



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2022 – 06:13 PM EDT

PDB ID : 7U39
Title : Structure of the apo form of Streptomyces venezuelae GlgX, the glycogen de-branching enzyme
Authors : Schumacher, M.A.
Deposited on : 2022-02-26
Resolution : 3.51 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

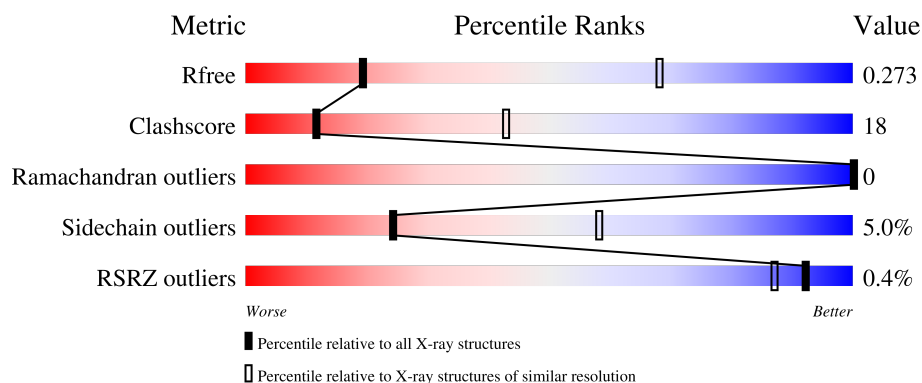
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. 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	709	 60% 37% ..
1	B	709	 59% 37% ..
1	C	709	 56% 41% ..
1	D	709	 60% 37% ..
1	E	709	 60% 36% ..

