



wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 12:45 AM GMT

PDB ID : 3KR4
Title : Structure of a protease 3
Authors : McGowan, S.; Whisstock, J.C.
Deposited on : 2009-11-17
Resolution : 2.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

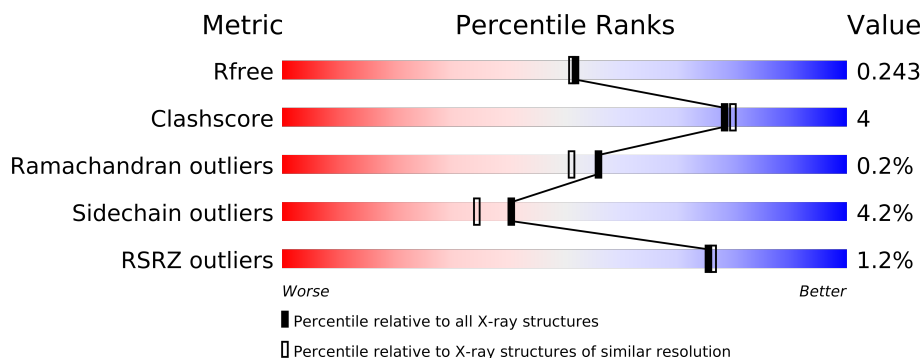
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	528	
1	B	528	
1	C	528	
1	D	528	
1	E	528	
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 that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CO3	A	1002	-	X
4	BES	A	1003	-	X
4	BES	B	1003	-	X
4	BES	D	1003	-	X
4	BES	E	1003	-	X
4	BES	F	1003	-	X
4	BES	G	1003	-	X
4	BES	H	1003	-	X
4	BES	J	1003	-	X
4	BES	K	1003	-	X
4	BES	L	1003	-	X
5	MG	A	1004	-	X
5	MG	B	1004	-	X
5	MG	C	1004	-	X
5	MG	D	1004	-	X
5	MG	E	1004	-	X
5	MG	F	1004	-	X
5	MG	G	1004	-	X
5	MG	H	1004	-	X
5	MG	I	1004	-	X
5	MG	J	1004	-	X
5	MG	K	1004	-	X
5	MG	L	1004	-	X
6	SO4	A	24	-	X
6	SO4	E	22	-	X
6	SO4	F	21	-	X
6	SO4	G	23	-	X
6	SO4	J	20	-	X
6	SO4	L	25	-	X
7	1PE	A	19	-	X
7	1PE	A	20	-	X
7	1PE	B	61	-	X
7	1PE	B	62	-	X
7	1PE	D	44	-	X
7	1PE	D	67	-	X
7	1PE	E	43	-	X
7	1PE	F	33	-	X
7	1PE	G	12	-	X
7	1PE	G	30	-	X
7	1PE	G	48	-	X
7	1PE	G	58	-	X
7	1PE	H	65	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	1PE	J	45	-	X
7	1PE	K	42	-	X
7	1PE	K	50	-	X
7	1PE	L	56	-	X
7	1PE	L	612	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 53016 atoms, of which 0 are hydrogen and 0 are deuterium.

