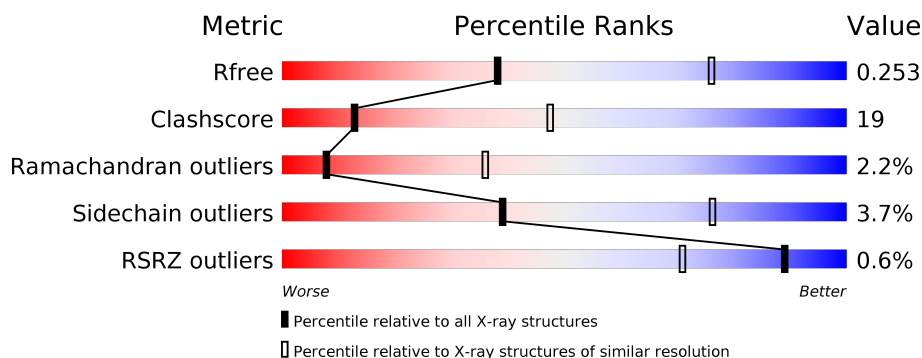
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.






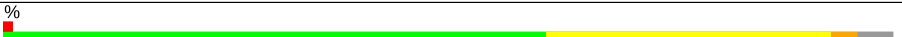
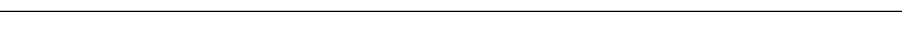
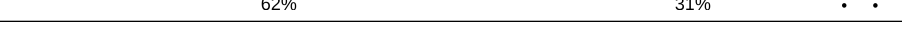
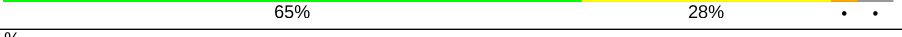


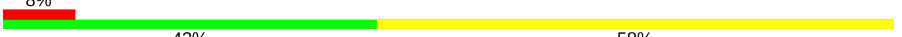

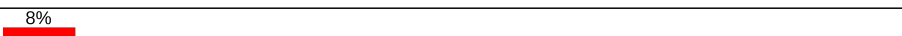

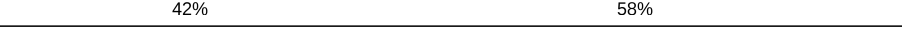

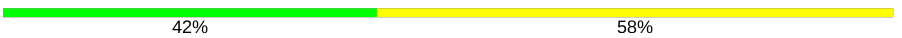



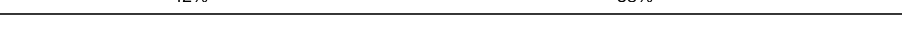


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	547	<div> <div></div> <div>65%28% . .</div> </div>
1	B	547	<div> <div></div> <div>65%28% . .</div> </div>
1	C	547	<div> <div>%</div> <div>63%30% . .</div> </div>
1	D	547	<div> <div></div> <div>61%32% . .</div> </div>
1	E	547	<div> <div>%</div> <div>65%28% . .</div> </div>
1	F	547	<div> <div>%</div> <div>64%29% . .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	
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 [i](#)

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

Continued on next page...