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Mol	Chain	Length	Quality of chain
1	F	709	<div><div><div>%</div><div><div></div><div>62%</div><div>34%</div><div></div></div><div>..</div></div></div>
1	G	709	<div><div><div>2%</div><div><div></div><div>60%</div><div>36%</div><div></div></div><div>..</div></div></div>
1	H	709	<div><div><div></div><div><div></div><div>60%</div><div>37%</div><div></div></div><div>..</div></div></div>
1	I	709	<div><div><div></div><div><div></div><div>59%</div><div>39%</div><div></div></div><div>..</div></div></div>
1	J	709	<div><div><div>%</div><div><div></div><div>58%</div><div>39%</div><div></div></div><div>..</div></div></div>
1	K	709	<div><div><div>%</div><div><div></div><div>60%</div><div>37%</div><div></div></div><div>..</div></div></div>
1	L	709	<div><div><div></div><div><div></div><div>58%</div><div>39%</div><div></div></div><div>..</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 67324 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 Glycogen debranching enzyme GlgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	0	0
			5567	3499	1002	1042	24			
1	B	705	Total	C	N	O	S	0	0	0
			5595	3514	1013	1044	24			
1	C	699	Total	C	N	O	S	0	0	0
			5551	3487	1003	1037	24			
1	D	700	Total	C	N	O	S	0	0	0
			5566	3495	1007	1041	23			
1	E	700	Total	C	N	O	S	0	0	0
			5567	3497	1003	1044	23			
1	F	698	Total	C	N	O	S	0	0	0
			5549	3486	1003	1037	23			
1	G	698	Total	C	N	O	S	0	0	0
			5554	3490	1004	1037	23			
1	H	701	Total	C	N	O	S	0	0	0
			5570	3499	1009	1038	24			
1	I	701	Total	C	N	O	S	0	0	0
			5583	3506	1012	1042	23			
1	J	700	Total	C	N	O	S	0	0	0
			5557	3491	1001	1041	24			
1	K	701	Total	C	N	O	S	0	0	0
			5583	3506	1012	1042	23			
1	L	701	Total	C	N	O	S	0	0	0
			5564	3494	1004	1043	23			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A5P2ALW6
A	-1	SER	-	expression tag	UNP A0A5P2ALW6
A	0	HIS	-	expression tag	UNP A0A5P2ALW6
A	103	VAL	ILE	conflict	UNP A0A5P2ALW6
A	192	ARG	LYS	conflict	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	296	ALA	SER	conflict	UNP A0A5P2ALW6
A	297	ASP	ASN	conflict	UNP A0A5P2ALW6
A	303	MET	THR	conflict	UNP A0A5P2ALW6
A	682	GLN	GLU	conflict	UNP A0A5P2ALW6
B	-2	GLY	-	expression tag	UNP A0A5P2ALW6
B	-1	SER	-	expression tag	UNP A0A5P2ALW6
B	0	HIS	-	expression tag	UNP A0A5P2ALW6
B	103	VAL	ILE	conflict	UNP A0A5P2ALW6
B	192	ARG	LYS	conflict	UNP A0A5P2ALW6
B	296	ALA	SER	conflict	UNP A0A5P2ALW6
B	297	ASP	ASN	conflict	UNP A0A5P2ALW6
B	303	MET	THR	conflict	UNP A0A5P2ALW6
B	682	GLN	GLU	conflict	UNP A0A5P2ALW6
C	-2	GLY	-	expression tag	UNP A0A5P2ALW6
C	-1	SER	-	expression tag	UNP A0A5P2ALW6
C	0	HIS	-	expression tag	UNP A0A5P2ALW6
C	103	VAL	ILE	conflict	UNP A0A5P2ALW6
C	192	ARG	LYS	conflict	UNP A0A5P2ALW6
C	296	ALA	SER	conflict	UNP A0A5P2ALW6
C	297	ASP	ASN	conflict	UNP A0A5P2ALW6
C	303	MET	THR	conflict	UNP A0A5P2ALW6
C	682	GLN	GLU	conflict	UNP A0A5P2ALW6
D	-2	GLY	-	expression tag	UNP A0A5P2ALW6
D	-1	SER	-	expression tag	UNP A0A5P2ALW6
D	0	HIS	-	expression tag	UNP A0A5P2ALW6
D	103	VAL	ILE	conflict	UNP A0A5P2ALW6
D	192	ARG	LYS	conflict	UNP A0A5P2ALW6
D	296	ALA	SER	conflict	UNP A0A5P2ALW6
D	297	ASP	ASN	conflict	UNP A0A5P2ALW6
D	303	MET	THR	conflict	UNP A0A5P2ALW6
D	682	GLN	GLU	conflict	UNP A0A5P2ALW6
E	-2	GLY	-	expression tag	UNP A0A5P2ALW6
E	-1	SER	-	expression tag	UNP A0A5P2ALW6
E	0	HIS	-	expression tag	UNP A0A5P2ALW6
E	103	VAL	ILE	conflict	UNP A0A5P2ALW6
E	192	ARG	LYS	conflict	UNP A0A5P2ALW6
E	296	ALA	SER	conflict	UNP A0A5P2ALW6
E	297	ASP	ASN	conflict	UNP A0A5P2ALW6
E	303	MET	THR	conflict	UNP A0A5P2ALW6
E	682	GLN	GLU	conflict	UNP A0A5P2ALW6
F	-2	GLY	-	expression tag	UNP A0A5P2ALW6
F	-1	SER	-	expression tag	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP A0A5P2ALW6
F	103	VAL	ILE	conflict	UNP A0A5P2ALW6
F	192	ARG	LYS	conflict	UNP A0A5P2ALW6
F	296	ALA	SER	conflict	UNP A0A5P2ALW6
F	297	ASP	ASN	conflict	UNP A0A5P2ALW6
F	303	MET	THR	conflict	UNP A0A5P2ALW6
F	682	GLN	GLU	conflict	UNP A0A5P2ALW6
G	-2	GLY	-	expression tag	UNP A0A5P2ALW6
G	-1	SER	-	expression tag	UNP A0A5P2ALW6
G	0	HIS	-	expression tag	UNP A0A5P2ALW6
G	103	VAL	ILE	conflict	UNP A0A5P2ALW6
G	192	ARG	LYS	conflict	UNP A0A5P2ALW6
G	296	ALA	SER	conflict	UNP A0A5P2ALW6
G	297	ASP	ASN	conflict	UNP A0A5P2ALW6
G	303	MET	THR	conflict	UNP A0A5P2ALW6
G	682	GLN	GLU	conflict	UNP A0A5P2ALW6
H	-2	GLY	-	expression tag	UNP A0A5P2ALW6
H	-1	SER	-	expression tag	UNP A0A5P2ALW6
H	0	HIS	-	expression tag	UNP A0A5P2ALW6
H	103	VAL	ILE	conflict	UNP A0A5P2ALW6
H	192	ARG	LYS	conflict	UNP A0A5P2ALW6
H	296	ALA	SER	conflict	UNP A0A5P2ALW6
H	297	ASP	ASN	conflict	UNP A0A5P2ALW6
H	303	MET	THR	conflict	UNP A0A5P2ALW6
H	682	GLN	GLU	conflict	UNP A0A5P2ALW6
I	-2	GLY	-	expression tag	UNP A0A5P2ALW6
I	-1	SER	-	expression tag	UNP A0A5P2ALW6
I	0	HIS	-	expression tag	UNP A0A5P2ALW6
I	103	VAL	ILE	conflict	UNP A0A5P2ALW6
I	192	ARG	LYS	conflict	UNP A0A5P2ALW6
I	296	ALA	SER	conflict	UNP A0A5P2ALW6
I	297	ASP	ASN	conflict	UNP A0A5P2ALW6
I	303	MET	THR	conflict	UNP A0A5P2ALW6
I	682	GLN	GLU	conflict	UNP A0A5P2ALW6
J	-2	GLY	-	expression tag	UNP A0A5P2ALW6
J	-1	SER	-	expression tag	UNP A0A5P2ALW6
J	0	HIS	-	expression tag	UNP A0A5P2ALW6
J	103	VAL	ILE	conflict	UNP A0A5P2ALW6
J	192	ARG	LYS	conflict	UNP A0A5P2ALW6
J	296	ALA	SER	conflict	UNP A0A5P2ALW6
J	297	ASP	ASN	conflict	UNP A0A5P2ALW6
J	303	MET	THR	conflict	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	682	GLN	GLU	conflict	UNP A0A5P2ALW6
K	-2	GLY	-	expression tag	UNP A0A5P2ALW6
K	-1	SER	-	expression tag	UNP A0A5P2ALW6
K	0	HIS	-	expression tag	UNP A0A5P2ALW6
K	103	VAL	ILE	conflict	UNP A0A5P2ALW6
K	192	ARG	LYS	conflict	UNP A0A5P2ALW6
K	296	ALA	SER	conflict	UNP A0A5P2ALW6
K	297	ASP	ASN	conflict	UNP A0A5P2ALW6
K	303	MET	THR	conflict	UNP A0A5P2ALW6
K	682	GLN	GLU	conflict	UNP A0A5P2ALW6
L	-2	GLY	-	expression tag	UNP A0A5P2ALW6
L	-1	SER	-	expression tag	UNP A0A5P2ALW6
L	0	HIS	-	expression tag	UNP A0A5P2ALW6
L	103	VAL	ILE	conflict	UNP A0A5P2ALW6
L	192	ARG	LYS	conflict	UNP A0A5P2ALW6
L	296	ALA	SER	conflict	UNP A0A5P2ALW6
L	297	ASP	ASN	conflict	UNP A0A5P2ALW6
L	303	MET	THR	conflict	UNP A0A5P2ALW6
L	682	GLN	GLU	conflict	UNP A0A5P2ALW6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	56	Total O 56 56	0	0
2	B	56	Total O 56 56	0	0
2	C	63	Total O 63 63	0	0
2	D	43	Total O 43 43	0	0
2	E	42	Total O 42 42	0	0
2	F	43	Total O 43 43	0	0
2	G	27	Total O 27 27	0	0
2	H	41	Total O 41 41	0	0
2	I	38	Total O 38 38	0	0
2	J	38	Total O 38 38	0	0

