



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:15 PM GMT

PDB ID : 4R6T  
Title : Structure of the m17 leucyl aminopeptidase from malaria complexed with a hydroxamic acid-based inhibitor  
Authors : Drinkwater, N.; McGowan, S.  
Deposited on : 2014-08-26  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

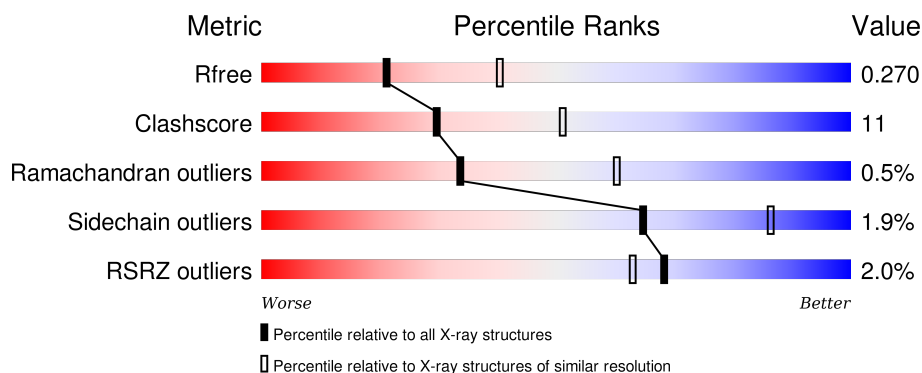
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	528	<div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	B	528	<div>6%</div> <div>73%</div> <div>23%</div> <div>..</div>
1	C	528	<div>2%</div> <div>73%</div> <div>24%</div> <div>..</div>
1	D	528	<div>71%</div> <div>25%</div> <div>..</div>
1	E	528	<div>75%</div> <div>22%</div> <div>..</div>

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Mol	Chain	Length	Quality of chain
1	F	528	
1	G	528	
1	H	528	
1	I	528	
1	J	528	
1	K	528	
1	L	528	

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
3	CO3	C	1002	-	-	-	X
3	CO3	D	1002	-	-	-	X
3	CO3	F	1002	-	-	-	X
3	CO3	G	1002	-	-	-	X
3	CO3	H	1002	-	-	-	X
4	SO4	A	1009	-	-	-	X
4	SO4	B	1004	-	-	X	-
4	SO4	C	1005	-	-	-	X
4	SO4	G	1004	-	-	-	X
4	SO4	G	1005	-	-	-	X
4	SO4	J	1007	-	-	-	X
4	SO4	J	1008	-	-	-	X
4	SO4	L	1005	-	-	-	X
4	SO4	L	1008	-	-	-	X
5	R5T	F	1005	-	-	-	X
5	R5T	I	1004	-	-	-	X
5	R5T	L	1006	-	-	-	X
6	1PE	C	1009	-	-	-	X
6	1PE	C	1010	-	-	X	X
6	1PE	E	1006	-	-	X	-
6	1PE	E	1007	-	-	-	X
6	1PE	G	1007	-	-	-	X
6	1PE	I	1006	-	-	-	X
6	1PE	K	1008	-	-	-	X
7	DMS	G	1009	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 49091 atoms, of which 6 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 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	1	0
			3945	2537	632	757	19			
1	B	511	Total	C	N	O	S	0	0	0
			3869	2489	626	735	19			
1	C	518	Total	C	N	O	S	0	0	0
			3949	2541	637	752	19			
1	D	513	Total	C	N	O	S	0	0	0
			3918	2524	630	745	19			
1	E	513	Total	C	N	O	S	0	0	0
			3913	2521	626	746	20			
1	F	508	Total	C	N	O	S	0	0	0
			3785	2438	610	718	19			
1	G	514	Total	C	N	O	S	0	0	0
			3944	2537	630	758	19			
1	H	511	Total	C	N	O	S	0	0	0
			3878	2495	625	739	19			
1	I	516	Total	C	N	O	S	0	0	0
			3908	2516	629	744	19			
1	J	512	Total	C	N	O	S	0	0	0
			3910	2519	630	742	19			
1	K	509	Total	C	N	O	S	0	0	0
			3879	2500	622	738	19			
1	L	509	Total	C	N	O	S	0	0	0
			3823	2457	614	733	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	607	HIS	-	EXPRESSION TAG	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
F	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
F	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	610	HIS	-	EXPRESSION TAG	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	611	HIS	-	EXPRESSION TAG	UNP Q8IL11

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

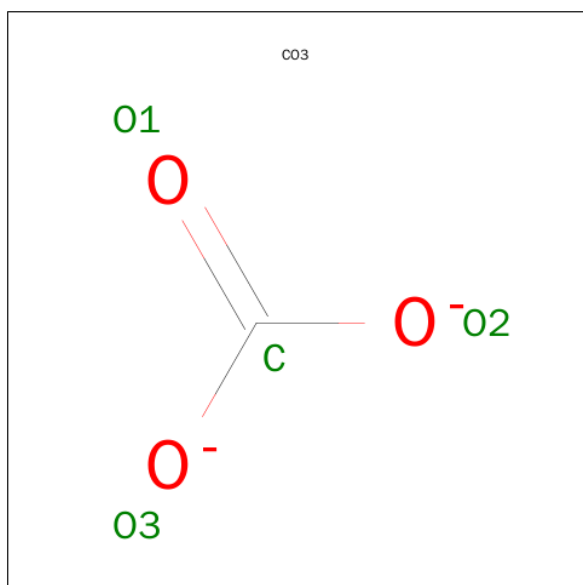
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



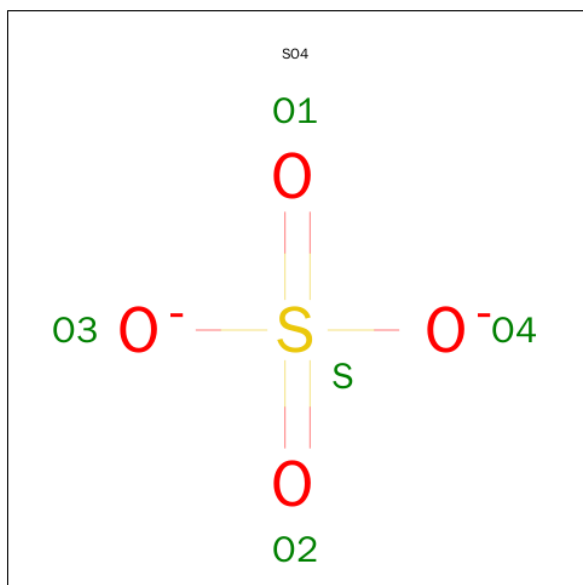
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 1	O 3	0	0
3	B	1	Total 4	C 1	O 3	0	0
3	C	1	Total 4	C 1	O 3	0	0
3	D	1	Total 4	C 1	O 3	0	0
3	E	1	Total 4	C 1	O 3	0	0
3	F	1	Total 4	C 1	O 3	0	0
3	G	1	Total 4	C 1	O 3	0	0
3	H	1	Total 4	C 1	O 3	0	0
3	I	1	Total 4	C 1	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	C	O	0	0
			4	1	3		
3	K	1	Total	C	O	0	0
			4	1	3		
3	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