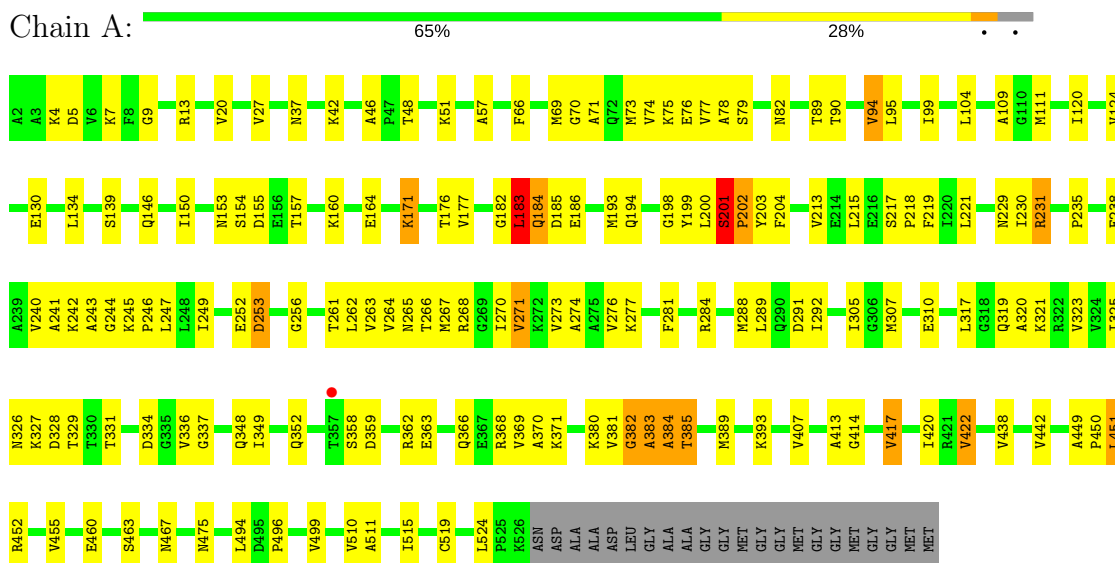
Continued from previous page...

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

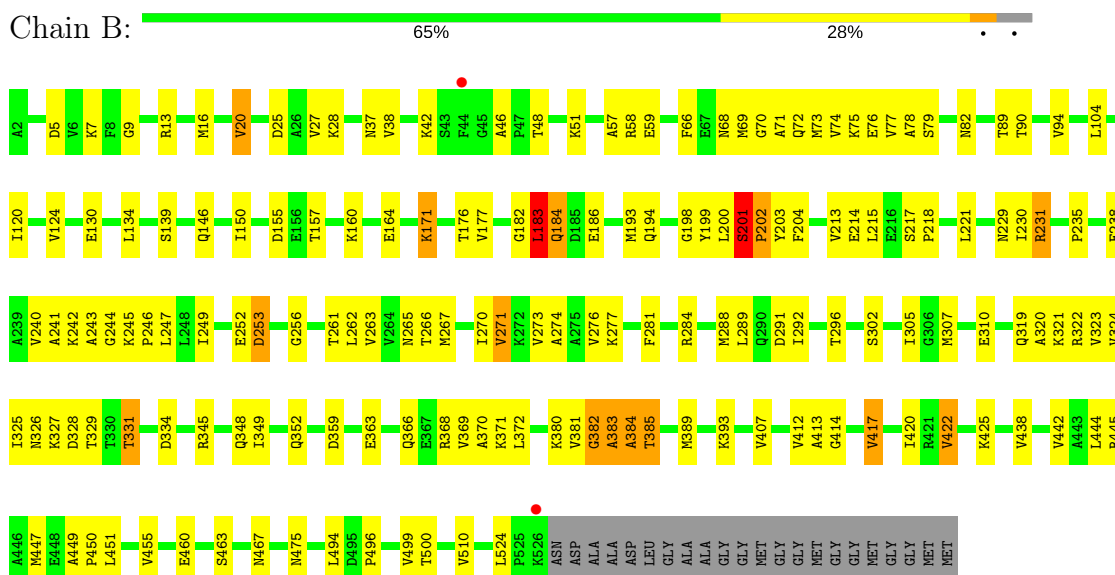
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