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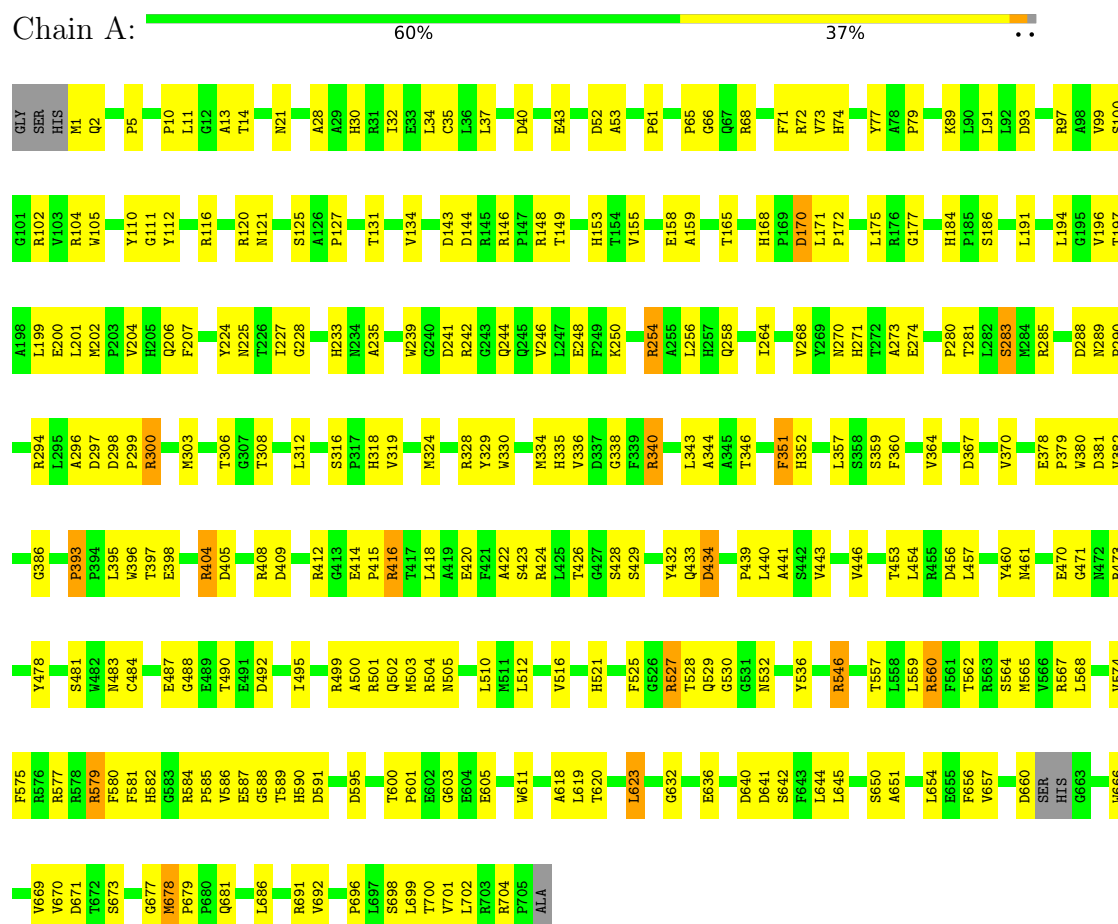
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	37	Total	O	0	0
			37	37		
2	L	34	Total	O	0	0
			34	34		

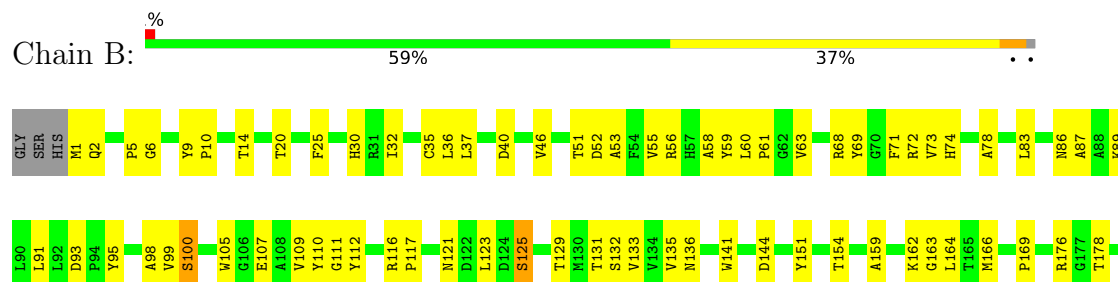
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Glycogen debranching enzyme GlgX



