



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 07:03 PM EDT

PDB ID : 3LJ5
Title : Full Length Bacteriophage P22 Portal Protein
Authors : Olia, A.S.; Cingolani, G.
Deposited on : 2010-01-25
Resolution : 7.50 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)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

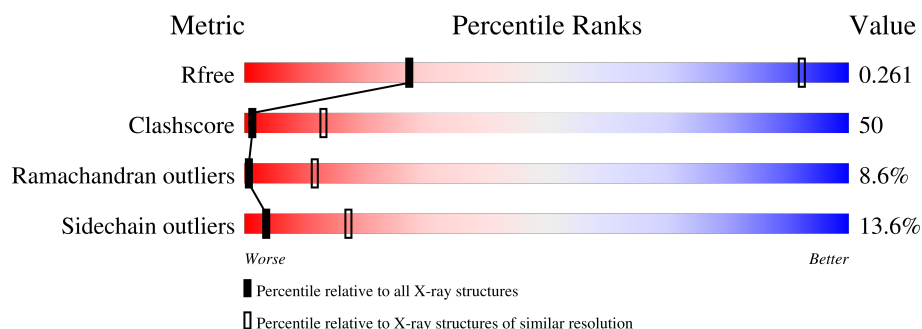
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.50 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	725	38% 45% 12% • 5%
1	B	725	39% 45% 12% • 5%
1	C	725	39% 44% 12% • 5%
1	D	725	38% 45% 12% • 5%
1	E	725	37% 45% 12% • 5%
1	F	725	39% 44% 12% • 5%
1	G	725	37% 47% 12% 5%

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Mol	Chain	Length	Quality of chain
1	H	725	<div><div></div><div>38%</div><div>45%</div><div>12%</div><div>5%</div></div>
1	I	725	<div><div></div><div>39%</div><div>44%</div><div>12%</div><div>• 5%</div></div>
1	J	725	<div><div></div><div>39%</div><div>44%</div><div>12%</div><div>• 5%</div></div>
1	K	725	<div><div></div><div>39%</div><div>43%</div><div>12%</div><div>• 5%</div></div>
1	L	725	<div><div></div><div>40%</div><div>43%</div><div>12%</div><div>• 5%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 61512 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.

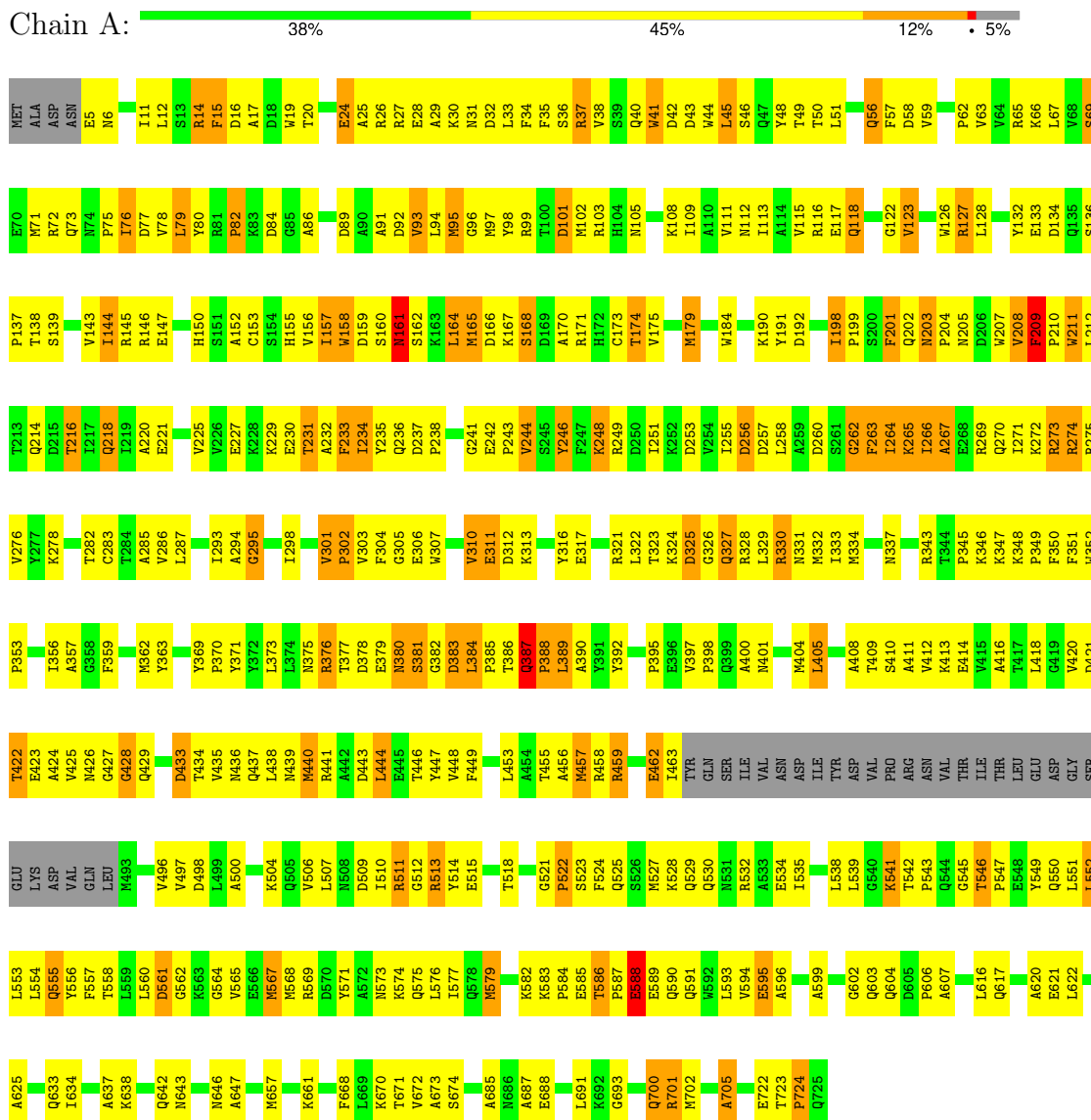
- Molecule 1 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	B	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	C	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	D	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	E	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	F	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	G	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	H	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	I	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	J	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	K	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			
1	L	692	Total	C	N	O	S	0	0	0
			5126	3204	900	1002	20			

