



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:43 PM GMT

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
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

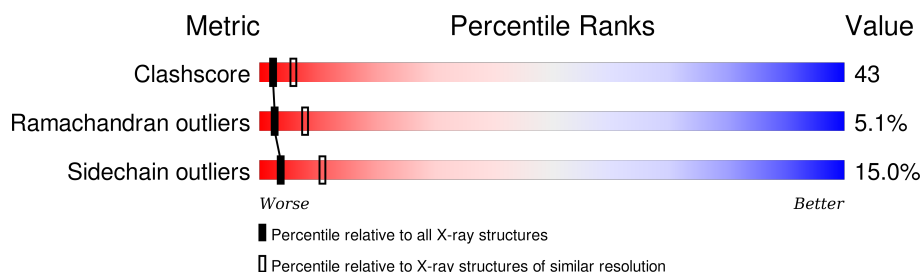
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	
1	G	548	

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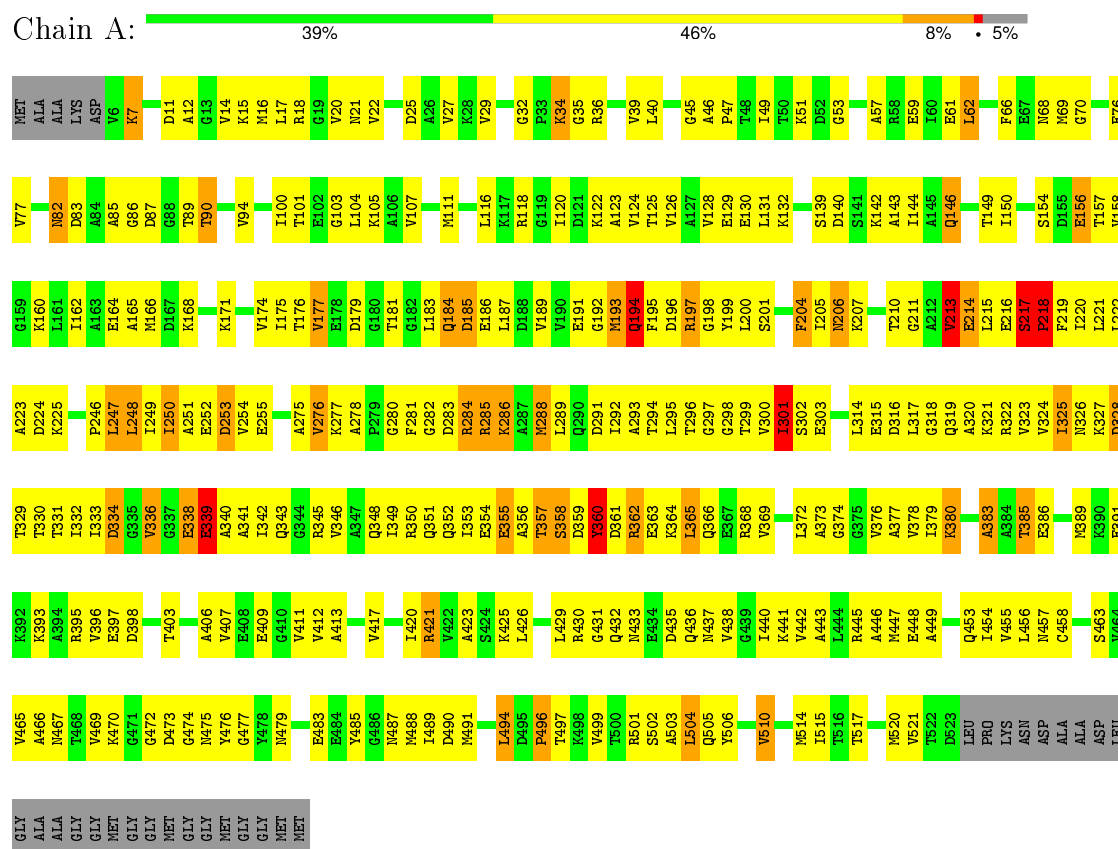
Chain	Residue	Modelled	Actual	Comment	Reference
F	13	GLY	ARG	CONFLICT	UNP P06139
F	126	VAL	ALA	CONFLICT	UNP P06139
F	267	MET	ILE	CONFLICT	UNP P06139
G	13	GLY	ARG	CONFLICT	UNP P06139
G	126	VAL	ALA	CONFLICT	UNP P06139
G	267	MET	ILE	CONFLICT	UNP P06139

