



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:20 am GMT

PDB ID : 5CBM
Title : Crystal structure of PfA-M17 with virtual ligand inhibitor
Authors : Ruggeri, C.; Drinkwater, N.; McGowan, S.
Deposited on : 2015-07-01
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

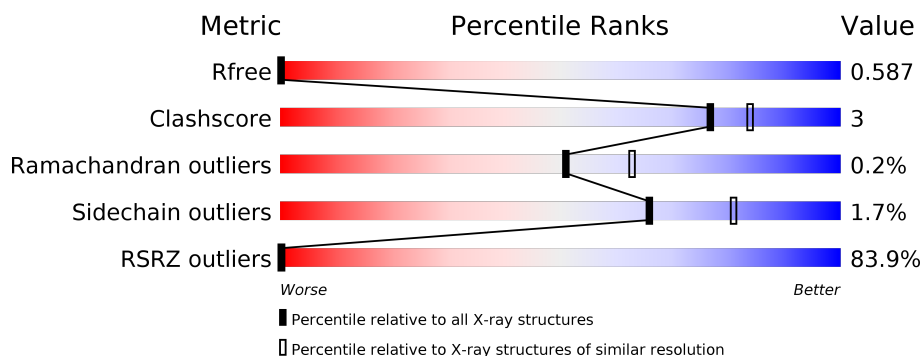
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>88%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	B	519	<div> <div>84%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
1	C	519	<div> <div>86%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	D	519	<div> <div>77%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
1	E	519	<div> <div>82%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>
1	F	519	<div> <div>82%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	519	<div>87%</div> <div>90%</div> <div>10%</div>
1	H	519	<div>86%</div> <div>90%</div> <div>9%</div>
1	I	519	<div>84%</div> <div>92%</div> <div>7%</div>
1	J	519	<div>78%</div> <div>87%</div> <div>11%</div>
1	K	519	<div>83%</div> <div>92%</div> <div>6%</div>
1	L	519	<div>81%</div> <div>90%</div> <div>8%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	D	701	-	-	-	X
2	CO3	E	701	-	-	-	X
2	CO3	J	701	-	-	-	X
2	CO3	K	701	-	-	-	X
4	4ZN	B	704	-	-	-	X
4	4ZN	D	704	-	-	-	X
4	4ZN	E	704	-	-	-	X
4	4ZN	F	704	-	-	-	X
4	4ZN	G	704	-	-	-	X
4	4ZN	H	704	-	-	-	X
4	4ZN	L	704	-	-	-	X
5	1PE	A	705	-	-	-	X
5	1PE	B	705	-	-	-	X
5	1PE	D	706	-	-	-	X
5	1PE	G	705	-	-	-	X
5	1PE	G	706	-	-	-	X
5	1PE	G	707	-	-	-	X
5	1PE	H	706	-	-	-	X
5	1PE	I	706	-	-	-	X
5	1PE	J	705	-	-	-	X
5	1PE	J	707	-	-	-	X
5	1PE	K	706	-	-	-	X
5	1PE	L	705	-	-	-	X
7	SO4	A	711	-	-	-	X
7	SO4	A	712	-	-	X	X
7	SO4	C	708	-	-	-	X
7	SO4	C	710	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	C	711	-	-	-	X
7	SO4	E	709	-	-	-	X
7	SO4	F	707	-	-	-	X
7	SO4	G	711	-	-	X	X
7	SO4	K	708	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 50850 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 M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			3971	2547	639	766	19			
1	B	516	Total	C	N	O	S	0	0	0
			3902	2509	633	740	20			
1	C	517	Total	C	N	O	S	0	0	0
			3941	2532	637	753	19			
1	D	514	Total	C	N	O	S	0	0	0
			3920	2526	633	741	20			
1	E	509	Total	C	N	O	S	0	0	0
			3893	2509	624	741	19			
1	F	511	Total	C	N	O	S	0	0	0
			3851	2477	622	733	19			
1	G	519	Total	C	N	O	S	0	0	0
			3974	2554	640	760	20			
1	H	517	Total	C	N	O	S	1	0	0
			3902	2508	632	743	19			
1	I	517	Total	C	N	O	S	0	0	0
			3951	2540	637	754	20			
1	J	514	Total	C	N	O	S	0	0	0
			3926	2529	633	744	20			
1	K	509	Total	C	N	O	S	0	0	0
			3884	2504	623	738	19			
1	L	511	Total	C	N	O	S	0	0	0
			3848	2475	622	732	19			

There are 36 discrepancies between the modelled and reference sequences:

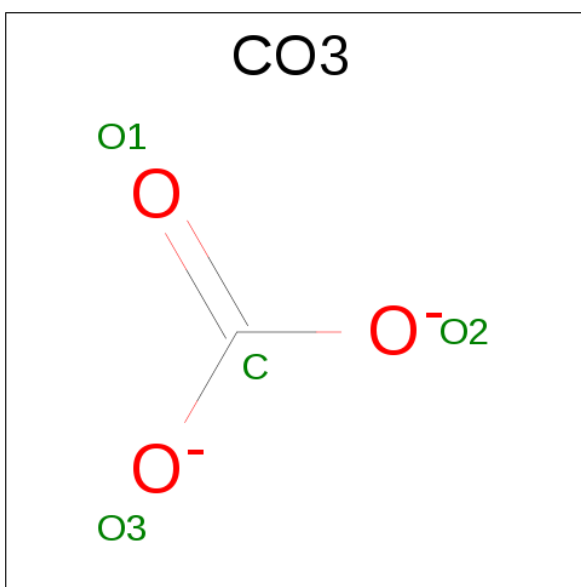
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	546	GLN	ASN	engineered mutation	UNP A0A024V0B1

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).

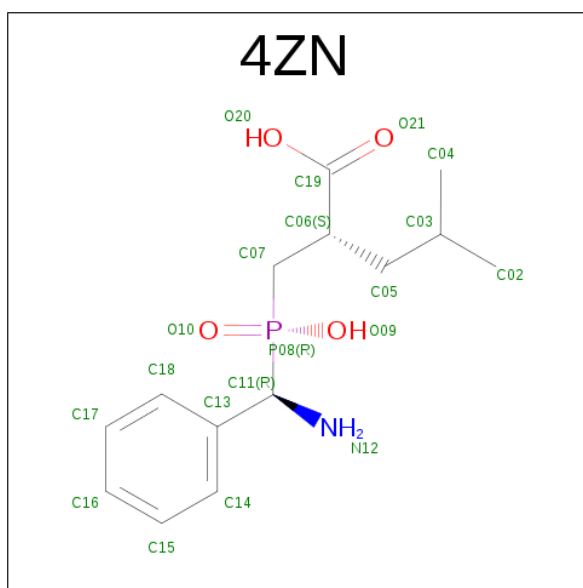


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		
2	G	1	Total	C	O	0	0
			4	1	3		
2	H	1	Total	C	O	0	0
			4	1	3		
2	I	1	Total	C	O	0	0
			4	1	3		
2	J	1	Total	C	O	0	0
			4	1	3		
2	K	1	Total	C	O	0	0
			4	1	3		
2	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

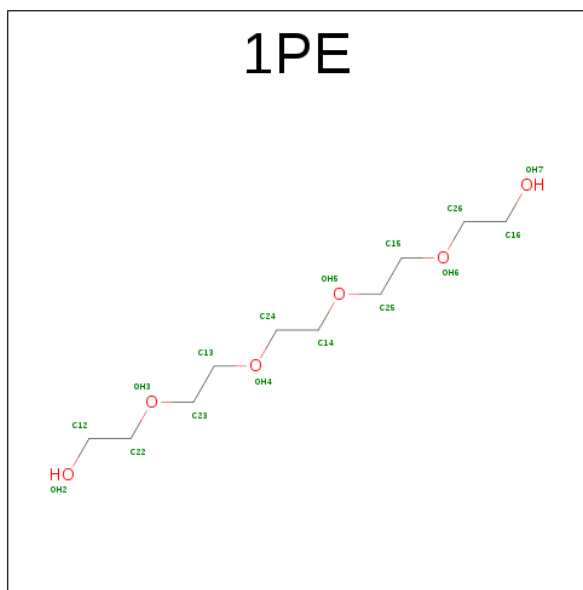
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total 2 Zn 2 2	0	0
3	J	2	Total 2 Zn 2 2	0	0
3	D	2	Total 2 Zn 2 2	0	0
3	K	2	Total 2 Zn 2 2	0	0
3	E	2	Total 2 Zn 2 2	0	0
3	H	2	Total 2 Zn 2 2	0	0
3	B	2	Total 2 Zn 2 2	0	0
3	I	2	Total 2 Zn 2 2	0	0
3	C	2	Total 2 Zn 2 2	0	0
3	A	2	Total 2 Zn 2 2	0	0
3	L	2	Total 2 Zn 2 2	0	0
3	F	2	Total 2 Zn 2 2	0	0