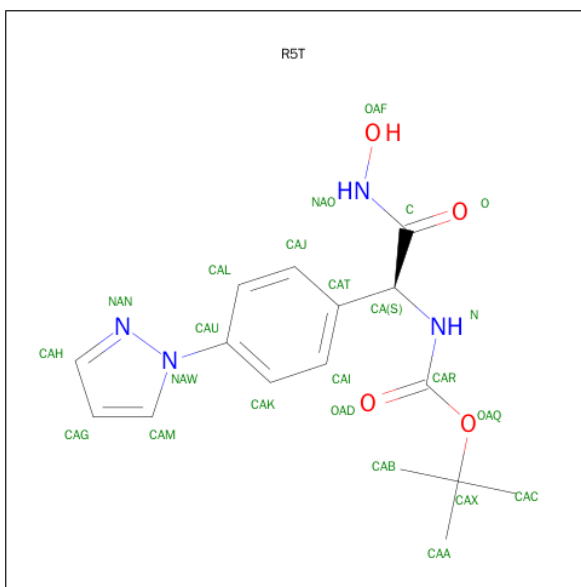
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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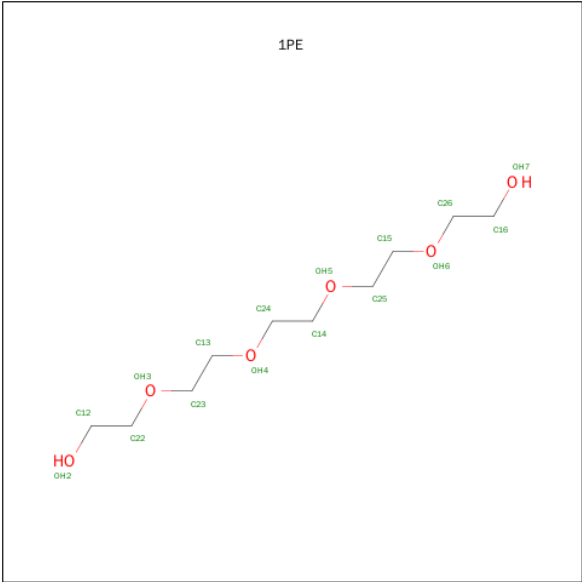
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total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

- Molecule 5 is TERT-BUTYL {(1S)-2-(HYDROXYAMINO)-2-OXO-1-[4-(1H-PYRAZOL-1-YL)PHENYL]ETHYL}CARBAMATE (three-letter code: R5T) (formula: C<sub>16</sub>H<sub>20</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			24	16	4	4		
5	B	1	Total	C	N	O	0	0
			24	16	4	4		
5	C	1	Total	C	N	O	0	0
			24	16	4	4		
5	D	1	Total	C	N	O	0	0
			24	16	4	4		
5	E	1	Total	C	N	O	0	0
			24	16	4	4		
5	F	1	Total	C	N	O	0	0
			24	16	4	4		
5	G	1	Total	C	N	O	0	0
			24	16	4	4		
5	H	1	Total	C	N	O	0	0
			24	16	4	4		
5	I	1	Total	C	N	O	0	0
			24	16	4	4		
5	J	1	Total	C	N	O	0	0
			24	16	4	4		
5	K	1	Total	C	N	O	0	0
			24	16	4	4		
5	L	1	Total	C	N	O	0	0
			21	13	4	4		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



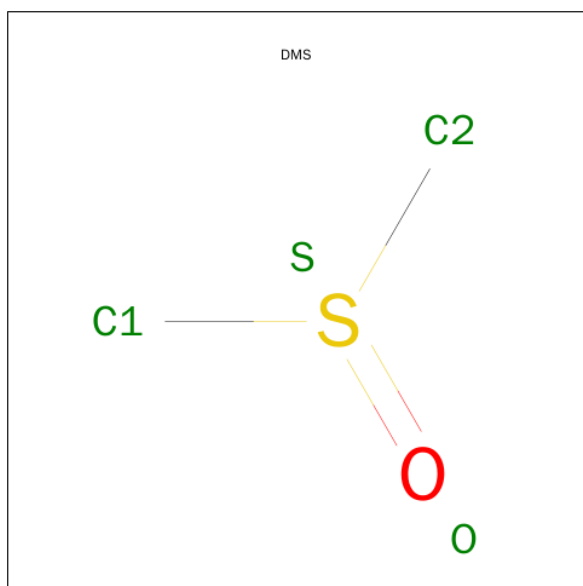
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	B	1	Total	C	O	0	0
			14	9	5		
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			12	8	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	C	1	Total	C	O	0	0
			8	5	3		
6	D	1	Total	C	O	0	0
			9	6	3		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			13	9	4		
6	E	1	Total	C	O	0	0
			8	6	2		
6	F	1	Total	C	O	0	0
			8	6	2		
6	F	1	Total	C	O	0	0
			8	6	2		
6	G	1	Total	C	O	0	0
			7	5	2		
6	G	1	Total	C	O	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			13	9	4		
6	I	1	Total	C	O	0	0
			8	5	3		
6	J	1	Total	C	O	0	0
			9	6	3		
6	J	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			13	9	4		
6	L	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	G	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	160	Total	O	0	0
			160	160		
8	B	130	Total	O	0	0
			130	130		

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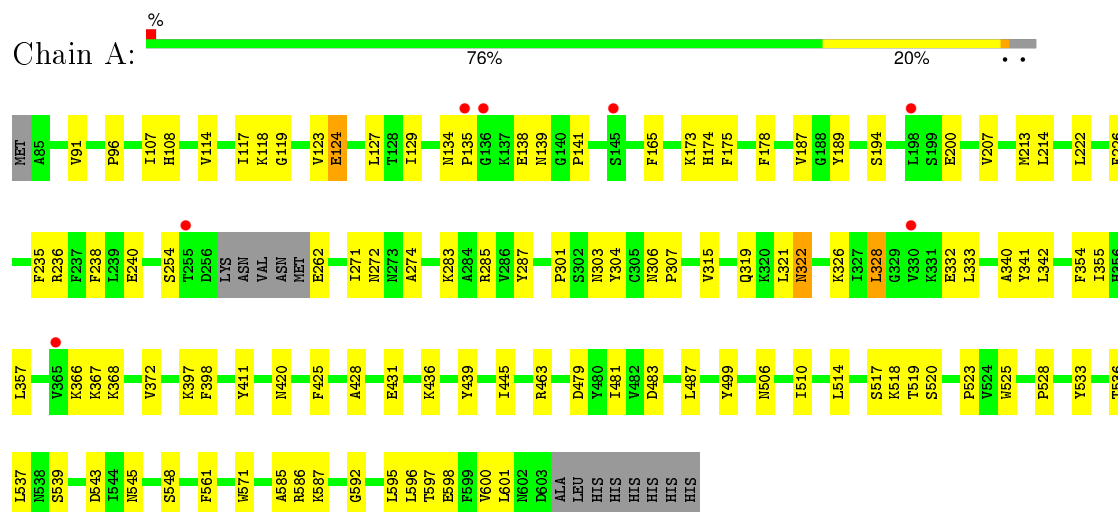
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	169	Total 169	O 169	0	0
8	D	151	Total 151	O 151	0	0
8	E	132	Total 132	O 132	0	0
8	F	94	Total 94	O 94	0	0
8	G	149	Total 149	O 149	0	0
8	H	117	Total 117	O 117	0	0
8	I	164	Total 164	O 164	0	0
8	J	154	Total 154	O 154	0	0
8	K	157	Total 157	O 157	0	0
8	L	114	Total 114	O 114	0	0

