



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:43 PM 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20026982

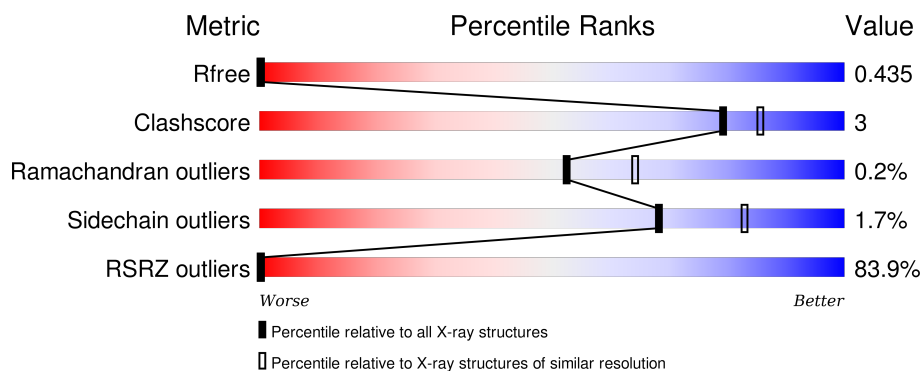
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>87%</div> <div> <div>92%</div> <div>8%</div> </div> </div>
1	B	519	<div> <div>84%</div> <div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	519	<div> <div>87%</div> <div> <div>91%</div> <div>9%</div> </div> </div>
1	D	519	<div> <div>77%</div> <div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	E	519	<div> <div>82%</div> <div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	<div>82%</div> <div>90%</div> <div>8%</div>
1	G	519	<div>86%</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>79%</div> <div>87%</div> <div>11%</div>
1	K	519	<div>82%</div> <div>92%</div> <div>6%</div>
1	L	519	<div>82%</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	708	-	-	-	X
7	SO4	A	711	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	A	712	-	-	X	X
7	SO4	C	708	-	-	-	X
7	SO4	C	710	-	-	-	X
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:

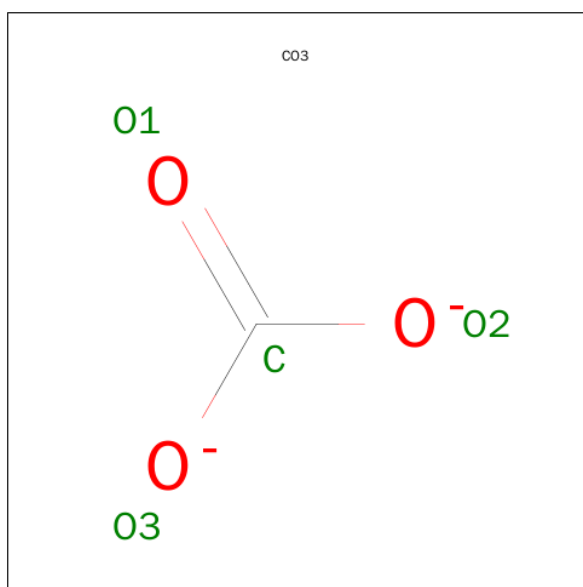
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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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: CO<sub>3</sub>).

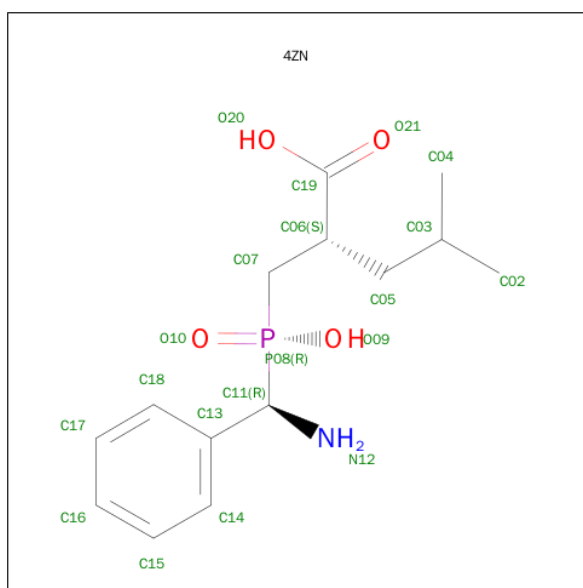


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		
2	G	1	Total	C	O	0	0
			4	1	3		
2	H	1	Total	C	O	0	0
			4	1	3		
2	I	1	Total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

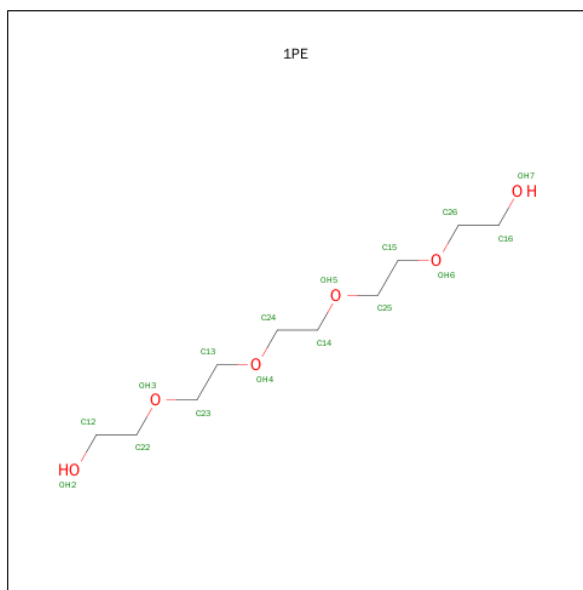
- Molecule 4 is (2S)-2-[[[(R)-[(R)-amino(phenyl)methyl](hydroxy)phosphoryl]methyl]-4-methylpentanoic acid (three-letter code: 4ZN) (formula: C<sub>14</sub>H<sub>22</sub>NO<sub>4</sub>P).