- Molecule 4 is (2S)-2-[[[(R)-[(R)-amino(phenyl)methyl](hydroxy)phosphoryl]methyl]-4-methylpentanoic acid (three-letter code: 4ZN) (formula: C₁₄H₂₂NO₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			20	14	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			20	14	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	I	1	Total	C	N	O	P	0	0
			12	8	1	2	1		
4	J	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			14	10	1	2	1		
4	L	1	Total	C	N	O	P	0	0
			16	10	1	4	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



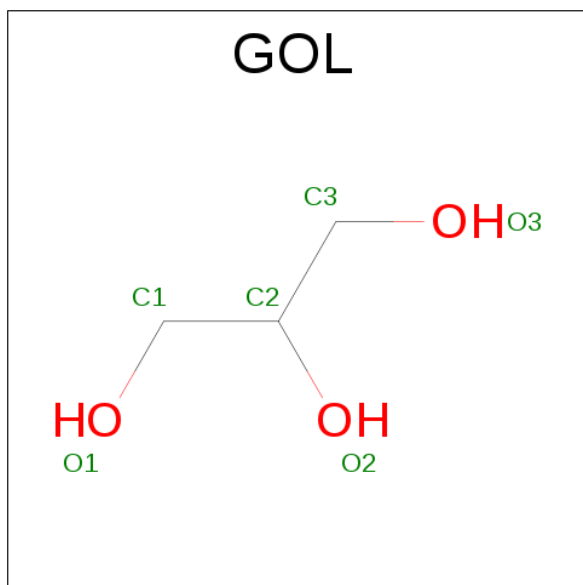
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 6 3	0	0
5	A	1	Total C O 12 8 4	0	0
5	B	1	Total C O 10 7 3	0	0
5	B	1	Total C O 10 7 3	0	0
5	C	1	Total C O 13 9 4	0	0
5	C	1	Total C O 9 6 3	0	0
5	D	1	Total C O 10 7 3	0	0
5	D	1	Total C O 10 7 3	0	0
5	E	1	Total C O 12 8 4	0	0
5	E	1	Total C O 12 8 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	G	1	Total C O 9 6 3	0	0
5	G	1	Total C O 6 4 2	0	0
5	G	1	Total C O 6 4 2	0	0
5	H	1	Total C O 10 7 3	0	0
5	H	1	Total C O 10 7 3	0	0
5	I	1	Total C O 12 8 4	0	0
5	I	1	Total C O 11 8 3	0	0
5	J	1	Total C O 11 7 4	0	0
5	J	1	Total C O 11 7 4	0	0
5	J	1	Total C O 10 6 4	0	0
5	K	1	Total C O 12 8 4	0	0

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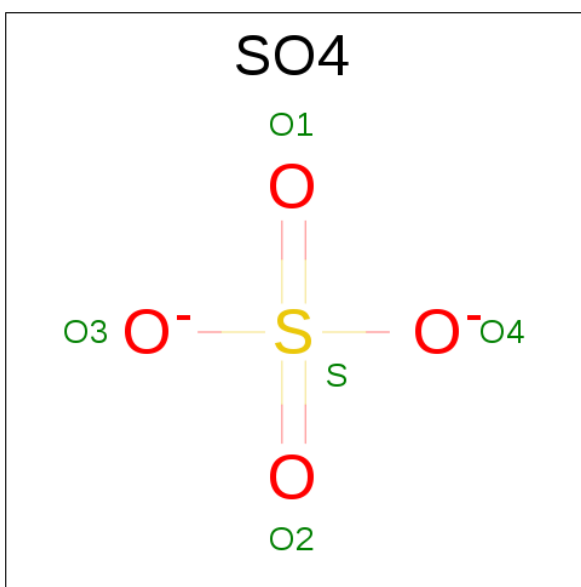
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			12	8	4		
5	L	1	Total	C	O	0	0
			7	4	3		
5	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	G	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	I	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	J	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	K	1	Total O S 5 4 1	0	0
7	L	1	Total O S 5 4 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	265	Total O 265 265	0	0
8	B	246	Total O 246 246	0	0
8	C	277	Total O 277 277	0	0
8	D	283	Total O 283 283	0	0
8	E	322	Total O 322 322	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	245	Total 245	O 245	0	0
8	G	281	Total 281	O 281	0	0
8	H	220	Total 220	O 220	0	0
8	I	272	Total 272	O 272	0	0
8	J	287	Total 287	O 287	0	0
8	K	283	Total 283	O 283	0	0
8	L	240	Total 240	O 240	0	0

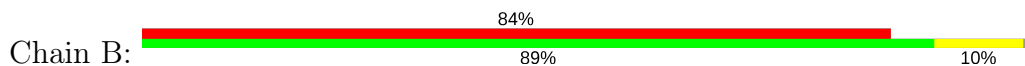
3 Residue-property plots

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 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: M17 family aminopeptidase



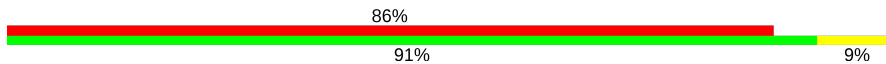
• Molecule 1: M17 family aminopeptidase



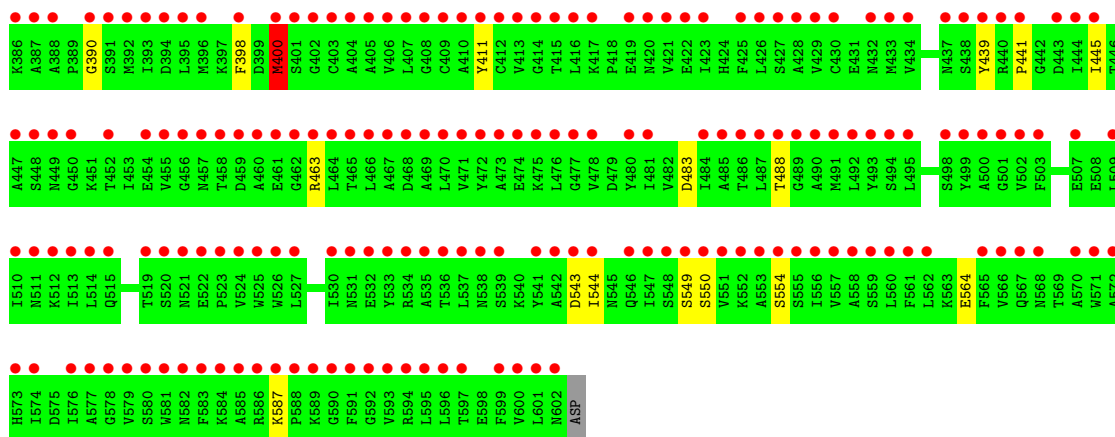
V579	S517	G456	I393	G329	L267	V286	S146
S580	K518	G457	D394	V330	G268	V207	S147
W581	T519	T458	L395	V330	V269	L208	S148
N582	S520	N460	N396	E332	Y270	S209	N149
F583	N521	A460	K397	L333	K397	L210	D150
K584	E522	F461	F398	E334	N272	V211	K151
A585		G462	D399	E335	N273	T212	K152
S586	W525	R463	M400	L336	A274	L214	V153
K587	W526	L464	S401	K337	D275	L215	S154
P588	L527	T465	G402	N338	T276	H215	E155
K589	P528	L466	G403	G339	Y277	D216	P96
G590	L529	A467	A404	L340	K278	L217	T97
F591	L530	D468	A405	Y341	E279	K218	S98
G592	N531	A469	L406	L342	E280	L219	S99
V593	E532	L470	L407	S343		S220	P100
R594	V533	V471	G408	V344	A284	K221	I101
L595	R534	Y472	G409	G345	R285	L222	M162
L596	A535	A473	A410	K346	Y286	T223	E163
T597	T536	E474	Y411	G347	Y287	V224	K164
E598	L537	K475	G412	S348	Y288	V225	F165
F599	N538	L476	V413	N349	F289	E227	N166
V600	S539	G477	G414	V350	G290	F227	V167
L601	K540	G478	T415	P351	T291	L228	H168
M602	Y541	D479	L416	N352	Y292	N229	K169
	A542	Y480	K417	K353	Y293	V230	G170
ASP	D543	L481	P418	F354	A294	D231	I110
	L544	V482	E419	L355	S295	K232	K111
	N545	D483	M420	H356	Q296	N233	V112
	Q546	L484	V421	L357	L297	L234	K113
	L547	A485	E422	T358	L298	F235	H114
S548	S548	T486	L423	V359	A299	R236	Y115
S549	S549	L487	H424	K360	F237	K177	D116
S550	T488	F425	S361	S361	P301	F238	I117
V551	G489	L426	K362	S362	S302	N179	K118
K552	A490	S427	G363	S363	N303	E240	G119
A553		A428	G364	D364	Y304	N180	G120
S554	Y493	W429	V365	V365	C305	T241	C121
S555	S494		K366		K182	L242	C122
L556	L495	N433			N306	F243	N123
V557	G496	V434	K367		P307	Y244	E124
A558	T497	S435	S435	I369	V308	E245	E125
S559	S498			A370	S309	G246	G126
L560	Y499		V372	L371	L310	W247	L127
F561	A500	S438	G373		S311	T248	L128
L562	G501	R440	K374	G374	N312	D249	I129
K563	V502	P441	G375	A314	A313	E250	F130
E564	F503	G442	L376	V315	R251	K191	L131
F565	G504	D443	T377	G315	F252	C192	V132
V566	N505	L444	F378	E316	K253	G193	N133
Q567	N506	L445		A318	S254	L194	N134
	E507				T255	P135	N135
A570	S508		G381	Q319	ASP	A196	G136
N571	L509	A447	G382	K320	K257	K137	K137
A572	I510	S448	Y383	L391	N258	L198	E138
H573	N511	N449	N384	N322	V259	S199	N139
L574	K512	G450	L386	L323	E260	G140	G140
D575	I513	K451	K386	E324	M261	A201	P141
L576	I513	T452	A387	Y325	E262	D202	K142
W577	L514	L453		K326	V263	M203	V143
A577	Q515	E454	S591	I327	L264	K204	I144
E578	S516	W455	N202	L208		S205	S145

