



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:05 PM GMT

PDB ID : 1IOK  
Title : CRYSTAL STRUCTURE OF CHAPERONIN-60 FROM PARACOCCLUS  
DENITRIFICANS  
Authors : Fukami, T.A.; Yohda, M.; Taguchi, H.; Yoshida, M.; Miki, K.  
Deposited on : 2001-03-16  
Resolution : 3.20 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  
<http://wwpdb.org/validation/2016/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  
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

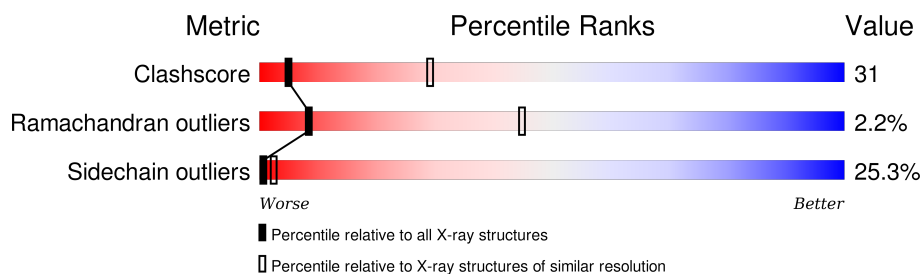
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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. 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	545	<div> <div>36%</div> <div>42%</div> <div>10%</div> <div>12%</div> </div>
1	B	545	<div> <div>37%</div> <div>42%</div> <div>10%</div> <div>12%</div> </div>
1	C	545	<div> <div>37%</div> <div>41%</div> <div>10%</div> <div>12%</div> </div>
1	D	545	<div> <div>37%</div> <div>42%</div> <div>10%</div> <div>12%</div> </div>
1	E	545	<div> <div>37%</div> <div>41%</div> <div>10%</div> <div>12%</div> </div>
1	F	545	<div> <div>37%</div> <div>41%</div> <div>10%</div> <div>12%</div> </div>
1	G	545	<div> <div>37%</div> <div>41%</div> <div>10%</div> <div>12%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25095 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 CHAPERONIN 60.

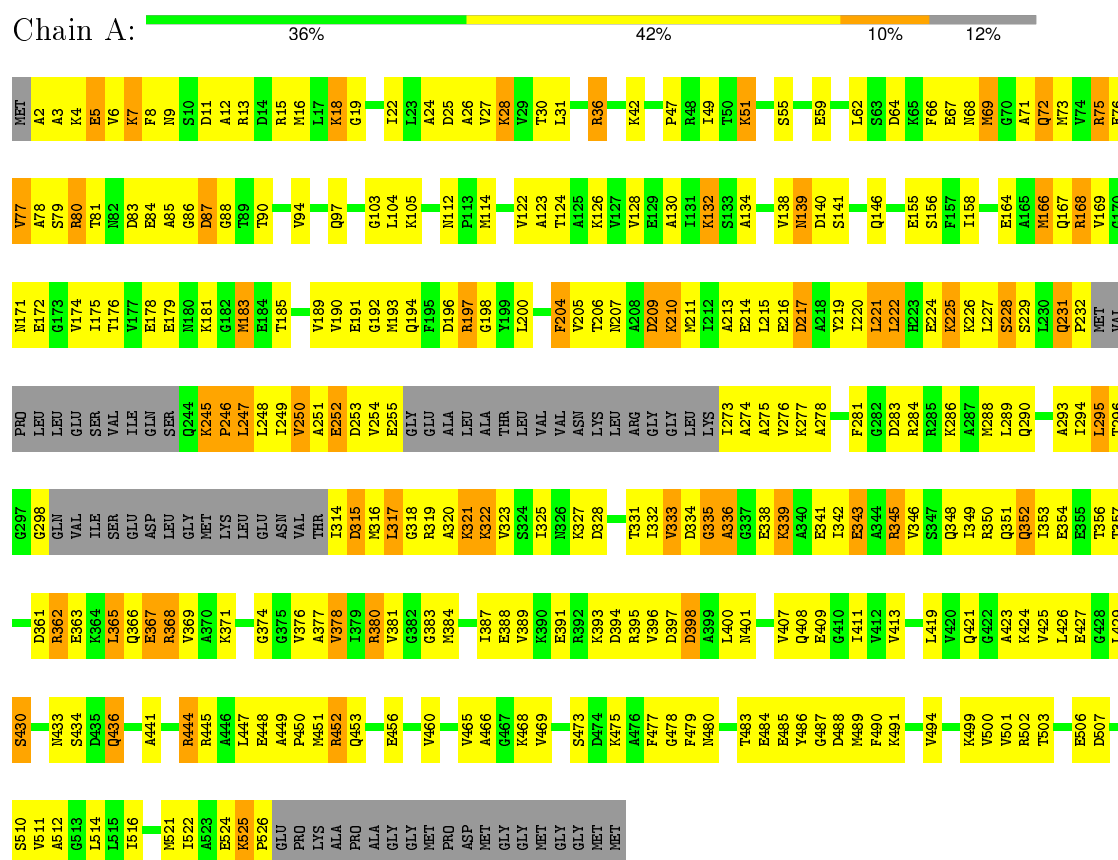
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	B	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	C	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	D	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	E	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	F	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	G	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			

