



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 06:12 am BST

PDB ID : 1GRL  
Title : THE CRYSTAL STRUCTURE OF THE BACTERIAL CHAPERONIN  
GROEL AT 2.8 ANGSTROMS  
Authors : Braig, K.; Otwinowski, Z.; Hegde, R.; Boisvert, D.C.; Joachimiak, A.; Horwich,  
A.L.; Sigler, P.B.  
Deposited on : 1995-03-07  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

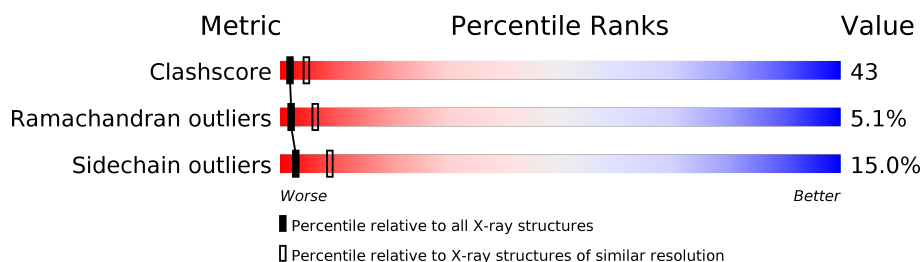
# 1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	<div> <div>39%</div> <div>46%</div> <div>8%</div> <div>5%</div> </div>
1	B	548	<div> <div>39%</div> <div>46%</div> <div>8%</div> <div>5%</div> </div>
1	C	548	<div> <div>39%</div> <div>46%</div> <div>8%</div> <div>5%</div> </div>
1	D	548	<div> <div>38%</div> <div>47%</div> <div>7%</div> <div>5%</div> </div>
1	E	548	<div> <div>39%</div> <div>47%</div> <div>8%</div> <div>5%</div> </div>
1	F	548	<div> <div>39%</div> <div>46%</div> <div>8%</div> <div>5%</div> </div>
1	G	548	<div> <div>39%</div> <div>47%</div> <div>7%</div> <div>5%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29274 atoms, of which 5278 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	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	B	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	C	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	D	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	E	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	F	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	G	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	CONFLICT	UNP P06139
A	126	VAL	ALA	CONFLICT	UNP P06139
A	267	MET	ILE	CONFLICT	UNP P06139
B	13	GLY	ARG	CONFLICT	UNP P06139
B	126	VAL	ALA	CONFLICT	UNP P06139
B	267	MET	ILE	CONFLICT	UNP P06139
C	13	GLY	ARG	CONFLICT	UNP P06139
C	126	VAL	ALA	CONFLICT	UNP P06139
C	267	MET	ILE	CONFLICT	UNP P06139
D	13	GLY	ARG	CONFLICT	UNP P06139
D	126	VAL	ALA	CONFLICT	UNP P06139
D	267	MET	ILE	CONFLICT	UNP P06139
E	13	GLY	ARG	CONFLICT	UNP P06139
E	126	VAL	ALA	CONFLICT	UNP P06139
E	267	MET	ILE	CONFLICT	UNP P06139

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Chain	Residue	Modelled	Actual	Comment	Reference
F	13	GLY	ARG	CONFLICT	UNP P06139
F	126	VAL	ALA	CONFLICT	UNP P06139
F	267	MET	ILE	CONFLICT	UNP P06139
G	13	GLY	ARG	CONFLICT	UNP P06139
G	126	VAL	ALA	CONFLICT	UNP P06139
G	267	MET	ILE	CONFLICT	UNP P06139