• Molecule 1: M17 family aminopeptidase

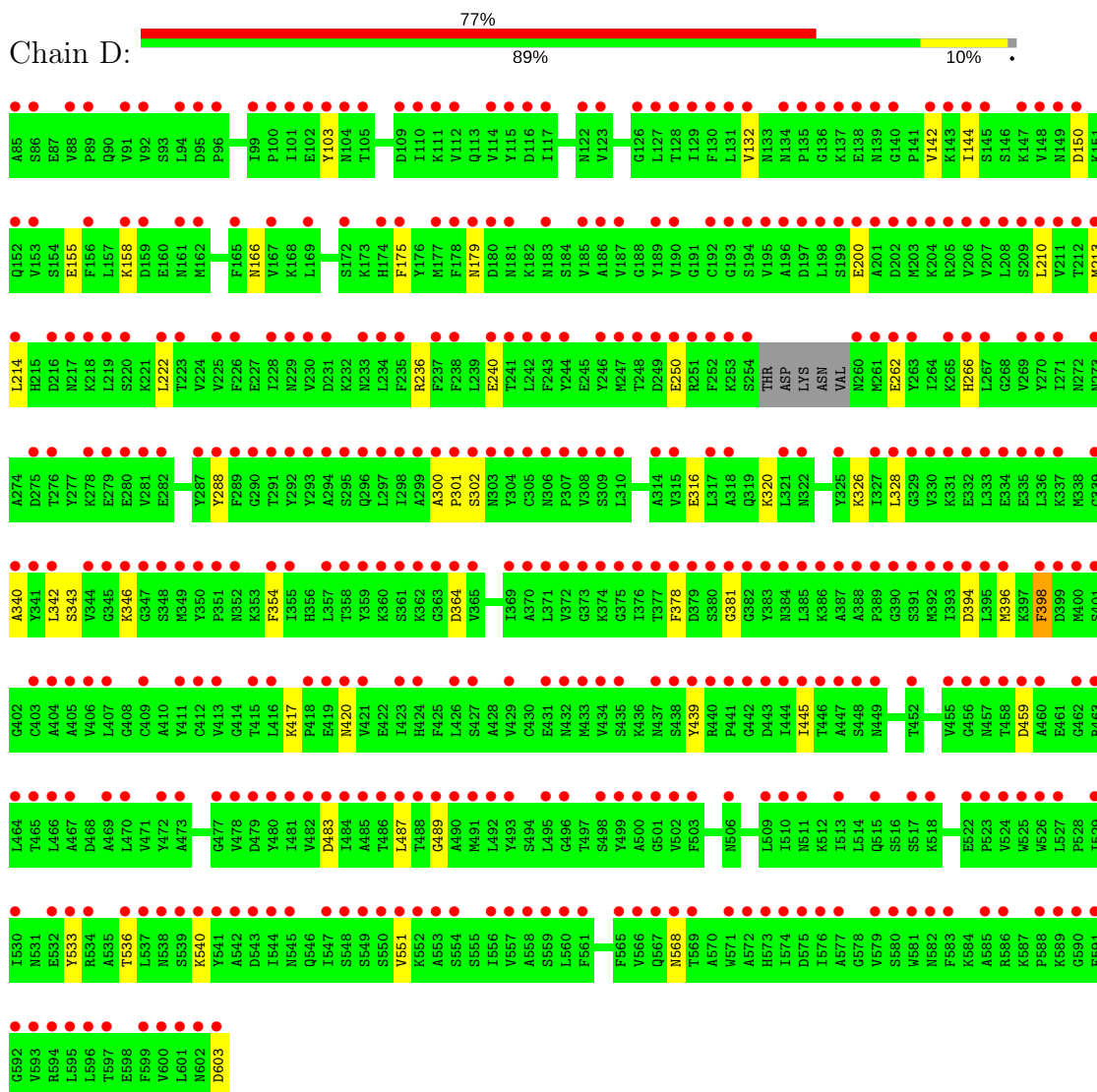
Chain C:



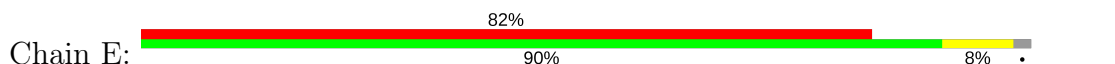
ALA	S145	V206	H266	K326	S146	V207	L267	L327	S147	V208	L268	L328	S148	V209	L269	V330	S149	V210	Y270	V331	S150	V211	L271	V332	S151	V212	L272	E332	S152	V213	N273	L333	S153	V214	A274	E334	S154	V215	D275	E335	S155	V216	L276	L336	S156	V217	Y277	K337	S157	V218	K278	H338	S158	V219	E279	A340	S159	V220	E280	A341	S160	V221	L281	Y341	S161	V222	Y282	L342	S162	V223	K283	L343	S163	V224	K284	V344	S164	V225	R285	V345	S165	V226	Y286	K346	S166	V227	Y287	G347	S167	V228	Y288	S348	S168	V229	F289	K349	S169	V230	G290	Y350	S170	V231	T291	P351	S171	V232	Y292	N352	S172	V233	Y293	K353	S173	V234	A294	F354	S174	V235	S295	L355	S175	V236	Q296	H356	S176	V237	L297	L357	S177	V238	L298	T358	S178	V239	A299	Y359	S179	V240	S300	K360	S180	V241	P301	S361	S181	V242	S302	L362	S182	V243	N303	G363	S183	V244	Y304	D364	S184	V245	C305	V365	S185	V246	N306	K366	S186	V247	P307	K367	S187	V248	V308	H368	S188	V249	S309	L369	S189	V250	L310	A370	S190	V251	S311	L371	S191	V252	N312	V372	S192	V253	A313	G373	S193	V254	A314	L374	S194	V255	V315	G375	S195	V256	E316	L376	S196	V257	L317	T377	S197	V258	A318	F378	S198	V259	Q319	D379	S199	V260	K320	S380	S200	V261	L321	G381	S201	V262	N322	G382	S202	V263	L323	Y383	S203	V264	E324	N384	S204	V265	Y285	L385	S205	V266	Y286	L386	S206	V267	Y287	L387	S207	V268	Y288	L388	S208	V269	Y289	L389	S209	V270	Y290	L390	S210	V271	Y291	L391	S211	V272	Y292	L392	S212	V273	Y293	L393	S213	V274	Y294	L394	S214	V275	Y295	L395	S215	V276	Y296	L396	S216	V277	Y297	L397	S217	V278	Y298	L398	S218	V279	Y299	L399	S219	V280	Y300	L400	S220	V281	Y301	L401	S221	V282	Y302	L402	S222	V283	Y303	L403	S223	V284	Y304	L404	S224	V285	Y305	L405	S225	V286	Y306	L406	S226	V287	Y307	L407	S227	V288	Y308	L408	S228	V289	Y309	L409	S229	V290	Y310	L410	S230	V291	Y311	L411	S231	V292	Y312	L412	S232	V293	Y313	L413	S233	V294	Y314	L414	S234	V295	Y315	L415	S235	V296	Y316	L416	S236	V297	Y317	L417	S237	V298	Y318	L418	S238	V299	Y319	L419	S239	V300	Y320	L420	S240	V301	Y321	L421	S241	V302	Y322	L422	S242	V303	Y323	L423	S243	V304	Y324	L424	S244	V305	Y325	L425	S245	V306	Y326	L426	S246	V307	Y327	L427	S247	V308	Y328	L428	S248	V309	Y329	L429	S249	V310	Y330	L430	S250	V311	Y331	L431	S251	V312	Y332	L432	S252	V313	Y333	L433	S253	V314	Y334	L434	S254	V315	Y335	L435	S255	V316	Y336	L436	S256	V317	Y337	L437	S257	V318	Y338	L438	S258	V319	Y339	L439	S259	V320	Y340	L440	S260	V321	Y341	L441	S261	V322	Y342	L442	S262	V323	Y343	L443	S263	V324	Y344	L444	S264	V325	Y345	L445	S265	V326	Y346	L446	S266	V327	Y347	L447	S267	V328	Y348	L448	S268	V329	Y349	L449	S269	V330	Y350	L450	S270	V331	Y351	L451	S271	V332	Y352	L452	S272	V333	Y353	L453	S273	V334	Y354	L454	S274	V335	Y355	L455	S275	V336	Y356	L456	S276	V337	Y357	L457	S277	V338	Y358	L458	S278	V339	Y359	L459	S279	V340	Y360	L460	S280	V341	Y361	L461	S281	V342	Y362	L462	S282	V343	Y363	L463	S283	V344	Y364	L464	S284	V345	Y365	L465	S285	V346	Y366	L466	S286	V347	Y367	L467	S287	V348	Y368	L468	S288	V349	Y369	L469	S289	V350	Y370	L470	S290	V351	Y371	L471	S291	V352	Y372	L472	S292	V353	Y373	L473	S293	V354	Y374	L474	S294	V355	Y375	L475	S295	V356	Y376	L476	S296	V357	Y377	L477	S297	V358	Y378	L478	S298	V359	Y379	L479	S299	V360	Y380	L480	S300	V361	Y381	L481	S301	V362	Y382	L482	S302	V363	Y383	L483	S303	V364	Y384	L484	S304	V365	Y385	L485	S305	V366	Y386	L486	S306	V367	Y387	L487	S307	V368	Y388	L488	S308	V369	Y389	L489	S309	V370	Y390	L490	S310	V371	Y391	L491	S311	V372	Y392	L492	S312	V373	Y393	L493	S313	V374	Y394	L494	S314	V375	Y395	L495	S315	V376	Y396	L496	S316	V377	Y397	L497	S317	V378	Y398	L498	S318	V379	Y399	L499	S319	V380	Y400	L500	S320	V381	Y401	L501	S321	V382	Y402	L502	S322	V383	Y403	L503	S323	V384	Y404	L504	S324	V385	Y405	L505	S325	V386	Y406	L506	S326	V387	Y407	L507	S327	V388	Y408	L508	S328	V389	Y409	L509	S329	V390	Y410	L510	S330	V391	Y411	L511	S331	V392	Y412	L512	S332	V393	Y413	L513	S333	V394	Y414	L514	S334	V395	Y415	L515	S335	V396	Y416	L516	S336	V397	Y417	L517	S337	V398	Y418	L518	S338	V399	Y419	L519	S339	V400	Y420	L520	S340	V401	Y421	L521	S341	V402	Y422	L522	S342	V403	Y423	L523	S343	V404	Y424	L524	S344	V405	Y425	L525	S345	V406	Y426	L526	S346	V407	Y427	L527	S347	V408	Y428	L528	S348	V409	Y429	L529	S349	V410	Y430	L530	S350	V411	Y431	L531	S351	V412	Y432	L532	S352	V413	Y433	L533	S353	V414	Y434	L534	S354	V415	Y435	L535	S355	V416	Y436	L536	S356	V417	Y437	L537	S357	V418	Y438	L538	S358	V419	Y439	L539	S359	V420	Y440	L540	S360	V421	Y441	L541	S361	V422	Y442	L542	S362	V423	Y443	L543	S363	V424	Y444	L544	S364	V425	Y445	L545	S365	V426	Y446	L546	S366	V427	Y447	L547	S367	V428	Y448	L548	S368	V429	Y449	L549	S369	V430	Y450	L550	S370	V431	Y451	L551	S371	V432	Y452	L552	S372	V433	Y453	L553	S373	V434	Y454	L554	S374	V435	Y455	L555	S375	V436	Y456	L556	S376	V437	Y457	L557	S377	V438	Y458	L558	S378	V439	Y459	L559	S379	V440	Y460	L560	S380	V441	Y461	L561	S381	V442	Y462	L562	S382	V443	Y463	L563	S383	V444	Y464	L564	S384	V445	Y465	L565	S385	V446	Y466	L566	S386	V447	Y467	L567	S387	V448	Y468	L568	S388	V449	Y469	L569	S389	V450	Y470	L570	S390	V451	Y471	L571	S391	V452	Y472	L572	S392	V453	Y473	L573	S393	V454	Y474	L574	S394	V455	Y475	L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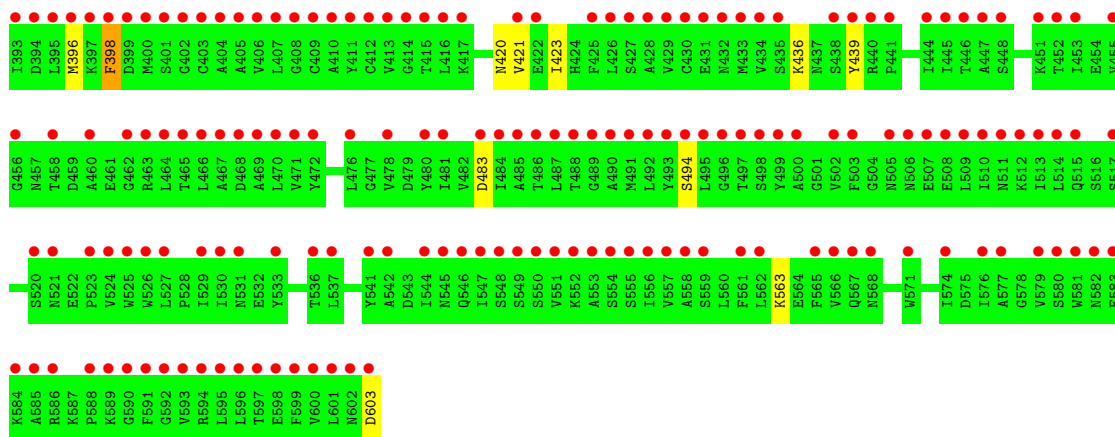
• Molecule 1: M17 family aminopeptidase