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<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



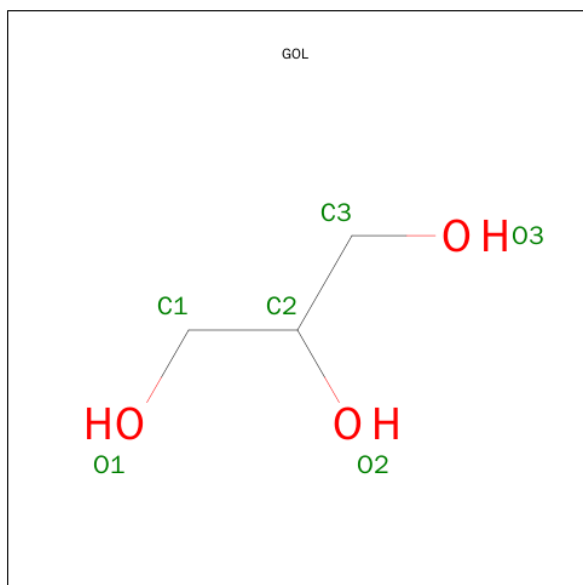
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	6	3		
5	A	1	Total	C	O	0	0
			12	8	4		
5	B	1	Total	C	O	0	0
			10	7	3		
5	B	1	Total	C	O	0	0
			10	7	3		
5	C	1	Total	C	O	0	0
			13	9	4		
5	C	1	Total	C	O	0	0
			9	6	3		
5	D	1	Total	C	O	0	0
			10	7	3		
5	D	1	Total	C	O	0	0
			10	7	3		
5	E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

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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 5	O 4	S 1	0	0
7	F	1	Total 5	O 4	S 1	0	0
7	F	1	Total 5	O 4	S 1	0	0
7	G	1	Total 5	O 4	S 1	0	0
7	G	1	Total 5	O 4	S 1	0	0
7	G	1	Total 5	O 4	S 1	0	0
7	G	1	Total 5	O 4	S 1	0	0
7	I	1	Total 5	O 4	S 1	0	0
7	I	1	Total 5	O 4	S 1	0	0
7	J	1	Total 5	O 4	S 1	0	0
7	J	1	Total 5	O 4	S 1	0	0
7	K	1	Total 5	O 4	S 1	0	0
7	K	1	Total 5	O 4	S 1	0	0
7	L	1	Total 5	O 4	S 1	0	0

- Molecule 8 is water.

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

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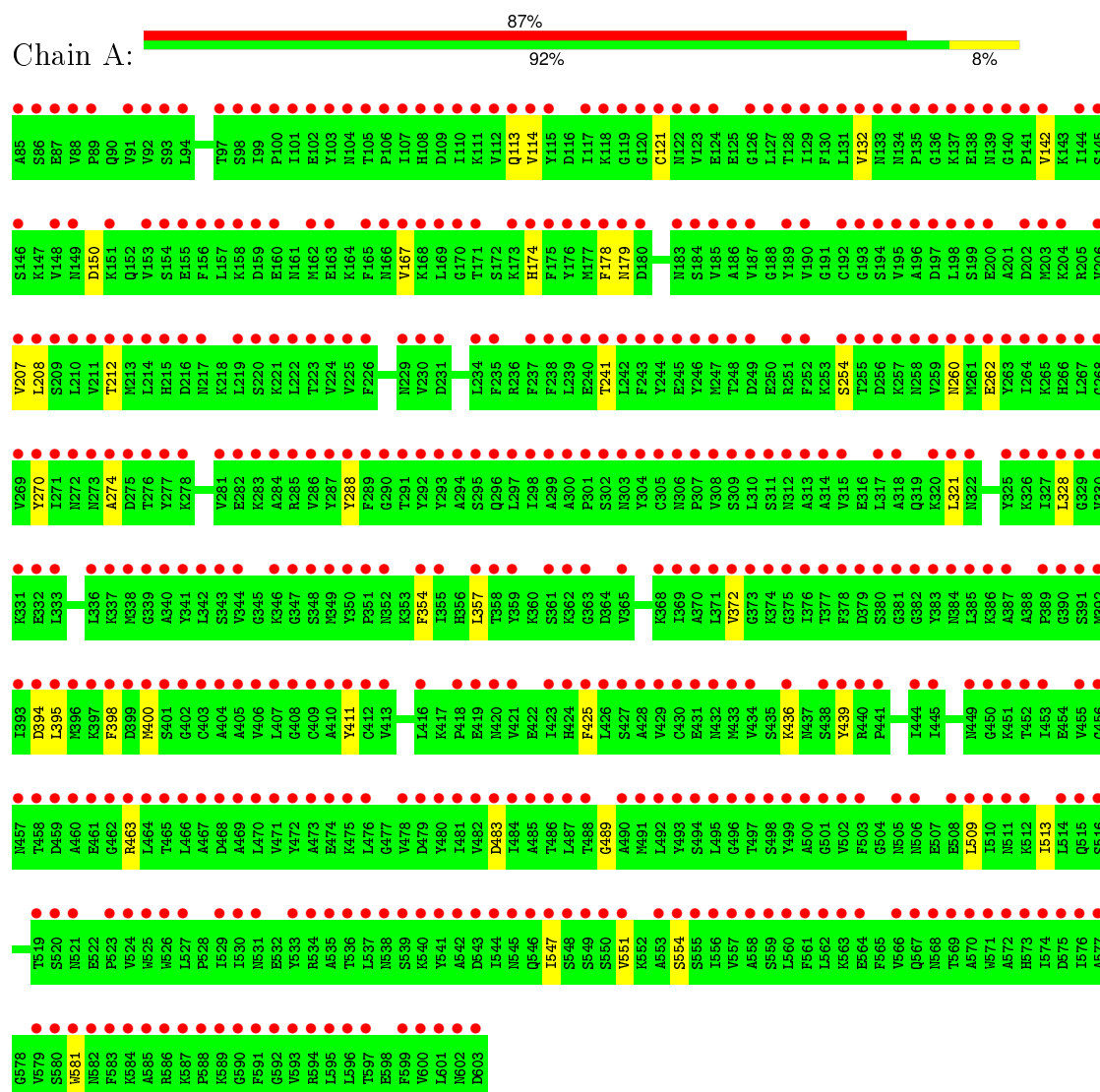
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	245	Total 245	O 245	0	0
8	G	281	Total 281	O 281	0	0
8	H	220	Total 220	O 220	0	0
8	I	272	Total 272	O 272	0	0
8	J	287	Total 287	O 287	0	0
8	K	283	Total 283	O 283	0	0
8	L	240	Total 240	O 240	0	0

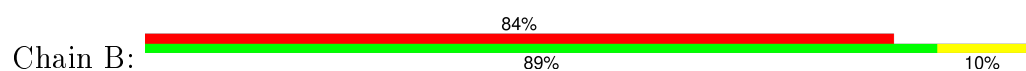
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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