3 Residue-property plots

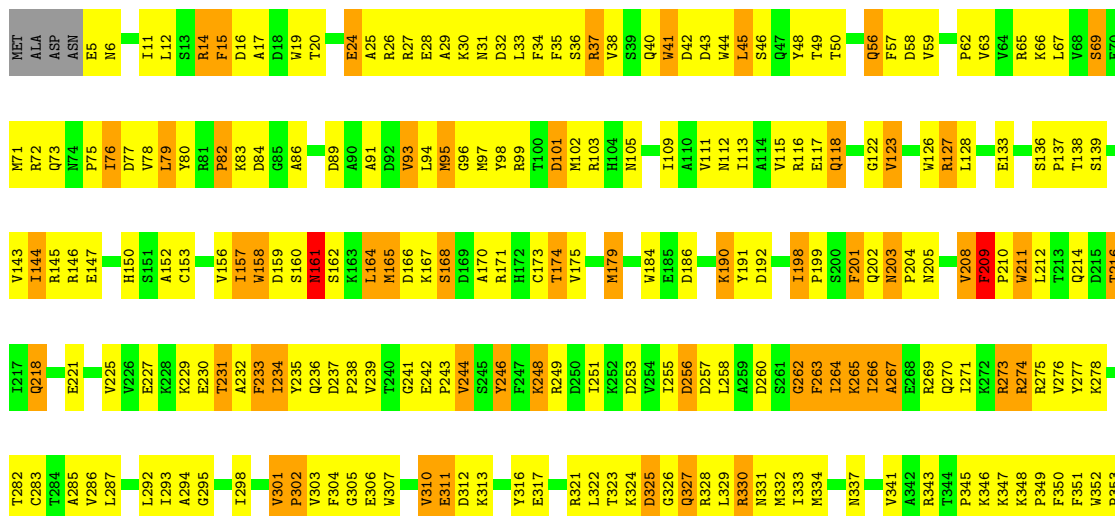
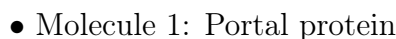
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