### 3 Residue-property plots

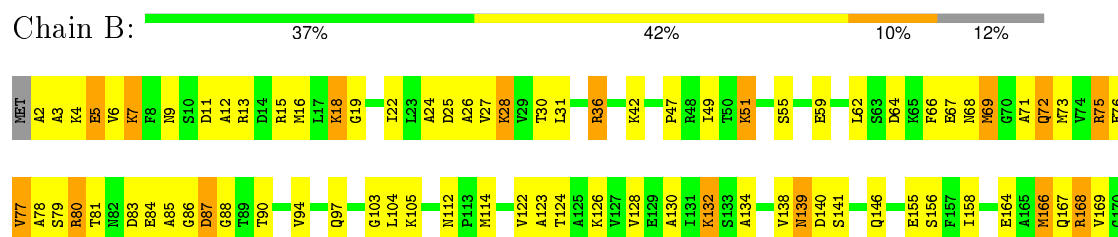
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

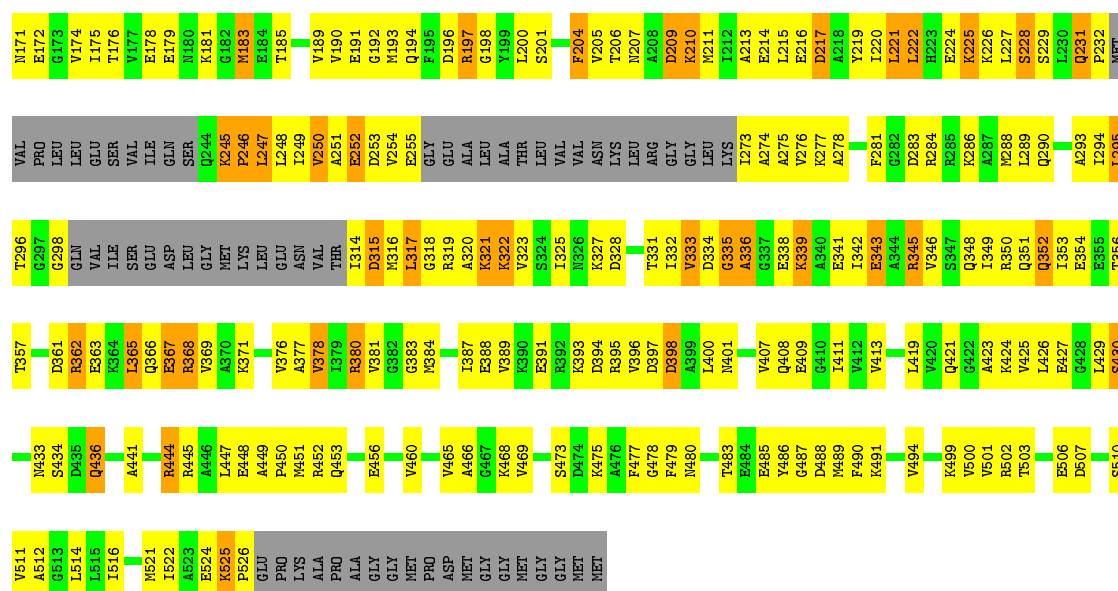
Note EDS was not executed.

