



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:33 am GMT

PDB ID : 1OEL
Title : CONFORMATIONAL VARIABILITY IN THE REFINED STRUCTURE OF
THE CHAPERONIN GROEL AT 2.8 ANGSTROM RESOLUTION
Authors : Braig, K.; Adams, P.D.; Brunger, A.T.
Deposited on : 1995-11-21
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

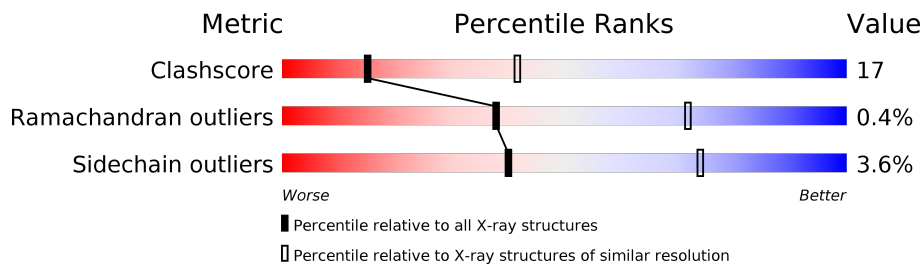
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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.

Note EDS was not executed.

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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27078 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 (HSP60 CLASS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	B	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	C	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	D	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	E	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	F	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			
1	G	524	Total	C	N	O	S	0	0	0
			3847	2393	662	773	19			

There are 14 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is water.

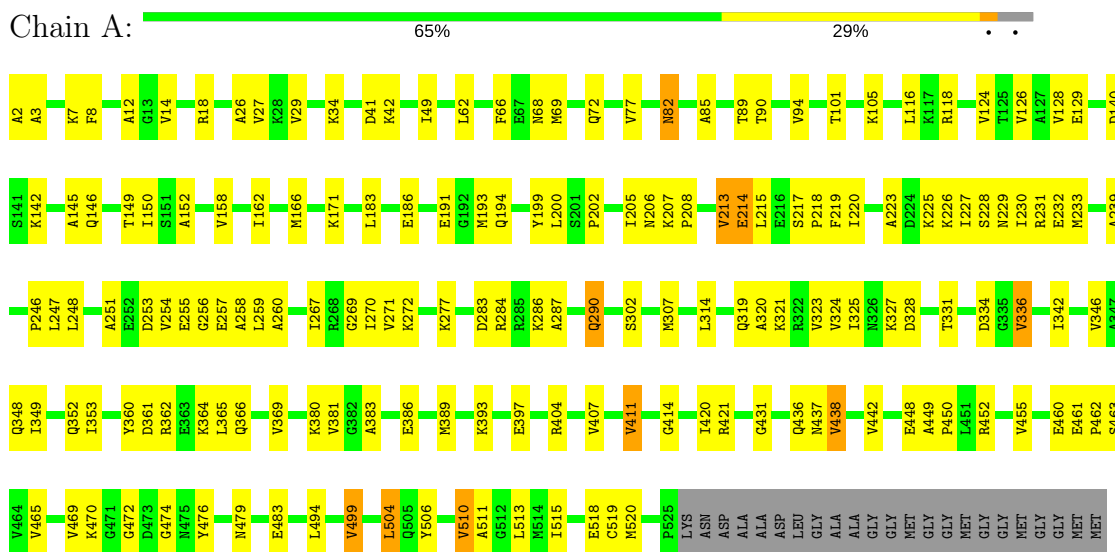
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total 18	O 18	0	0
2	B	23	Total 23	O 23	0	0
2	C	17	Total 17	O 17	0	0
2	D	18	Total 18	O 18	0	0
2	E	36	Total 36	O 36	0	0
2	F	18	Total 18	O 18	0	0
2	G	19	Total 19	O 19	0	0

3 Residue-property plots

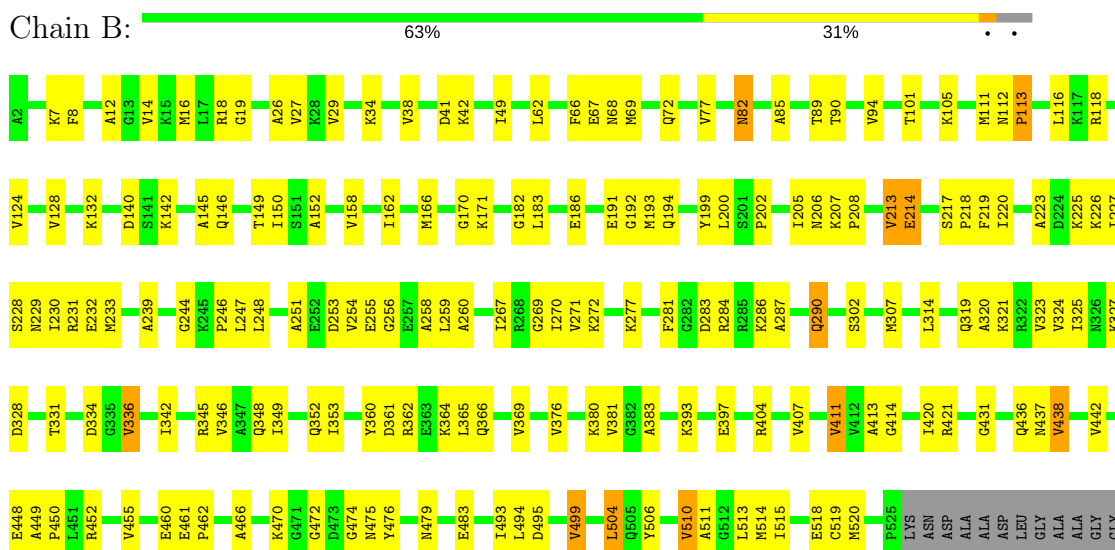
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