• Molecule 1: Glycogen debranching enzyme GlgX

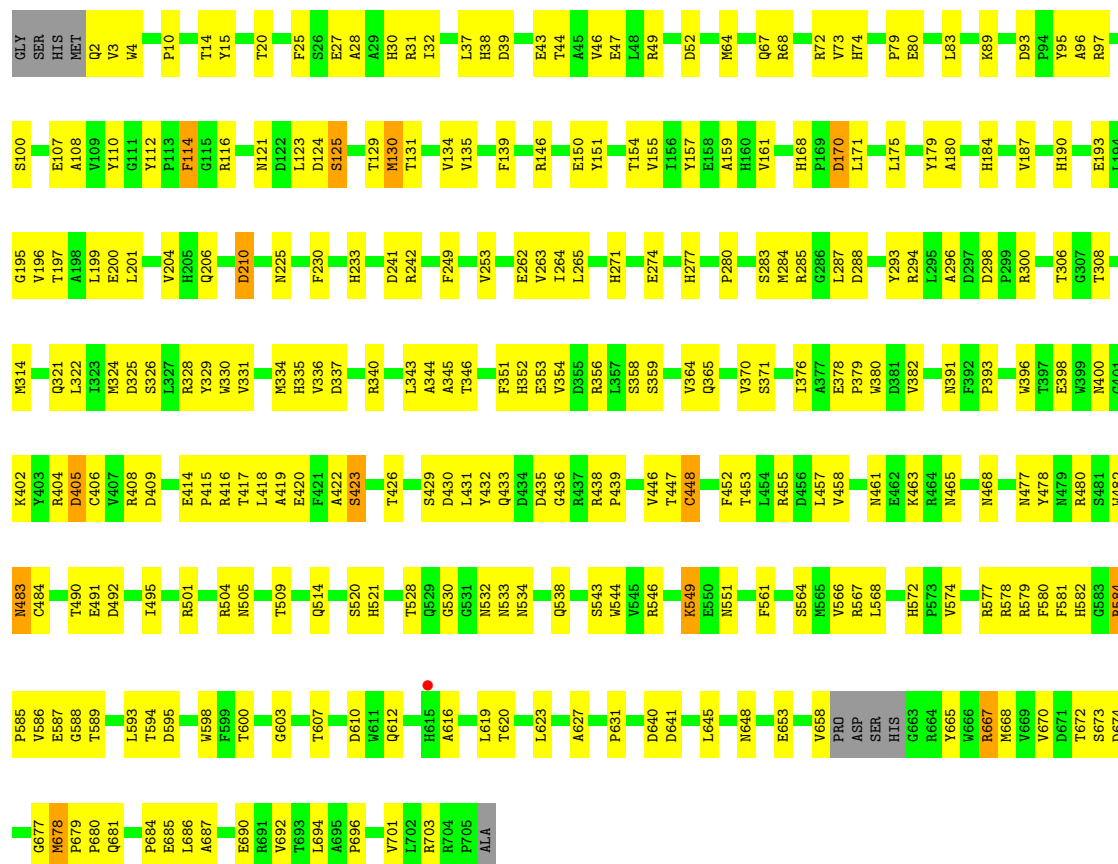






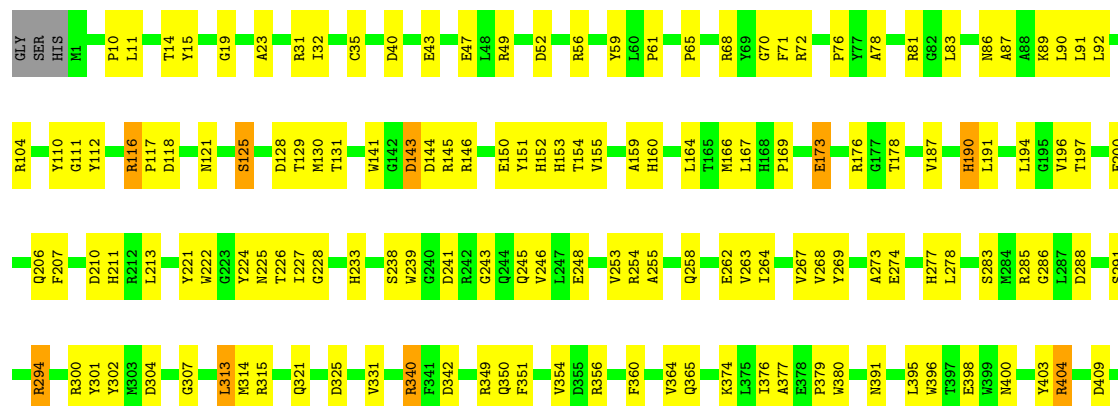
• Molecule 1: Glycogen debranching enzyme GlgX

Chain D: 60% 37% ..