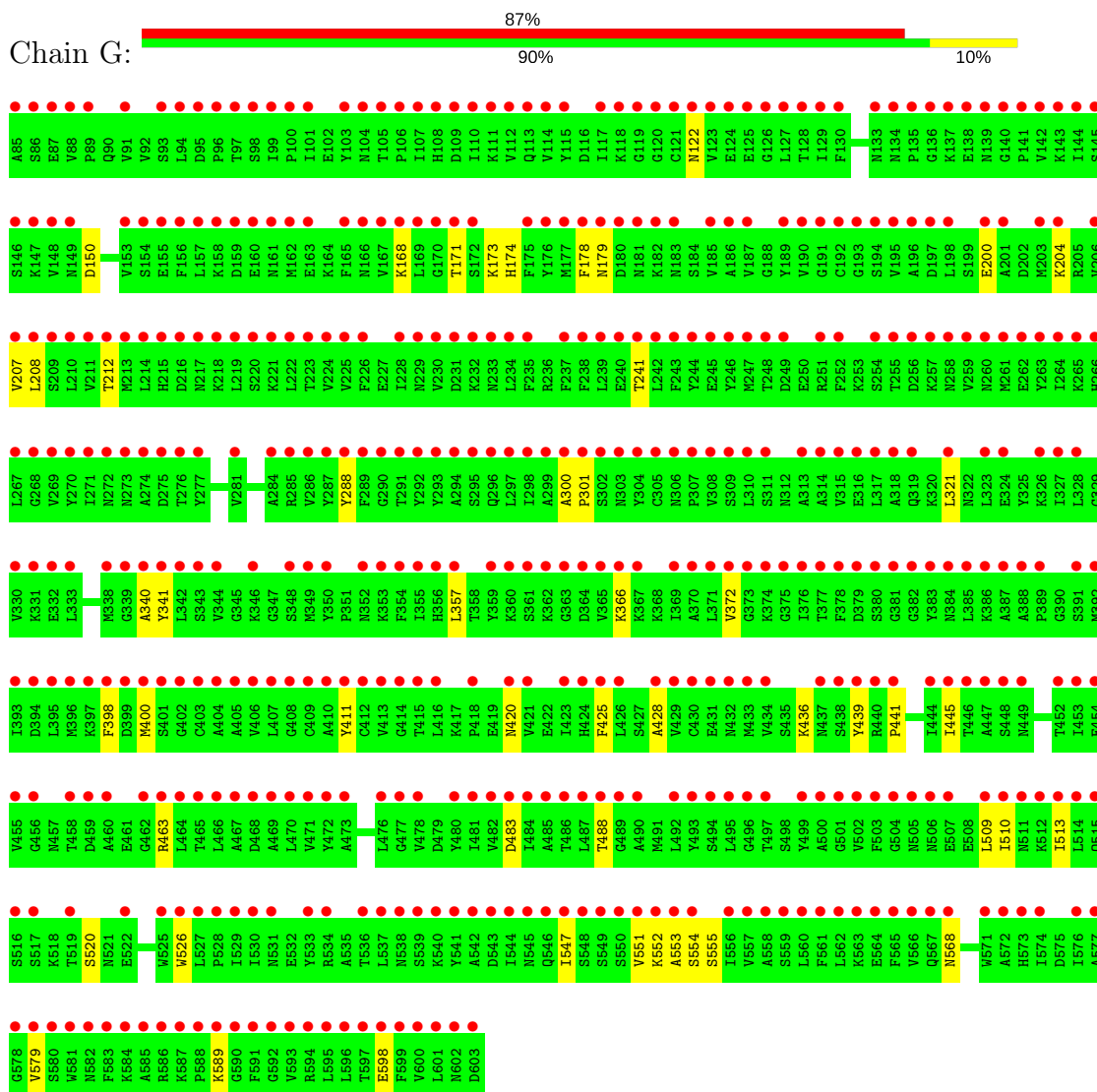
• Molecule 1: M17 family aminopeptidase



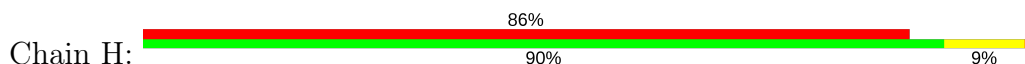




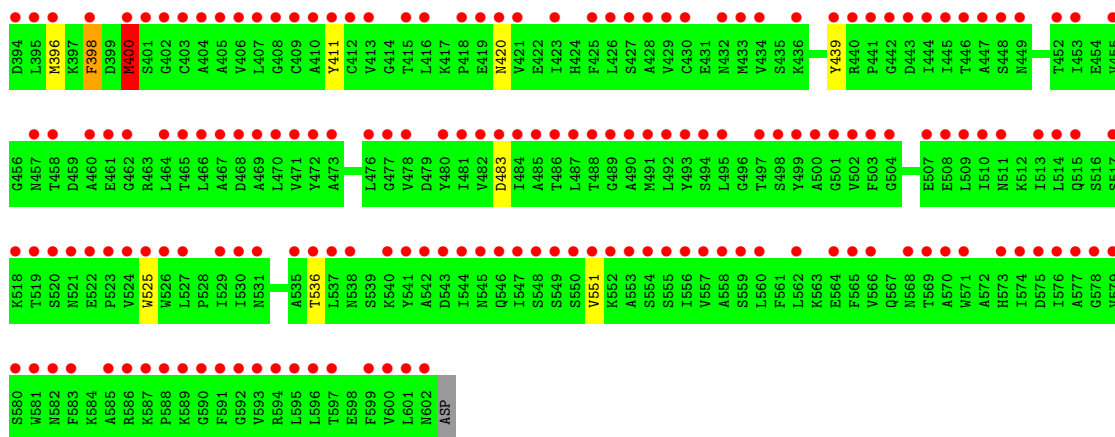
• Molecule 1: M17 family aminopeptidase



• Molecule 1: M17 family aminopeptidase



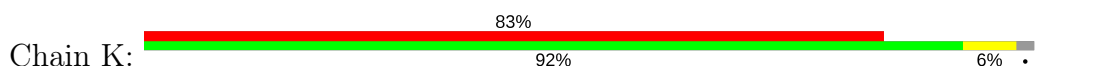




● Molecule 1: M17 family aminopeptidase



● Molecule 1: M17 family aminopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.09Å 177.73Å 230.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.30 48.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.98-2.30) 99.9 (48.98-2.30)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.182 , 0.235 0.579 , 0.587	Depositor DCC
R_{free} test set	15699 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	50850	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.6001e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CO3, 1PE, SO4, 4ZN

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	0.43	0/4052	0.55	0/5502
1	B	0.40	0/3979	0.52	0/5405
1	C	0.43	0/4019	0.55	1/5456 (0.0%)
1	D	0.44	0/3997	0.54	0/5422
1	E	0.43	0/3969	0.56	1/5384 (0.0%)
1	F	0.40	0/3928	0.53	0/5342
1	G	0.42	0/4052	0.53	0/5497
1	H	0.39	0/3979	0.52	0/5407
1	I	0.41	0/4029	0.54	1/5466 (0.0%)
1	J	0.43	0/4003	0.54	0/5430
1	K	0.42	0/3960	0.58	1/5372 (0.0%)
1	L	0.41	0/3925	0.54	0/5338
All	All	0.42	0/47892	0.54	4/65021 (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	K	0	2
1	L	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	99	ILE	C-N-CD	-13.20	91.55	120.60
1	I	400	MET	CA-CB-CG	-7.64	100.31	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	400	MET	CA-CB-CG	-6.05	103.01	113.30
1	C	400	MET	CA-CB-CG	-5.85	103.35	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	551	VAL	Peptide
1	K	99	ILE	Peptide
1	L	551	VAL	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	3971	0	3875	26	0
1	B	3902	0	3787	29	0
1	C	3941	0	3855	25	0
1	D	3920	0	3851	31	0
1	E	3893	0	3820	26	0
1	F	3851	0	3726	21	0
1	G	3974	0	3899	31	0
1	H	3902	0	3774	31	0
1	I	3951	0	3877	22	0
1	J	3926	0	3854	45	0
1	K	3884	0	3805	18	0
1	L	3848	0	3716	32	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	16	0	9	2	0
4	B	16	0	9	3	0
4	C	16	0	9	1	0
4	D	20	0	20	3	0
4	E	20	0	19	2	0
4	F	16	0	9	0	0
4	G	16	0	9	0	0
4	H	16	0	9	1	0
4	I	12	0	7	0	0
4	J	16	0	9	2	0
4	K	14	0	9	1	0
4	L	16	0	9	1	0
5	A	21	0	22	0	0
5	B	20	0	20	3	0
5	C	22	0	24	1	0
5	D	20	0	20	2	0
5	E	24	0	28	2	0
5	F	10	0	13	0	0
5	G	21	0	20	4	0
5	H	20	0	20	1	0
5	I	23	0	26	2	0
5	J	32	0	39	12	0
5	K	24	0	28	2	0
5	L	17	0	21	6	0
6	A	6	0	8	0	0
7	A	25	0	0	2	0
7	B	5	0	0	0	0
7	C	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	5	0	0	1	0
7	E	15	0	0	1	0
7	F	10	0	0	0	0
7	G	20	0	0	2	0
7	I	10	0	0	0	0
7	J	10	0	0	0	0
7	K	10	0	0	0	0
7	L	5	0	0	0	0
8	A	265	0	0	3	0
8	B	246	0	0	3	0
8	C	277	0	0	2	0
8	D	283	0	0	5	0
8	E	322	0	0	5	0
8	F	245	0	0	4	0
8	G	281	0	0	0	0
8	H	220	0	0	2	0
8	I	272	0	0	3	0
8	J	287	0	0	5	0
8	K	283	0	0	1	0
8	L	240	0	0	4	0
All	All	50850	0	46255	326	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 3.