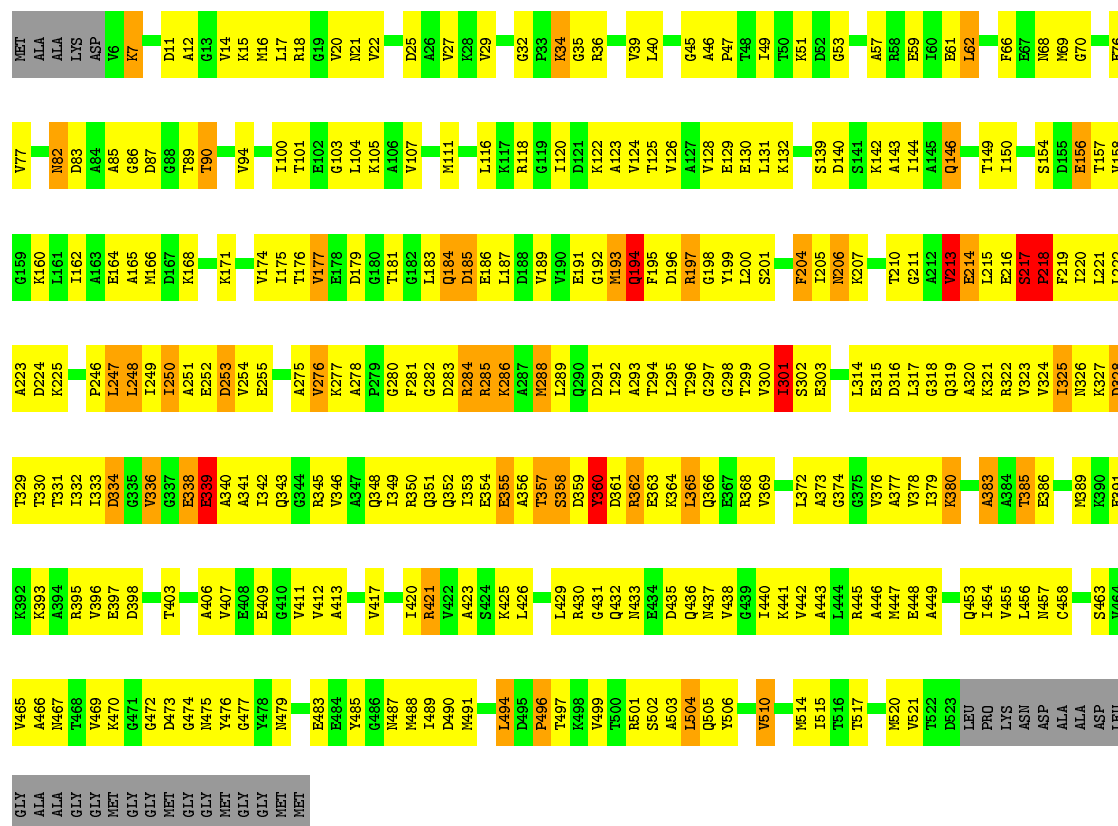
### 3 Residue-property plots

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. 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. 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.

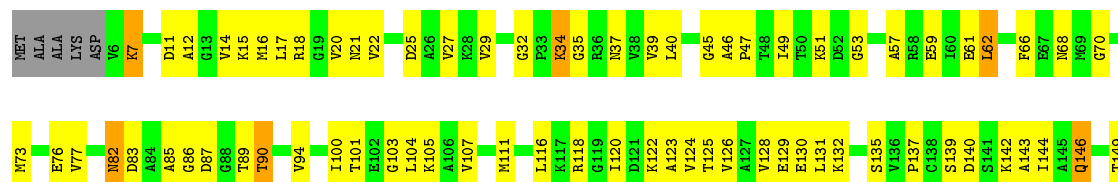
#### • Molecule 1: GROEL (HSP60 CLASS)

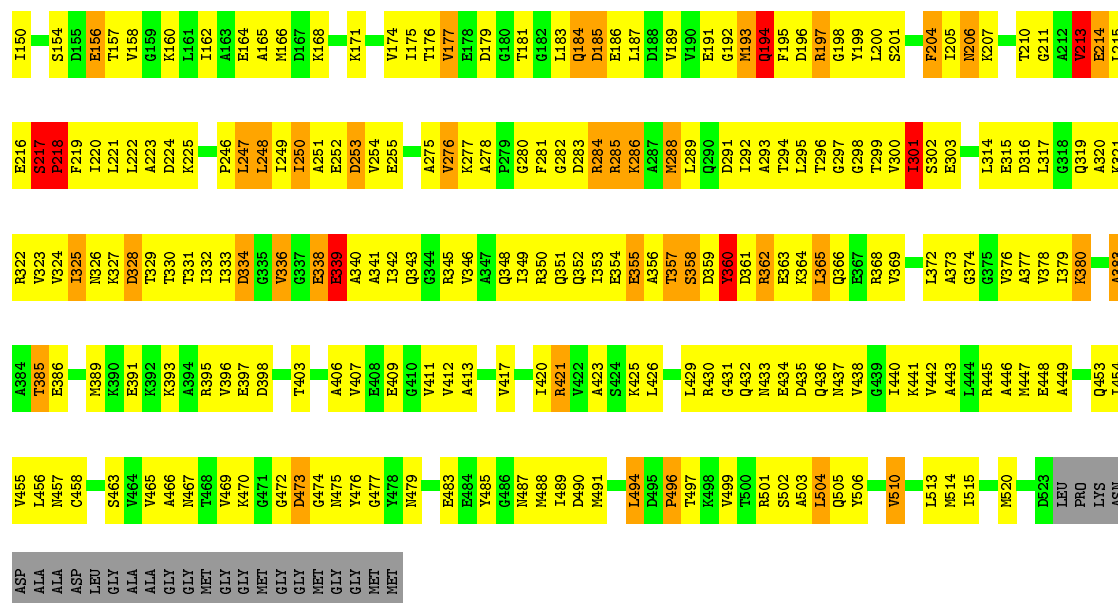
Chain A: 