3 Residue-property plots

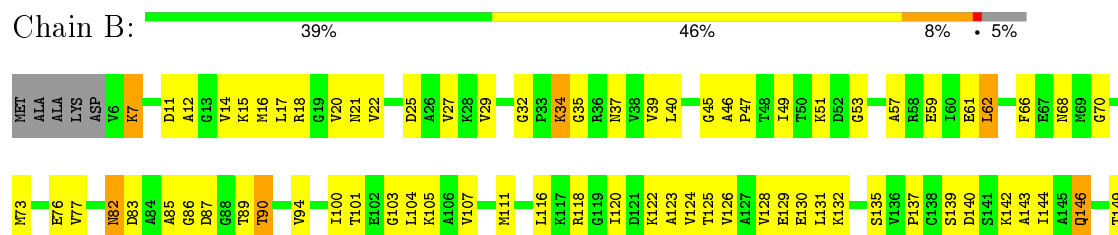
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

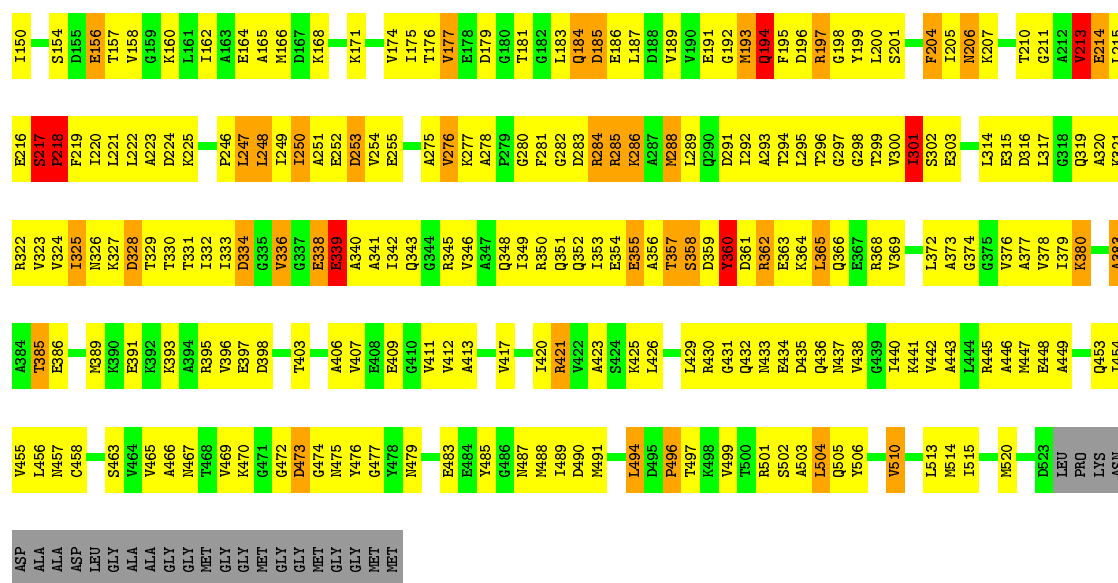
Note EDS was not executed.

• Molecule 1: GROEL (HSP60 CLASS)