The worst 5 of 326 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:J:320:LYS:HZ1	5:J:706:1PE:H151	1.30	0.96
1:J:489:GLY:N	4:J:704:4ZN:O20	2.06	0.88
1:L:532:GLU:HB2	5:L:705:1PE:H142	1.55	0.87
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.65	0.78
1:B:320:LYS:HZ1	5:B:706:1PE:H241	1.50	0.77

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	518/519 (100%)	501 (97%)	16 (3%)	1 (0%)	51	63
1	B	512/519 (99%)	495 (97%)	16 (3%)	1 (0%)	51	63
1	C	515/519 (99%)	499 (97%)	15 (3%)	1 (0%)	51	63
1	D	510/519 (98%)	496 (97%)	13 (2%)	1 (0%)	51	63
1	E	503/519 (97%)	493 (98%)	10 (2%)	0	100	100
1	F	507/519 (98%)	490 (97%)	17 (3%)	0	100	100
1	G	517/519 (100%)	503 (97%)	14 (3%)	0	100	100
1	H	513/519 (99%)	500 (98%)	11 (2%)	2 (0%)	38	47
1	I	515/519 (99%)	505 (98%)	8 (2%)	2 (0%)	38	47
1	J	510/519 (98%)	496 (97%)	12 (2%)	2 (0%)	38	47
1	K	503/519 (97%)	490 (97%)	10 (2%)	3 (1%)	28	34
1	L	507/519 (98%)	491 (97%)	14 (3%)	2 (0%)	38	47
All	All	6130/6228 (98%)	5959 (97%)	156 (2%)	15 (0%)	51	63

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	VAL
1	H	138	GLU
1	K	100	PRO
1	K	551	VAL
1	K	552	LYS

5.3.2 Protein sidechains [i](#)

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	423/447 (95%)	417 (99%)	6 (1%)	71	85
1	B	407/447 (91%)	403 (99%)	4 (1%)	80	90
1	C	418/447 (94%)	406 (97%)	12 (3%)	48	64
1	D	413/447 (92%)	405 (98%)	8 (2%)	62	78
1	E	413/447 (92%)	410 (99%)	3 (1%)	87	94
1	F	402/447 (90%)	391 (97%)	11 (3%)	50	67
1	G	422/447 (94%)	415 (98%)	7 (2%)	66	81
1	H	406/447 (91%)	397 (98%)	9 (2%)	57	74
1	I	420/447 (94%)	414 (99%)	6 (1%)	71	85
1	J	414/447 (93%)	408 (99%)	6 (1%)	71	85
1	K	410/447 (92%)	406 (99%)	4 (1%)	80	90
1	L	400/447 (90%)	394 (98%)	6 (2%)	70	83
All	All	4948/5364 (92%)	4866 (98%)	82 (2%)	66	81