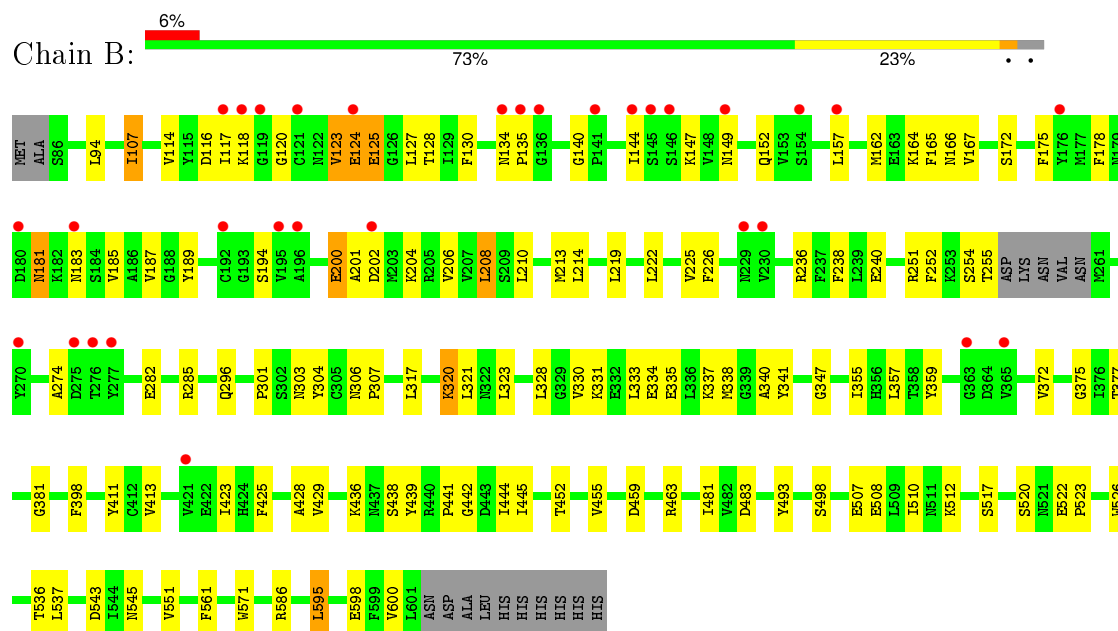
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: M17 leucyl aminopeptidase



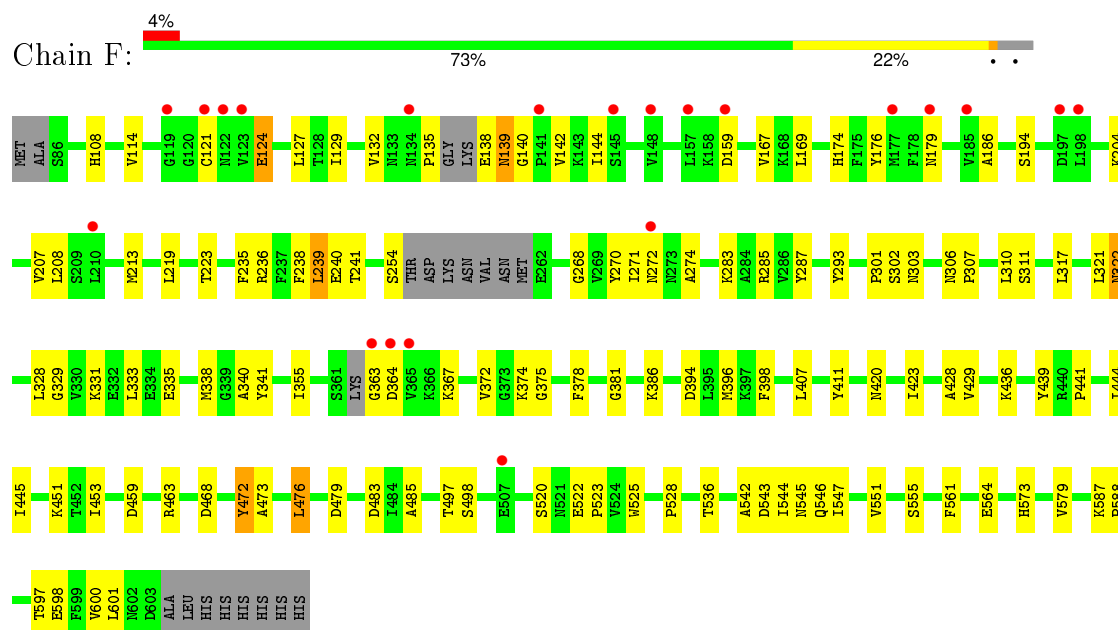
#### • Molecule 1: M17 leucyl aminopeptidase



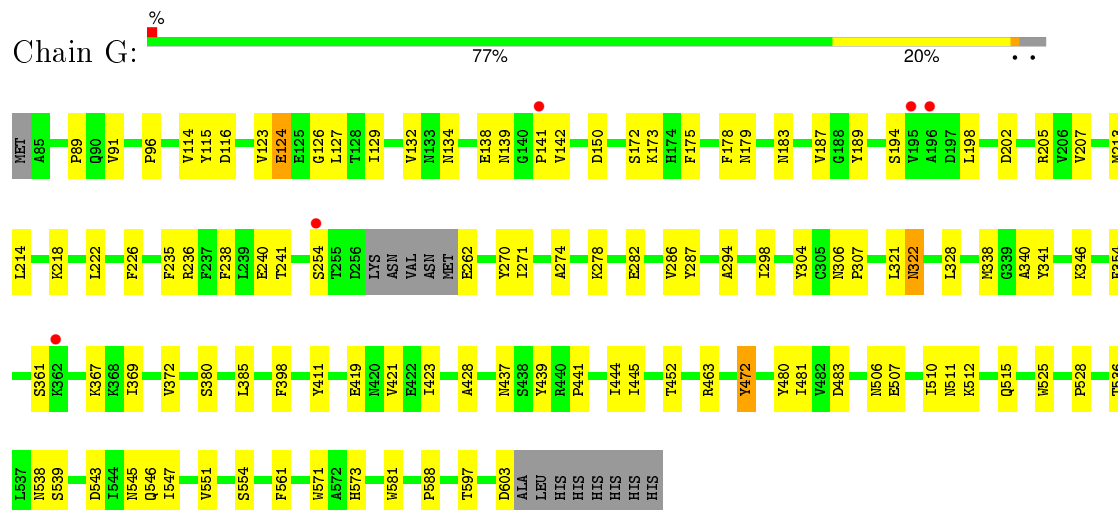
#### • Molecule 1: M17 leucyl aminopeptidase