#### • Molecule 1: CHAPERONIN 60

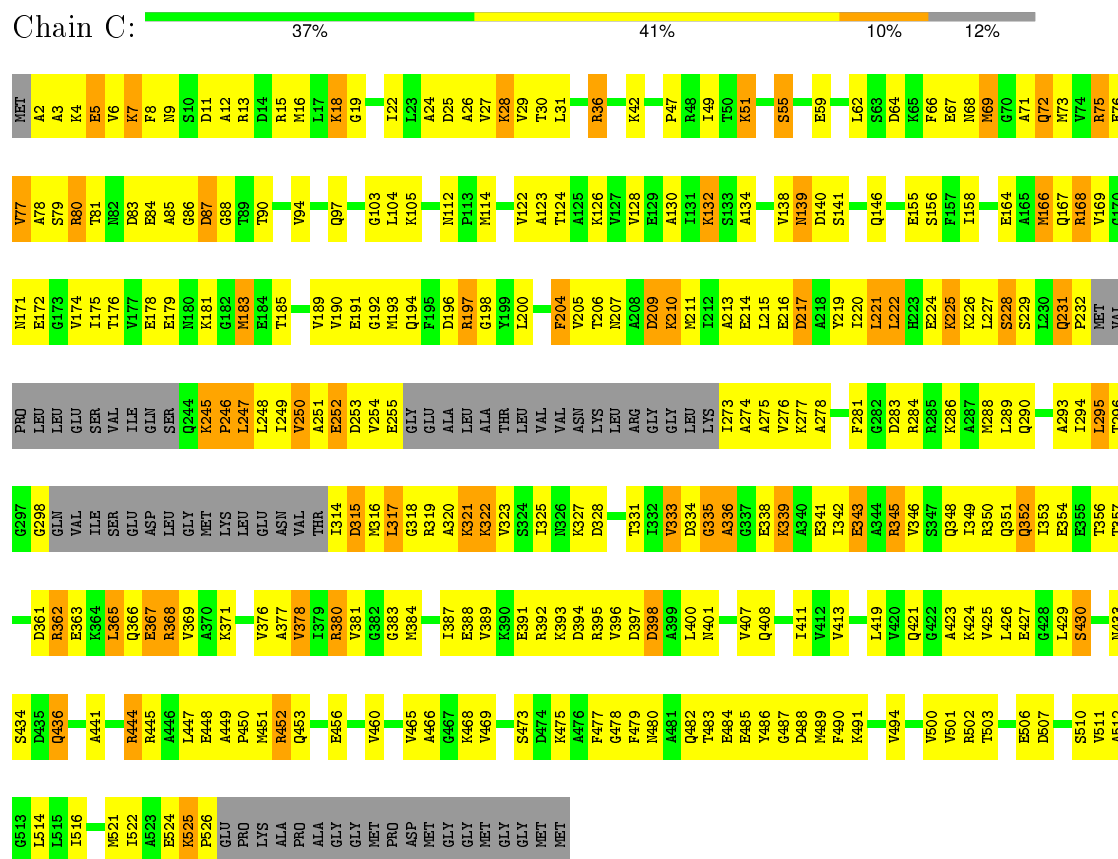


#### • Molecule 1: CHAPERONIN 60

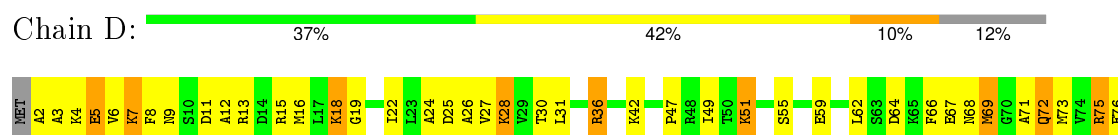


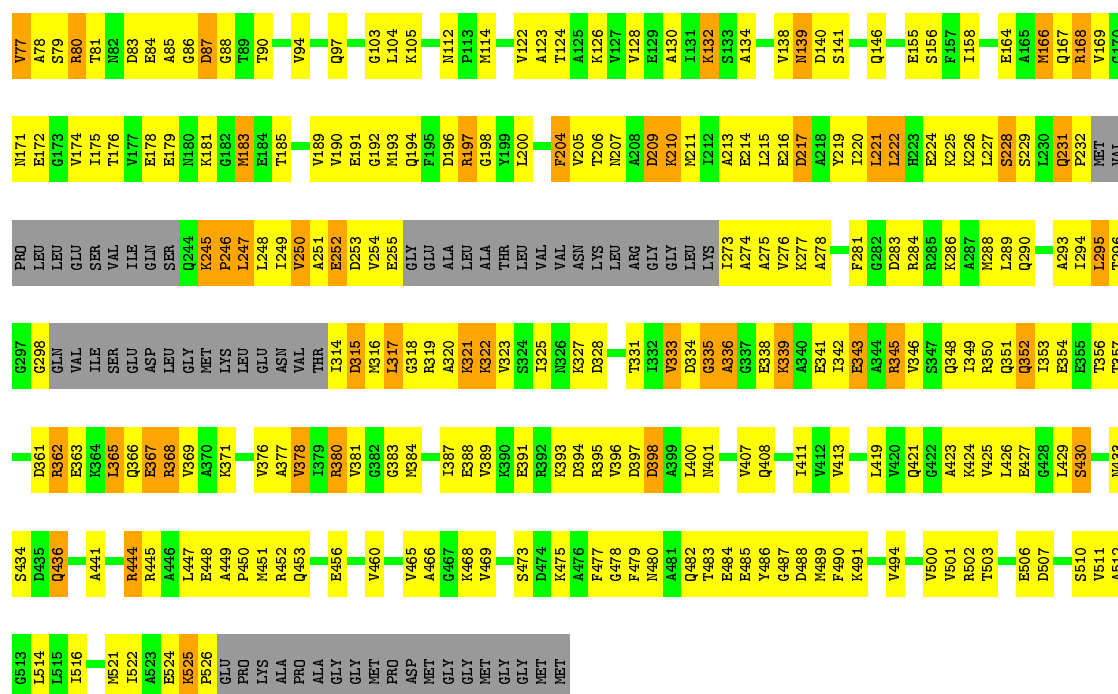


• Molecule 1: CHAPERONIN 60



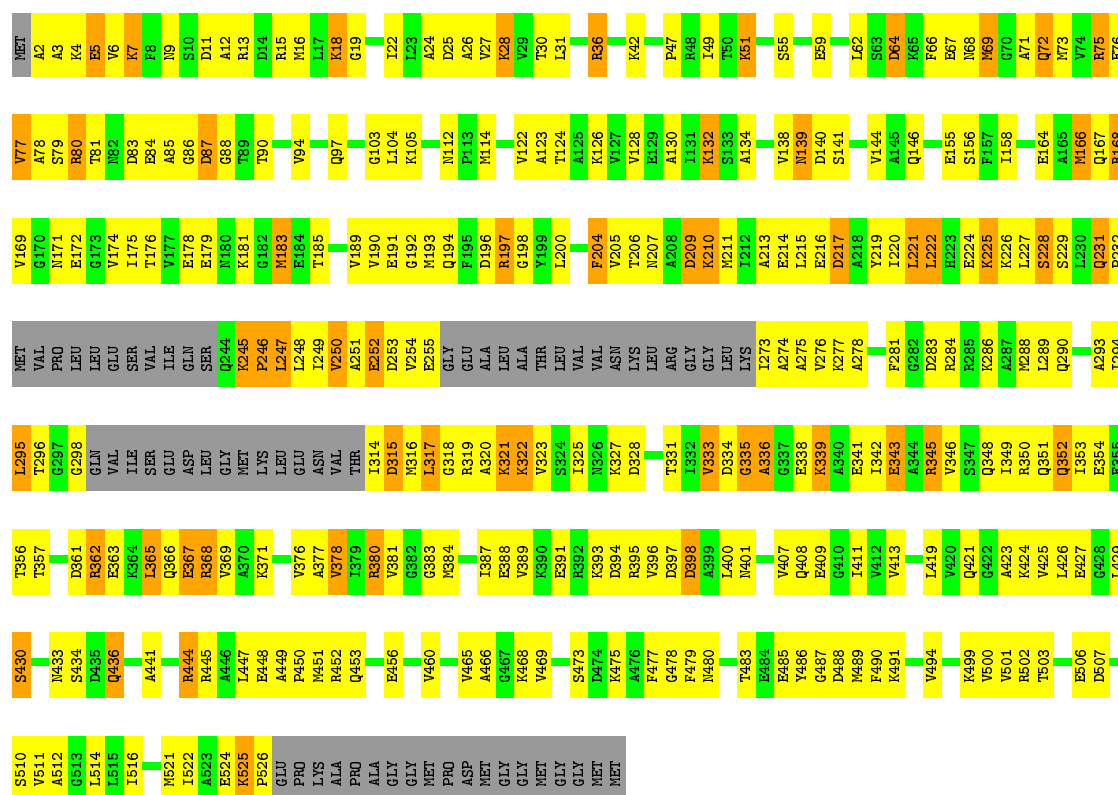
• Molecule 1: CHAPERONIN 60





# • Molecule 1: CHAPERONIN 60

Chain E: 37% 41% 10% 12%



# • Molecule 1: CHAPERONIN 60

Chain F: 37% 41% 10% 12%

Q436	D361	G297	PRO	N171	V77	MET
A441	R362	G298	LEU	E172	A78	A2
R444	E363	GLN	LEU	G173	S79	A3
R445	E364	VAL	GLU	V174	R80	K4
A446	R365	ILE	SER	T176	T81	E5
E447	Q366	SER	VAL	N82	V6	V6
A448	Q367	GLU	ILE	D83	K7	K7
A449	E368	ASP	GLN	E177	F8	F8
M450	R369	LEU	SER	E178	N9	N9
R452	V369	GLY	Q244	E179	A85	A85
R453	A370	MET	K245	H180	G86	S10
E456	K371	LYS	P246	K181	D87	D11
V460	G374	LEU	L247	G182	A12	A12
A465	G375	GLU	L248	M183	B13	B13
G467	V376	ASN	L249	E184	D14	D14
D474	A377	THR	V250	T185	R15	R15
K475	V378	THR	A251	V189	M16	M16
A476	K380	D315	E252	L17	K18	K18
S473	V381	R316	D253	E191	G19	G19
D474	G382	L317	V254	G192	T22	T22
K475	G383	R319	E255	K105	L23	L23
A476	M384	GLU	GLY	L104	A24	A24
E481	I387	A320	ALA	D196	D25	D25
Q482	E388	K322	LEU	E197	A26	A26
E483	V389	V323	ALA	G198	V27	V27
E484	G390	S324	THR	Y199	K28	K28
E485	K391	K326	VAL	F204	L31	L31
E486	D394	K327	ASN	V205	R36	R36
E487	V396	D328	LEU	T206	K42	K42
E488	D397	T331	ARG	N207	K42	K42
E489	I400	I332	GLY	D209	P47	P47
E490	M401	V333	GLY	K210	R48	R48
E491	V407	D334	LEU	N211	I49	I49
E494	Q408	G335	LYS	T212	T50	T50
E500	I411	A336	I273	A213	K51	K51
E501	V412	G337	A274	E214	S55	S55
E502	V413	E338	A275	E216	E59	E59
E503	I419	K339	V276	D217	L62	L62
E506	V420	A340	K277	A218	S63	S63