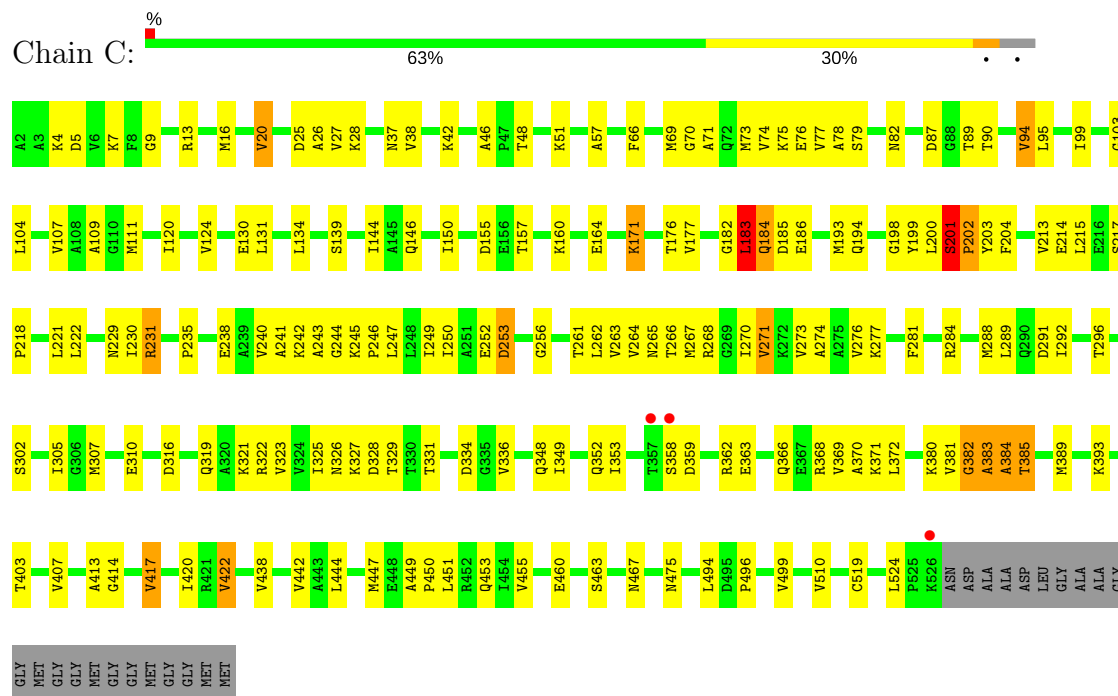
• Molecule 1: groEL protein



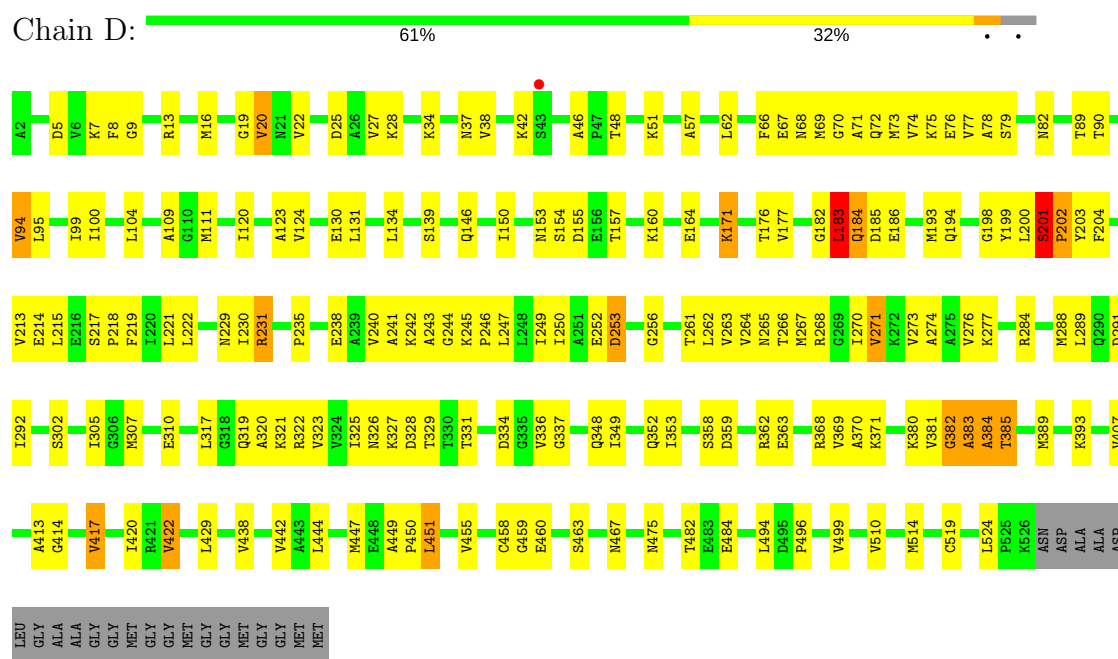
• Molecule 1: groEL protein



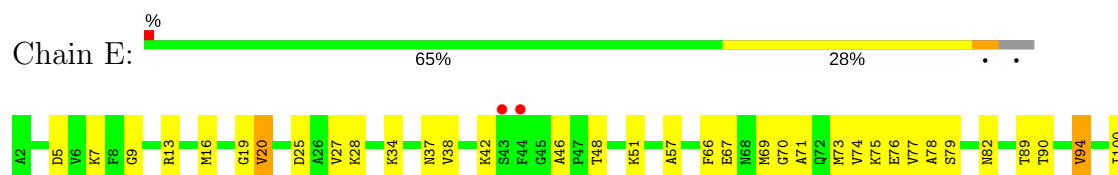
- Molecule 1: groEL protein

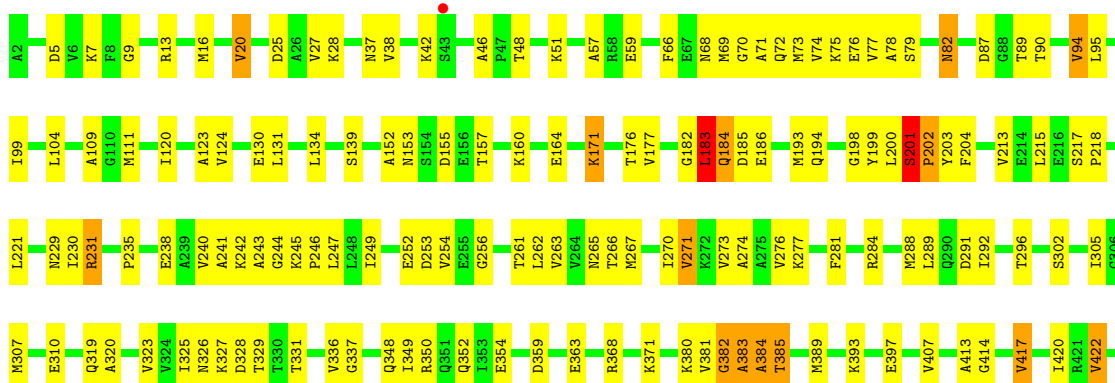


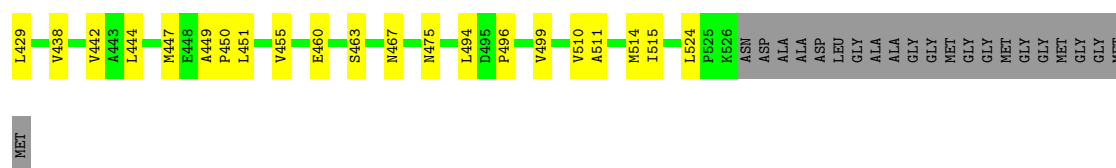
- Molecule 1: groEL protein



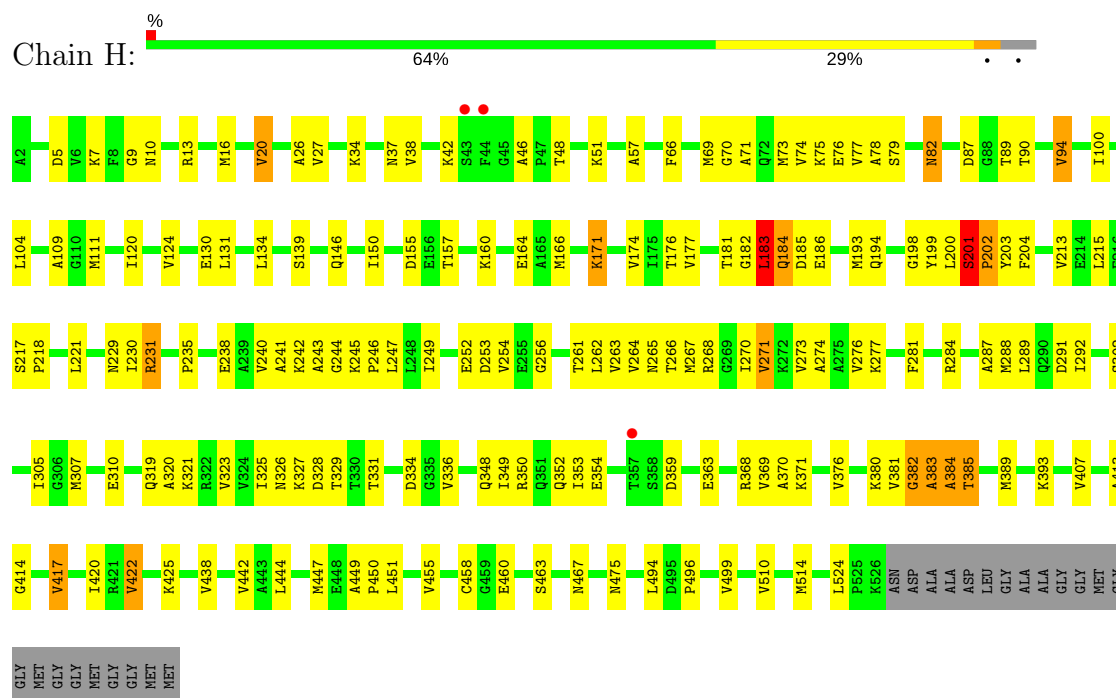
- Molecule 1: groEL protein



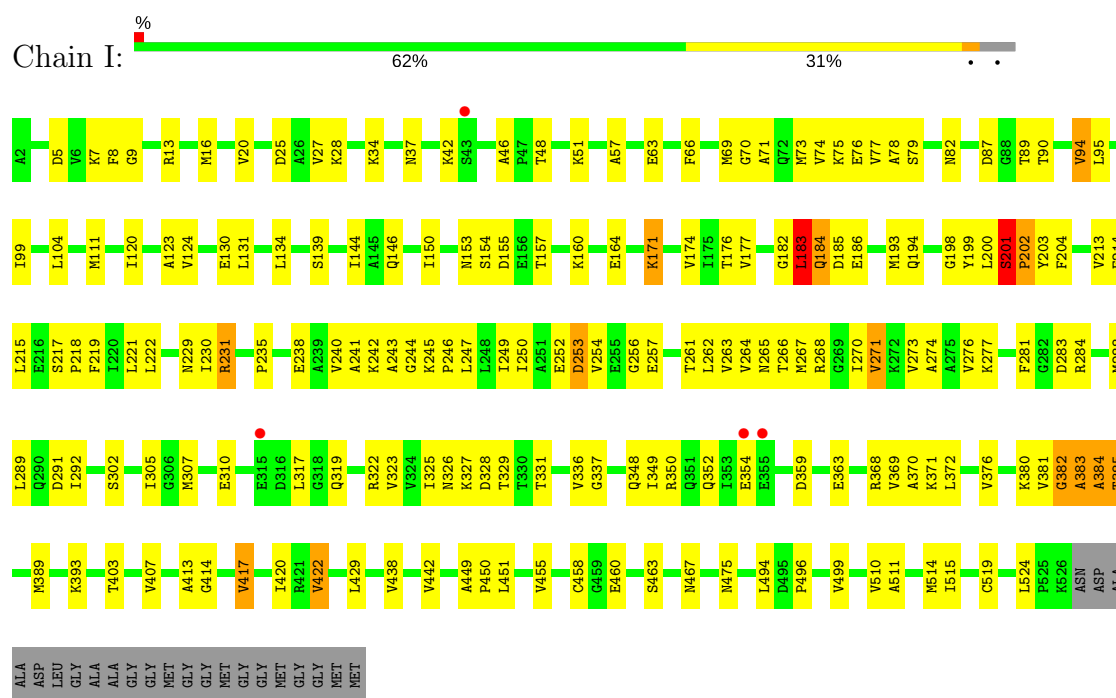




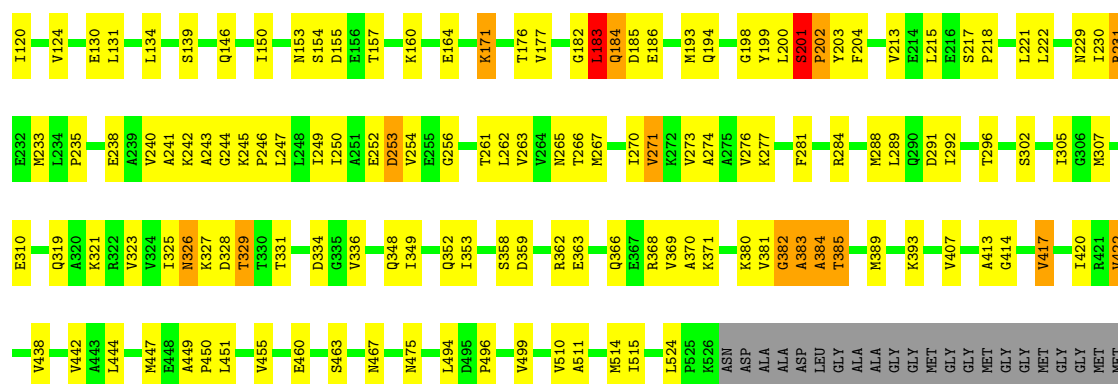
- Molecule 1: groEL protein



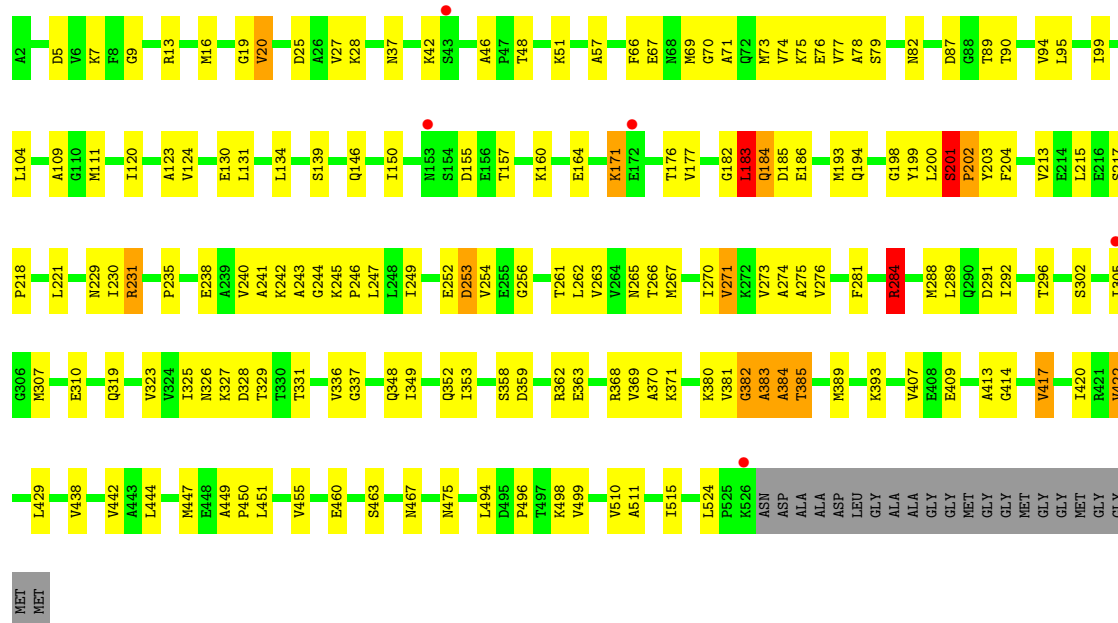
- Molecule 1: groEL protein



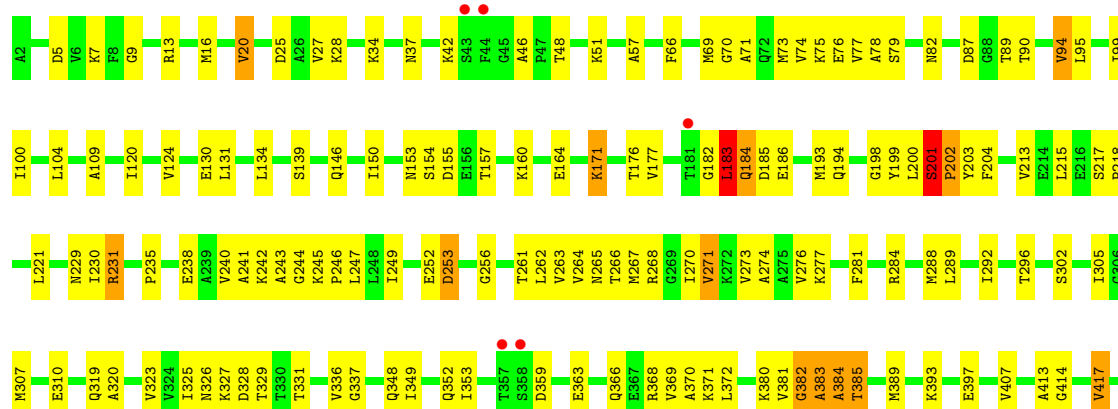