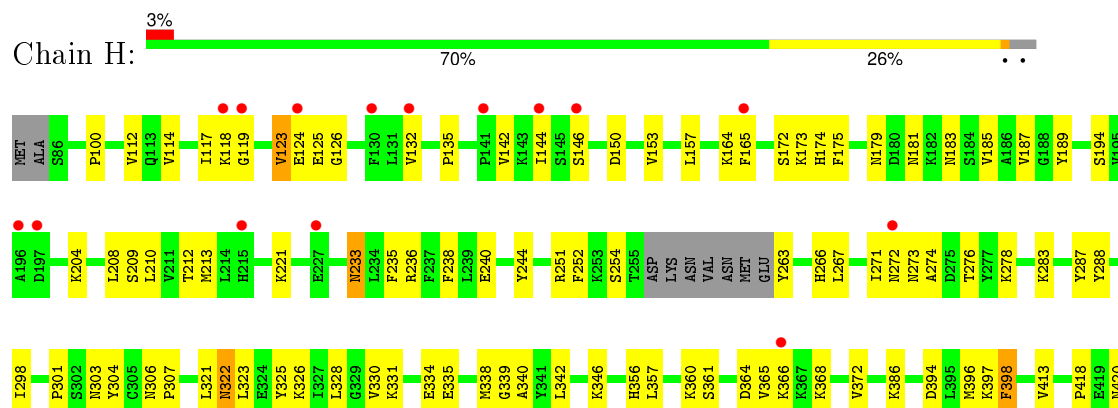
- Molecule 1: M17 leucyl aminopeptidase

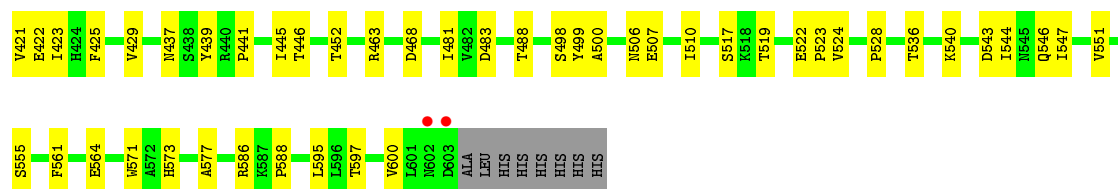


- Molecule 1: M17 leucyl aminopeptidase

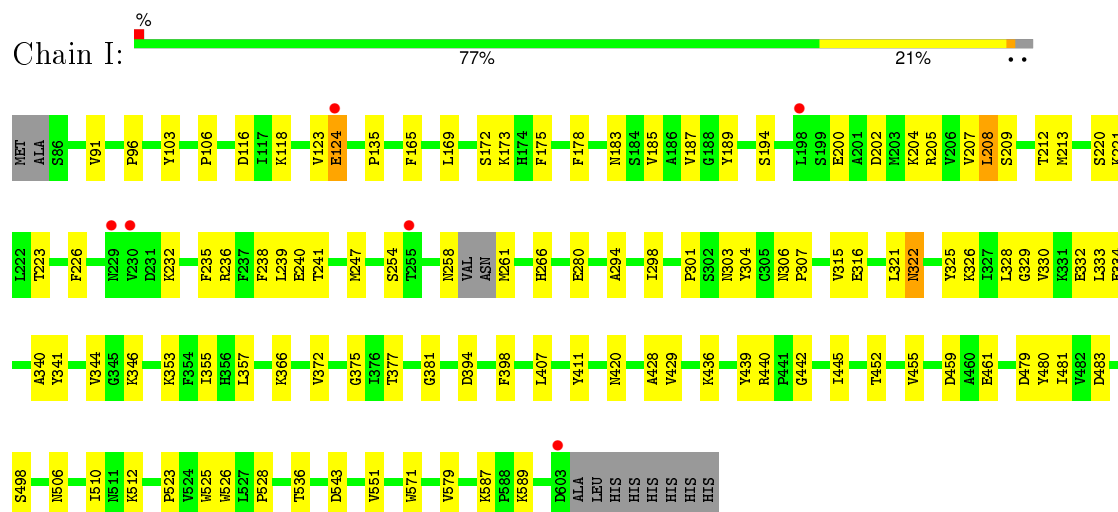


- Molecule 1: M17 leucyl aminopeptidase

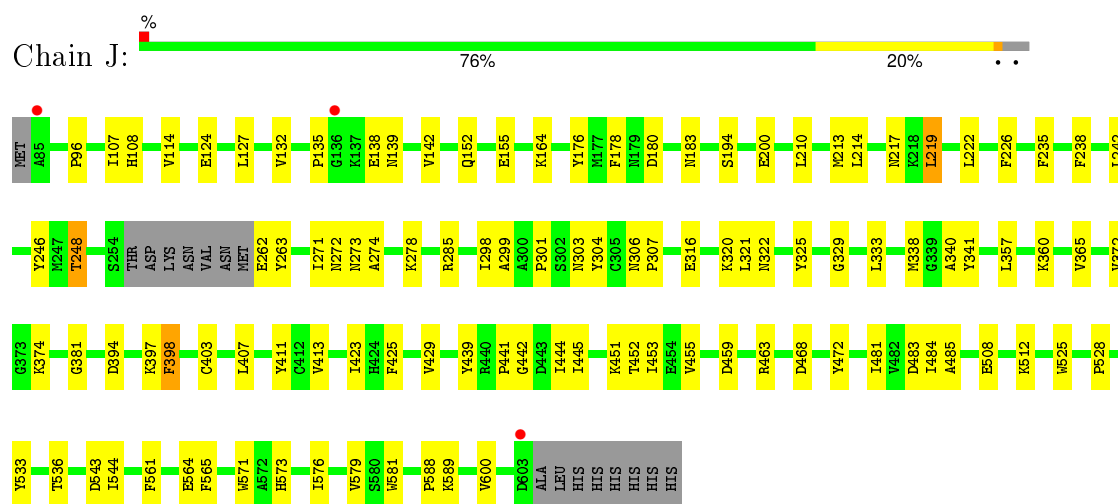




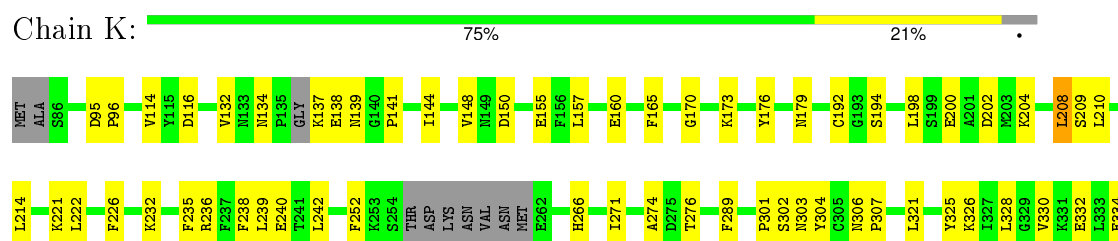
• Molecule 1: M17 leucyl aminopeptidase

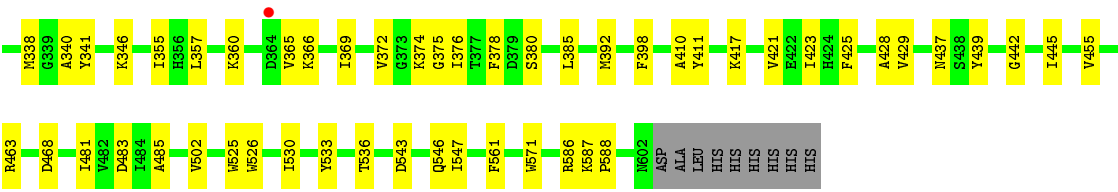


• Molecule 1: M17 leucyl aminopeptidase

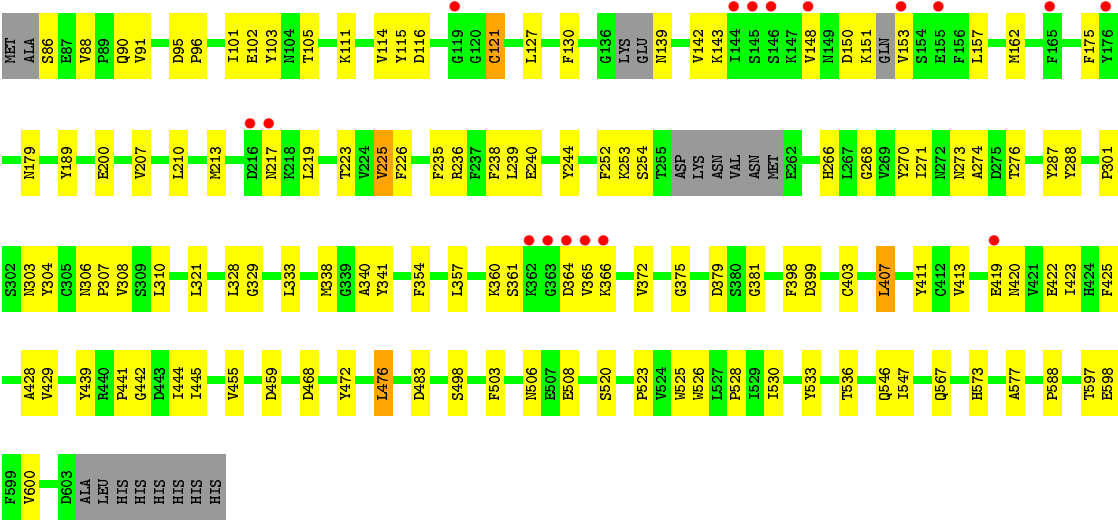


• Molecule 1: M17 leucyl aminopeptidase





• Molecule 1: M17 leucyl aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.90Å 175.93Å 231.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.60 46.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.1 (46.70-2.60) 77.7 (46.70-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.211 , 0.269 0.215 , 0.270	Depositor DCC
$R_{free}$ test set	9435 reflections (5.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.4	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	7 of 189505 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	49091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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 45.00 % 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 1.4075e-04. 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: ZN, CO3, 1PE, DMS, SO4, R5T

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	0.22	0/4025	0.38	0/5459
1	B	0.23	0/3946	0.41	0/5361
1	C	0.21	0/4027	0.39	0/5465
1	D	0.22	0/3995	0.39	0/5420
1	E	0.23	0/3989	0.39	0/5412
1	F	0.21	0/3860	0.39	0/5254
1	G	0.21	0/4021	0.38	0/5453
1	H	0.21	0/3955	0.39	0/5373
1	I	0.21	0/3985	0.39	0/5410
1	J	0.22	0/3987	0.38	0/5409
1	K	0.21	0/3955	0.38	0/5368
1	L	0.22	0/3897	0.41	0/5298
All	All	0.22	0/47642	0.39	0/64682

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3945	0	3876	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3869	0	3760	106	0
1	C	3949	0	3873	100	1
1	D	3918	0	3847	107	0
1	E	3913	0	3830	85	2
1	F	3785	0	3598	102	0
1	G	3944	0	3875	85	0
1	H	3878	0	3776	112	0
1	I	3908	0	3800	84	1
1	J	3910	0	3840	84	0
1	K	3879	0	3795	78	1