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	518	Total	C	N	O	S	3	1	0
			3983	2558	639	766	20			
1	B	518	Total	C	N	O	S	0	0	0
			3936	2531	637	748	20			
1	C	518	Total	C	N	O	S	0	1	0
			3955	2545	638	753	19			
1	D	516	Total	C	N	O	S	0	0	0
			3946	2541	638	747	20			
1	E	510	Total	C	N	O	S	0	0	0
			3896	2509	626	743	18			
1	F	510	Total	C	N	O	S	0	0	0
			3873	2492	623	739	19			
1	G	516	Total	C	N	O	S	0	0	0
			3996	2564	650	762	20			
1	H	509	Total	C	N	O	S	0	1	0
			3943	2534	641	749	19			
1	I	518	Total	C	N	O	S	0	1	0
			4008	2570	652	767	19			
1	J	513	Total	C	N	O	S	0	1	0
			3963	2545	641	757	20			
1	K	509	Total	C	N	O	S	0	1	0
			3935	2528	638	750	19			
1	L	513	Total	C	N	O	S	0	1	0
			3944	2532	635	758	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	ENGINEERED	UNP Q8IL11
A	515	GLN	ASN	ENGINEERED	UNP Q8IL11
A	546	GLN	ASN	ENGINEERED	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	UNP Q8IL11
B	515	GLN	ASN	ENGINEERED	UNP Q8IL11
B	546	GLN	ASN	ENGINEERED	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	UNP Q8IL11
C	515	GLN	ASN	ENGINEERED	UNP Q8IL11
C	546	GLN	ASN	ENGINEERED	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	UNP Q8IL11
D	515	GLN	ASN	ENGINEERED	UNP Q8IL11
D	546	GLN	ASN	ENGINEERED	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	UNP Q8IL11
E	515	GLN	ASN	ENGINEERED	UNP Q8IL11
E	546	GLN	ASN	ENGINEERED	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	UNP Q8IL11
F	515	GLN	ASN	ENGINEERED	UNP Q8IL11

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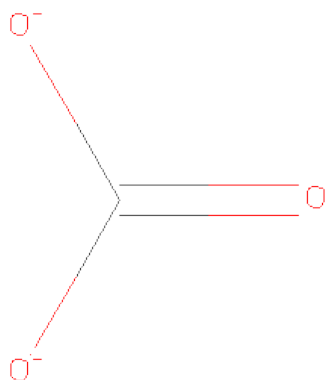
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	ENGINEERED	UNP Q8IL11
F	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	611	HIS	-	EXPRESSION TAG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

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

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

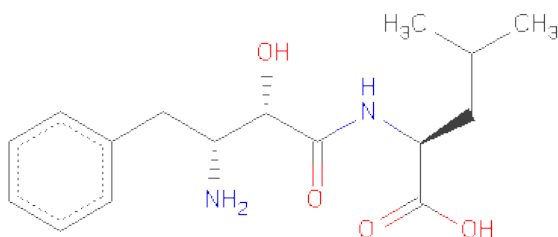
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	K	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOICACID (three-letter code: BES) (formula: C₁₆H₂₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	16	2	4		
4	B	1	Total	C	N	O	0	0
			22	16	2	4		
4	C	1	Total	C	N	O	0	0
			22	16	2	4		
4	D	1	Total	C	N	O	0	0
			22	16	2	4		
4	E	1	Total	C	N	O	0	0
			22	16	2	4		
4	F	1	Total	C	N	O	0	0
			22	16	2	4		
4	G	1	Total	C	N	O	0	0
			22	16	2	4		
4	H	1	Total	C	N	O	0	0
			22	16	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total	C	N	O	0	0
			22	16	2	4		
4	J	1	Total	C	N	O	0	0
			22	16	2	4		
4	K	1	Total	C	N	O	0	0
			22	16	2	4		
4	L	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

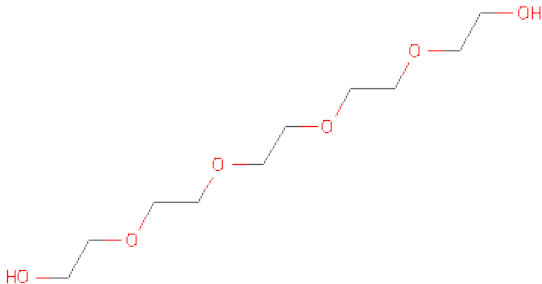
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			8	5	3		
7	F	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			9	6	3		
7	G	1	Total	C	O	0	0
			7	4	3		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			15	10	5		
7	H	1	Total	C	O	0	0
			10	7	3		
7	H	1	Total	C	O	0	0
			10	7	3		
7	I	1	Total	C	O	0	0
			15	10	5		
7	I	1	Total	C	O	0	0
			11	8	3		
7	I	1	Total	C	O	0	0
			7	5	2		
7	J	1	Total	C	O	0	0
			11	7	4		
7	J	1	Total	C	O	0	0
			10	6	4		
7	J	1	Total	C	O	0	0
			10	7	3		
7	K	1	Total	C	O	0	0
			12	8	4		
7	K	1	Total	C	O	0	0
			12	8	4		
7	K	1	Total	C	O	0	0
			11	7	4		
7	K	1	Total	C	O	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			10	6	4		
7	L	1	Total	C	O	0	0
			12	8	4		
7	L	1	Total	C	O	0	0
			11	7	4		

- Molecule 8 is water.