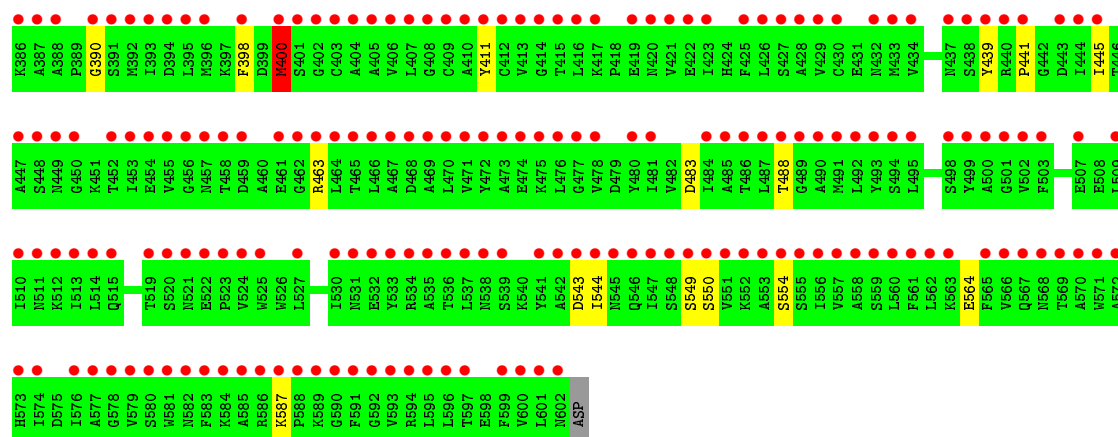


- Molecule 1: M17 family aminopeptidase

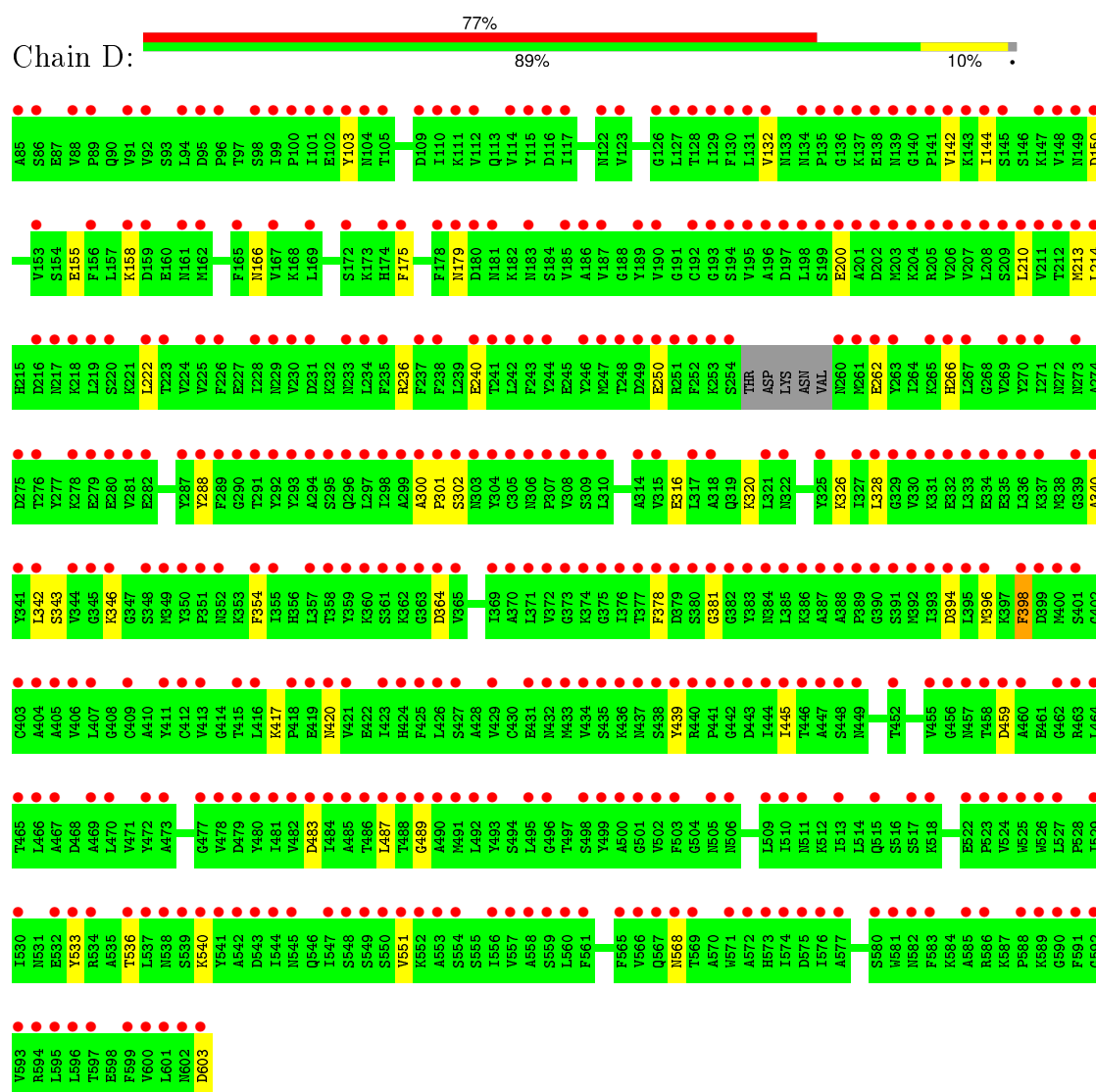




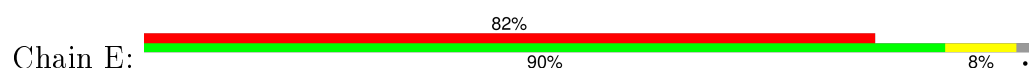


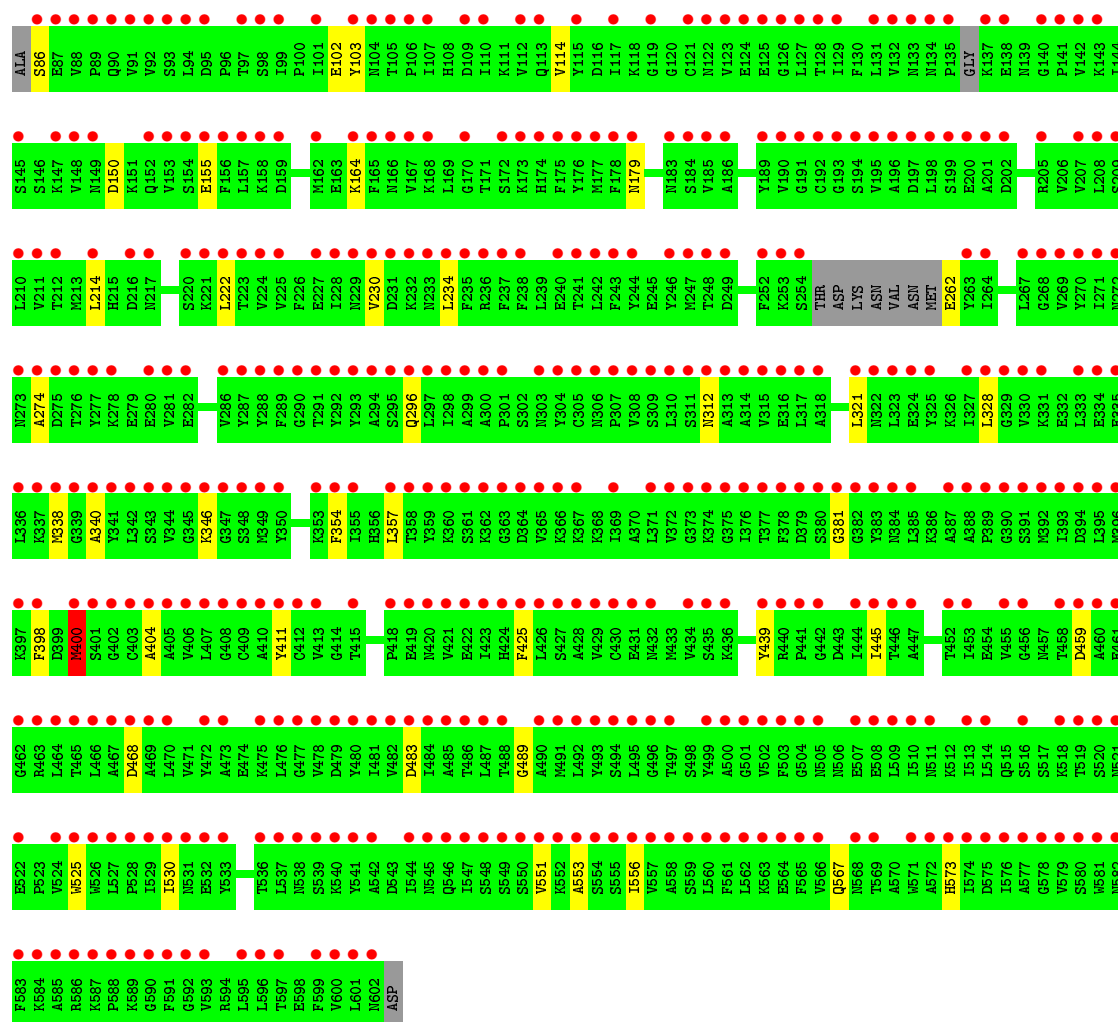


• Molecule 1: M17 family aminopeptidase



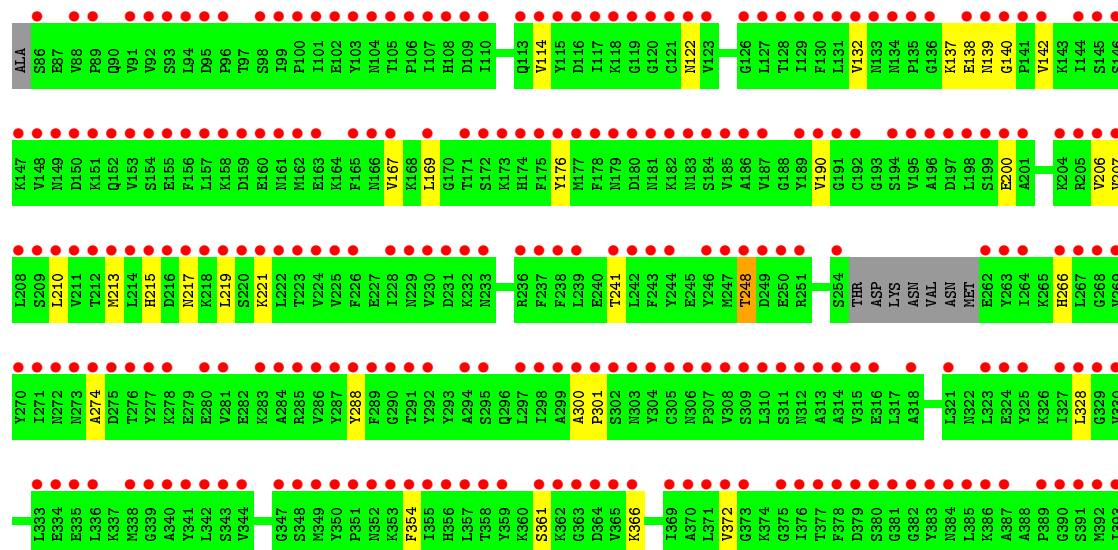
• Molecule 1: M17 family aminopeptidase



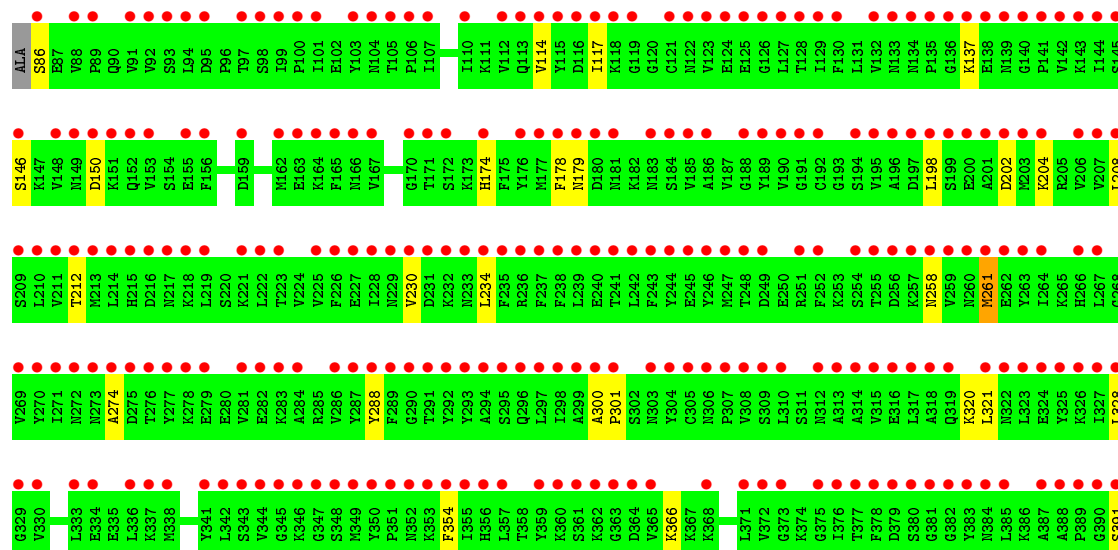
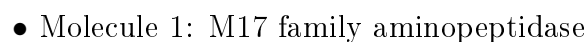