- Molecule 1: groEL protein

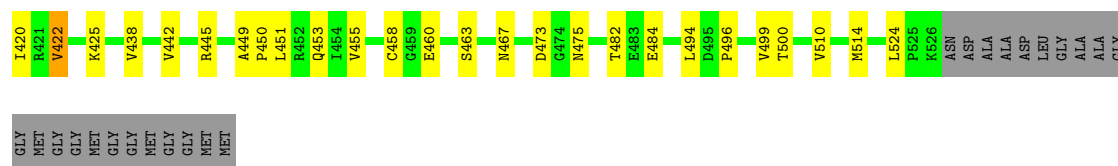


• Molecule 1: groEL protein



• Molecule 1: groEL protein





- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate



- Molecule 2: 12-residue peptide substrate

Chain U:  42% 58%



- Molecule 2: 12-residue peptide substrate

Chain V:  42% 58%



- Molecule 2: 12-residue peptide substrate

Chain W:  42% 58%



- Molecule 2: 12-residue peptide substrate

Chain X:  42% 58%



- Molecule 2: 12-residue peptide substrate

Chain Y:  42% 58%



- Molecule 2: 12-residue peptide substrate

Chain Z:  75% 25%



- Molecule 2: 12-residue peptide substrate

Chain 1:  8% 42% 58%



- Molecule 2: 12-residue peptide substrate

Chain 2:  42% 58%

S601
W602
W603
T604
T605
P606
W607
G608
P609
L610
H611
P612

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.41Å 260.69Å 148.69Å 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 2.98Å)	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 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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

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 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	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
2	V	104	0	91	9	0