1	L	3823	0	3664	98	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	20	0	0	0	0
4	B	10	0	0	2	0
4	C	15	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	1	0
4	G	10	0	0	0	0
4	H	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	10	0	0	0	0
4	K	15	0	0	1	0
4	L	15	0	0	1	0
5	A	24	0	20	0	0
5	B	24	0	19	0	0
5	C	24	0	20	0	0
5	D	24	0	19	1	0
5	E	24	0	19	0	0
5	F	24	0	19	1	0
5	G	24	0	19	1	0
5	H	24	0	19	1	0
5	I	24	0	20	0	0
5	J	24	0	19	0	0
5	K	24	0	19	0	0
5	L	21	0	10	1	0
6	A	9	0	10	2	0
6	B	21	0	26	6	0
6	C	29	0	32	13	0
6	D	9	0	10	1	0
6	E	33	0	36	10	0
6	F	16	0	16	2	0
6	G	17	0	16	2	0
6	I	21	0	22	3	0
6	J	21	0	22	3	0
6	K	13	0	14	1	0
6	L	8	0	8	0	0
7	G	4	6	6	2	0
8	A	160	0	0	5	0
8	B	130	0	0	1	0
8	C	169	0	0	1	0
8	D	151	0	0	5	0
8	E	132	0	0	4	0
8	F	94	0	0	1	0
8	G	149	0	0	9	1
8	H	117	0	0	5	0
8	I	164	0	0	7	0
8	J	154	0	0	3	0
8	K	157	0	0	3	0
8	L	114	0	0	5	0
All	All	49085	6	45974	1047	3

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 11.

The worst 5 of 1047 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:L:157:LEU:HA	1:L:162:MET:HE3	1.42	0.99
1:G:545:ASN:ND2	8:G:1180:HOH:O	1.98	0.97
1:I:366:LYS:HE2	1:I:420:ASN:HB3	1.47	0.94
1:F:174:HIS:HB3	1:F:213:MET:HE1	1.48	0.94
1:L:360:LYS:HD2	1:L:422:GLU:HG3	1.52	0.90

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:479:ASP:OD1	1:K:366:LYS:NZ[4_456]	2.18	0.02
1:C:479:ASP:OD1	1:E:366:LYS:NZ[4_455]	2.19	0.01
1:E:124:GLU:OE1	8:G:1223:HOH:O[3_645]	2.19	0.01

## 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	511/528 (97%)	495 (97%)	12 (2%)	4 (1%)	24	46
1	B	507/528 (96%)	487 (96%)	18 (4%)	2 (0%)	39	65
1	C	516/528 (98%)	500 (97%)	13 (2%)	3 (1%)	30	56
1	D	509/528 (96%)	493 (97%)	13 (3%)	3 (1%)	30	56
1	E	507/528 (96%)	492 (97%)	13 (3%)	2 (0%)	39	65
1	F	500/528 (95%)	483 (97%)	14 (3%)	3 (1%)	30	56
1	G	510/528 (97%)	494 (97%)	13 (2%)	3 (1%)	30	56
1	H	507/528 (96%)	488 (96%)	16 (3%)	3 (1%)	30	56
1	I	512/528 (97%)	497 (97%)	13 (2%)	2 (0%)	39	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	508/528 (96%)	494 (97%)	12 (2%)	2 (0%)	39	65
1	K	503/528 (95%)	488 (97%)	14 (3%)	1 (0%)	52	77
1	L	501/528 (95%)	488 (97%)	13 (3%)	0	100	100
All	All	6091/6336 (96%)	5899 (97%)	164 (3%)	28 (0%)	34	60