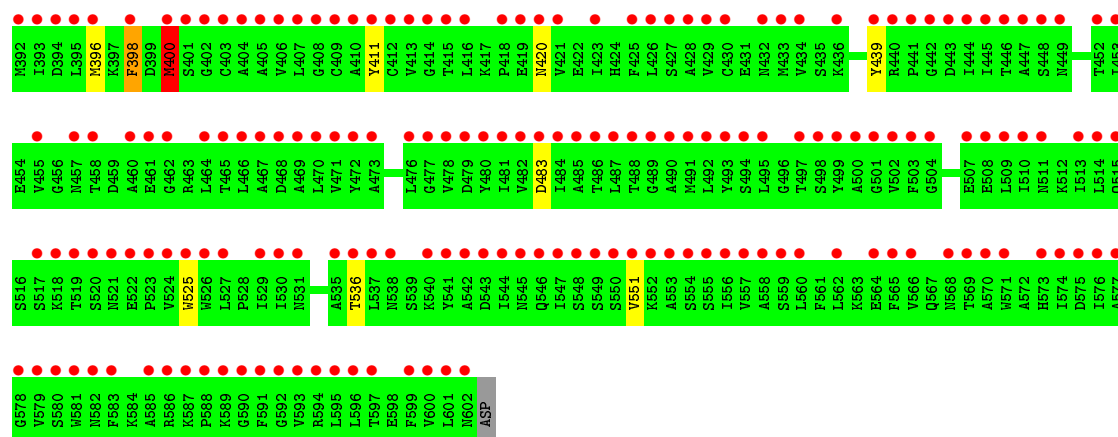
• Molecule 1: M17 family aminopeptidase

Chain F:

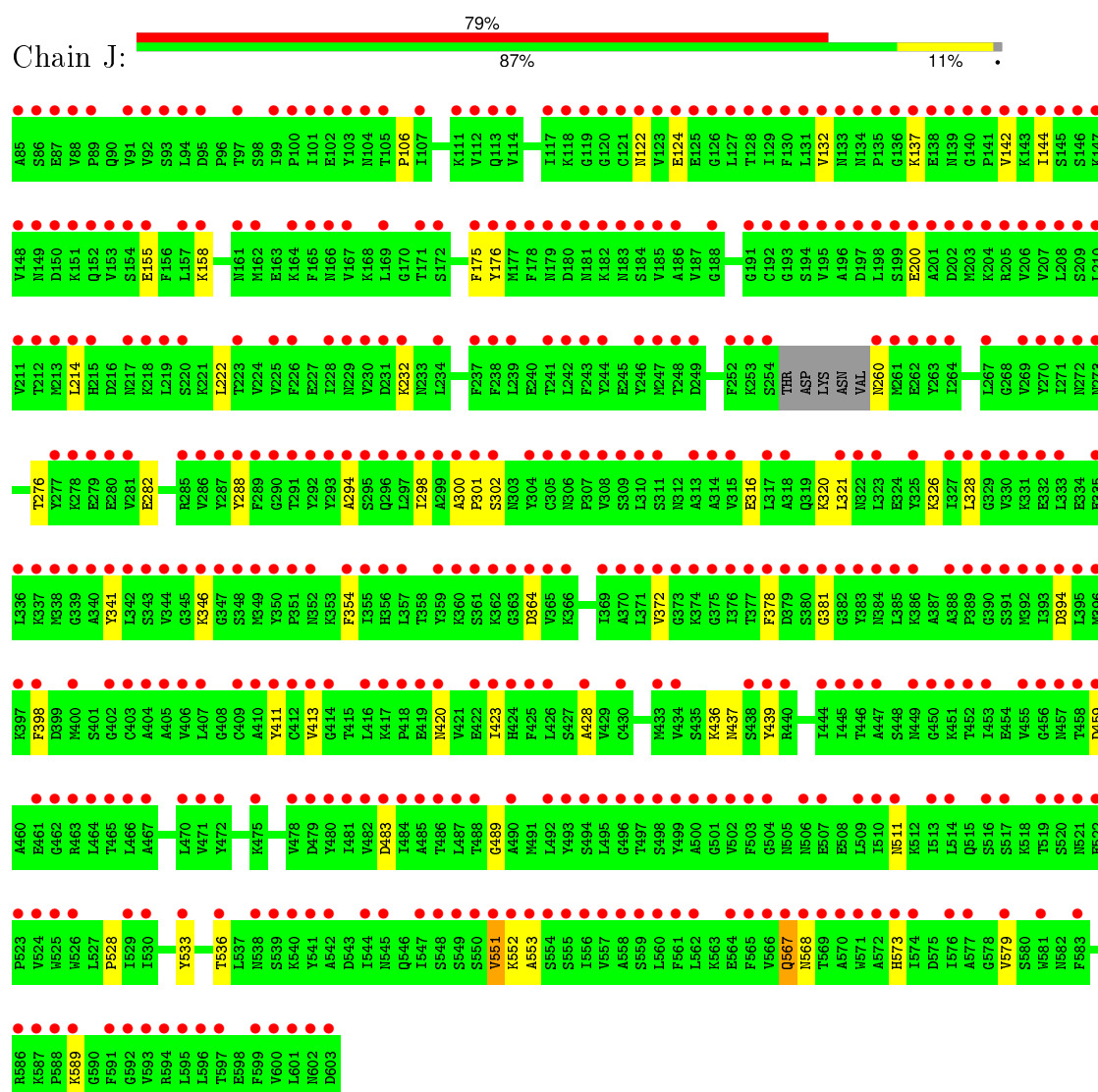








• Molecule 1: M17 family aminopeptidase



• Molecule 1: M17 family aminopeptidase



W581	N521	K397	T458	
N582	E522	F398	D459	
F583	P523	D399	A460	
K584	V524	M400	E461	
A585	W525	S401	G462	
R586	W526	G402	R463	
K587	L527	C403	L464	
P588	P528	A404	T465	
K589	I529	A405	L466	
G590	I530	V406	A467	
F591	N531	L407	D468	
G592	E532	G408	A469	
V593	Y533	C409	L470	
R594	R534	A410	V471	
L595	A535	Y411	V472	
L596	T536	C412	A473	
L597	T537	V413	G477	
E598	N538	G414	V478	
	S539	T415	D479	
F599	K540	L416	Y480	
V600	Y541	K417	V481	
L601	A542	P418	V482	
N602	D543	E419	V483	
D603	I544	N420	D483	
	N545	V421	I484	
	Q546	E422	A485	
	I547	I423	T486	
	S548	H424	L487	
	S549	F425	T488	
	S550	L426	G489	
	V551	S427	A490	
	K552	A428	M491	
	A553	V429	L492	
	S554	C430	Y493	
	S555	E431	S494	
	I556	N432	L495	
	V557	M433	G496	
	A558	V434	T497	
	S559	S435	S498	
	L560	K436	Y499	
	F561	M437	A500	
	L562	S438	G501	
	K563	Y439	V502	
	E564	R440	F503	
	F565	P441	M506	
	V566	G442	E507	
	Q567	D443	E508	
	N568	I444	L509	
	T569	I445	I510	
	A570	T446	N511	
	M571	A447	K512	
	A572		I513	
	H573		L514	
	I574		G450	
	D575		T452	
	I576		I453	
	I577		E454	
	G578		V455	
	V579		G456	
	S580		N457	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.182 , 0.235 0.422 , 0.435	Depositor DCC
$R_{free}$ test set	2920 reflections (0.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 24.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	112 of 315398 reflections (0.036%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	50850	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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%)	52	64
1	B	512/519 (99%)	495 (97%)	16 (3%)	1 (0%)	52	64
1	C	515/519 (99%)	499 (97%)	15 (3%)	1 (0%)	52	64
1	D	510/519 (98%)	496 (97%)	13 (2%)	1 (0%)	52	64
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%)	39	48
1	I	515/519 (99%)	505 (98%)	8 (2%)	2 (0%)	39	48
1	J	510/519 (98%)	496 (97%)	12 (2%)	2 (0%)	39	48
1	K	503/519 (97%)	490 (97%)	10 (2%)	3 (1%)	30	36
1	L	507/519 (98%)	491 (97%)	14 (3%)	2 (0%)	39	48
All	All	6130/6228 (98%)	5959 (97%)	156 (2%)	15 (0%)	52	64

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%)	74	86
1	B	407/447 (91%)	403 (99%)	4 (1%)	82	91
1	C	418/447 (94%)	406 (97%)	12 (3%)	50	66
1	D	413/447 (92%)	405 (98%)	8 (2%)	65	81
1	E	413/447 (92%)	410 (99%)	3 (1%)	88	95
1	F	402/447 (90%)	391 (97%)	11 (3%)	52	70
1	G	422/447 (94%)	415 (98%)	7 (2%)	68	83
1	H	406/447 (91%)	397 (98%)	9 (2%)	60	77
1	I	420/447 (94%)	414 (99%)	6 (1%)	74	86
1	J	414/447 (93%)	408 (99%)	6 (1%)	74	86
1	K	410/447 (92%)	406 (99%)	4 (1%)	82	91
1	L	400/447 (90%)	394 (98%)	6 (2%)	72	85
All	All	4948/5364 (92%)	4866 (98%)	82 (2%)	68	83

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	12,22,28	1.52	2 (16%)
5	1PE	A	705	-	8,8,15	0.76	0	7,7,14	0.33	0
5	1PE	A	706	-	11,11,15	0.80	0	10,10,14	0.34	0
6	GOL	A	707	-	5,5,5	0.44	0	5,5,5	0.22	0
7	SO4	A	708	-	4,4,4	0.12	0	6,6,6	0.16	0
7	SO4	A	709	-	4,4,4	0.10	0	6,6,6	0.17	0
7	SO4	A	710	-	4,4,4	0.12	0	6,6,6	0.28	0
7	SO4	A	711	-	4,4,4	0.12	0	6,6,6	0.21	0
7	SO4	A	712	-	4,4,4	0.24	0	6,6,6	0.53	0
2	CO3	B	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	B	704	3	10,16,20	0.77	0	12,22,28	2.65	5 (41%)
5	1PE	B	705	-	9,9,15	0.71	0	8,8,14	0.38	0
5	1PE	B	706	-	9,9,15	0.73	0	8,8,14	0.46	0
7	SO4	B	707	-	4,4,4	0.22	0	6,6,6	0.31	0