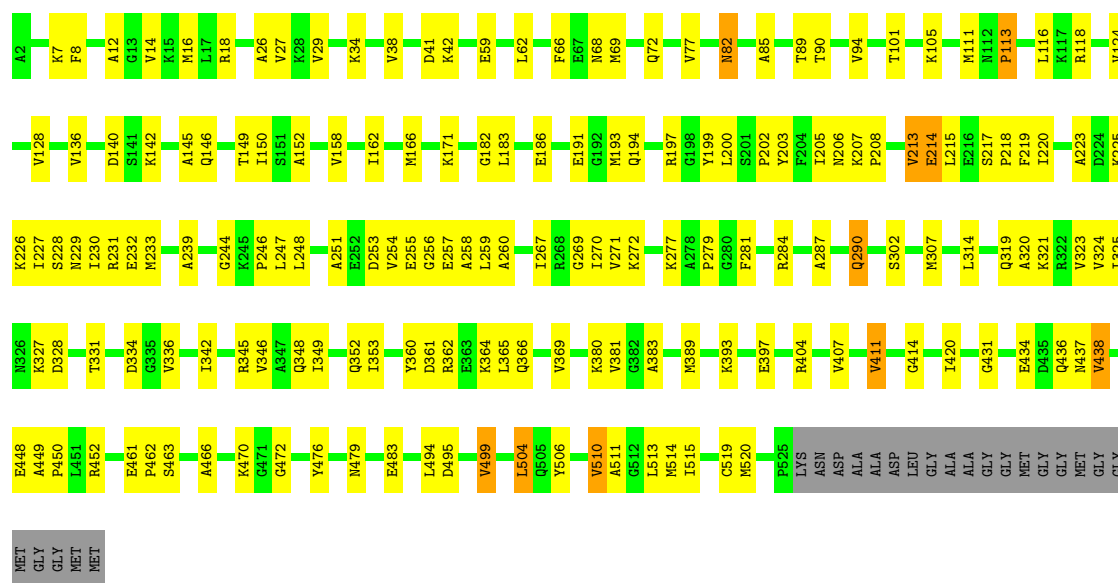
• Molecule 1: GROEL (HSP60 CLASS)



• Molecule 1: GROEL (HSP60 CLASS)