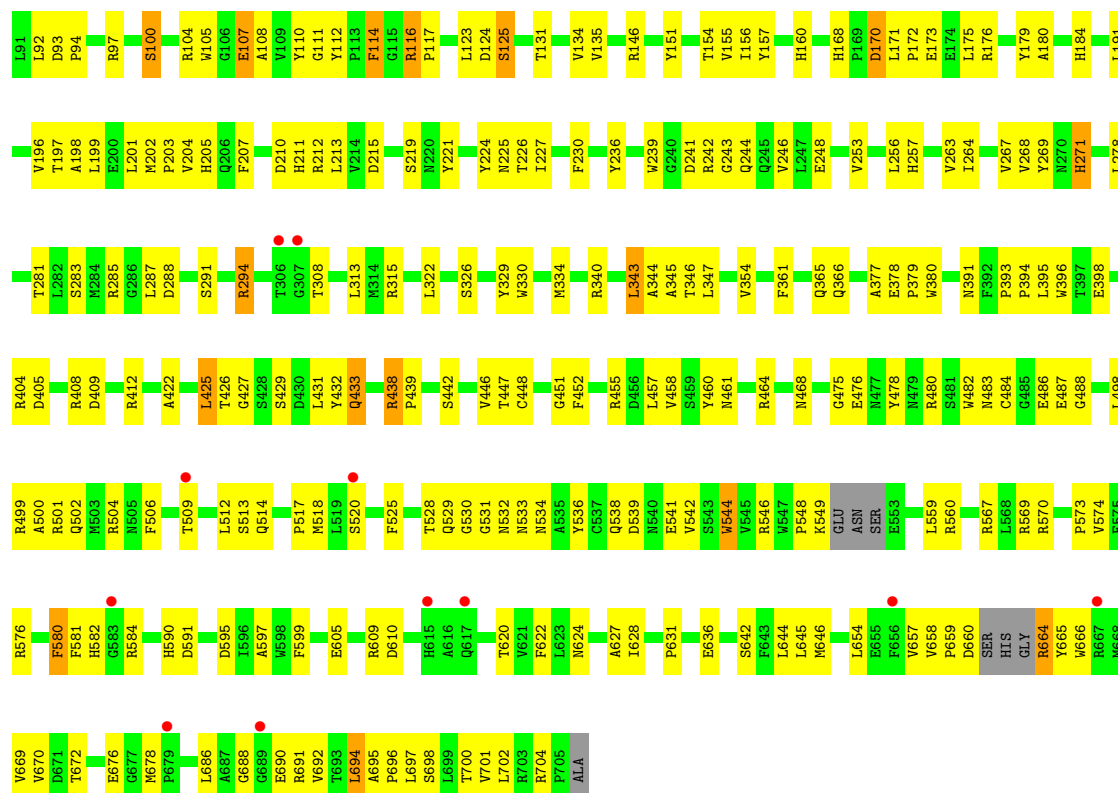


• Molecule 1: Glycogen debranching enzyme GlgX

Chain E: 60% 36% ..