2	W	104	0	91	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 19.

The worst 5 of 2085 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: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	Interatomic distance (Å)	Clash overlap (Å)
1:G:354:GLU:OE1	1:J:432:GLN:O[2_655]	1.90	0.30
1:H:166:MET:O	1:L:359:ASP:OD2[1_455]	2.13	0.07
1:C:316:ASP:OD1	1:J:311:LYS:NZ[1_554]	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%)	7	35
1	B	523/547 (96%)	496 (95%)	15 (3%)	12 (2%)	7	35
1	C	523/547 (96%)	493 (94%)	18 (3%)	12 (2%)	7	35
1	D	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	7	35
1	E	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	7	35
1	F	523/547 (96%)	492 (94%)	19 (4%)	12 (2%)	7	35
1	G	523/547 (96%)	495 (95%)	17 (3%)	11 (2%)	8	38
1	H	523/547 (96%)	495 (95%)	17 (3%)	11 (2%)	8	38
1	I	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	7	35
1	J	523/547 (96%)	493 (94%)	18 (3%)	12 (2%)	7	35
1	K	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	7	35
1	L	523/547 (96%)	494 (94%)	17 (3%)	12 (2%)	7	35
1	M	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	7	35
1	N	523/547 (96%)	495 (95%)	16 (3%)	12 (2%)	7	35
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	10/12 (83%)	10 (100%)	0	0	100	100
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%)	8	36