2	CO3	C	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	C	704	3	10,16,20	1.47	1 (10%)	12,22,28	1.08	1 (8%)
5	1PE	C	705	-	12,12,15	0.81	0	11,11,14	0.55	0
5	1PE	C	706	-	8,8,15	0.79	0	7,7,14	0.30	0
7	SO4	C	707	-	4,4,4	0.16	0	6,6,6	0.11	0
7	SO4	C	708	-	4,4,4	0.10	0	6,6,6	0.36	0
7	SO4	C	709	-	4,4,4	0.19	0	6,6,6	0.40	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	0.21	0	6,6,6	0.24	0
7	SO4	C	711	-	4,4,4	0.23	0	6,6,6	0.39	0
2	CO3	D	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	D	704	3	13,20,20	1.42	2 (15%)	18,28,28	2.51	5 (27%)
5	1PE	D	705	-	9,9,15	0.83	0	8,8,14	0.46	0
5	1PE	D	706	-	9,9,15	0.77	0	8,8,14	0.34	0
7	SO4	D	707	-	4,4,4	0.19	0	6,6,6	0.20	0
2	CO3	E	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	E	704	3	13,20,20	0.72	1 (7%)	18,28,28	2.07	6 (33%)
5	1PE	E	705	-	11,11,15	0.84	0	10,10,14	0.39	0
5	1PE	E	706	-	11,11,15	0.72	0	10,10,14	0.32	0
7	SO4	E	707	-	4,4,4	0.20	0	6,6,6	0.14	0
7	SO4	E	708	-	4,4,4	0.22	0	6,6,6	0.25	0
7	SO4	E	709	-	4,4,4	0.13	0	6,6,6	0.09	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	12,22,28	1.69	3 (25%)
5	1PE	F	705	-	9,9,15	0.70	0	8,8,14	0.40	0
7	SO4	F	706	-	4,4,4	0.17	0	6,6,6	0.20	0
7	SO4	F	707	-	4,4,4	0.10	0	6,6,6	0.09	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	12,22,28	1.89	3 (25%)
5	1PE	G	705	-	8,8,15	0.71	0	7,7,14	0.34	0
5	1PE	G	706	-	5,5,15	0.61	0	4,4,14	0.59	0
5	1PE	G	707	-	5,5,15	0.69	0	4,4,14	0.42	0
7	SO4	G	708	-	4,4,4	0.18	0	6,6,6	0.19	0
7	SO4	G	709	-	4,4,4	0.18	0	6,6,6	0.33	0
7	SO4	G	710	-	4,4,4	0.12	0	6,6,6	0.19	0
7	SO4	G	711	-	4,4,4	0.29	0	6,6,6	0.49	0
2	CO3	H	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	H	704	3	10,16,20	1.73	2 (20%)	12,22,28	1.40	2 (16%)
5	1PE	H	705	-	9,9,15	0.77	0	8,8,14	0.27	0
5	1PE	H	706	-	9,9,15	0.76	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	7,12,20	0.69	0	10,17,28	0.77	0
5	1PE	I	705	-	11,11,15	0.77	0	10,10,14	0.39	0
5	1PE	I	706	-	10,10,15	0.72	0	9,9,14	0.45	0
7	SO4	I	707	-	4,4,4	0.18	0	6,6,6	0.17	0
7	SO4	I	708	-	4,4,4	0.12	0	6,6,6	0.08	0
2	CO3	J	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	J	704	3	10,16,20	1.44	1 (10%)	12,22,28	1.27	1 (8%)
5	1PE	J	705	-	10,10,15	0.70	0	9,9,14	0.41	0
5	1PE	J	706	-	10,10,15	0.73	0	9,9,14	0.48	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	1PE	J	707	-	9,9,15	0.62	0	8,8,14	0.34	0
7	SO4	J	708	-	4,4,4	0.25	0	6,6,6	0.21	0
7	SO4	J	709	-	4,4,4	0.40	0	6,6,6	0.17	0
2	CO3	K	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	4ZN	K	704	3	11,14,20	0.80	1 (9%)	14,19,28	1.82	2 (14%)
5	1PE	K	705	-	11,11,15	0.73	0	10,10,14	0.26	0
5	1PE	K	706	-	11,11,15	0.75	0	10,10,14	0.44	0
7	SO4	K	707	-	4,4,4	0.23	0	6,6,6	0.10	0
7	SO4	K	708	-	4,4,4	0.08	0	6,6,6	0.28	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	12,22,28	1.49	1 (8%)
5	1PE	L	705	-	6,6,15	0.72	0	5,5,14	0.39	0
5	1PE	L	706	-	9,9,15	0.63	0	8,8,14	0.43	0
7	SO4	L	707	-	4,4,4	0.24	0	6,6,6	0.18	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
7	SO4	C	708	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
5	1PE	J	705	-	-	0/8/8/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 8 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	D	704	4ZN	P08-O10	4.16	1.57	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	704	4ZN	O09-P08-O10	-6.55	102.90	114.00
4	B	704	4ZN	O09-P08-O10	-6.48	103.02	114.00
4	K	704	4ZN	O09-P08-O10	-4.92	105.67	114.00
4	G	704	4ZN	O09-P08-O10	-4.27	106.76	114.00
4	L	704	4ZN	O09-P08-O10	-4.01	107.20	114.00