E507	Q421	E341	A278	Y219	D64	D64
E510	Q422	I342	F281	L220	F66	F66
E511	E423	E343	G282	L221	E67	E67
E512	V425	R345	D283	L222	N68	N68
E513	V426	V346	R284	L223	M69	M69
E514	V427	S347	R285	E224	G70	G70
E515	V428	Q348	K286	K225	A71	A71
E516	V429	I349	A287	K226	Q72	Q72
E517	V430	R350	M288	L227	M73	M73
E518	V431	R351	L289	L227	V74	V74
E519	V432	T503	Q290	Q352	R75	R75
E520	V433	V425	Q290	Q352	E76	E76
E521	V434	E506	A293	L353		
E522	V435	D507	I294	I353		
E523	V436	S510	L296	I353		
E524	V437	S511	T296	I353		
E525	V438	S512	T296	I353		
E526	V439	S513	T296	I353		
E527	V440	S514	T296	I353		
E528	V441	S515	T296	I353		
E529	V442	S516	T296	I353		
E530	V443	S517	T296	I353		
E531	V444	S518	T296	I353		
E532	V445	S519	T296	I353		
E533	V446	S520	T296	I353		
E534	V447	S521	T296	I353		
E535	V448	S522	T296	I353		
E536	V449	S523	T296	I353		
E537	V450	S524	T296	I353		
E538	V451	S525	T296	I353		
E539	V452	S526	T296	I353		
E540	V453	S527	T296	I353		
E541	V454	S528	T296	I353		
E542	V455	S529	T296	I353		
E543	V456	S530	T296	I353		
E544	V457	S531	T296	I353		
E545	V458	S532	T296	I353		
E546	V459	S533	T296	I353		
E547	V460	S534	T296	I353		
E548	V461	S535	T296	I353		
E549	V462	S536	T296	I353		
E550	V463	S537	T296	I353		
E551	V464	S538	T296	I353		
E552	V465	S539	T296	I353		
E553	V466	S540	T296	I353		
E554	V467	S541	T296	I353		
E555	V468	S542	T296	I353		
E556	V469	S543	T296	I353		
E557	V470	S544	T296	I353		
E558	V471	S545	T296	I353		
E559	V472	S546	T296	I353		
E560	V473	S547	T296	I353		
E561	V474	S548	T296	I353		
E562	V475	S549	T296	I353		
E563	V476	S550	T296	I353		
E564	V477	S551	T296	I353		
E565	V478	S552	T296	I353		
E566	V479	S553	T296	I353		
E567	V480	S554	T296	I353		