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ASN
1	B	124	GLU
1	D	254	SER
1	D	322	ASN
1	E	139	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	421/455 (92%)	417 (99%)	4 (1%)	82	94
1	B	405/455 (89%)	394 (97%)	11 (3%)	52	79
1	C	418/455 (92%)	407 (97%)	11 (3%)	54	80
1	D	414/455 (91%)	405 (98%)	9 (2%)	60	83
1	E	414/455 (91%)	406 (98%)	8 (2%)	65	86
1	F	383/455 (84%)	375 (98%)	8 (2%)	61	85
1	G	421/455 (92%)	418 (99%)	3 (1%)	88	96
1	H	408/455 (90%)	400 (98%)	8 (2%)	63	85
1	I	408/455 (90%)	402 (98%)	6 (2%)	72	90
1	J	413/455 (91%)	405 (98%)	8 (2%)	65	86
1	K	410/455 (90%)	404 (98%)	6 (2%)	72	90
1	L	394/455 (87%)	384 (98%)	10 (2%)	55	81
All	All	4909/5460 (90%)	4817 (98%)	92 (2%)	65	86

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	439	TYR
1	G	398	PHE
1	L	225	VAL
1	E	472	TYR
1	F	398	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	174	HIS
1	L	266	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 24 are monoatomic - leaving 68 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	$\# Z  > 2$
3	CO3	A	1002	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	1004	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	A	1005	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	1006	-	4,4,4	0.24	0	6,6,6	0.08	0
5	R5T	A	1007	2	23,25,25	2.33	5 (21%)	32,35,35	2.62	7 (21%)
6	1PE	A	1008	-	8,8,15	0.48	0	7,7,14	0.26	0
4	SO4	A	1009	-	4,4,4	0.24	0	6,6,6	0.08	0
3	CO3	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	B	1004	-	4,4,4	0.21	0	6,6,6	0.07	0
4	SO4	B	1005	-	4,4,4	0.23	0	6,6,6	0.09	0
5	R5T	B	1006	2	23,25,25	2.32	5 (21%)	32,35,35	2.68	8 (25%)
6	1PE	B	1007	-	13,13,15	0.46	0	12,12,14	0.40	0
6	1PE	B	1008	-	6,6,15	0.43	0	5,5,14	0.32	0
3	CO3	C	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	C	1004	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	C	1005	-	4,4,4	0.26	0	6,6,6	0.06	0
4	SO4	C	1006	-	4,4,4	0.23	0	6,6,6	0.09	0
5	R5T	C	1007	2	23,25,25	2.36	5 (21%)	32,35,35	2.67	6 (18%)
6	1PE	C	1008	-	11,11,15	0.47	0	10,10,14	0.27	0
6	1PE	C	1009	-	8,8,15	0.48	0	7,7,14	0.29	0
6	1PE	C	1010	-	7,7,15	0.43	0	6,6,14	0.28	0
3	CO3	D	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
5	R5T	D	1004	2	23,25,25	2.26	5 (21%)	32,35,35	2.73	10 (31%)
6	1PE	D	1005	-	8,8,15	0.49	0	7,7,14	0.27	0
3	CO3	E	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
5	R5T	E	1004	2	23,25,25	2.33	5 (21%)	32,35,35	2.62	9 (28%)
6	1PE	E	1005	-	11,11,15	0.46	0	10,10,14	0.27	0
6	1PE	E	1006	-	12,12,15	0.48	0	11,11,14	0.34	0
6	1PE	E	1007	-	7,7,15	0.48	0	6,6,14	0.44	0
4	SO4	E	1008	-	4,4,4	0.23	0	6,6,6	0.08	0
3	CO3	F	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	F	1004	-	4,4,4	0.22	0	6,6,6	0.10	0
5	R5T	F	1005	2	23,25,25	2.33	5 (21%)	32,35,35	2.50	8 (25%)
6	1PE	F	1006	-	7,7,15	0.49	0	6,6,14	0.33	0
6	1PE	F	1007	-	7,7,15	0.51	0	6,6,14	0.25	0
4	SO4	F	1008	-	4,4,4	0.23	0	6,6,6	0.08	0
3	CO3	G	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	G	1004	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	G	1005	-	4,4,4	0.24	0	6,6,6	0.09	0
5	R5T	G	1006	2	23,25,25	2.29	5 (21%)	32,35,35	2.65	7 (21%)
6	1PE	G	1007	-	6,6,15	0.50	0	5,5,14	0.27	0
6	1PE	G	1008	-	9,9,15	0.46	0	8,8,14	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	DMS	G	1009	-	3,3,3	0.64	0	3,3,3	0.42	0
3	CO3	H	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	H	1004	-	4,4,4	0.22	0	6,6,6	0.08	0
5	R5T	H	1005	2	23,25,25	2.24	6 (26%)	32,35,35	2.58	9 (28%)
3	CO3	I	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
5	R5T	I	1004	2	23,25,25	2.28	5 (21%)	32,35,35	2.63	7 (21%)
6	1PE	I	1005	-	12,12,15	0.48	0	11,11,14	0.26	0
6	1PE	I	1006	-	7,7,15	0.44	0	6,6,14	0.28	0
3	CO3	J	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
5	R5T	J	1004	2	23,25,25	2.28	5 (21%)	32,35,35	2.71	8 (25%)
6	1PE	J	1005	-	8,8,15	0.48	0	7,7,14	0.31	0
6	1PE	J	1006	-	11,11,15	0.48	0	10,10,14	0.25	0
4	SO4	J	1007	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	J	1008	-	4,4,4	0.23	0	6,6,6	0.08	0
3	CO3	K	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	K	1004	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	K	1005	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	K	1006	-	4,4,4	0.23	0	6,6,6	0.08	0
5	R5T	K	1007	2	23,25,25	2.30	4 (17%)	32,35,35	2.78	8 (25%)
6	1PE	K	1008	-	12,12,15	0.47	0	11,11,14	0.26	0
3	CO3	L	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	L	1004	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	L	1005	-	4,4,4	0.23	0	6,6,6	0.08	0
5	R5T	L	1006	2	20,22,25	2.43	5 (25%)	26,29,35	2.96	8 (30%)
6	1PE	L	1007	-	7,7,15	0.53	0	6,6,14	0.23	0
4	SO4	L	1008	-	4,4,4	0.23	0	6,6,6	0.08	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
3	CO3	A	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
5	R5T	A	1007	2	-	0/23/23/23	0/2/2/2
6	1PE	A	1008	-	-	0/6/6/13	0/0/0/0
4	SO4	A	1009	-	-	0/0/0/0	0/0/0/0
3	CO3	B	1002	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
5	R5T	B	1006	2	-	0/23/23/23	0/2/2/2
6	1PE	B	1007	-	-	0/11/11/13	0/0/0/0
6	1PE	B	1008	-	-	0/4/4/13	0/0/0/0
3	CO3	C	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1006	-	-	0/0/0/0	0/0/0/0
5	R5T	C	1007	2	-	0/23/23/23	0/2/2/2
6	1PE	C	1008	-	-	0/9/9/13	0/0/0/0
6	1PE	C	1009	-	-	0/6/6/13	0/0/0/0
6	1PE	C	1010	-	-	0/5/5/13	0/0/0/0
3	CO3	D	1002	-	-	0/0/0/0	0/0/0/0
5	R5T	D	1004	2	-	0/23/23/23	0/2/2/2
6	1PE	D	1005	-	-	0/6/6/13	0/0/0/0
3	CO3	E	1002	-	-	0/0/0/0	0/0/0/0
5	R5T	E	1004	2	-	0/23/23/23	0/2/2/2
6	1PE	E	1005	-	-	0/9/9/13	0/0/0/0
6	1PE	E	1006	-	-	0/10/10/13	0/0/0/0
6	1PE	E	1007	-	-	0/5/5/13	0/0/0/0
4	SO4	E	1008	-	-	0/0/0/0	0/0/0/0
3	CO3	F	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1004	-	-	0/0/0/0	0/0/0/0
5	R5T	F	1005	2	-	0/23/23/23	0/2/2/2
6	1PE	F	1006	-	-	0/5/5/13	0/0/0/0
6	1PE	F	1007	-	-	0/5/5/13	0/0/0/0
4	SO4	F	1008	-	-	0/0/0/0	0/0/0/0
3	CO3	G	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	G	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	G	1005	-	-	0/0/0/0	0/0/0/0
5	R5T	G	1006	2	-	0/23/23/23	0/2/2/2
6	1PE	G	1007	-	-	0/4/4/13	0/0/0/0
6	1PE	G	1008	-	-	0/7/7/13	0/0/0/0
7	DMS	G	1009	-	-	0/0/0/0	0/0/0/0
3	CO3	H	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	H	1004	-	-	0/0/0/0	0/0/0/0
5	R5T	H	1005	2	-	0/23/23/23	0/2/2/2
3	CO3	I	1002	-	-	0/0/0/0	0/0/0/0
5	R5T	I	1004	2	-	0/23/23/23	0/2/2/2
6	1PE	I	1005	-	-	0/10/10/13	0/0/0/0
6	1PE	I	1006	-	-	0/5/5/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CO3	J	1002	-	-	0/0/0/0	0/0/0/0
5	R5T	J	1004	2	-	0/23/23/23	0/2/2/2
6	1PE	J	1005	-	-	0/6/6/13	0/0/0/0
6	1PE	J	1006	-	-	0/9/9/13	0/0/0/0
4	SO4	J	1007	-	-	0/0/0/0	0/0/0/0
4	SO4	J	1008	-	-	0/0/0/0	0/0/0/0
3	CO3	K	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	K	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	K	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	K	1006	-	-	0/0/0/0	0/0/0/0
5	R5T	K	1007	2	-	0/23/23/23	0/2/2/2
6	1PE	K	1008	-	-	0/10/10/13	0/0/0/0
3	CO3	L	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	L	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	L	1005	-	-	0/0/0/0	0/0/0/0
5	R5T	L	1006	2	-	0/20/20/23	0/2/2/2
6	1PE	L	1007	-	-	0/5/5/13	0/0/0/0
4	SO4	L	1008	-	-	0/0/0/0	0/0/0/0