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	219	LEU
1	G	288	TYR
1	K	439	TYR
1	F	248	THR
1	F	398	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	122	ASN
1	J	181	ASN
1	G	149	ASN
1	B	181	ASN
1	H	139	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 102 ligands modelled in this entry, 24 are monoatomic - leaving 78 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CO3	A	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	A	704	3	10,16,20	0.40	0	14,22,28	1.45	3 (21%)
5	1PE	A	705	-	8,8,15	0.75	0	7,7,14	0.34	0
5	1PE	A	706	-	11,11,15	0.79	0	10,10,14	0.33	0
6	GOL	A	707	-	5,5,5	0.43	0	5,5,5	0.20	0
7	SO4	A	708	-	4,4,4	0.21	0	6,6,6	0.23	0
7	SO4	A	709	-	4,4,4	0.23	0	6,6,6	0.10	0
7	SO4	A	710	-	4,4,4	0.25	0	6,6,6	0.34	0
7	SO4	A	711	-	4,4,4	0.25	0	6,6,6	0.21	0
7	SO4	A	712	-	4,4,4	0.23	0	6,6,6	0.56	0
2	CO3	B	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	B	704	3	10,16,20	0.76	0	14,22,28	2.93	6 (42%)
5	1PE	B	705	-	9,9,15	0.70	0	8,8,14	0.38	0
5	1PE	B	706	-	9,9,15	0.72	0	8,8,14	0.46	0
7	SO4	B	707	-	4,4,4	0.16	0	6,6,6	0.27	0
2	CO3	C	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	C	704	3	10,16,20	1.50	1 (10%)	14,22,28	0.69	0
5	1PE	C	705	-	12,12,15	0.80	0	11,11,14	0.55	0
5	1PE	C	706	-	8,8,15	0.78	0	7,7,14	0.30	0
7	SO4	C	707	-	4,4,4	0.15	0	6,6,6	0.11	0
7	SO4	C	708	-	4,4,4	0.24	0	6,6,6	0.27	0
7	SO4	C	709	-	4,4,4	0.32	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	C	710	-	4,4,4	0.33	0	6,6,6	0.24	0
7	SO4	C	711	-	4,4,4	0.30	0	6,6,6	0.37	0
2	CO3	D	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	D	704	3	14,20,20	1.41	2 (14%)	18,28,28	2.35	5 (27%)
5	1PE	D	705	-	9,9,15	0.82	0	8,8,14	0.48	0
5	1PE	D	706	-	9,9,15	0.76	0	8,8,14	0.34	0
7	SO4	D	707	-	4,4,4	0.25	0	6,6,6	0.24	0
2	CO3	E	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	E	704	3	14,20,20	0.71	1 (7%)	18,28,28	2.17	6 (33%)
5	1PE	E	705	-	11,11,15	0.83	0	10,10,14	0.38	0
5	1PE	E	706	-	11,11,15	0.71	0	10,10,14	0.31	0
7	SO4	E	707	-	4,4,4	0.17	0	6,6,6	0.14	0
7	SO4	E	708	-	4,4,4	0.19	0	6,6,6	0.23	0
7	SO4	E	709	-	4,4,4	0.29	0	6,6,6	0.11	0
2	CO3	F	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	F	704	3	10,16,20	0.56	0	14,22,28	1.41	2 (14%)
5	1PE	F	705	-	9,9,15	0.69	0	8,8,14	0.38	0
7	SO4	F	706	-	4,4,4	0.25	0	6,6,6	0.15	0
7	SO4	F	707	-	4,4,4	0.28	0	6,6,6	0.13	0
2	CO3	G	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	G	704	3	10,16,20	0.47	0	14,22,28	1.54	3 (21%)
5	1PE	G	705	-	8,8,15	0.71	0	7,7,14	0.33	0
5	1PE	G	706	-	5,5,15	0.61	0	4,4,14	0.58	0
5	1PE	G	707	-	5,5,15	0.69	0	4,4,14	0.43	0
7	SO4	G	708	-	4,4,4	0.22	0	6,6,6	0.12	0
7	SO4	G	709	-	4,4,4	0.15	0	6,6,6	0.22	0
7	SO4	G	710	-	4,4,4	0.25	0	6,6,6	0.15	0
7	SO4	G	711	-	4,4,4	0.18	0	6,6,6	0.50	0
2	CO3	H	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	H	704	3	10,16,20	1.76	2 (20%)	14,22,28	1.08	2 (14%)
5	1PE	H	705	-	9,9,15	0.76	0	8,8,14	0.26	0
5	1PE	H	706	-	9,9,15	0.75	0	8,8,14	0.20	0
2	CO3	I	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	I	704	3	8,12,20	1.57	1 (12%)	12,17,28	1.73	1 (8%)
5	1PE	I	705	-	11,11,15	0.76	0	10,10,14	0.40	0
5	1PE	I	706	-	10,10,15	0.71	0	9,9,14	0.46	0
7	SO4	I	707	-	4,4,4	0.17	0	6,6,6	0.19	0
7	SO4	I	708	-	4,4,4	0.18	0	6,6,6	0.10	0
2	CO3	J	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	J	704	3	10,16,20	1.47	1 (10%)	14,22,28	1.03	1 (7%)
5	1PE	J	705	-	10,10,15	0.69	0	9,9,14	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1PE	J	706	-	10,10,15	0.72	0	9,9,14	0.46	0
5	1PE	J	707	-	9,9,15	0.61	0	8,8,14	0.32	0
7	SO4	J	708	-	4,4,4	0.14	0	6,6,6	0.30	0
7	SO4	J	709	-	4,4,4	0.15	0	6,6,6	0.12	0
2	CO3	K	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	K	704	3	11,14,20	0.81	1 (9%)	15,19,28	1.43	2 (13%)
5	1PE	K	705	-	11,11,15	0.72	0	10,10,14	0.25	0
5	1PE	K	706	-	11,11,15	0.74	0	10,10,14	0.45	0
7	SO4	K	707	-	4,4,4	0.21	0	6,6,6	0.12	0
7	SO4	K	708	-	4,4,4	0.17	0	6,6,6	0.25	0
2	CO3	L	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	L	704	3	10,16,20	0.53	0	14,22,28	1.00	0
5	1PE	L	705	-	6,6,15	0.72	0	5,5,14	0.36	0
5	1PE	L	706	-	9,9,15	0.63	0	8,8,14	0.41	0
7	SO4	L	707	-	4,4,4	0.16	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO3	A	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	A	704	3	-	0/9/16/23	0/1/1/1
5	1PE	A	705	-	-	0/6/6/13	0/0/0/0
5	1PE	A	706	-	-	0/9/9/13	0/0/0/0
6	GOL	A	707	-	-	0/4/4/4	0/0/0/0
7	SO4	A	708	-	-	0/0/0/0	0/0/0/0
7	SO4	A	709	-	-	0/0/0/0	0/0/0/0
7	SO4	A	710	-	-	0/0/0/0	0/0/0/0
7	SO4	A	711	-	-	0/0/0/0	0/0/0/0
7	SO4	A	712	-	-	0/0/0/0	0/0/0/0
2	CO3	B	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	B	704	3	-	0/9/16/23	0/1/1/1
5	1PE	B	705	-	-	0/7/7/13	0/0/0/0
5	1PE	B	706	-	-	0/7/7/13	0/0/0/0
7	SO4	B	707	-	-	0/0/0/0	0/0/0/0
2	CO3	C	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	C	704	3	-	0/9/16/23	0/1/1/1
5	1PE	C	705	-	-	0/10/10/13	0/0/0/0
5	1PE	C	706	-	-	0/6/6/13	0/0/0/0
7	SO4	C	707	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SO4	C	708	-	-	0/0/0/0	0/0/0/0
7	SO4	C	709	-	-	0/0/0/0	0/0/0/0
7	SO4	C	710	-	-	0/0/0/0	0/0/0/0
7	SO4	C	711	-	-	0/0/0/0	0/0/0/0
2	CO3	D	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	D	704	3	-	0/13/23/23	0/1/1/1
5	1PE	D	705	-	-	0/7/7/13	0/0/0/0
5	1PE	D	706	-	-	0/7/7/13	0/0/0/0
7	SO4	D	707	-	-	0/0/0/0	0/0/0/0
2	CO3	E	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	E	704	3	-	0/13/23/23	0/1/1/1
5	1PE	E	705	-	-	0/9/9/13	0/0/0/0
5	1PE	E	706	-	-	0/9/9/13	0/0/0/0
7	SO4	E	707	-	-	0/0/0/0	0/0/0/0
7	SO4	E	708	-	-	0/0/0/0	0/0/0/0
7	SO4	E	709	-	-	0/0/0/0	0/0/0/0
2	CO3	F	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	F	704	3	-	0/9/16/23	0/1/1/1
5	1PE	F	705	-	-	0/7/7/13	0/0/0/0
7	SO4	F	706	-	-	0/0/0/0	0/0/0/0
7	SO4	F	707	-	-	0/0/0/0	0/0/0/0
2	CO3	G	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	G	704	3	-	0/9/16/23	0/1/1/1
5	1PE	G	705	-	-	0/6/6/13	0/0/0/0
5	1PE	G	706	-	-	0/3/3/13	0/0/0/0
5	1PE	G	707	-	-	0/3/3/13	0/0/0/0
7	SO4	G	708	-	-	0/0/0/0	0/0/0/0
7	SO4	G	709	-	-	0/0/0/0	0/0/0/0
7	SO4	G	710	-	-	0/0/0/0	0/0/0/0
7	SO4	G	711	-	-	0/0/0/0	0/0/0/0
2	CO3	H	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	H	704	3	-	0/9/16/23	0/1/1/1
5	1PE	H	705	-	-	0/7/7/13	0/0/0/0
5	1PE	H	706	-	-	0/7/7/13	0/0/0/0
2	CO3	I	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	I	704	3	-	0/5/10/23	0/1/1/1
5	1PE	I	705	-	-	0/9/9/13	0/0/0/0
5	1PE	I	706	-	-	0/8/8/13	0/0/0/0
7	SO4	I	707	-	-	0/0/0/0	0/0/0/0
7	SO4	I	708	-	-	0/0/0/0	0/0/0/0
2	CO3	J	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	J	704	3	-	0/9/16/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	J	705	-	-	0/8/8/13	0/0/0/0
5	1PE	J	706	-	-	0/8/8/13	0/0/0/0
5	1PE	J	707	-	-	0/7/7/13	0/0/0/0
7	SO4	J	708	-	-	0/0/0/0	0/0/0/0
7	SO4	J	709	-	-	0/0/0/0	0/0/0/0
2	CO3	K	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	K	704	3	-	0/9/14/23	0/1/1/1
5	1PE	K	705	-	-	0/9/9/13	0/0/0/0
5	1PE	K	706	-	-	0/9/9/13	0/0/0/0
7	SO4	K	707	-	-	0/0/0/0	0/0/0/0
7	SO4	K	708	-	-	0/0/0/0	0/0/0/0
2	CO3	L	701	-	-	0/0/0/0	0/0/0/0
4	4ZN	L	704	3	-	0/9/16/23	0/1/1/1
5	1PE	L	705	-	-	0/4/4/13	0/0/0/0
5	1PE	L	706	-	-	0/7/7/13	0/0/0/0
7	SO4	L	707	-	-	0/0/0/0	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	704	4ZN	P08-C07	2.13	1.81	1.79
4	K	704	4ZN	P08-C07	2.21	1.81	1.79
4	H	704	4ZN	P08-C07	2.61	1.82	1.79
4	D	704	4ZN	P08-C07	2.86	1.82	1.79
4	I	704	4ZN	P08-O10	4.02	1.57	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	704	4ZN	O09-P08-O10	-5.42	107.35	113.96
4	B	704	4ZN	O10-P08-C11	-3.57	104.65	111.45
4	E	704	4ZN	O10-P08-C11	-3.19	105.38	111.45
4	G	704	4ZN	O10-P08-C11	-3.11	105.52	111.45
4	D	704	4ZN	C13-C11-N12	-2.91	104.80	112.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	704	4ZN	2	0
7	A	712	SO4	2	0
4	B	704	4ZN	3	0
5	B	706	1PE	3	0
4	C	704	4ZN	1	0
5	C	706	1PE	1	0
7	C	708	SO4	1	0
7	C	711	SO4	1	0
4	D	704	4ZN	3	0
5	D	705	1PE	2	0
7	D	707	SO4	1	0
4	E	704	4ZN	2	0
5	E	705	1PE	1	0
5	E	706	1PE	1	0
7	E	707	SO4	1	0
5	G	705	1PE	1	0
5	G	706	1PE	2	0
5	G	707	1PE	1	0
7	G	711	SO4	2	0
4	H	704	4ZN	1	0
5	H	705	1PE	1	0
5	I	705	1PE	1	0
5	I	706	1PE	1	0
4	J	704	4ZN	2	0
5	J	705	1PE	4	0
5	J	706	1PE	5	0
5	J	707	1PE	3	0
4	K	704	4ZN	1	0
5	K	706	1PE	2	0
4	L	704	4ZN	1	0
5	L	705	1PE	5	0
5	L	706	1PE	1	0

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 [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	519/519 (100%)	3.50	458 (88%) 0 0	14, 23, 41, 61	3 (0%)
1	B	516/519 (99%)	3.61	435 (84%) 0 0	13, 25, 56, 73	5 (0%)
1	C	517/519 (99%)	3.28	446 (86%) 0 0	13, 23, 43, 60	3 (0%)
1	D	514/519 (99%)	2.98	400 (77%) 0 0	14, 23, 38, 58	1 (0%)
1	E	509/519 (98%)	3.18	425 (83%) 0 0	13, 22, 35, 48	2 (0%)
1	F	511/519 (98%)	3.48	426 (83%) 0 0	16, 26, 54, 71	9 (1%)
1	G	519/519 (100%)	3.41	449 (86%) 0 0	14, 23, 40, 55	5 (0%)
1	H	517/519 (99%)	3.67	448 (86%) 0 0	14, 27, 58, 73	5 (0%)
1	I	517/519 (99%)	3.32	434 (83%) 0 0	13, 25, 46, 63	5 (0%)
1	J	514/519 (99%)	3.09	404 (78%) 0 0	13, 23, 39, 55	6 (1%)
1	K	509/519 (98%)	3.23	433 (85%) 0 0	15, 23, 37, 62	3 (0%)
1	L	511/519 (98%)	3.48	421 (82%) 0 0	15, 25, 52, 62	6 (1%)
All	All	6173/6228 (99%)	3.35	5179 (83%) 0 0	13, 24, 49, 73	53 (0%)

The worst 5 of 5179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	136	GLY	13.9
1	F	121	CYS	12.8
1	J	603	ASP	12.3
1	L	197	ASP	11.4
1	F	138	GLU	11.2