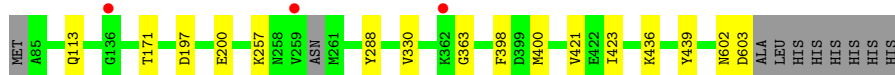
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	423	Total	O	0	0
			423	423		
8	B	361	Total	O	0	0
			361	361		
8	C	427	Total	O	0	0
			427	427		
8	D	411	Total	O	0	0
			411	411		
8	E	442	Total	O	0	0
			442	442		
8	F	373	Total	O	0	0
			373	373		
8	G	421	Total	O	0	0
			421	421		
8	H	389	Total	O	0	0
			389	389		
8	I	414	Total	O	0	0
			414	414		
8	J	403	Total	O	0	0
			403	403		
8	K	438	Total	O	0	0
			438	438		
8	L	356	Total	O	0	0
			356	356		

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 ($RSRZ > 2$). 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.

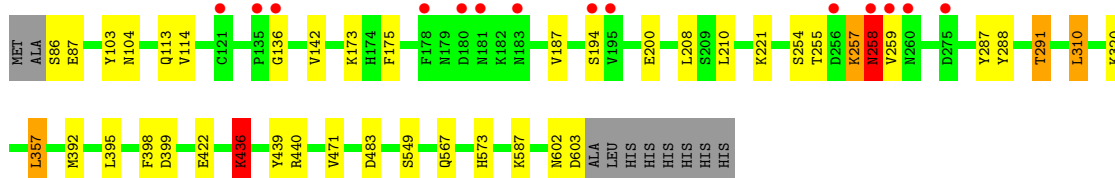
- Molecule 1: M17 leucyl aminopeptidase

Chain A: 



- Molecule 1: M17 leucyl aminopeptidase

Chain B: 



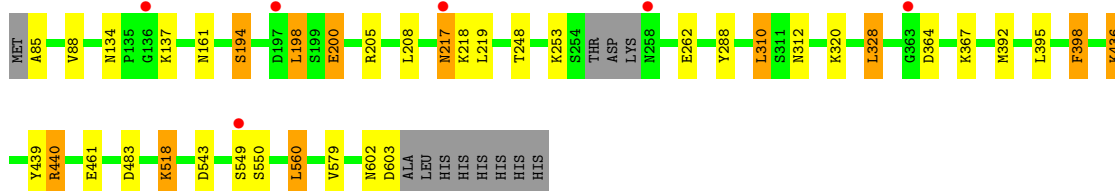
- Molecule 1: M17 leucyl aminopeptidase

Chain C: 



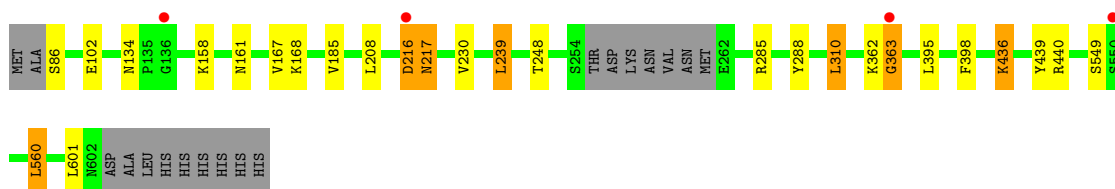
- Molecule 1: M17 leucyl aminopeptidase

Chain D: 