• Molecule 1: Portal protein



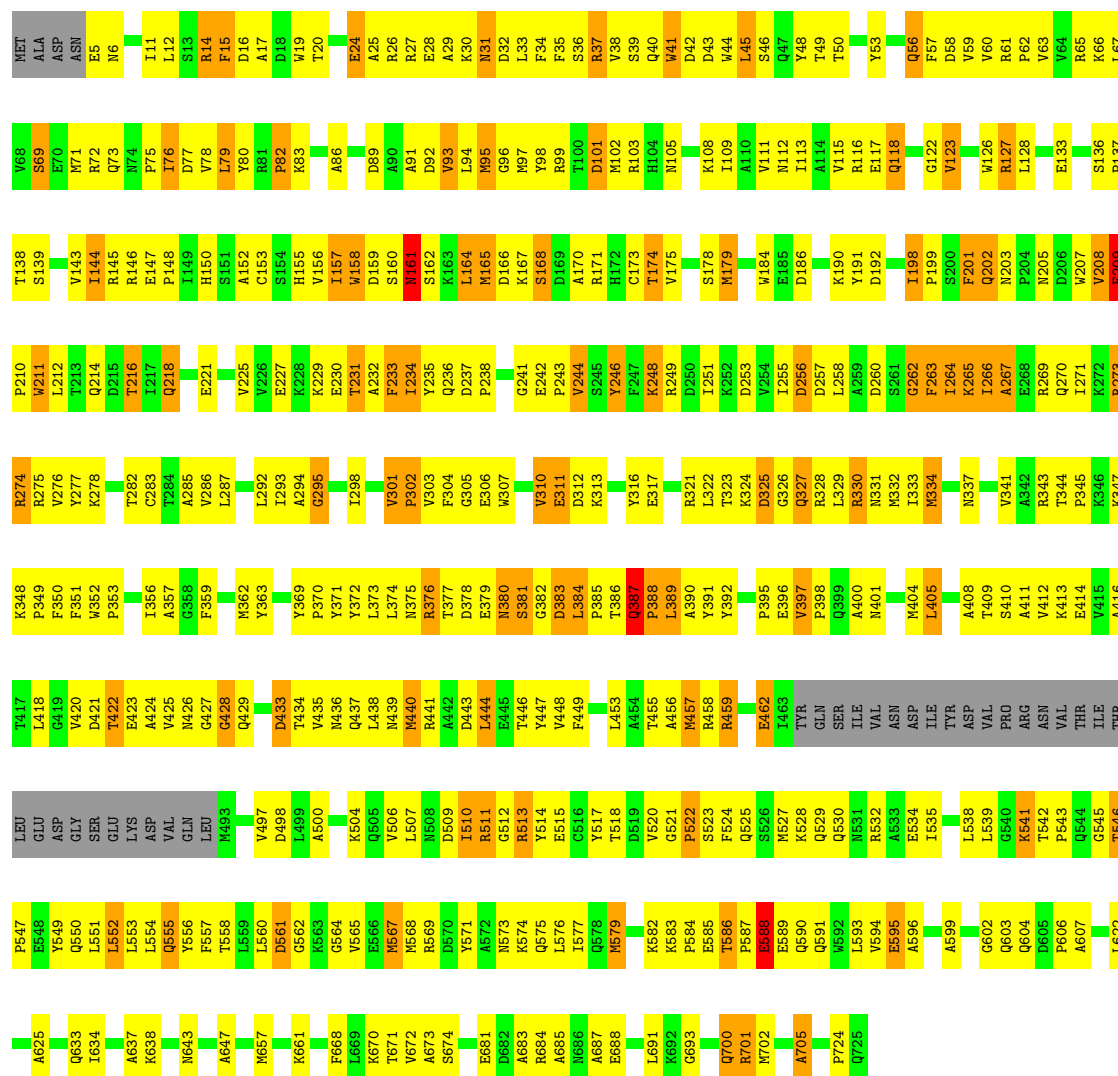
• Molecule 1: Portal protein





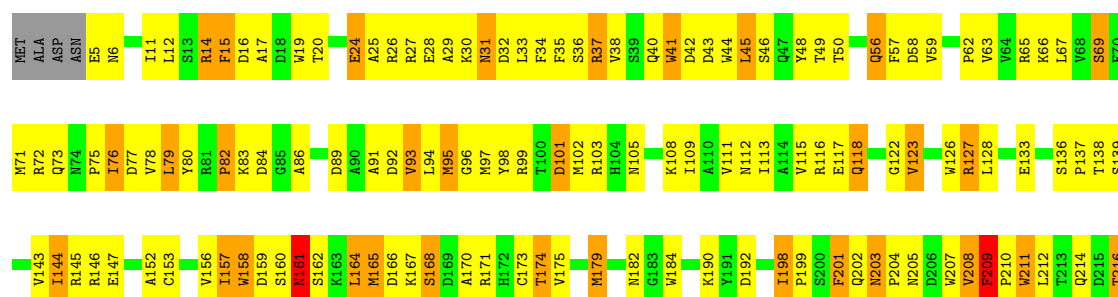
• Molecule 1: Portal protein

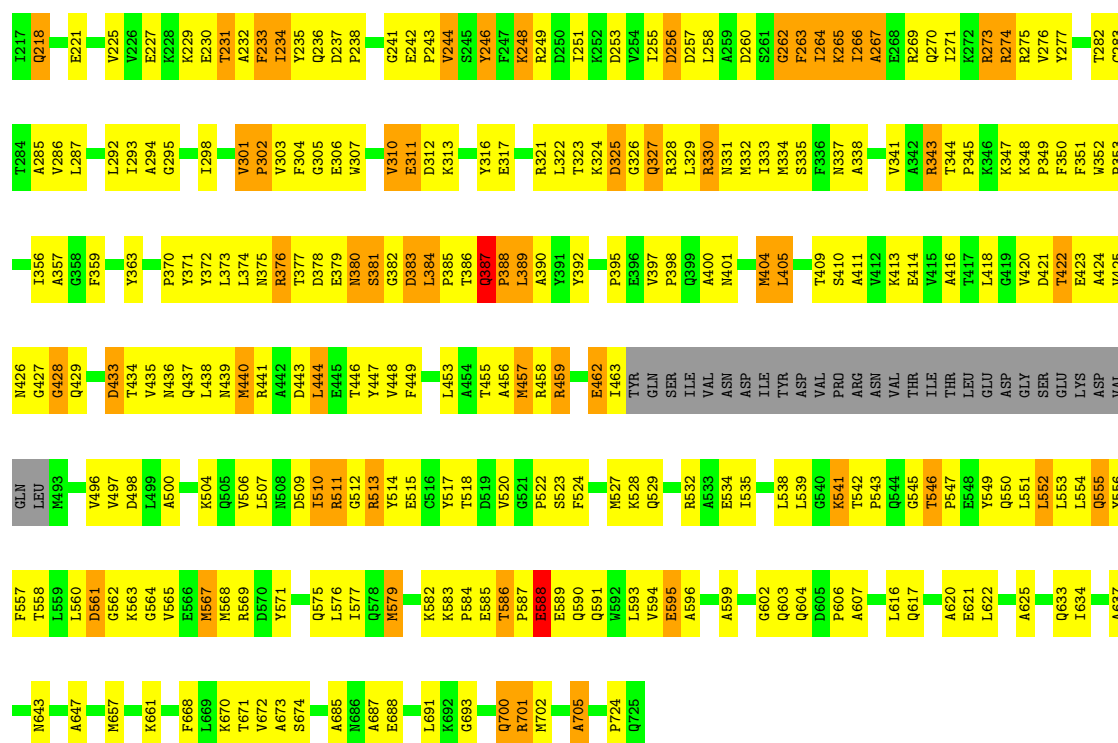
Chain E:  37% 45% 12% • 5%



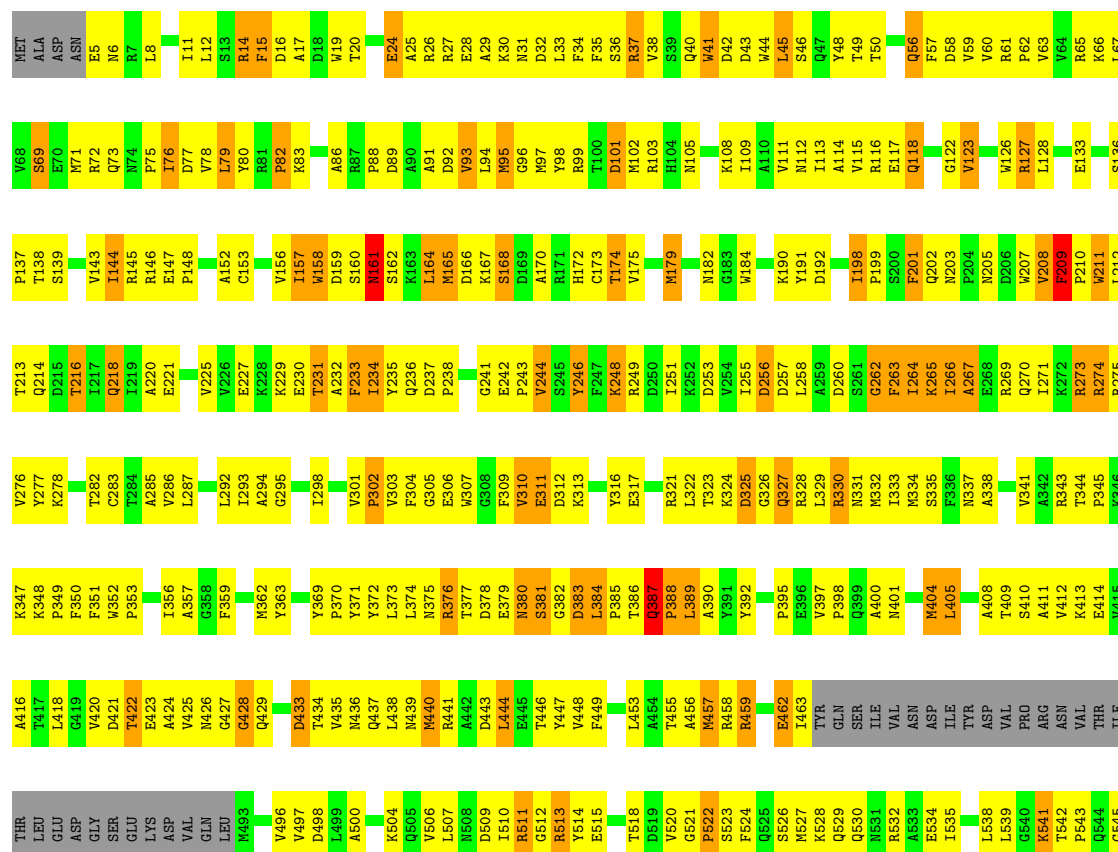
• Molecule 1: Portal protein

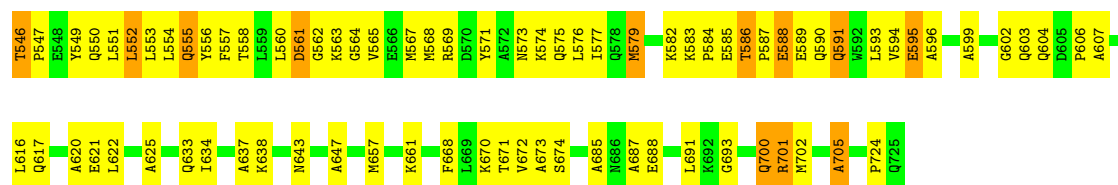
Chain F:  39% 44% 12% • 5%





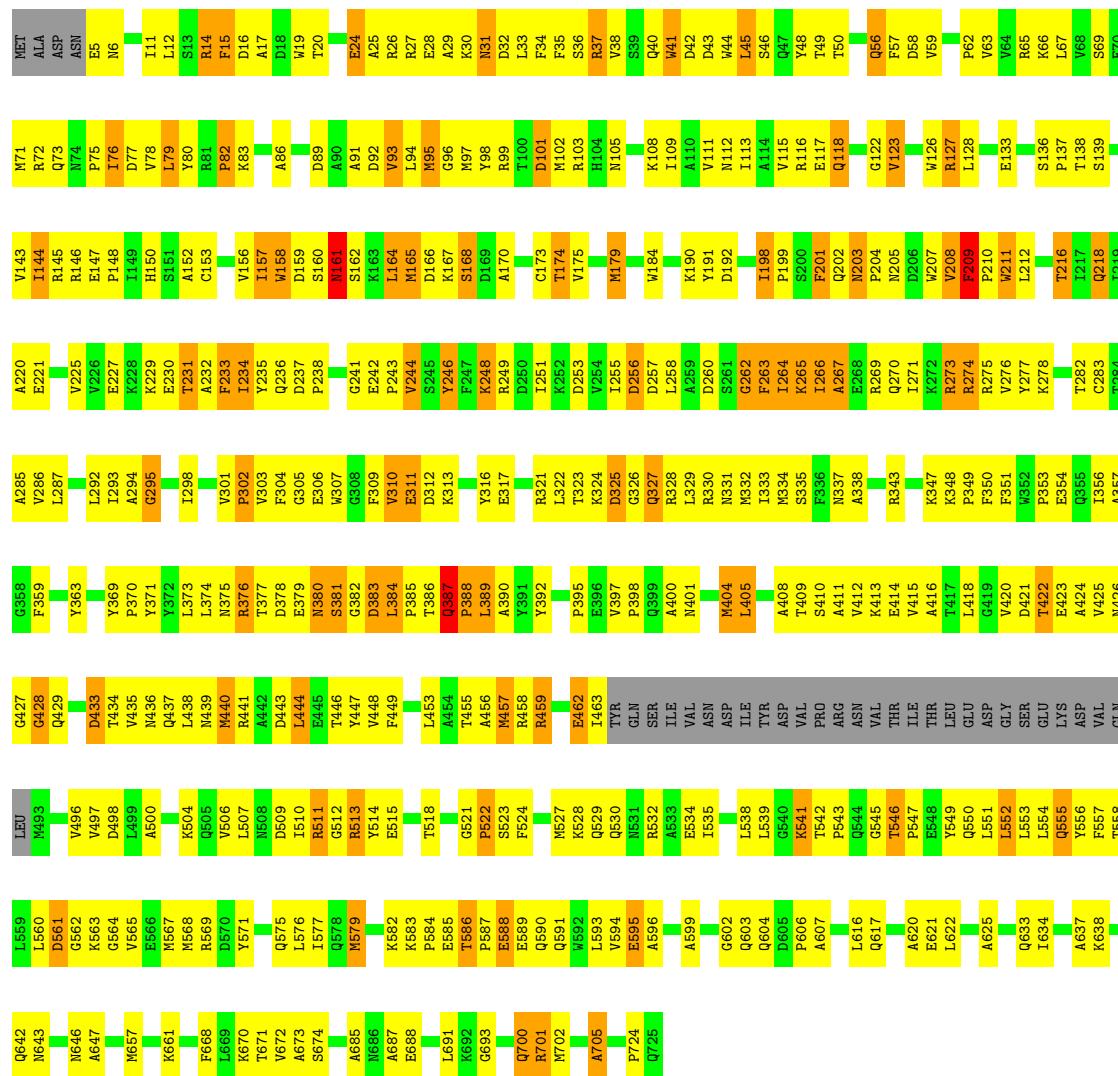
Chain G: 37% 47% 12% 5%





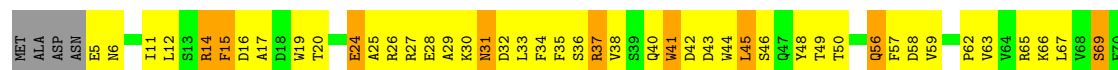
• Molecule 1: Portal protein

Chain H: 38% 45% 12% 5%



• Molecule 1: Portal protein

Chain I: 39% 44% 12% 5%

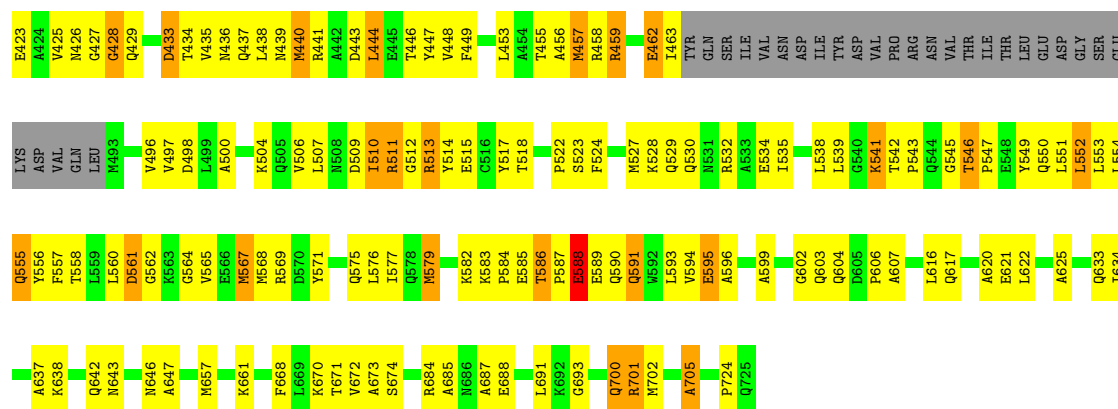


M71	I144	I219	C283	I356	V425	VAL	F557	A637	F570	F350
R72	R145	A220	T284	A357	N426	GLN	T558	K638	M71	F351
Q73	R146	E221	A285	A358	G427	LEU	L559	N643	R72	W352
N74	R147		G286	F359	Q429	M493	L560		Q73	P353