E568	V481	S555	T296	I353		
E569	V482	S556	T296	I353		
E570	V483	S557	T296	I353		
E571	V484	S558	T296	I353		
E572	V485	S559	T296	I353		
E573	V486	S560	T296	I353		
E574	V487	S561	T296	I353		
E575	V488	S562	T296	I353		
E576	V489	S563	T296	I353		
E577	V490	S564	T296	I353		
E578	V491	S565	T296	I353		
E579	V492	S566	T296	I353		
E580	V493	S567	T296	I353		
E581	V494	S568	T296	I353		
E582	V495	S569	T296	I353		
E583	V496	S570	T296	I353		
E584	V497	S571	T296	I353		
E585	V498	S572	T296	I353		
E586	V499	S573	T296	I353		
E587	V500	S574	T296	I353		
E588	V501	S575	T296	I353		
E589	V502	S576	T296	I353		
E590	V503	S577	T296	I353		
E591	V504	S578	T296	I353		
E592	V505	S579	T296	I353		
E593	V506	S580	T296	I353		
E594	V507	S581	T296	I353		
E595	V508	S582	T296	I353		
E596	V509	S583	T296	I353		
E597	V510	S584	T296	I353		
E598	V511	S585	T296	I353		
E599	V512	S586	T296	I353		
E600	V513	S587	T296	I353		
E601	V514	S588	T296	I353		
E602	V515	S589	T296	I353		
E603	V516	S590	T296	I353		
E604	V517	S591	T296	I353		
E605	V518	S592	T296	I353		
E606	V519	S593	T296	I353		
E607	V520	S594	T296	I353		
E608	V521	S595	T296	I353		
E609	V522	S596	T296	I353		
E610	V523	S597	T296	I353		
E611	V524	S598	T296	I353		
E612	V525	S599	T296	I353		
E613	V526	S600	T296	I353		
E614	V527	S601	T296	I353		
E615	V528	S602	T296	I353		
E616	V529	S603	T296	I353		
E617	V530	S604	T296	I353		
E618	V531	S605	T296	I353		
E619	V532	S606	T296	I353		
E620	V533	S607	T296	I353		
E621	V534	S608	T296	I353		
E622	V535	S609	T296	I353		
E623	V536	S610	T296	I353		
E624	V537	S611	T296	I353		
E625	V538	S612	T296	I353		
E626	V539	S613	T296	I353		
E627	V540	S614	T296	I353		
E628	V541	S615	T296	I353		