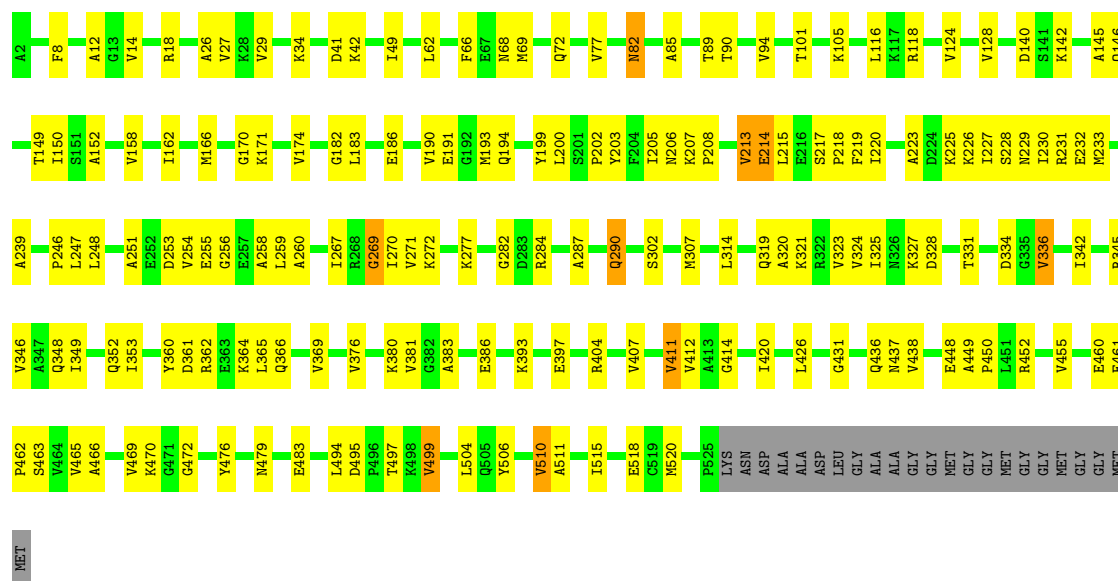


Chain E: 65% 29% • •



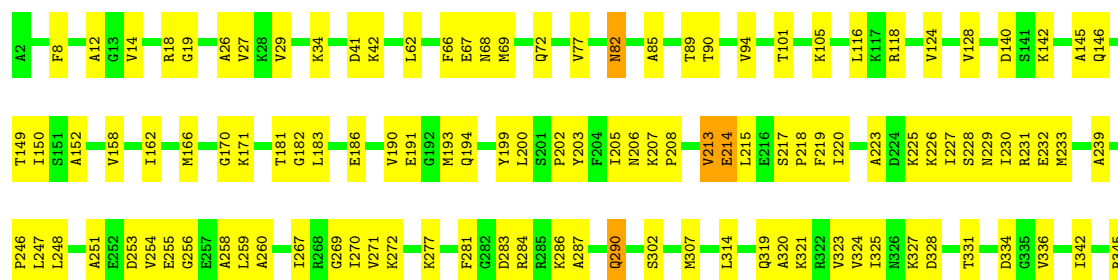
• Molecule 1: GROEL (HSP60 CLASS)

Chain F: 65% 29%



• Molecule 1: GROEL (HSP60 CLASS)

Chain G: 65% 29%



V346	A347	Q348	I349	Q352	I353	Y360	D361	R362	E363	K364	L365	Q366	Y369	K380	V381	G382	A383	K389	K393	E397	R404	V407	V411	Q414	I420	R421	G431	Q436	M437	V438	E448	A449	P450	L451	R452	S463	V464	V465	A466	V469	K470	G471	
G472	D473	G474	N475	Y476	N479	E483	I493	L494	V499	L504	Q505	Y506	V510	A511	G512	L513	M514	I515	E518	C519	M520	P525	LYS	ASN	ASP	ALA	ALA	ASP	LEU	GLY	ALA	ALA	GLY	GLY	MET	GLY	GLY	MET	MET	GLY	GLY	MET	MET

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	178.38Å 204.98Å 280.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	72.2 (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.227 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27078	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/3875	0.57	0/5234
1	B	0.41	0/3875	0.57	0/5234
1	C	0.39	0/3875	0.57	0/5234
1	D	0.40	0/3875	0.56	0/5234
1	E	0.41	0/3875	0.57	0/5234
1	F	0.39	0/3875	0.56	0/5234
1	G	0.39	0/3875	0.56	0/5234
All	All	0.40	0/27125	0.57	0/36638

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3847	0	3966	133	0
1	B	3847	0	3966	139	0
1	C	3847	0	3966	135	0
1	D	3847	0	3966	140	0
1	E	3847	0	3966	134	0
1	F	3847	0	3966	134	0
1	G	3847	0	3966	134	0
2	A	18	0	0	0	0
2	B	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	17	0	0	0	0
2	D	18	0	0	1	0
2	E	36	0	0	0	0
2	F	18	0	0	0	0
2	G	19	0	0	0	0
All	All	27078	0	27762	918	0

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 17.

The worst 5 of 918 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:E:166:MET:HG2	1:E:171:LYS:HA	1.58	0.86
1:F:166:MET:HG2	1:F:171:LYS:HA	1.59	0.85
1:A:166:MET:HG2	1:A:171:LYS:HA	1.58	0.84
1:D:166:MET:HG2	1:D:171:LYS:HA	1.61	0.83
1:G:166:MET:HG2	1:G:171:LYS:HA	1.60	0.83

There are no symmetry-related clashes.

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	522/547 (95%)	497 (95%)	23 (4%)	2 (0%)	38	72
1	B	522/547 (95%)	498 (95%)	22 (4%)	2 (0%)	38	72
1	C	522/547 (95%)	496 (95%)	24 (5%)	2 (0%)	38	72
1	D	522/547 (95%)	497 (95%)	23 (4%)	2 (0%)	38	72
1	E	522/547 (95%)	497 (95%)	24 (5%)	1 (0%)	51	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	522/547 (95%)	497 (95%)	22 (4%)	3 (1%)	28 62
1	G	522/547 (95%)	497 (95%)	24 (5%)	1 (0%)	51 83
All	All	3654/3829 (95%)	3479 (95%)	162 (4%)	13 (0%)	38 72

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	426	LEU
1	C	426	LEU
1	C	269	GLY
1	E	269	GLY
1	F	269	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	403/413 (98%)	389 (96%)	14 (4%)	41 75
1	B	403/413 (98%)	388 (96%)	15 (4%)	39 73
1	C	403/413 (98%)	389 (96%)	14 (4%)	41 75
1	D	403/413 (98%)	388 (96%)	15 (4%)	39 73
1	E	403/413 (98%)	388 (96%)	15 (4%)	39 73
1	F	403/413 (98%)	389 (96%)	14 (4%)	41 75
1	G	403/413 (98%)	389 (96%)	14 (4%)	41 75
All	All	2821/2891 (98%)	2720 (96%)	101 (4%)	40 74

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	PRO
1	D	504	LEU
1	G	232	GLU
1	D	199	TYR

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Mol	Chain	Res	Type
1	D	290	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	68	ASN
1	D	453	GLN
1	G	348	GLN
1	D	194	GLN
1	D	352	GLN

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.