P75	P148	V225	L287			V496	D561	A647	N74	I356
I76	I149	V226		Y363	D433	V497	G562	H657	I76	A357
D77	H150	E227	L292		T434	D498	K563		D77	G358
V78	S151	K228	I293	Y369	V435	D499	G564	H657	V78	A285
L79	A152	K229	A294	P370	V436	A500	G565	K661	L79	W352
Y80	C153	E230	G295	Y371	Q437		G566		N74	I356
R81		T231			L438		M567	F668	I76	A357
P82	V156	A232	L298	L372	L438	K504	G568	F668	D77	G358
	I157	F233		L373	M439	G505	B569	K670	V78	A285
A86	M158	I234	V301	L374	M440	V506	B570		R81	C153
	D159	Q236	P302	N375	R441	L507	Y571		P82	V156
D89	S160	Q236	F303	K376	A442	L508	A572	V672	A86	
A90	N161	D237	F304	T377	D443	D509	N573	A673	D89	S160
A91	S162	P238	G305	T378	L444	T510	K574	S674	A90	S162
D92	K163	V239	E306	E379	E445	R511	O575		A91	S162
V93	L164	T240	V307	N380	T446	G512	L576	A685	D92	K163
L94	M165	G241	G308	S381	Y447	R513	L577	H686	V93	L164