E629	V542	S616	T296	I353		
E630	V543	S617	T296	I353		
E631	V544	S618	T296	I353		
E632	V545	S619	T296	I353		
E633	V546	S620	T296	I353		
E634	V547	S621	T296	I353		
E635	V548	S622	T296	I353		
E636	V549	S623	T296	I353		
E637	V550	S624	T296	I353		
E638	V551	S625	T296	I353		
E639	V552	S626	T296	I353		
E640	V553	S627	T296	I353		
E641	V554	S628	T296	I353		
E642	V555	S629	T296	I353		
E643	V556	S630	T296	I353		
E644	V557	S631	T296	I353		
E645	V558	S632	T296	I353		
E646	V559	S633	T296	I353		
E647	V560	S634	T296	I353		
E648	V561	S635	T296	I353		
E649	V562	S636	T296	I353		
E650	V563	S637	T296	I353		
E651	V564	S638	T296	I353		
E652	V565	S639	T296	I353		
E653	V566	S640	T296	I353		
E654	V567	S641	T296	I353		
E655	V568	S642	T296	I353		
E656	V569	S643	T296	I353		
E657	V570	S644	T296	I353		
E658	V571	S645	T296	I353		
E659	V572	S646	T296	I353		
E660	V573	S647	T296	I353		
E661	V574	S648	T296	I353		
E662	V575	S649	T296	I353		
E663	V576	S650	T296	I353		
E664	V577	S651	T296	I353		
E665	V578	S652	T296	I353		
E666	V579	S653	T296	I353		
E667	V580	S654	T296	I353		
E668	V581	S655	T296	I353		
E669	V582	S656	T296	I353		
E670	V583	S657	T296	I353		
E671	V584	S658	T296	I353		
E672	V585	S659	T296	I353		
E673	V586	S660	T296	I353		
E674	V587	S661	T296	I353		
E675	V588	S662	T296	I353		
E676	V589	S663	T296	I353		
E677	V590	S664	T296	I353		
E678	V591	S665	T296	I353		
E679	V592	S666	T296	I353		
E680	V593	S667	T296	I353		
E681	V594	S668	T296	I353		
E682	V595	S669	T296	I353		
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E691	V604	S678	T296	I353		
E692	V605	S679	T296	I353		
E693	V606	S680	T296	I353		
E694	V607	S681	T296	I353		
E695	V608	S682	T296	I353		
E696	V609	S683				