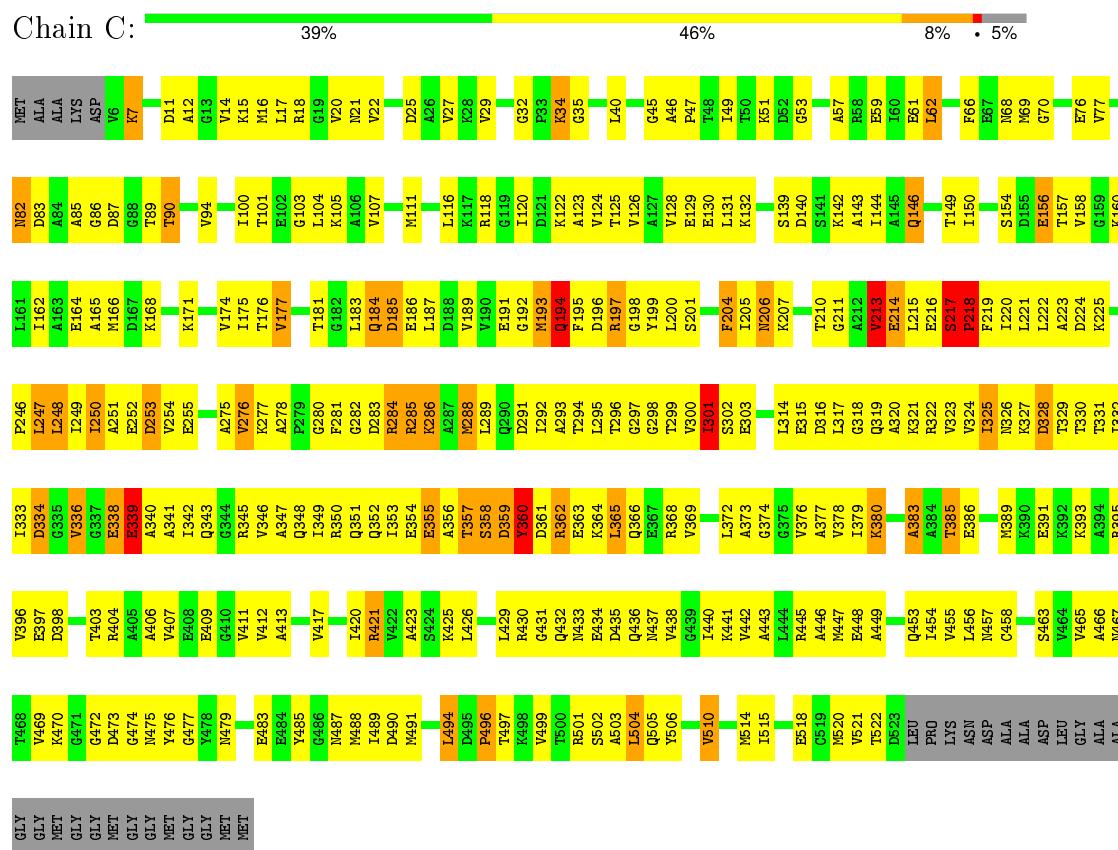


• Molecule 1: GROEL (HSP60 CLASS)

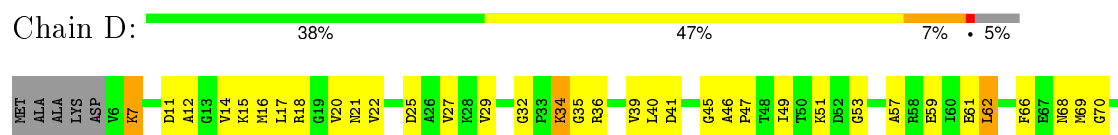




• Molecule 1: GROEL (HSP60 CLASS)



• Molecule 1: GROEL (HSP60 CLASS)





MET	M82	K160	D224	T330	A394	N467	GLY
ALA	M82	L161	K225	T331	R395	T468	GLY
ALA	D83	I162		T332	V396	T469	MET
LYS	A84	A163	P246	T333	V397	K470	GLY
ASP	A85	E164	L247	T334	D398	G471	GLY
V6	G86	A165	L248	G335	T403	G472	MET
K7	D87	M166	L249	V336		D473	GLY
	G88	D167	L250	G337		G474	GLY
	T89	K168	L251	E338	A406	G475	MET
D11	T90		E252	E339	V407	Y476	GLY
A12			D253	A340	E408	Y477	GLY
G13			E254	A341	E409	Y478	MET
V14	V94	K171	V254	A342	G410	N479	MET
K15			E255	Q343	V411		
M16	I100	V174		Q344	V412		
L17	T101	I175	A275	G345	A413	E483	
R18	E102	T176	V276	R345	A414	E484	
G19	G103	E178	K277	V346	V417	Y485	
V20	L104	D179	A278	A347		Y486	
N21	K105	G180	P279	Q348	I420	N487	
V22	A106	T181	G280	Q349	R421	M488	
	V107	G182	F281	R350	V422	D490	
D25	M111	L183	D282	Q351	A423	M491	
A26		Q184	D283	Q352	S424	G492	
V27	L116	D185	R284	I353	K425	I493	
K28	K117	E186	K285	E354	L426	L494	
V29	R118	L187	K286	E355		D495	
	R119	D188	A287	A356	L429	P496	
G32	K119	T189	M288	T357	R430	D498	
K34	I120	P33	L289	R358	R431	K498	
G35	D121	E191	Q290	G359	Q431	T497	
R36	K122	G192	D291	R361	Q432	V499	
	A123	M193	L292	D362	N433	T500	
L40	V124	Q194	D293	R363	E434	R501	
	V126	F195	T294	E363	D435	S502	
G45	A127	D196	L295	K364	Q436	A503	
A46	L128	R197	T296	L365	N437	L504	
P47	E129	G198	G297	Q366	V438	Q505	
T48	E130	Y199	C298	E367	G439	Y506	
L49	L131		T299	R368	I440	V510	
T50	K132		V300		K441	M514	
K51		F204	I301	L372	V442	I515	
D52	S139	I205	E303	A373	A443		
G53	D140	K206		G374	L444	M520	
A57	S141	K207	L314	V376	R445	V521	
R58	K142		E315	A377	A446	D522	
E59	A143	T210	D316	V378	M447	T522	
I60	I144	G211	L317	I379	E448	D523	
E61	A145	A212	G318	K380	A449	LEU	
L62	Q146	V213	Q319		Q453	P80	
		E214	A320	A383	I454	LYS	
F66	T149	L215	K321	A384	V455	ASN	
E67	I150	E216	R322	T385	L456	ASP	
N68	S154	S217	V323	E386	N457	ALA	
N69	D155	P218	V324	C458	C458	ALA	
G70	E156	F219	I325			ASP	
	T157	I220	N326	K389	S463	LEU	
V158	G159	L221	K327	K390	V464	GLY	
E76		L222	D328	E391	V465	ALA	
V77		A223	T329	K393	A466	ALA	