M95	D166	E242	F309	D382	V448	Y514	L578	E688	L94	M165
G96	K167	P243	V310	D383	F449	E515	M579		M95	D166
M97	S168	V244	E311	L384					E28	K167
Y98	D169	S245	D312	T385	L453	T518	K582	L691	A29	D166
R99	A170	Y246	K313	T386	A454		K583	K692	K30	K167
I100		F247		Q387	A456	G521	P584	G693	R31	S168
D101	C173	K248	Y316	P388	A456	P522	E585		D32	D169
M102	T174	R249	E317	L389	M457	P523	T586	Q700	R26	S160
R103	V175	D250	R458		R459	F524	R701	M702	E27	L164
H104		I251	R321	Y392		M527	S588		F34	S245
N105	M179	K252	L322		E462	K528	E589	A599	M102	G96
		D253	L323	P395	I463	Q590	Q591		R103	G96
K108	W184	V254	D325	E396	TYR	Q592	W592	P724	V38	S39
I109		I255	G326	P397	GLN	N531	L593	Q725	Q40	N105
A110	K190	D256	Q327	P398	SER	R532	V594		W41	K108
V111	Y191	D257	R328	Q399	ILE	A533	E595		D42	I109
N112	D192	L258	R329	A400	VAL	E534	A596		D43	A110
I113		A259	R330	M401	ASN	L536			W44	V111