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	286.36 Å   286.36 Å   153.46 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.204 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	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	0.32	0/3609	0.48	0/4855
1	B	0.33	0/3609	0.48	0/4855
1	C	0.32	0/3609	0.49	0/4855
1	D	0.34	0/3609	0.48	0/4855
1	E	0.33	0/3609	0.48	0/4855
1	F	0.32	0/3609	0.49	0/4855
1	G	0.33	0/3609	0.48	0/4855
All	All	0.33	0/25263	0.48	0/33985

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	3585	0	3657	233	0
1	B	3585	0	3657	231	0
1	C	3585	0	3657	229	0
1	D	3585	0	3657	228	0
1	E	3585	0	3657	231	0
1	F	3585	0	3657	235	0
1	G	3585	0	3657	231	0
All	All	25095	0	25599	1574	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 31.

The worst 5 of 1574 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:D:139:ASN:HD22	1:D:140:ASP:H	1.17	0.93
1:G:139:ASN:HD22	1:G:140:ASP:H	1.16	0.92
1:C:139:ASN:HD22	1:C:140:ASP:H	1.17	0.92
1:C:36:ARG:HG2	1:C:36:ARG:HH11	1.35	0.92
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.35	0.91

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	474/545 (87%)	404 (85%)	59 (12%)	11 (2%)	8	44
1	B	474/545 (87%)	405 (85%)	59 (12%)	10 (2%)	9	46
1	C	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	9	46
1	D	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	9	46
1	E	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	9	46
1	F	474/545 (87%)	404 (85%)	58 (12%)	12 (2%)	7	41
1	G	474/545 (87%)	405 (85%)	59 (12%)	10 (2%)	9	46
All	All	3318/3815 (87%)	2830 (85%)	415 (12%)	73 (2%)	8	45

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	85	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	228	SER
1	A	378	VAL
1	B	9	ASN

### 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	372/421 (88%)	278 (75%)	94 (25%)	1	2
1	B	372/421 (88%)	279 (75%)	93 (25%)	1	2
1	C	372/421 (88%)	277 (74%)	95 (26%)	1	2
1	D	372/421 (88%)	279 (75%)	93 (25%)	1	2
1	E	372/421 (88%)	278 (75%)	94 (25%)	1	2
1	F	372/421 (88%)	278 (75%)	94 (25%)	1	2
1	G	372/421 (88%)	277 (74%)	95 (26%)	1	2
All	All	2604/2947 (88%)	1946 (75%)	658 (25%)	1	2

5 of 658 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	80	ARG
1	D	430	SER
1	G	225	LYS
1	D	156	SER
1	D	281	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	68	ASN
1	D	352	GLN
1	G	153	ASN
1	D	72	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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.