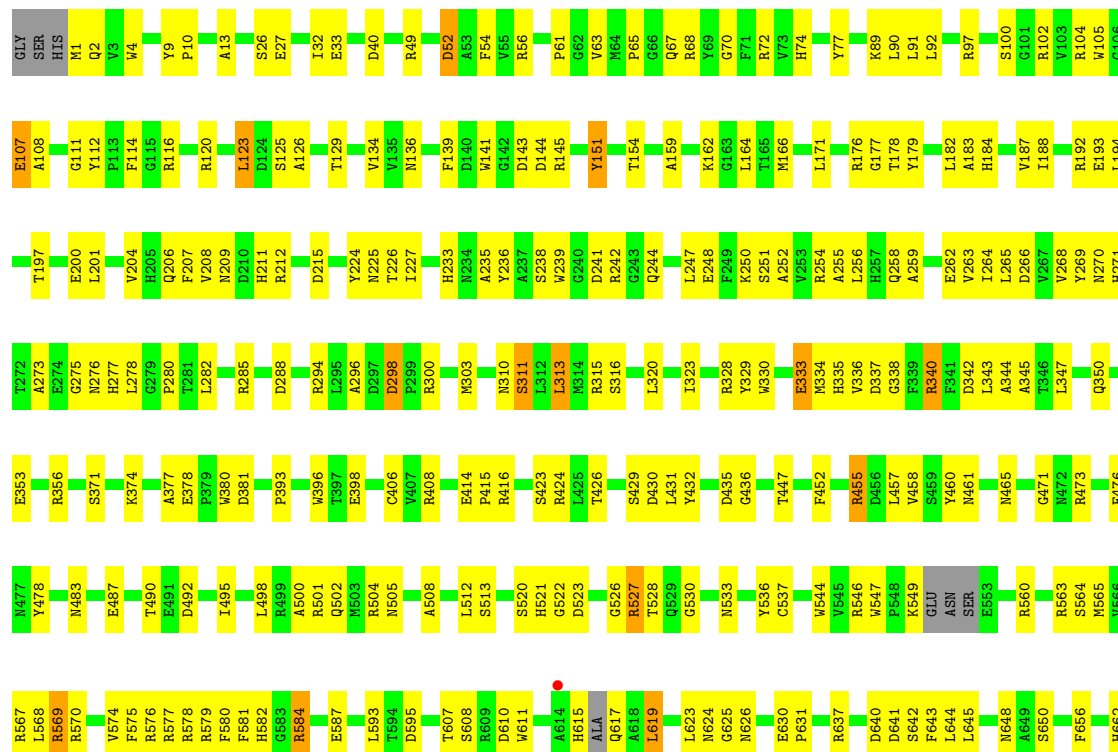


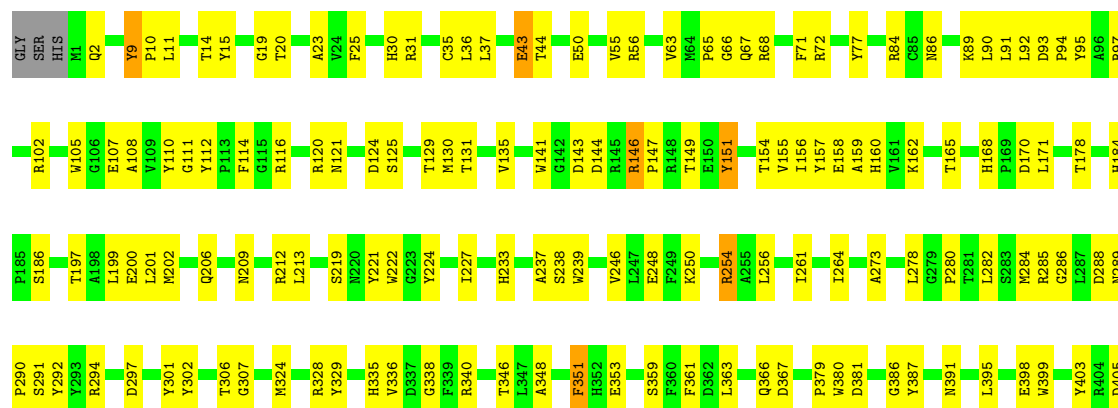


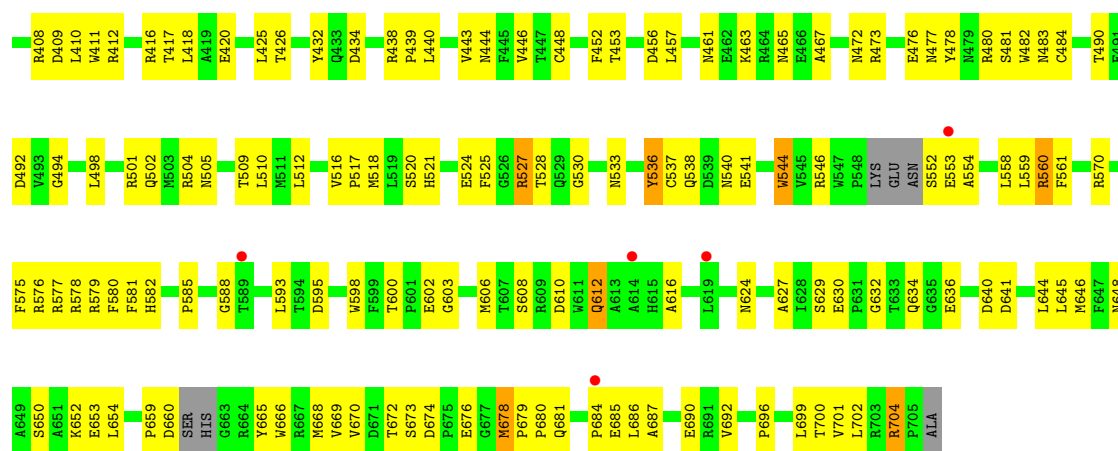


• Molecule 1: Glycogen debranching enzyme GlgX

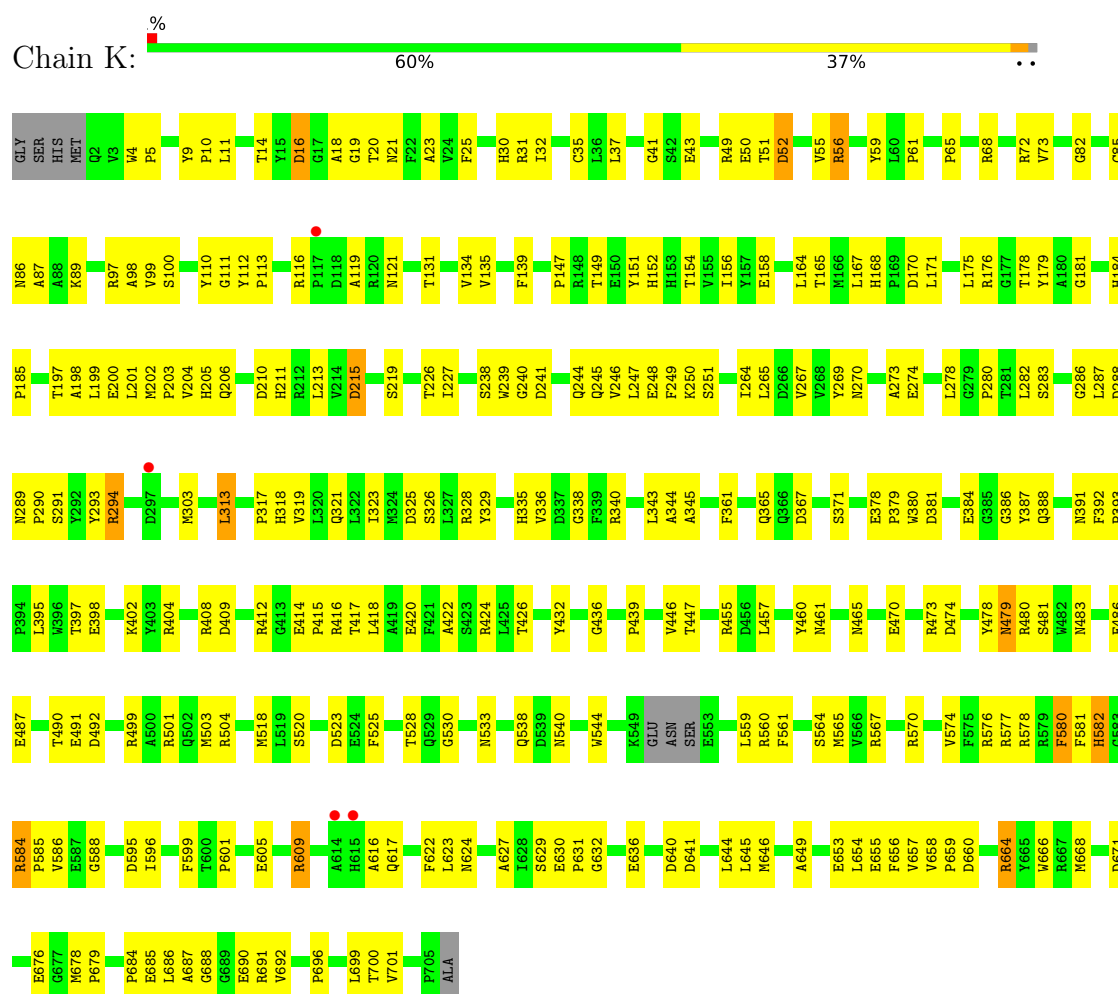
Chain H: 60% 37%



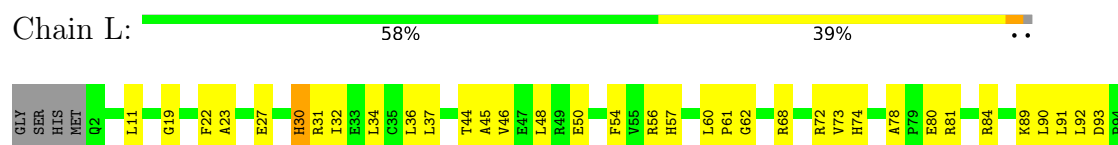




• Molecule 1: Glycogen debranching enzyme GlgX



• Molecule 1: Glycogen debranching enzyme GlgX



L654	E655	F656	P659	D660	SER	HIS	G663	R664	M668	V669	V670	D671	T672	S673	D674	P675	R678	P679	P680	Q681	P684	A687	G688	G689	L694	A695	P696	L697	S698	L699	T700	V701	L702	R703	R704	P705	ALA																
P573	V574	F575	R576	R579	F580	F581	H582	G583	R584	P585	V586	T589	H590	T594	D595	I596	A597	W598	P601	E605	D610	W611	Q612	A618	L619	T620	V621	F622	L623	N624	G625	N626	E630	P631	G632	E636	R637	I638	A639	D640	D641	L644	L645	R646	F647	N648	K652	F653					
S481	W482	N483	C484	G485	E486	E487	G488	F489	T490	E491	D492	R499	A500	R501	Q502	N505	F506	L507	A508	L512	S513	Q514	G515	V516	S520	H521	G522	D523	R527	T528	Q529	G530	N533	Y536	V545	R546	W547	E550	ASN	S552	L559	R560	F561	T562	R563	L568	H572						
E398		R404	D405	C406	V407	R408	D409	R416	T417	L418	A419	E420	T426	R315	G427	S428	S429	D430	L431	Y432	Q433	D434	D435	P439	L440	A441	S442	V443	N444	F445	V446	T447	C448	H449	F452	T453	L454	R455	V458	S459	Y460	N461	E462	K463	E470	R473	D474	G475	E476	N477	Y478	N479	R480
G286	L287	Y293		D297	T306	G307	T308	S311	L312	L313	R314	R315	G316	M324	D337	L343	A344	A345	T346	L347	Q350	F351	V354	D355	R356	L357	F361	D362	L363	Y364	Q365	Q366	V370	K374	E378	P379	W380	D381	V382	G386	N391	F392	P393	W396	T397								
Y95	A96	R97	A98	V99	R102	W105	Y110	G111	Y112	R116	P117	D118	D124	S125	T129	M130	V135	D143	T149	E150	Y151	H152	H153	Y157	E158	A159	H160	V161	K162	G163	L164	H168	F169	D170	L171	P172	L175	R176	G177	A180	G181	H184	P185	S186	V187								