#### • Molecule 1: GROEL (HSP60 CLASS)

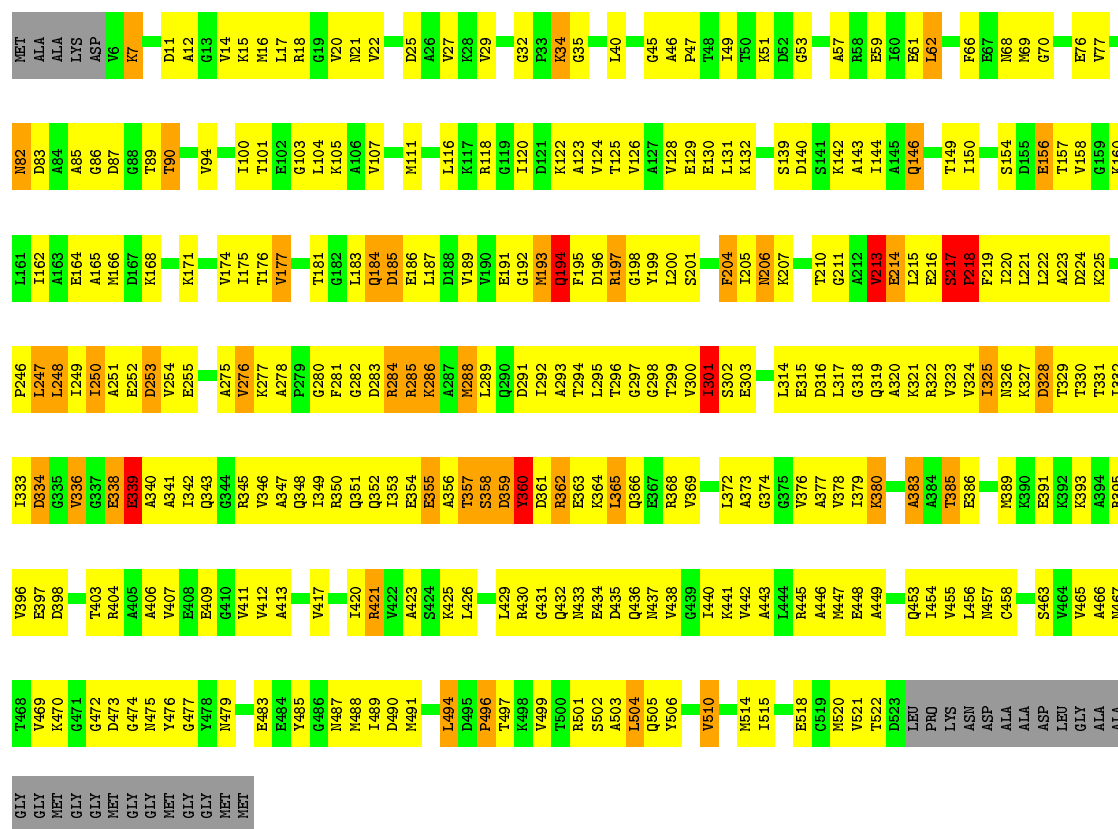
Chain B: 





• Molecule 1: GROEL (HSP60 CLASS)