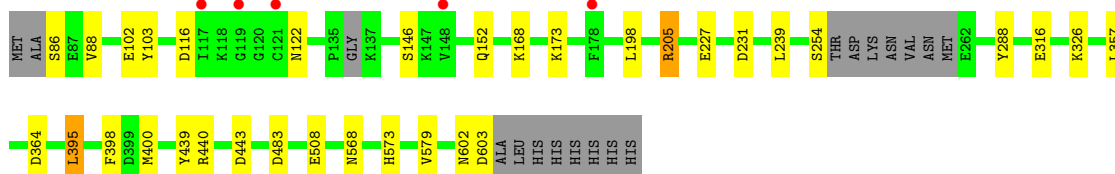
- Molecule 1: M17 leucyl aminopeptidase

Chain E: 



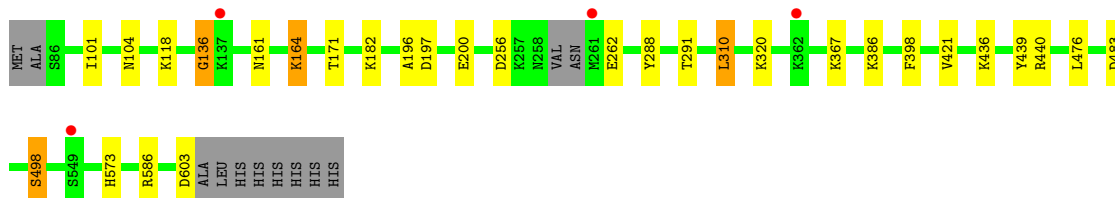
- Molecule 1: M17 leucyl aminopeptidase

Chain F:



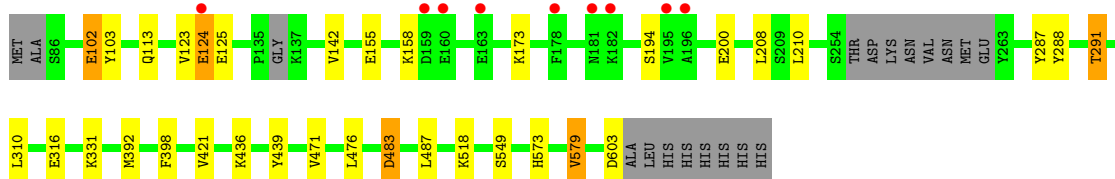
- Molecule 1: M17 leucyl aminopeptidase

Chain G:



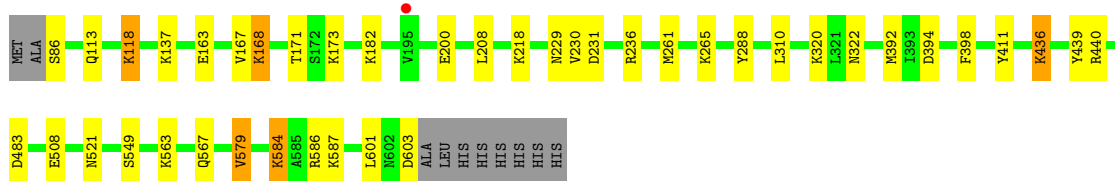
- Molecule 1: M17 leucyl aminopeptidase

Chain H:



- Molecule 1: M17 leucyl aminopeptidase

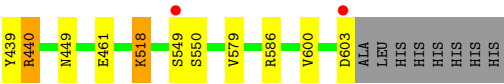
Chain I:



- Molecule 1: M17 leucyl aminopeptidase

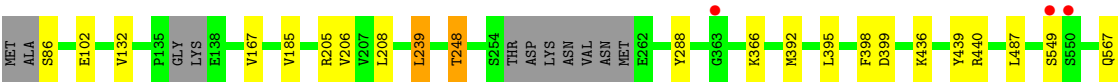
Chain J:





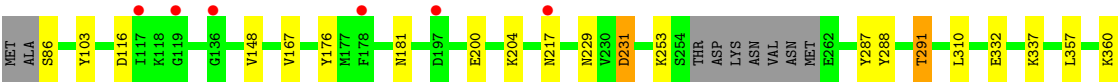
● Molecule 1: M17 leucyl aminopeptidase

Chain K:



● Molecule 1: M17 leucyl aminopeptidase

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.56Å 178.12Å 230.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 2.00 43.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.15-2.00) 98.3 (43.13-2.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.192 , 0.242 0.195 , 0.243	Depositor DCC
R_{free} test set	23578 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.1	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	5 of 469041 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53016	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 47.00 % 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 1.0558e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: CO3, ZN, MG, 1PE, SO4, BES