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	SO4	C	711	5/5	0.31	1.44	19.87	41,45,53,55	0
7	SO4	F	707	5/5	0.39	0.82	9.81	55,57,61,75	0
5	1PE	B	705	10/16	0.32	0.68	9.54	36,40,51,51	0
7	SO4	C	710	5/5	0.71	0.84	8.50	34,38,58,62	0
7	SO4	A	711	5/5	0.22	0.70	7.84	56,56,63,81	0
5	1PE	L	705	7/16	0.45	0.87	7.08	30,34,39,41	0
5	1PE	H	706	10/16	0.54	0.60	6.12	30,40,46,47	0
2	CO3	D	701	4/4	0.75	0.58	5.92	16,17,18,18	0
7	SO4	E	709	5/5	0.50	0.45	4.50	47,51,64,76	0
7	SO4	C	708	5/5	-0.03	0.66	4.48	53,57,64,72	0
2	CO3	K	701	4/4	0.68	0.51	4.17	19,19,19,21	0
2	CO3	E	701	4/4	0.83	0.48	3.90	16,18,18,21	0
7	SO4	A	712	5/5	0.73	0.63	3.59	36,42,50,54	0
7	SO4	G	711	5/5	0.52	0.62	3.34	46,48,51,55	0
5	1PE	D	706	10/16	0.60	0.46	3.22	27,36,40,41	0
5	1PE	K	706	12/16	0.48	0.38	2.94	26,36,43,48	0
7	SO4	K	708	5/5	0.21	0.52	2.94	58,60,74,75	0
2	CO3	J	701	4/4	0.80	0.47	2.70	15,16,17,20	0
5	1PE	I	706	11/16	0.46	0.41	2.16	26,35,48,53	0
5	1PE	A	705	9/16	0.63	0.54	2.13	25,32,36,39	0
5	1PE	J	707	10/16	0.46	0.44	1.92	27,34,42,52	0
2	CO3	I	701	4/4	0.87	0.38	1.91	15,15,16,17	0
4	4ZN	D	704	20/20	0.55	0.43	1.86	13,20,27,31	3
5	1PE	G	705	9/16	0.49	0.52	1.67	25,32,39,40	0
5	1PE	G	706	6/16	0.69	0.42	1.64	34,37,41,42	0
4	4ZN	B	704	16/20	0.55	0.43	1.55	11,19,24,31	3
5	1PE	G	707	6/16	0.49	0.47	1.54	31,35,39,39	0
5	1PE	C	706	9/16	0.67	0.34	1.35	26,29,35,36	0
5	1PE	F	705	10/16	0.40	0.39	1.19	26,37,45,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	1PE	L	706	10/16	0.65	0.39	1.17	31,38,45,48	0
5	1PE	J	705	11/16	0.25	0.44	1.15	33,40,50,52	0
5	1PE	E	706	12/16	0.53	0.38	0.96	25,33,43,44	0
4	4ZN	F	704	16/20	0.52	0.42	0.93	17,21,27,31	3
4	4ZN	G	704	16/20	0.51	0.44	0.92	14,17,22,23	4
4	4ZN	E	704	20/20	0.70	0.42	0.87	16,20,27,28	7
4	4ZN	L	704	16/20	0.53	0.44	0.86	14,18,23,27	3
2	CO3	C	701	4/4	0.52	0.40	0.78	15,16,18,18	0
4	4ZN	H	704	16/20	0.69	0.41	0.71	12,18,28,32	3
4	4ZN	C	704	16/20	0.69	0.37	0.62	15,18,23,24	4
4	4ZN	K	704	14/20	0.56	0.39	0.54	14,20,28,33	0
7	SO4	E	707	5/5	0.91	0.36	0.34	21,21,23,24	0
4	4ZN	I	704	12/20	0.70	0.34	0.25	16,18,22,23	0
2	CO3	B	701	4/4	0.74	0.33	0.18	16,16,16,20	0
2	CO3	L	701	4/4	0.60	0.38	0.14	16,17,18,19	0
7	SO4	G	709	5/5	0.92	0.33	-0.02	16,19,20,22	0
7	SO4	A	708	5/5	0.61	0.40	-0.03	44,47,50,58	0
4	4ZN	A	704	16/20	0.60	0.37	-0.12	15,17,22,23	3
7	SO4	J	708	5/5	0.95	0.29	-0.15	21,22,24,25	0
7	SO4	A	709	5/5	0.73	0.36	-0.17	53,57,75,78	0
2	CO3	H	701	4/4	0.67	0.34	-0.19	15,16,17,19	0
4	4ZN	J	704	16/20	0.72	0.30	-0.37	14,17,21,27	3
7	SO4	I	708	5/5	0.68	0.29	-0.57	74,74,83,91	0
2	CO3	G	701	4/4	0.62	0.33	-0.61	13,14,17,19	0
7	SO4	A	710	5/5	0.73	0.33	-0.62	36,40,54,59	0
2	CO3	F	701	4/4	0.56	0.31	-0.67	19,19,19,20	0
7	SO4	B	707	5/5	0.93	0.24	-1.11	17,19,23,24	0
2	CO3	A	701	4/4	0.72	0.29	-1.64	15,18,19,20	0
3	ZN	L	702	1/1	0.61	0.22	-1.68	18,18,18,18	0
7	SO4	G	710	5/5	0.75	0.21	-2.11	35,43,55,58	0
3	ZN	I	702	1/1	0.22	0.14	-2.56	19,19,19,19	0
3	ZN	C	702	1/1	0.54	0.17	-2.62	19,19,19,19	0
3	ZN	B	703	1/1	0.90	0.08	-3.16	15,15,15,15	0
3	ZN	K	703	1/1	0.92	0.14	-3.18	16,16,16,16	0
3	ZN	H	703	1/1	0.69	0.10	-3.25	15,15,15,15	0
3	ZN	C	703	1/1	0.74	0.12	-3.27	15,15,15,15	0
3	ZN	L	703	1/1	0.88	0.11	-3.31	17,17,17,17	0
3	ZN	F	702	1/1	0.58	0.14	-3.46	22,22,22,22	0
3	ZN	K	702	1/1	0.91	0.08	-3.55	19,19,19,19	0
3	ZN	J	703	1/1	0.72	0.10	-3.63	15,15,15,15	0
3	ZN	H	702	1/1	0.74	0.08	-3.82	17,17,17,17	0
3	ZN	B	702	1/1	0.87	0.06	-3.84	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	D	703	1/1	0.82	0.10	-4.12	17,17,17,17	0
3	ZN	I	703	1/1	0.61	0.07	-4.42	19,19,19,19	0
3	ZN	G	702	1/1	0.70	0.10	-4.65	18,18,18,18	0
3	ZN	G	703	1/1	0.82	0.09	-4.76	15,15,15,15	0
3	ZN	E	702	1/1	0.96	0.07	-4.85	17,17,17,17	0
3	ZN	J	702	1/1	0.71	0.09	-4.97	19,19,19,19	0
3	ZN	F	703	1/1	0.97	0.08	-4.98	18,18,18,18	0
3	ZN	A	703	1/1	0.82	0.10	-5.10	14,14,14,14	0
3	ZN	A	702	1/1	0.67	0.16	-5.43	18,18,18,18	0
3	ZN	D	702	1/1	0.73	0.11	-6.28	17,17,17,17	0
3	ZN	E	703	1/1	0.73	0.08	-10.11	17,17,17,17	0
7	SO4	K	707	5/5	0.78	0.32	-	53,54,58,71	0
7	SO4	C	709	5/5	0.34	0.59	-	55,55,63,82	0
5	1PE	K	705	12/16	0.37	0.37	-	29,41,46,47	0
5	1PE	A	706	12/16	-0.04	0.89	-	33,46,50,51	0
7	SO4	G	708	5/5	0.85	0.33	-	41,43,46,58	0
7	SO4	J	709	5/5	0.56	0.80	-	30,33,41,44	5
5	1PE	J	706	11/16	0.43	0.40	-	36,43,47,52	0
7	SO4	C	707	5/5	0.53	0.47	-	57,57,57,58	0
5	1PE	D	705	10/16	0.01	0.52	-	27,37,45,48	0
7	SO4	L	707	5/5	0.80	0.39	-	62,63,64,66	0
5	1PE	I	705	12/16	0.53	0.30	-	35,40,43,47	0
5	1PE	C	705	13/16	0.41	0.35	-	27,41,52,52	0
5	1PE	B	706	10/16	0.47	0.57	-	41,45,54,56	0
7	SO4	D	707	5/5	0.74	0.36	-	42,43,57,58	0
7	SO4	F	706	5/5	0.86	0.40	-	44,46,54,58	0
7	SO4	E	708	5/5	0.80	0.38	-	42,42,54,56	0
5	1PE	E	705	12/16	0.31	0.45	-	29,39,44,45	0
6	GOL	A	707	6/6	0.27	0.58	-	37,37,45,54	0
5	1PE	H	705	10/16	0.36	0.62	-	35,44,50,53	0
7	SO4	I	707	5/5	0.67	0.33	-	52,58,61,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.