Chain C: 39% 46% 8% • 5%

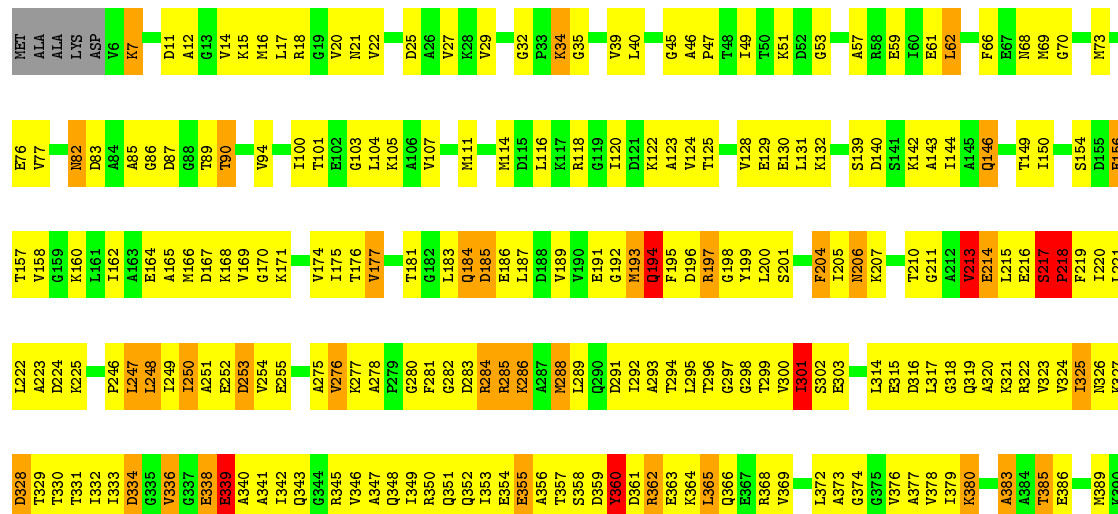


• Molecule 1: GROEL (HSP60 CLASS)

Chain D: 38% 47% 7% • 5%



V465	K392	D328	L222	E156	E76
K393	T329	A223	A223	T157	V77
N467	T330	D224	D224	T158	ALA
T468	R395	T331	K225	G159	LYS
V469	V396	T332		K160	D83
K470	E397	T333	P246	L161	A84
D398	D394	D334	L247	I162	A85
			L248	A163	G86
T403	G335	V336	T249	E164	D87
		G337	T250	A165	G88
A406	V407	E338	A251	M166	T89
N475	V408	E339	E252	D167	G13
Y476	E407	A340	D253	K168	V14
G477	G410	T342	E254		K15
N478	V411	G343	E255	K171	L17
E483	V412	G344	A275		R18
E484	A413	R345	V276	V174	I100
Y485		V346	K277	I175	T101
N487	V417	A347	A278	T176	E102
L489	I420	G348	G280		G103
D490	R421	R350	F281	T181	K21
D491	V422	Q351	G282	G182	K105
M491	A423	Q352	D283	L183	V107
G492	S424	R353	K284	Q184	
I493	K425	E354	R285	E186	M111
L494	L426	E355	K286	E187	N112
D495		A356	A287	D188	L116
P496	L429	T357	R288	V189	R117
T497	R430	S358	L289	G190	R118
K498	G431	D359	Q290	E191	G119
V499	Q432	T360	D291	G192	R36
T500	N433	D361	T292	M193	D121
R501	E434	R362	A293	K122	N37
S502	D435	E363	T294	G194	N38
A503	Q436	K364	L295	D196	V39
L504	N437	L365	T296	R197	L40
Q505	V438	Q366	G297	G198	
Y506	G439	E367	G298	V199	G45
	I440	R368	T299	L200	I49
V510	K441		V300	S201	T50
	V442	L372	R301		K51
L513	A443	A373	S302	P204	E52
M514	L444	G374	E303	K132	G53
I515	R445	G375		N206	A133
T516	A446	V376	L314	K207	
	M447	A377	E315		R58
M520	E448	T378	D316	T210	E59
	A449	L379	G318	G211	L60
		K380	G319	A212	K142
D523	Q453	A383	Q319	V213	A143
LEU	I454	E384	A320	E214	I144
PRO	V455	A384	K321	L215	A145
LYS	L456	T385	R322	E216	Q146
ASN	N457	E386	V323	S217	E67
ASP	C458		V324	P218	N68
ALA		M389	I325	F219	G70
		ALA	T326	T220	I150
ASP	S463	R390	K326	L221	S154
LEU	V466	F231	T222	P155	