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	0.85	0/4063	0.76	0/5508
1	B	0.81	2/4014 (0.0%)	0.79	8/5450 (0.1%)
1	C	0.84	0/4036	0.80	4/5477 (0.1%)
1	D	0.84	0/4023	0.81	8/5454 (0.1%)
1	E	0.86	0/3973	0.83	9/5392 (0.2%)
1	F	0.83	0/3949	0.81	5/5364 (0.1%)
1	G	0.86	2/4073 (0.0%)	0.77	6/5513 (0.1%)
1	H	0.80	2/4022 (0.0%)	0.78	3/5445 (0.1%)
1	I	0.84	0/4089	0.83	6/5539 (0.1%)
1	J	0.86	0/4043	0.81	4/5476 (0.1%)
1	K	0.87	2/4014 (0.0%)	0.83	7/5438 (0.1%)
1	L	0.85	0/4024	0.81	4/5460 (0.1%)
All	All	0.84	8/48323 (0.0%)	0.80	64/65516 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	262	GLU	CB-CG	-5.83	1.41	1.52
1	K	206	VAL	CB-CG2	-5.61	1.41	1.52
1	B	422	GLU	CD-OE1	-5.53	1.19	1.25
1	K	206	VAL	CB-CG1	-5.39	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	421	VAL	CB-CG2	-5.33	1.41	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	440	ARG	NE-CZ-NH2	-15.18	112.71	120.30
1	I	440	ARG	NE-CZ-NH2	-13.93	113.34	120.30
1	B	440	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	L	440	ARG	NE-CZ-NH2	-12.05	114.28	120.30
1	F	440	ARG	NE-CZ-NH2	-11.99	114.31	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	257	LYS	Peptide
1	G	136	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3983	0	8	5	0
1	B	3936	0	4	20	0
1	C	3955	0	8	13	0
1	D	3946	0	8	18	0
1	E	3896	0	4	9	0
1	F	3873	0	2	15	0
1	G	3996	0	11	9	0
1	H	3943	0	4	8	0
1	I	4008	0	4	16	0
1	J	3963	0	4	20	0
1	K	3935	0	4	11	0
1	L	3944	0	19	19	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	22	0	22	0	0
4	B	22	0	22	1	0
4	C	22	0	22	2	0
4	D	22	0	22	1	0
4	E	22	0	0	0	0
4	F	22	0	22	0	0
4	G	22	0	22	0	0
4	H	22	0	22	2	0
4	I	22	0	22	1	0
4	J	22	0	22	1	0
4	K	22	0	22	2	0
4	L	22	0	22	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	15	0	0	0	0
6	B	5	0	0	0	0
6	D	10	0	0	0	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
6	G	10	0	0	1	0
6	J	10	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	2	0
7	A	21	0	22	0	0
7	B	30	0	30	4	0
7	C	22	0	24	3	0
7	D	38	0	38	4	0
7	E	32	0	36	2	0
7	F	30	0	39	2	0
7	G	43	0	47	2	0
7	H	20	0	20	2	0
7	I	33	0	37	6	0
7	J	31	0	36	5	0
7	K	41	0	44	1	0
7	L	33	0	40	5	0
8	A	423	0	0	4	0
8	B	361	0	0	10	0
8	C	427	0	0	10	0
8	D	411	0	0	8	0
8	E	442	0	0	7	0
8	F	373	0	0	8	0
8	G	421	0	0	5	0
8	H	389	0	0	0	0
8	I	414	0	0	14	0
8	J	403	0	0	10	0
8	K	438	0	0	9	0
8	L	356	0	0	11	0
All	All	53016	0	735	176	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 176 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:320:LYS:NZ	7:D:63:1PE:H142	1.80	0.97
1:B:320:LYS:NZ	7:B:61:1PE:H132	1.82	0.92
7:I:22:1PE:H252	8:I:4748:HOH:O	1.74	0.88
1:K:392:MET:CE	4:K:1003:BES:H10	2.11	0.80
1:B:257:LYS:CB	1:B:258:ASN:CB	2.61	0.78