I188	G189	H190	L194	T197	E200	L201	H205	Q206	N209	D210	H211	R212	S219	R220	Y221	Y224	R225	T226	G228	H233	R242	Q245	V246	L247	E248	F249	K250	R254	A255	L256	H257	T264	L265	D266	V267	V268	Y269	T272	A273	E274	P280	T281	R285										

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	181.50Å 204.86Å 195.72Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	67.92 – 3.51 67.92 – 3.66	Depositor EDS
% Data completeness (in resolution range)	83.5 (67.92-3.51) 83.5 (67.92-3.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.276 0.209 , 0.273	Depositor DCC
R_{free} test set	1920 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.912	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 20.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.037 for -h,-l,-k 0.035 for -h,l,k 0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	67324	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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	0.30	0/5720	0.58	4/7785 (0.1%)
1	B	0.30	0/5750	0.56	5/7825 (0.1%)
1	C	0.31	0/5700	0.54	0/7752
1	D	0.30	0/5718	0.55	1/7779 (0.0%)
1	E	0.31	0/5719	0.56	0/7781
1	F	0.30	0/5701	0.54	2/7757 (0.0%)
1	G	0.30	0/5706	0.53	0/7763
1	H	0.31	0/5723	0.54	0/7785
1	I	0.29	0/5737	0.54	0/7805
1	J	0.31	0/5709	0.56	2/7768 (0.0%)
1	K	0.30	0/5737	0.56	0/7805
1	L	0.30	0/5715	0.54	3/7776 (0.0%)
All	All	0.30	0/68635	0.55	17/93381 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	L	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ASP	N-CA-C	-8.64	87.67	111.00
1	J	673	SER	C-N-CA	-7.04	104.10	121.70
1	A	298	ASP	CB-CA-C	6.68	123.76	110.40
1	A	546	ARG	C-N-CA	-6.09	106.48	121.70
1	B	673	SER	C-N-CA	-6.05	106.57	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	586	VAL	Peptide
1	B	661	SER	Peptide
1	B	678	MET	Peptide
1	D	678	MET	Peptide
1	E	678	MET	Peptide