LEU	V465	E391
GLY	A466	K392
ALA	M467	K393
GLA	T468	A394
GLY	V469	K395
MET	K470	V396
GLY	G471	E397
GLY	G472	D398
GLY	G473	
MET	G474	T403
GLY	M475	
GLY	V476	A406
MET	G477	V407
GLY	V478	E408
GLY	M479	E409
MET		G410
MET	E483	V411
	E484	V412
	V485	A413
	G486	
	M487	V417
	M488	
	I489	T420
	D490	R421
	M491	V422
	G492	A423
	I493	S424
	L494	K425
	D495	
	V496	L429
	T497	R430
	K498	G431
	V499	Q432
	T500	N433
	R501	E434
	S502	D435
	A503	Q436
	L504	N437
	Q505	V438
	Y506	G439
		T440
	V510	K441
		V442
	M514	A443
	I515	L444
		R445
	E518	A446
	G519	M447
	M520	E448
	V521	A449
	T522	
	D523	Q453
	LEU	T454
	PRO	V455
	LYS	L456
	ASN	N457
	ASP	C458
	ALA	
	ALA	S463
	ASP	V464

## 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, $\alpha$ , $\beta$ , $\gamma$	178.00 Å   203.00 Å   278.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.326 , 0.368	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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	0.62	0/3389	0.84	2/4571 (0.0%)
1	B	0.62	0/3389	0.84	2/4571 (0.0%)
1	C	0.62	0/3389	0.84	2/4571 (0.0%)
1	D	0.62	0/3389	0.84	2/4571 (0.0%)
1	E	0.62	0/3389	0.84	2/4571 (0.0%)
1	F	0.62	0/3389	0.84	2/4571 (0.0%)
1	G	0.62	0/3389	0.84	2/4571 (0.0%)
All	All	0.62	0/23723	0.84	14/31997 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	F	360	TYR	N-CA-C	6.51	128.57	111.00
1	B	360	TYR	N-CA-C	6.50	128.55	111.00
1	G	360	TYR	N-CA-C	6.50	128.55	111.00
1	D	360	TYR	N-CA-C	6.49	128.53	111.00
1	E	360	TYR	N-CA-C	6.49	128.52	111.00

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	3428	754	3441	314	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3428	754	3441	324	9
1	C	3428	754	3440	334	54
1	D	3428	754	3441	323	0
1	E	3428	754	3441	323	18
1	F	3428	754	3440	324	1
1	G	3428	754	3441	315	55
All	All	23996	5278	24085	2090	75

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 43.

The worst 5 of 2090 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:A:181:THR:O	1:G:282:GLY:CA	1.65	1.39
1:D:282:GLY:CA	1:E:181:THR:O	1.69	1.37
1:F:282:GLY:CA	1:G:181:THR:O	1.72	1.36
1:A:282:GLY:HA3	1:B:181:THR:O	1.28	1.30
1:A:386:GLU:OE2	1:G:285:ARG:NH2	1.71	1.23

The worst 5 of 75 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:C:358:SER:OG	1:G:169:VAL:CB[5_455]	0.65	1.55
1:C:358:SER:CB	1:G:169:VAL:CA[5_455]	0.74	1.46
1:C:358:SER:CA	1:G:169:VAL:CA[5_455]	0.89	1.31
1:C:359:ASP:N	1:G:170:GLY:H[5_455]	0.31	1.29
1:C:359:ASP:CB	1:G:167:ASP:CA[5_455]	0.97	1.23

## 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	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	6
1	B	449/548 (82%)	359 (80%)	67 (15%)	23 (5%)	2	6
1	C	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	6
1	D	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	6
1	E	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	6
1	F	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	6
1	G	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	6
All	All	3143/3836 (82%)	2507 (80%)	475 (15%)	161 (5%)	2	6

5 of 161 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	185	ASP
1	A	214	GLU
1	A	253	ASP
1	A	301	ILE

### 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	353/414 (85%)	300 (85%)	53 (15%)	3	9
1	B	353/414 (85%)	300 (85%)	53 (15%)	3	9
1	C	353/414 (85%)	300 (85%)	53 (15%)	3	9
1	D	353/414 (85%)	300 (85%)	53 (15%)	3	9
1	E	353/414 (85%)	300 (85%)	53 (15%)	3	9
1	F	353/414 (85%)	300 (85%)	53 (15%)	3	9
1	G	353/414 (85%)	300 (85%)	53 (15%)	3	9
All	All	2471/2898 (85%)	2100 (85%)	371 (15%)	3	9

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	87	ASP
1	D	421	ARG
1	G	218	PRO
1	D	146	GLN
1	D	283	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	68	ASN
1	D	453	GLN
1	G	146	GLN
1	D	72	GLN
1	D	194	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.