• Molecule 1: GROEL (HSP60 CLASS)

Chain G:  39% 47% 7% 5%

MET	E76	T157	L222	D328	E391	V465	LEU
ALA	V77	V158	A223	T329	F392	A466	GLY
ALA	M82	G159	D224	T330	K393	T468	ALA
LYS	D83	K160	K225	T331	A394	T469	ALA
ASP	A85	L161	P246	I332	V396	K470	GLY
V6	G86	I162	L247	I333	R395	G471	GLY
K7	D87	A163	L248	D334	E397	G472	MET
	G88	E164	L249	G335	D398	G473	GLY
D11	T90	A165	L250	E337	T403	G474	GLY
A12		M166	E251	E338	A406	G475	MET
G13	T89	K168	E252	A339	V407	Y476	GLY
V14		D169	D253	E340	E408	Y477	GLY
K15	V94	G170	V254	A341	E409	Y478	MET
M16		K171	E255	A342	G410	N479	MET
L17	I100			Q343	V411		
R18	T101	V174	A275	G344	V412	E483	
G19	E102	I175	V276	R345	A413	E484	
N21	G103	T176	K277	V346	A414	Y485	
V22	L104	V177	A278	A347	V417	Y486	
	K105		P279	Q348		N487	
D25	A106	T181	G280	Q349	I420	M488	
A26	V107	G182	F281	R350	V422	D490	
V27	M111	L183	D282	Q351	A423	M491	
K28		Q184	D283	Q352	S424	G492	
V29	L116	D185	R284	I353	K425	I493	
	K117	E186	K285	E354	S424	L494	
G32	M114	L187	R286	E355		D495	
K34	D115	T189	M288	T357	L429	P496	
G35	K116	R497	D188	K189	R430	T497	
V39	G119	V190	G191	D359	Q431	K498	
L40	I120	E191	D291	R361	Q432	T500	
	K121	M193	L292	D362	N433	R501	
G45	A123	F195	A293	R363	D435	S502	
A46	V124	D196	L295	E363	Q436	A503	
P47	T125	R197	T296	L365	N437	L504	
T48		G198	G297	Q366	V438	Q505	
L49	V128	Y199	C298	E367	G439	Y506	
T50	E129	L200	T299	R368	I440	V510	
K51	E130	K51	V300	V369	K441	M514	
D52	L131		I301		V442	I515	
G53	K132	F204	S302		A443		
	I205	I206	E303	L372	L444		
A57	S139	K207	L314	A373	R445	E518	
R58	D140	K206	E315	G374	A446	C519	
E59	K142		D316	V376	M447	M520	
I60	S141	T210	L317	A377	E448	V521	
E61	A143	G211	G318	I379	A449	T522	
L62	A145	A212	Q319		Q453	D523	
	Q146	V213	A320	A383	I454	LEU	
F66	T149	E214	K321	A384	V455	P80	
E67	I150	E216	R322	T385	L456	LYS	
N68	D155	S217	V323	E386	N457	ASN	
N69	G70	P218	V324	E386	C458	ASP	
	S154	F219	I325			ALA	
V158	E156	I220	N326	K389	S463	ALA	
		L221	K327	K390	V464	ASP	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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	8
1	B	449/548 (82%)	359 (80%)	67 (15%)	23 (5%)	2	8
1	C	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	D	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	E	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	F	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	G	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
All	All	3143/3836 (82%)	2507 (80%)	475 (15%)	161 (5%)	2	8

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	11
1	B	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	C	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	D	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	E	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	F	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	G	353/414 (85%)	300 (85%)	53 (15%)	3	11
All	All	2471/2898 (85%)	2100 (85%)	371 (15%)	3	11

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.