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%)	39	76
1	B	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	C	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	D	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	E	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	F	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	G	405/414 (98%)	389 (96%)	16 (4%)	36	74
1	H	405/414 (98%)	389 (96%)	16 (4%)	36	74
1	I	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	J	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	K	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	L	405/414 (98%)	390 (96%)	15 (4%)	39	76
1	M	405/414 (98%)	389 (96%)	16 (4%)	36	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	405/414 (98%)	390 (96%)	15 (4%)	39	76
2	1	11/11 (100%)	11 (100%)	0	100	100
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%)	39	76

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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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%)	-0.46	1 (0%) 94 85	12, 36, 70, 88	0
1	B	525/547 (95%)	-0.43	2 (0%) 92 77	12, 36, 70, 88	0
1	C	525/547 (95%)	-0.49	3 (0%) 89 71	12, 36, 69, 88	0
1	D	525/547 (95%)	-0.47	1 (0%) 94 85	12, 36, 69, 88	0
1	E	525/547 (95%)	-0.45	4 (0%) 86 64	12, 36, 69, 88	0
1	F	525/547 (95%)	-0.46	5 (0%) 82 58	13, 36, 69, 88	0
1	G	525/547 (95%)	-0.48	1 (0%) 94 85	11, 35, 69, 88	0
1	H	525/547 (95%)	-0.45	3 (0%) 89 71	12, 36, 71, 88	0
1	I	525/547 (95%)	-0.44	4 (0%) 86 64	12, 36, 71, 88	0
1	J	525/547 (95%)	-0.49	4 (0%) 86 64	13, 37, 69, 88	0
1	K	525/547 (95%)	-0.46	2 (0%) 92 77	12, 36, 70, 88	0
1	L	525/547 (95%)	-0.47	2 (0%) 92 77	12, 36, 69, 88	0
1	M	525/547 (95%)	-0.50	5 (0%) 82 58	12, 37, 70, 88	0
1	N	525/547 (95%)	-0.46	5 (0%) 82 58	12, 36, 70, 88	0
2	1	12/12 (100%)	-0.04	1 (8%) 12 4	42, 55, 70, 74	0
2	2	12/12 (100%)	-0.08	0 100 100	43, 55, 71, 74	0
2	O	12/12 (100%)	-0.09	1 (8%) 12 4	43, 55, 70, 74	0
2	P	12/12 (100%)	-0.18	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%)	0.16	0 100 100	43, 55, 70, 74	0
2	S	12/12 (100%)	0.21	1 (8%) 12 4	43, 54, 70, 74	0
2	T	12/12 (100%)	-0.38	0 100 100	43, 54, 70, 74	0
2	U	12/12 (100%)	0.03	0 100 100	43, 54, 70, 74	0
2	V	12/12 (100%)	0.01	0 100 100	43, 54, 71, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	12/12 (100%)	-0.17	0 100 100	44, 55, 71, 74	0
2	X	12/12 (100%)	-0.18	0 100 100	43, 55, 70, 74	0
2	Y	12/12 (100%)	0.08	0 100 100	44, 55, 70, 74	0
2	Z	12/12 (100%)	-0.10	0 100 100	43, 55, 70, 74	0
All	All	7518/7826 (96%)	-0.46	45 (0%) 89 71	11, 37, 71, 88	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	44	PHE	4.2
1	J	43	SER	4.0
1	I	43	SER	3.7
1	M	526	LYS	3.6
1	G	43	SER	3.5

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.