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1004	R5T	CAT-CA	-7.91	1.39	1.52
5	F	1005	R5T	CAT-CA	-7.90	1.39	1.52
5	K	1007	R5T	CAT-CA	-7.78	1.39	1.52
5	J	1004	R5T	CAT-CA	-7.59	1.39	1.52
5	L	1006	R5T	CAT-CA	-7.57	1.39	1.52

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1007	R5T	CAX-OAQ-CAR	-6.19	111.06	121.05
5	L	1006	R5T	CAX-OAQ-CAR	-5.43	108.92	115.63
5	J	1004	R5T	CAX-OAQ-CAR	-4.68	113.49	121.05
5	H	1005	R5T	CAX-OAQ-CAR	-4.35	114.03	121.05
5	D	1004	R5T	OAD-CAR-N	-4.19	117.54	124.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	CO3	1	0
6	A	1008	1PE	2	0
4	B	1004	SO4	2	0
6	B	1007	1PE	6	0
6	C	1008	1PE	2	0
6	C	1010	1PE	11	0
5	D	1004	R5T	1	0
6	D	1005	1PE	1	0
6	E	1005	1PE	3	0
6	E	1006	1PE	8	0
4	F	1004	SO4	1	0
5	F	1005	R5T	1	0
6	F	1006	1PE	2	0
5	G	1006	R5T	1	0
6	G	1008	1PE	2	0
7	G	1009	DMS	2	0
4	H	1004	SO4	1	0
5	H	1005	R5T	1	0
6	I	1005	1PE	3	0
6	J	1006	1PE	3	0
4	K	1005	SO4	1	0
6	K	1008	1PE	1	0
5	L	1006	R5T	1	0
4	L	1008	SO4	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	514/528 (97%)	-0.19	7 (1%) 78 74	27, 41, 65, 95	0
1	B	511/528 (96%)	0.19	31 (6%) 25 18	29, 48, 80, 113	1 (0%)
1	C	518/528 (98%)	-0.11	10 (1%) 70 64	27, 43, 72, 111	0
1	D	513/528 (97%)	-0.22	2 (0%) 93 91	28, 40, 63, 100	0
1	E	513/528 (97%)	-0.19	2 (0%) 93 91	31, 43, 64, 97	0
1	F	508/528 (96%)	0.07	21 (4%) 41 33	30, 48, 82, 101	0
1	G	514/528 (97%)	-0.19	5 (0%) 84 81	30, 42, 68, 103	0
1	H	511/528 (96%)	0.07	17 (3%) 50 43	29, 46, 79, 102	1 (0%)
1	I	516/528 (97%)	-0.17	6 (1%) 81 77	27, 42, 72, 127	0
1	J	512/528 (96%)	-0.16	3 (0%) 90 88	31, 43, 66, 95	0
1	K	509/528 (96%)	-0.20	1 (0%) 95 95	32, 44, 63, 89	0
1	L	509/528 (96%)	0.02	17 (3%) 50 43	34, 49, 79, 144	0
All	All	6148/6336 (97%)	-0.09	122 (1%) 68 63	27, 44, 73, 144	2 (0%)

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	363	GLY	9.6
1	F	157	LEU	4.9
1	H	124	GLU	4.8
1	J	85	ALA	4.7
1	E	363	GLY	4.6