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	515/528 (98%)	503 (98%)	12 (2%)	0	100	100
1	B	516/528 (98%)	502 (97%)	11 (2%)	3 (1%)	33	24
1	C	517/528 (98%)	509 (98%)	8 (2%)	0	100	100
1	D	512/528 (97%)	492 (96%)	18 (4%)	2 (0%)	43	36
1	E	506/528 (96%)	493 (97%)	10 (2%)	3 (1%)	33	24
1	F	504/528 (96%)	487 (97%)	17 (3%)	0	100	100
1	G	512/528 (97%)	500 (98%)	11 (2%)	1 (0%)	56	51
1	H	504/528 (96%)	493 (98%)	10 (2%)	1 (0%)	56	51
1	I	517/528 (98%)	507 (98%)	10 (2%)	0	100	100
1	J	510/528 (97%)	496 (97%)	14 (3%)	0	100	100
1	K	504/528 (96%)	495 (98%)	9 (2%)	0	100	100
1	L	510/528 (97%)	501 (98%)	9 (2%)	0	100	100
All	All	6127/6336 (97%)	5978 (98%)	139 (2%)	10 (0%)	56	51

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	124	GLU

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Mol	Chain	Res	Type
1	B	136	GLY
1	B	258	ASN
1	B	259	VAL
1	E	362	LYS

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	427/455 (94%)	417 (98%)	10 (2%)	63	63
1	B	414/455 (91%)	395 (95%)	19 (5%)	37	30
1	C	419/455 (92%)	401 (96%)	18 (4%)	40	33
1	D	418/455 (92%)	397 (95%)	21 (5%)	34	27
1	E	413/455 (91%)	398 (96%)	15 (4%)	47	42
1	F	409/455 (90%)	391 (96%)	18 (4%)	39	32
1	G	437/455 (96%)	422 (97%)	15 (3%)	49	45
1	H	431/455 (95%)	409 (95%)	22 (5%)	33	26
1	I	437/455 (96%)	411 (94%)	26 (6%)	28	20
1	J	432/455 (95%)	415 (96%)	17 (4%)	43	38
1	K	428/455 (94%)	415 (97%)	13 (3%)	53	50
1	L	424/455 (93%)	404 (95%)	20 (5%)	36	29
All	All	5089/5460 (93%)	4875 (96%)	214 (4%)	40	34