	I198	D260	N331	M404	ASP		A599	G602	Q47	A114
V115	P199	S261	M332	L405	ILE	L638		Q603	T49	V115
E117	R116	F201	I333	A408	TYR	L539	G604	Q604	T50	R116
Q118	F202	Q202	M334	T409	ASP	G540	P541	P605	Q56	E117
	N203	N203	S335	VAL	PRO	K541	T542	P606	F57	Q118
G122	P204	N205	F336	A411	ARG	P543	P543	A607	D58	G122
V123	D206	N205	A338	V412	ASN	Q544	G545		V59	V123
	W207	W207	E268	VAL	THR	T546	T546	L616	V60	W126
W126	R127	V208	R269	E414	THR	P547			R61	R127
R127	F209	F209	I271	V415	THR	E548	A620		P62	L128
L128	P210	W211	K272	A416	GLU	Y549	L622		V63	L128
	E133	L212	R273	T417	GLU	L551	L622		V64	E133
		L212	R273	L418	GLY	L552		A625	R65	
S136	T213	Q214	R275	G419	ASP	L553			K66	S136
P137	Q214	D215	R276	W420	GLY	L553			L67	P137
T138	D215	D215	Y277	D421	SER	L553	Q633		V68	T138
S139	T216	T216	K278	T422	GLU	L554	L634		S69	S139
	I217			E423	LYS	Q555				
V143	Q218	T282		A424	ASP	V556				