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	5567	0	5245	200	0
1	B	5595	0	5282	204	0
1	C	5551	0	5244	228	0
1	D	5566	0	5256	179	0
1	E	5567	0	5253	194	0
1	F	5549	0	5234	173	0
1	G	5554	0	5246	186	0
1	H	5570	0	5254	178	0
1	I	5583	0	5274	192	0
1	J	5557	0	5240	199	0
1	K	5583	0	5274	192	0
1	L	5564	0	5244	201	0
2	A	56	0	0	1	0
2	B	56	0	0	0	0
2	C	63	0	0	0	0
2	D	43	0	0	1	0
2	E	42	0	0	2	0
2	F	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	27	0	0	0	0
2	H	41	0	0	1	0
2	I	38	0	0	4	0
2	J	38	0	0	1	0
2	K	37	0	0	0	0
2	L	34	0	0	2	0
All	All	67324	0	63046	2278	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 18.

The worst 5 of 2278 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:H:102:ARG:HH12	1:H:208:VAL:HA	1.32	0.94
1:B:294:ARG:HH22	1:B:305:THR:HG23	1.32	0.94
1:C:493:VAL:HA	1:C:496:THR:HB	1.54	0.90
1:J:391:ASN:HD21	1:K:317:PRO:HG3	1.36	0.90
1:B:501:ARG:NH2	1:B:696:PRO:O	2.05	0.89

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	699/709 (99%)	620 (89%)	79 (11%)	0	100	100
1	B	703/709 (99%)	636 (90%)	67 (10%)	0	100	100
1	C	693/709 (98%)	614 (89%)	79 (11%)	0	100	100
1	D	696/709 (98%)	604 (87%)	92 (13%)	0	100	100
1	E	694/709 (98%)	628 (90%)	66 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	692/709 (98%)	617 (89%)	75 (11%)	0	100	100
1	G	692/709 (98%)	612 (88%)	80 (12%)	0	100	100
1	H	695/709 (98%)	623 (90%)	72 (10%)	0	100	100
1	I	697/709 (98%)	622 (89%)	75 (11%)	0	100	100
1	J	694/709 (98%)	622 (90%)	72 (10%)	0	100	100
1	K	697/709 (98%)	619 (89%)	78 (11%)	0	100	100
1	L	695/709 (98%)	617 (89%)	78 (11%)	0	100	100
All	All	8347/8508 (98%)	7434 (89%)	913 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	576/590 (98%)	551 (96%)	25 (4%)	29	62
1	B	580/590 (98%)	549 (95%)	31 (5%)	22	56
1	C	575/590 (98%)	546 (95%)	29 (5%)	24	58
1	D	578/590 (98%)	548 (95%)	30 (5%)	23	57
1	E	579/590 (98%)	548 (95%)	31 (5%)	22	56
1	F	576/590 (98%)	544 (94%)	32 (6%)	21	55
1	G	577/590 (98%)	544 (94%)	33 (6%)	20	54
1	H	577/590 (98%)	544 (94%)	33 (6%)	20	54
1	I	580/590 (98%)	557 (96%)	23 (4%)	31	64
1	J	577/590 (98%)	548 (95%)	29 (5%)	24	58
1	K	580/590 (98%)	554 (96%)	26 (4%)	27	62
1	L	577/590 (98%)	549 (95%)	28 (5%)	25	59
All	All	6932/7080 (98%)	6582 (95%)	350 (5%)	24	58

5 of 350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	455	ARG
1	J	527	ARG
1	H	584	ARG
1	I	455	ARG
1	K	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	483	ASN
1	L	365	GLN
1	C	391	ASN
1	C	365	GLN
1	L	391	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 monosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	703/709 (99%)	-0.31	0 100 100	26, 44, 73, 95	0
1	B	705/709 (99%)	-0.34	4 (0%) 89 81	27, 41, 69, 102	0
1	C	699/709 (98%)	-0.45	0 100 100	25, 41, 70, 93	0
1	D	700/709 (98%)	-0.44	1 (0%) 95 93	28, 45, 73, 112	0
1	E	700/709 (98%)	-0.34	3 (0%) 92 87	27, 46, 72, 106	0
1	F	698/709 (98%)	-0.35	4 (0%) 89 81	26, 43, 72, 98	0
1	G	698/709 (98%)	-0.08	11 (1%) 72 59	30, 56, 87, 113	0
1	H	701/709 (98%)	-0.35	3 (0%) 92 87	30, 43, 73, 96	0
1	I	701/709 (98%)	-0.39	1 (0%) 95 93	29, 45, 75, 96	0
1	J	700/709 (98%)	-0.34	5 (0%) 87 79	27, 44, 74, 103	0
1	K	701/709 (98%)	-0.30	4 (0%) 89 81	31, 49, 79, 122	0
1	L	701/709 (98%)	-0.32	1 (0%) 95 93	34, 50, 78, 102	0
All	All	8407/8508 (98%)	-0.33	37 (0%) 92 87	25, 45, 76, 122	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	615	HIS	4.4
1	F	615	HIS	3.9
1	G	306	THR	3.6
1	K	615	HIS	3.6
1	D	615	HIS	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 monosaccharides 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.