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

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
4	SO4	L	1008	5/5	0.88	0.40	14.60	104,105,109,109	0
4	SO4	L	1005	5/5	0.91	0.21	5.50	69,72,76,79	0
4	SO4	G	1005	5/5	0.95	0.34	4.77	76,82,82,88	0
6	1PE	C	1010	8/16	0.92	0.27	4.34	40,47,58,60	0
3	CO3	F	1002	4/4	0.95	0.20	3.84	35,45,48,51	0
3	CO3	D	1002	4/4	0.93	0.19	3.69	44,55,58,60	0
4	SO4	C	1005	5/5	0.94	0.29	3.67	84,85,89,105	0
5	R5T	I	1004	24/24	0.90	0.21	3.47	31,47,65,73	0
4	SO4	G	1004	5/5	0.92	0.20	3.35	83,90,90,95	0
6	1PE	K	1008	13/16	0.92	0.20	3.31	34,52,64,67	0
6	1PE	C	1009	9/16	0.85	0.23	2.97	48,62,78,79	0
6	1PE	E	1007	8/16	0.82	0.22	2.93	47,64,68,71	0
6	1PE	G	1007	7/16	0.89	0.22	2.79	56,58,68,72	0
6	1PE	I	1006	8/16	0.92	0.18	2.64	47,50,51,58	0
4	SO4	J	1007	5/5	0.84	0.33	2.52	126,131,132,133	0
3	CO3	C	1002	4/4	0.91	0.21	2.49	42,46,48,51	0
7	DMS	G	1009	4/4	0.94	0.25	2.46	39,53,74,76	0
5	R5T	F	1005	24/24	0.90	0.22	2.43	41,60,74,85	0
5	R5T	L	1006	21/24	0.90	0.19	2.39	34,49,58,61	0
3	CO3	G	1002	4/4	0.91	0.20	2.38	30,34,44,54	0
3	CO3	H	1002	4/4	0.99	0.20	2.32	28,39,44,53	0
4	SO4	A	1009	5/5	0.94	0.19	2.29	79,83,85,89	0
4	SO4	J	1008	5/5	0.86	0.28	2.22	118,119,124,127	0
3	CO3	E	1002	4/4	0.97	0.20	1.55	30,33,36,39	0
6	1PE	A	1008	9/16	0.95	0.18	1.51	41,45,51,53	0
5	R5T	K	1007	24/24	0.93	0.20	1.50	32,49,58,73	0
6	1PE	E	1005	12/16	0.89	0.18	1.45	42,60,68,70	0
5	R5T	A	1007	24/24	0.93	0.20	1.34	30,49,63,64	0
5	R5T	D	1004	24/24	0.93	0.19	1.21	26,44,55,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	R5T	B	1006	24/24	0.93	0.19	1.16	28,52,65,66	0
4	SO4	B	1005	5/5	0.91	0.16	1.04	85,86,92,93	0
4	SO4	A	1004	5/5	0.91	0.23	0.99	65,78,82,83	0
5	R5T	J	1004	24/24	0.94	0.18	0.98	33,52,85,89	0
3	CO3	A	1002	4/4	0.93	0.15	0.95	27,37,37,40	0
3	CO3	I	1002	4/4	0.96	0.16	0.91	26,31,31,45	0
3	CO3	J	1002	4/4	0.96	0.17	0.83	30,36,40,40	0
6	1PE	F	1007	8/16	0.94	0.19	0.78	32,44,49,56	0
6	1PE	D	1005	9/16	0.94	0.17	0.67	49,50,54,58	0
5	R5T	C	1007	24/24	0.95	0.17	0.63	31,47,55,57	0
5	R5T	G	1006	24/24	0.94	0.17	0.44	32,48,59,64	0
4	SO4	C	1006	5/5	0.81	0.19	0.29	115,118,121,124	0
5	R5T	H	1005	24/24	0.94	0.16	0.29	29,49,63,79	0
5	R5T	E	1004	24/24	0.95	0.17	0.11	31,62,70,75	0
6	1PE	J	1005	9/16	0.96	0.15	-0.27	36,39,52,57	0
4	SO4	K	1005	5/5	0.95	0.14	-0.28	70,72,77,89	0
6	1PE	B	1008	7/16	0.95	0.17	-0.36	42,49,51,57	0
3	CO3	B	1002	4/4	0.97	0.15	-0.39	28,28,29,34	0
6	1PE	G	1008	10/16	0.96	0.15	-0.40	39,48,61,65	0
4	SO4	K	1004	5/5	0.99	0.16	-0.54	34,34,44,44	0
3	CO3	K	1002	4/4	0.96	0.15	-0.65	33,48,58,60	0
4	SO4	B	1004	5/5	0.98	0.13	-0.93	31,32,36,39	0
6	1PE	F	1006	8/16	0.92	0.15	-0.96	40,50,55,59	0
4	SO4	H	1004	5/5	0.98	0.13	-0.98	26,26,40,49	0
3	CO3	L	1002	4/4	0.99	0.13	-1.13	33,37,39,47	0
4	SO4	A	1006	5/5	0.94	0.12	-1.42	71,74,79,83	0
6	1PE	L	1007	8/16	0.96	0.13	-1.77	38,58,60,62	0
2	ZN	J	1001	1/1	0.97	0.07	-2.92	52,52,52,52	0
2	ZN	F	1001	1/1	0.99	0.09	-3.11	48,48,48,48	0
2	ZN	K	1001	1/1	0.98	0.07	-3.42	37,37,37,37	0
2	ZN	L	1003	1/1	0.99	0.08	-3.50	52,52,52,52	0
2	ZN	B	1003	1/1	0.93	0.05	-3.61	41,41,41,41	0
2	ZN	J	1003	1/1	0.99	0.04	-3.66	47,47,47,47	0
4	SO4	F	1004	5/5	0.99	0.12	-3.70	29,30,37,43	0
2	ZN	A	1001	1/1	1.00	0.07	-3.74	40,40,40,40	0
2	ZN	C	1001	1/1	0.97	0.07	-3.89	42,42,42,42	0
2	ZN	C	1003	1/1	0.98	0.08	-3.94	43,43,43,43	0
2	ZN	E	1001	1/1	0.99	0.09	-3.96	40,40,40,40	0
2	ZN	K	1003	1/1	0.99	0.07	-3.97	48,48,48,48	0
2	ZN	A	1003	1/1	0.98	0.08	-4.21	56,56,56,56	0
2	ZN	G	1001	1/1	0.98	0.07	-4.22	42,42,42,42	0
2	ZN	B	1001	1/1	0.97	0.06	-4.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	F	1003	1/1	0.99	0.07	-4.36	50,50,50,50	0
2	ZN	E	1003	1/1	0.99	0.07	-4.42	48,48,48,48	0
2	ZN	D	1003	1/1	0.97	0.06	-4.49	49,49,49,49	0
2	ZN	I	1003	1/1	0.99	0.07	-5.12	46,46,46,46	0
2	ZN	G	1003	1/1	0.98	0.06	-5.28	44,44,44,44	0
2	ZN	I	1001	1/1	0.99	0.09	-5.48	45,45,45,45	0
2	ZN	L	1001	1/1	0.99	0.06	-6.47	42,42,42,42	0
2	ZN	D	1001	1/1	0.98	0.06	-6.49	43,43,43,43	0
2	ZN	H	1001	1/1	0.99	0.03	-6.56	44,44,44,44	0
2	ZN	H	1003	1/1	0.98	0.03	-8.59	44,44,44,44	0
6	1PE	C	1008	12/16	0.89	0.20	-	47,55,73,75	0
6	1PE	E	1006	13/16	0.90	0.15	-	43,52,59,60	0
4	SO4	A	1005	5/5	0.97	0.15	-	60,66,68,83	0
4	SO4	K	1006	5/5	0.96	0.17	-	62,64,69,77	0
4	SO4	E	1008	5/5	0.93	0.20	-	86,87,90,91	0
6	1PE	B	1007	14/16	0.80	0.26	-	54,69,82,82	0
4	SO4	L	1004	5/5	0.96	0.14	-	86,86,91,92	0
6	1PE	J	1006	12/16	0.82	0.25	-	49,73,83,87	0
4	SO4	C	1004	5/5	0.95	0.22	-	69,77,79,83	0
6	1PE	I	1005	13/16	0.91	0.22	-	51,59,62,64	0
4	SO4	F	1008	5/5	0.95	0.24	-	103,105,107,110	0

## 6.5 Other polymers

There are no such residues in this entry.