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	519/519 (100%)	3.49	451 (86%) 0 0	14, 23, 41, 61	3 (0%)
1	B	516/519 (99%)	3.62	434 (84%) 0 0	13, 25, 56, 73	5 (0%)
1	C	517/519 (99%)	3.28	451 (87%) 0 0	13, 23, 43, 60	3 (0%)
1	D	514/519 (99%)	2.97	401 (78%) 0 0	14, 23, 38, 58	1 (0%)
1	E	509/519 (98%)	3.19	424 (83%) 0 0	13, 22, 35, 48	2 (0%)
1	F	511/519 (98%)	3.47	426 (83%) 0 0	16, 26, 54, 71	9 (1%)
1	G	519/519 (100%)	3.39	446 (85%) 0 0	14, 23, 40, 55	5 (0%)
1	H	517/519 (99%)	3.67	447 (86%) 0 0	14, 27, 58, 73	5 (0%)
1	I	517/519 (99%)	3.32	438 (84%) 0 0	13, 25, 46, 63	5 (0%)
1	J	514/519 (99%)	3.09	411 (79%) 0 0	13, 23, 39, 55	6 (1%)
1	K	509/519 (98%)	3.22	428 (84%) 0 0	15, 23, 37, 62	3 (0%)
1	L	511/519 (98%)	3.47	424 (82%) 0 0	15, 25, 52, 62	6 (1%)
All	All	6173/6228 (99%)	3.35	5181 (83%) 0 0	13, 24, 49, 73	53 (0%)

The worst 5 of 5181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	136	GLY	13.2
1	J	603	ASP	12.6
1	F	121	CYS	12.0
1	L	363	GLY	12.0
1	H	261	MET	11.4