• Molecule 1: Portal protein

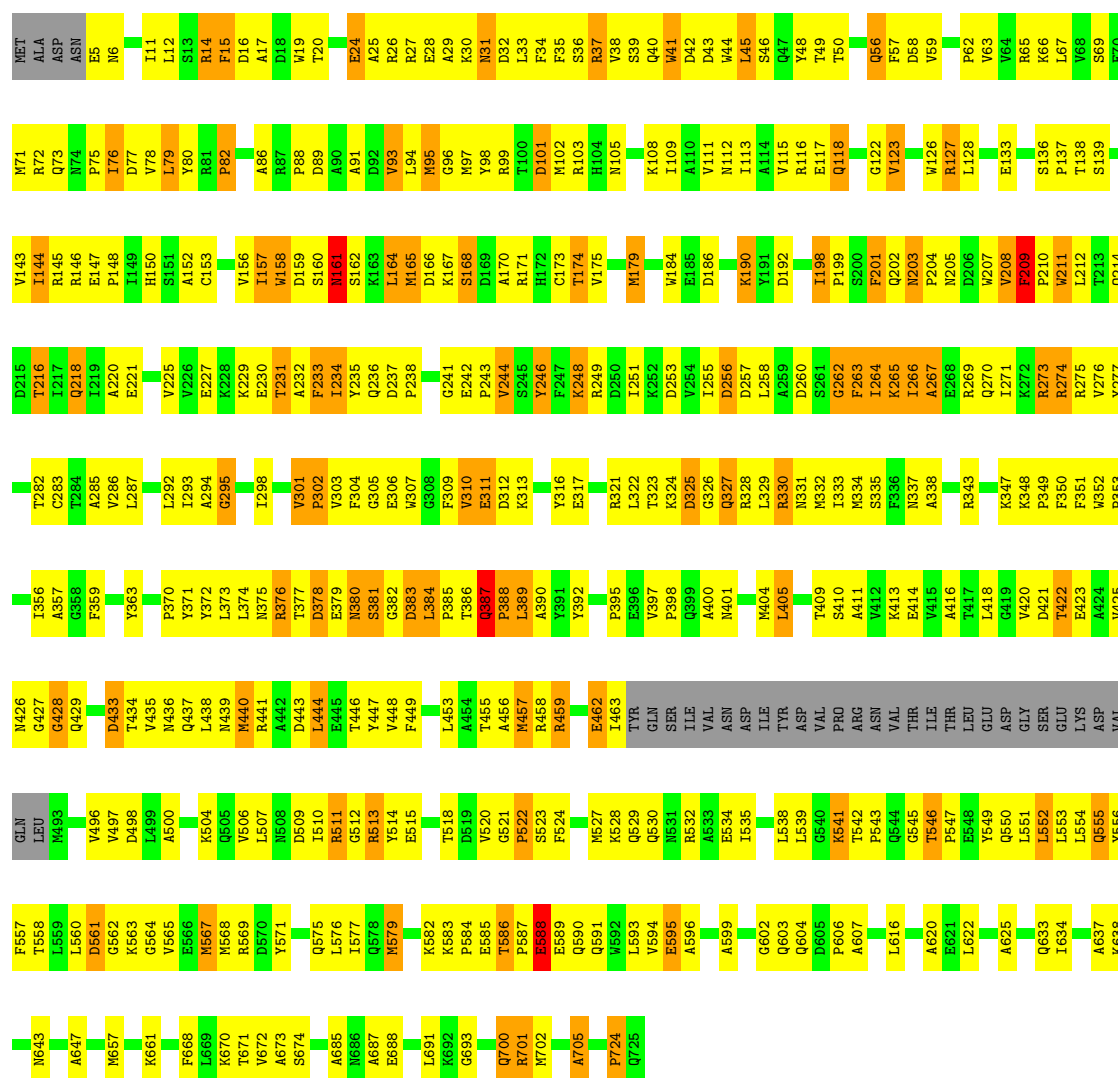
Chain J: 39% 44% 12% 5%

MET	E70	D215	Y277	F350
ALA	M71	T216	K278	F351
ASP	R72	I217	T282	W352
ASN	Q73	Q218	T282	P353
ASP	N74	I219	T284	I356
E5	P75	A220	A285	A357
N6	I76	E221	V286	G358
I11	D77	V225	L287	Y363
L12	V78	E227	L292	P370
S13	L79	E227	I293	Y371
G15	N80	V226	I293	Y372
F15	R81	S151	A294	L373
D16	P82	A152	G295	L374
A17	K83	C153		N375
D18		V156		R376
T20	A86	I157		T377
E24	D89	W158		D378
A25	A90	S160		G305
R26	A91	N161		N380
E27	D92	S162		S381
R27	V93	K163		G382
E28	L94	L164		D383
A29	M95	M165		L384
K30	N95	D166		N375
R31	G96	K167		R376
D32	M97	S168		T377
P33	Y98	D169		D378
L33	R99	A170		E379
F34	T100	A170		N380
M35	D101	C173		S381
R36	M102	G173		G382
S37	R103	T174		D383
V38	H104	V175		L384
S39	N105	M179		N375
Q40	K108	W184		R376
W41	I109	E185		T377
D42	A110	D186		D378
D43	V111			E379
W44	N112			N380
S46	I113			S381
L45	A114			G382
Y48	V115			D383
T49	R116			L384
T50	E117			N375
Q56	Q118			R376
F57	G122			T377
D58	V123			D378
P62	G122			E379
V60	N203			N380
R61	P204			S381
V63	N205			G382
V64	N206			D383
R65	D206			L384
K66	W207			N375
L67	V208			R376
V68	F209			T377
S69	P210			D378
	W211			E379
	L212			N380
	T213			G382
	T216			D383
	Q214			L384



• Molecule 1: Portal protein

Chain K: 39% 43% 12% • 5%



• Molecule 1: Portal protein

MET	A647	T558	GLN	G427	T356	T284	I219	R146	R72
	L559	A357	A285	G428	A357	V286	E221	E147	Q73
	L560	M493	F359	V430	F359	L287	E221	H150	N74
	D561	G562	V496	D433	X362	T293	V225	H151	I76
	K563	V497	D498	T434	X363	G295	K228	A152	D77
	V565	L499	V435	T435	P370	T298	K229	C153	V78
	M566	A500	Q436	Q437	X371	T301	E230	V156	L79
	K670	M568	L438	N439	X372	P302	T231	I157	I11
	T671	Q505	N440	N441	L373	V303	A232	H158	S13
	R672	D570	L507	R441	L374	F304	E233	M161	L12
F668	L669	N508	A442	N442	N375	F304	Y235	M162	R81
	M567	D443	N443	N444	R376	G305	Q236	K163	P82
	T671	D509	L444	L445	T377	E306	D237	L164	A90
	R672	R511	E445	E446	D376	X307	P238	M165	N91
	A673	G512	T446	T447	X380	F309	G241	D166	D89
	S674	R513	Y447	V448	N380	V310	E242	K167	A90
	Y571	Y514	F449	F449	G382	E311	P243	S168	A31
	Q575	E515	L453	L454	D383	D312	V244	A170	D18
	L576	T518	A454	A455	L384	K313	S245	C173	T20
	I577	G521	T455	T456	P385	Y316	F247	T174	E24
E688	M578	P522	A456	A456	T386	E317	K248	V175	A25
	Q579	S523	N457	N457	P388	R321	R249	M102	R26
	R580	F524	R458	R459	L389	L322	D250	R103	E28
	K682	M527	E462	E462	Y392	K324	K252	S178	A29
	P584	K528	L463	L463	P395	D325	V254	M182	R30
	E585	Q529	T463	T463	E396	G326	L255	G183	K37
	P587	Q530	GLN	GLN	Y397	Q327	D256	M184	V38
	E588	R531	SER	SER	P398	R328	D257	E185	S39
	E589	A533	ILE	ILE	Y398	L258	K329	D186	Q40
	Q590	E534	ASN	ASN	N401	R330	A259	K190	Q41
P724	Q591	I535	ASP	ASP	N404	K332	S261	D192	D42
	M592	L538	ILE	ILE	L405	T333	K334	G262	D43
	Q593	L539	T463	T463	L406	K335	K336	K263	D44
	L594	G540	ASP	ASP	T409	F336	I264	P199	W44
	V594	K541	VAL	VAL	S410	K337	K265	S200	V115
	E595	P542	PRO	PRO	A411	N337	I266	F201	Y191
	A596	P543	ARG	ARG	V412	A338	A267	E117	R116
	A599	Q544	ASN	ASN	K413	Y411	E268	Q202	E117
	G602	G545	VAL	VAL	E414	V341	R269	N203	S46
	Q603	T546	THR	THR	V415	A342	Q270	P204	Q37
Q604	L622	P547	ILE	ILE	A416	R343	I271	N205	R127
	E625	E548	THR	THR	T417	K347	K272	W207	L128
	A625	Y549	LEU	LEU	L418	R273	R274	V208	E133
	Q633	Q550	GLU	GLU	G419	K348	R275	R276	P62
	I634	L551	ASP	ASP	V420	P349	R277	F209	V63
	K637	L552	GLY	GLY	D421	F350	R278	P210	P137
	A637	L553	SER	SER	T422	G351	V276	W211	T138
	K638	L554	GLU	GLU	E423	P352	Y277	L212	S139
	A638	Q555	LVS	LVS	A424	K353	K278	Q202	L67
	S639	Q556	ASP	ASP	V425	E354	T216	T216	V68
W71	N643	F557	VAL	VAL	V426	R355	T282	I217	V143
	L644	E558	ASP	ASP	V427	E356	T283	Q318	E70
	E645	F559	VAL	VAL	V428	R357	T284	I218	E71
	L646	E560	ASP	ASP	V429	E357	T285	Q319	E72
	E647	F561</							