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	SO4	C	711	5/5	0.31	1.43	20.10	41,45,53,55	0
5	1PE	B	705	10/16	0.31	0.69	9.96	36,40,51,51	0
7	SO4	F	707	5/5	0.39	0.79	9.06	55,57,61,75	0
7	SO4	C	710	5/5	0.71	0.85	8.66	34,38,58,62	0
7	SO4	A	711	5/5	0.22	0.72	8.04	56,56,63,81	0
5	1PE	L	705	7/16	0.44	0.90	7.67	30,34,39,41	0
5	1PE	H	706	10/16	0.53	0.61	6.38	30,40,46,47	0
2	CO3	D	701	4/4	0.75	0.58	5.78	16,17,18,18	0
7	SO4	C	708	5/5	-0.01	0.66	4.67	53,57,64,72	0
7	SO4	E	709	5/5	0.50	0.46	4.44	47,51,64,76	0
7	SO4	A	712	5/5	0.73	0.66	3.99	36,42,50,54	0
2	CO3	E	701	4/4	0.83	0.48	3.76	16,18,18,21	0
5	1PE	K	706	12/16	0.47	0.39	3.22	26,36,43,48	0
7	SO4	G	711	5/5	0.53	0.60	3.09	46,48,51,55	0
5	1PE	D	706	10/16	0.58	0.46	3.08	27,36,40,41	0
2	CO3	K	701	4/4	0.68	0.47	3.06	19,19,19,21	0
7	SO4	K	708	5/5	0.22	0.51	2.79	58,60,74,75	0
2	CO3	J	701	4/4	0.79	0.46	2.78	15,16,17,20	0
5	1PE	I	706	11/16	0.46	0.42	2.28	26,35,48,53	0
5	1PE	J	707	10/16	0.46	0.44	1.94	27,34,42,52	0
5	1PE	A	705	9/16	0.63	0.55	1.94	25,32,36,39	0
2	CO3	I	701	4/4	0.88	0.38	1.91	15,15,16,17	0
4	4ZN	D	704	20/20	0.54	0.43	1.76	13,20,27,31	3
5	1PE	G	705	9/16	0.49	0.52	1.75	25,32,39,40	0
4	4ZN	B	704	16/20	0.55	0.43	1.59	11,19,24,31	3
5	1PE	G	706	6/16	0.70	0.41	1.58	34,37,41,42	0
5	1PE	C	706	9/16	0.67	0.35	1.57	26,29,35,36	0
5	1PE	F	705	10/16	0.40	0.39	1.39	26,37,45,52	0
5	1PE	G	707	6/16	0.49	0.45	1.34	31,35,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	1PE	L	706	10/16	0.66	0.39	1.21	31,38,45,48	0
4	4ZN	G	704	16/20	0.53	0.44	0.98	14,17,22,23	4
5	1PE	J	705	11/16	0.25	0.42	0.96	33,40,50,52	0
4	4ZN	F	704	16/20	0.53	0.42	0.95	17,21,27,31	3
5	1PE	E	706	12/16	0.53	0.38	0.90	25,33,43,44	0
4	4ZN	L	704	16/20	0.53	0.44	0.86	14,18,23,27	3
4	4ZN	E	704	20/20	0.69	0.42	0.84	16,20,27,28	7
4	4ZN	H	704	16/20	0.70	0.42	0.83	12,18,28,32	3
4	4ZN	C	704	16/20	0.69	0.38	0.73	15,18,23,24	4
4	4ZN	K	704	14/20	0.56	0.39	0.50	14,20,28,33	0
2	CO3	C	701	4/4	0.54	0.37	0.46	15,16,18,18	0
7	SO4	E	707	5/5	0.91	0.37	0.40	21,21,23,24	0
4	4ZN	I	704	12/20	0.69	0.34	0.29	16,18,22,23	0
2	CO3	B	701	4/4	0.74	0.33	0.23	16,16,16,20	0
7	SO4	A	708	5/5	0.60	0.43	0.21	44,47,50,58	0
2	CO3	L	701	4/4	0.60	0.37	0.12	16,17,18,19	0
7	SO4	G	709	5/5	0.92	0.33	0.03	16,19,20,22	0
7	SO4	J	708	5/5	0.95	0.31	-0.04	21,22,24,25	0
4	4ZN	A	704	16/20	0.60	0.37	-0.10	15,17,22,23	3
2	CO3	H	701	4/4	0.67	0.34	-0.17	15,16,17,19	0
7	SO4	A	709	5/5	0.73	0.35	-0.23	53,57,75,78	0
7	SO4	I	708	5/5	0.68	0.30	-0.35	74,74,83,91	0
4	4ZN	J	704	16/20	0.73	0.29	-0.49	14,17,21,27	3
7	SO4	A	710	5/5	0.73	0.33	-0.54	36,40,54,59	0
2	CO3	G	701	4/4	0.62	0.33	-0.63	13,14,17,19	0
2	CO3	F	701	4/4	0.56	0.30	-0.76	19,19,19,20	0
7	SO4	B	707	5/5	0.93	0.25	-1.11	17,19,23,24	0
2	CO3	A	701	4/4	0.72	0.29	-1.58	15,18,19,20	0
3	ZN	L	702	1/1	0.61	0.22	-1.67	18,18,18,18	0
7	SO4	G	710	5/5	0.75	0.21	-2.18	35,43,55,58	0
3	ZN	I	702	1/1	0.22	0.14	-2.52	19,19,19,19	0
3	ZN	C	702	1/1	0.53	0.17	-2.76	19,19,19,19	0
3	ZN	B	703	1/1	0.90	0.08	-3.18	15,15,15,15	0
3	ZN	K	703	1/1	0.92	0.14	-3.26	16,16,16,16	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	-3.30	17,17,17,17	0
3	ZN	H	703	1/1	0.69	0.10	-3.33	15,15,15,15	0
3	ZN	F	702	1/1	0.58	0.14	-3.48	22,22,22,22	0
3	ZN	K	702	1/1	0.91	0.09	-3.57	19,19,19,19	0
3	ZN	J	703	1/1	0.72	0.10	-3.68	15,15,15,15	0
3	ZN	H	702	1/1	0.73	0.08	-3.85	17,17,17,17	0
3	ZN	B	702	1/1	0.87	0.06	-3.86	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	D	703	1/1	0.82	0.10	-4.04	17,17,17,17	0
3	ZN	I	703	1/1	0.60	0.07	-4.19	19,19,19,19	0
3	ZN	E	702	1/1	0.95	0.07	-4.82	17,17,17,17	0
3	ZN	G	702	1/1	0.69	0.10	-4.85	18,18,18,18	0
3	ZN	G	703	1/1	0.82	0.09	-4.85	15,15,15,15	0
3	ZN	J	702	1/1	0.71	0.09	-4.89	19,19,19,19	0
3	ZN	F	703	1/1	0.97	0.08	-5.07	18,18,18,18	0
3	ZN	A	703	1/1	0.82	0.10	-5.13	14,14,14,14	0
3	ZN	A	702	1/1	0.67	0.16	-5.24	18,18,18,18	0
3	ZN	D	702	1/1	0.73	0.11	-5.56	17,17,17,17	0
3	ZN	E	703	1/1	0.73	0.08	-10.12	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	0.35	0.57	-	55,55,63,82	0
5	1PE	K	705	12/16	0.37	0.38	-	29,41,46,47	0
5	1PE	A	706	12/16	-0.04	0.87	-	33,46,50,51	0
7	SO4	G	708	5/5	0.85	0.34	-	41,43,46,58	0
7	SO4	J	709	5/5	0.57	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	0.52	0.47	-	57,57,57,58	0
5	1PE	D	705	10/16	0.01	0.53	-	27,37,45,48	0
7	SO4	L	707	5/5	0.80	0.35	-	62,63,64,66	0
5	1PE	I	705	12/16	0.53	0.31	-	35,40,43,47	0
5	1PE	C	705	13/16	0.42	0.35	-	27,41,52,52	0
5	1PE	B	706	10/16	0.46	0.58	-	41,45,54,56	0
7	SO4	D	707	5/5	0.74	0.35	-	42,43,57,58	0
7	SO4	F	706	5/5	0.86	0.36	-	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	0.46	-	29,39,44,45	0
6	GOL	A	707	6/6	0.26	0.59	-	37,37,45,54	0
5	1PE	H	705	10/16	0.34	0.63	-	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.