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	408.95Å 408.95Å 260.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.48 – 7.50 59.48 – 7.50	Depositor EDS
% Data completeness (in resolution range)	92.8 (59.48-7.50) 93.1 (59.48-7.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 7.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.187 , 0.263 0.181 , 0.261	Depositor DCC
R_{free} test set	1994 reflections (7.33%)	wwPDB-VP
Wilson B-factor (Å ²)	236.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 547.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	61512	wwPDB-VP
Average B, all atoms (Å ²)	297.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	B	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	C	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	D	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	E	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	F	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	G	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	H	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	I	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	J	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	K	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
1	L	0.50	11/5222 (0.2%)	0.58	1/7114 (0.0%)
All	All	0.50	132/62664 (0.2%)	0.58	12/85368 (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	A	0	1
1	B	0	1
1	C	0	1
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	K	0	1
1	L	0	1
All	All	0	12

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	165	MET	CG-SD	6.91	1.99	1.81
1	G	165	MET	CG-SD	6.91	1.99	1.81
1	J	165	MET	CG-SD	6.91	1.99	1.81
1	H	165	MET	CG-SD	6.90	1.99	1.81
1	I	165	MET	CG-SD	6.89	1.99	1.81

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	97	MET	CB-CG-SD	-6.24	93.67	112.40
1	E	97	MET	CB-CG-SD	-6.24	93.68	112.40
1	B	97	MET	CB-CG-SD	-6.24	93.68	112.40
1	A	97	MET	CB-CG-SD	-6.24	93.69	112.40
1	I	97	MET	CB-CG-SD	-6.24	93.69	112.40

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	THR	Peptide
1	B	231	THR	Peptide
1	C	231	THR	Peptide
1	D	231	THR	Peptide
1	E	231	THR	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	5126	0	4586	548	9
1	B	5126	0	4586	522	0
1	C	5126	0	4586	499	0
1	D	5126	0	4586	559	0
1	E	5126	0	4586	551	8
1	F	5126	0	4586	522	1
1	G	5126	0	4586	538	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	5126	0	4586	509	3
1	I	5126	0	4586	516	0
1	J	5126	0	4586	516	3
1	K	5126	0	4586	510	0
1	L	5126	0	4586	538	0
All	All	61512	0	55032	5771	12

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 50.

The worst 5 of 5771 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:58:ASP:OD2	1:L:322:LEU:CD1	1.73	1.35
1:G:322:LEU:HD12	1:H:58:ASP:OD2	1.23	1.34
1:I:322:LEU:HD12	1:J:58:ASP:OD2	1.26	1.34
1:F:322:LEU:HD12	1:G:58:ASP:OD2	1.19	1.32
1:H:322:LEU:HD12	1:I:58:ASP:OD2	1.19	1.31

The worst 5 of 12 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:H:49:THR:O	1:J:684:ARG:O[8_554]	1.56	0.64
1:A:49:THR:O	1:E:684:ARG:O[3_555]	1.86	0.34
1:A:48:TYR:O	1:E:687:ALA:CB[3_555]	1.89	0.31
1:H:49:THR:OG1	1:J:687:ALA:CB[8_554]	1.93	0.27
1:A:49:THR:CB	1:E:687:ALA:CB[3_555]	1.94	0.26

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	688/725 (95%)	507 (74%)	122 (18%)	59 (9%)	1	11
1	B	688/725 (95%)	507 (74%)	122 (18%)	59 (9%)	1	11
1	C	688/725 (95%)	508 (74%)	121 (18%)	59 (9%)	1	11
1	D	688/725 (95%)	506 (74%)	123 (18%)	59 (9%)	1	11
1	E	688/725 (95%)	507 (74%)	122 (18%)	59 (9%)	1	11
1	F	688/725 (95%)	507 (74%)	122 (18%)	59 (9%)	1	11
1	G	688/725 (95%)	507 (74%)	122 (18%)	59 (9%)	1	11
1	H	688/725 (95%)	506 (74%)	123 (18%)	59 (9%)	1	11
1	I	688/725 (95%)	507 (74%)	122 (18%)	59 (9%)	1	11
1	J	688/725 (95%)	507 (74%)	122 (18%)	59 (9%)	1	11
1	K	688/725 (95%)	508 (74%)	121 (18%)	59 (9%)	1	11
1	L	688/725 (95%)	507 (74%)	122 (18%)	59 (9%)	1	11
All	All	8256/8700 (95%)	6084 (74%)	1464 (18%)	708 (9%)	1	11

5 of 708 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	82	PRO
1	A	208	VAL
1	A	256	ASP
1	A	263	PHE

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	474/630 (75%)	410 (86%)	64 (14%)	4	17
1	B	474/630 (75%)	409 (86%)	65 (14%)	3	17
1	C	474/630 (75%)	410 (86%)	64 (14%)	4	17
1	D	474/630 (75%)	409 (86%)	65 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	474/630 (75%)	409 (86%)	65 (14%)	3	17
1	F	474/630 (75%)	409 (86%)	65 (14%)	3	17
1	G	474/630 (75%)	409 (86%)	65 (14%)	3	17
1	H	474/630 (75%)	410 (86%)	64 (14%)	4	17
1	I	474/630 (75%)	410 (86%)	64 (14%)	4	17
1	J	474/630 (75%)	410 (86%)	64 (14%)	4	17
1	K	474/630 (75%)	409 (86%)	65 (14%)	3	17
1	L	474/630 (75%)	410 (86%)	64 (14%)	4	17
All	All	5688/7560 (75%)	4914 (86%)	774 (14%)	3	17

5 of 774 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	79	LEU
1	I	518	THR
1	H	174	THR
1	H	69	SER
1	I	30	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 298 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	161	ASN
1	L	327	GLN
1	J	297	HIS
1	K	236	GLN
1	D	555	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.