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	400	MET
1	H	155	GLU
1	L	167	VAL
1	F	568	ASN
1	G	310	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	217	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 99 ligands modelled in this entry, 24 are monoatomic - leaving 75 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	$\# Z > 2$
6	SO4	A	1	-	4,4,4	0.38	0	6,6,6	0.22	0
2	CO3	A	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	A	1003	3,5	22,22,22	0.76	0	29,29,29	1.50	5 (17%)
7	1PE	A	19	-	8,8,15	2.21	1 (12%)	6,7,14	0.57	0
6	SO4	A	2	-	4,4,4	0.35	0	6,6,6	0.19	0
7	1PE	A	20	-	9,11,15	0.71	0	8,10,14	0.53	0
6	SO4	A	24	-	4,4,4	0.14	0	6,6,6	0.13	0
2	CO3	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	B	1003	3,5	22,22,22	0.66	0	29,29,29	1.53	7 (24%)
6	SO4	B	3	-	4,4,4	0.52	0	6,6,6	0.28	0
7	1PE	B	60	-	8,9,15	2.84	1 (12%)	6,8,14	0.56	0
7	1PE	B	61	-	8,9,15	3.35	1 (12%)	6,8,14	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	1PE	B	62	-	8,9,15	2.76	1 (12%)	6,8,14	0.50	0
2	CO3	C	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	C	1003	3,5	22,22,22	0.91	1 (4%)	29,29,29	1.41	4 (13%)
7	1PE	C	17	-	11,12,15	2.41	1 (9%)	9,11,14	0.57	0
7	1PE	C	18	-	8,8,15	2.80	1 (12%)	6,7,14	0.82	0
2	CO3	D	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	D	1003	3,5	22,22,22	0.74	0	29,29,29	0.99	2 (6%)
7	1PE	D	44	-	10,10,15	1.31	1 (10%)	7,9,14	0.80	0
6	SO4	D	5	-	4,4,4	0.41	0	6,6,6	0.33	0
7	1PE	D	63	-	8,9,15	2.98	1 (12%)	6,8,14	0.91	0
7	1PE	D	67	-	5,6,15	2.40	1 (20%)	3,5,14	0.20	0
6	SO4	D	7	-	4,4,4	0.70	0	6,6,6	0.69	0
7	1PE	D	9	-	8,9,15	2.46	1 (12%)	6,8,14	0.19	0
2	CO3	E	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	E	1003	3,5	22,22,22	0.81	0	29,29,29	1.26	2 (6%)
6	SO4	E	22	-	4,4,4	0.40	0	6,6,6	0.17	0
7	1PE	E	43	-	6,7,15	0.85	0	5,6,14	0.40	0
7	1PE	E	7	-	11,11,15	2.07	1 (9%)	9,10,14	0.68	0
7	1PE	E	8	-	11,11,15	1.93	1 (9%)	9,10,14	0.76	0
2	CO3	F	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	F	1003	3,5	22,22,22	0.72	0	29,29,29	1.38	5 (17%)
6	SO4	F	21	-	4,4,4	0.22	0	6,6,6	0.20	0
7	1PE	F	31	-	9,9,15	0.57	0	8,8,14	0.73	0
7	1PE	F	32	-	9,9,15	0.77	0	8,8,14	0.56	0
7	1PE	F	33	-	9,9,15	0.68	0	8,8,14	0.33	0
2	CO3	G	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	G	1003	3,5	22,22,22	0.90	1 (4%)	29,29,29	1.51	4 (13%)
7	1PE	G	12	-	6,8,15	0.57	0	5,7,14	0.33	0
6	SO4	G	17	-	4,4,4	0.23	0	6,6,6	0.33	0
6	SO4	G	23	-	4,4,4	0.26	0	6,6,6	0.21	0
7	1PE	G	30	-	6,6,15	0.95	0	5,5,14	0.80	0
7	1PE	G	47	-	5,5,15	2.38	1 (20%)	3,4,14	1.03	0
7	1PE	G	48	-	5,5,15	1.96	1 (20%)	3,4,14	1.27	0
7	1PE	G	58	-	14,14,15	1.98	1 (7%)	12,13,14	0.55	0
2	CO3	H	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	H	1003	3,5	22,22,22	0.69	0	29,29,29	1.31	4 (13%)
7	1PE	H	64	-	8,9,15	1.82	1 (12%)	6,8,14	0.64	0
7	1PE	H	65	-	8,9,15	3.27	1 (12%)	6,8,14	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CO3	I	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	I	1003	3,5	22,22,22	0.85	0	29,29,29	1.49	6 (20%)
7	1PE	I	21	-	14,14,15	0.79	0	12,13,14	0.80	0
7	1PE	I	22	-	10,10,15	2.78	2 (20%)	7,9,14	0.39	0
7	1PE	I	66	-	5,6,15	1.44	1 (20%)	3,5,14	0.48	0
2	CO3	J	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	J	1003	3,5	22,22,22	0.94	1 (4%)	29,29,29	1.49	4 (13%)
6	SO4	J	18	-	4,4,4	0.61	0	6,6,6	0.77	0
7	1PE	J	2	-	9,10,15	0.42	0	8,9,14	0.53	0
6	SO4	J	20	-	4,4,4	0.26	0	6,6,6	0.14	0
7	1PE	J	3	-	9,9,15	0.75	0	8,8,14	0.76	0
7	1PE	J	45	-	8,9,15	2.39	1 (12%)	6,8,14	0.34	0
2	CO3	K	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	K	1003	3,5	22,22,22	0.92	1 (4%)	29,29,29	1.47	5 (17%)
6	SO4	K	19	-	4,4,4	0.45	0	6,6,6	0.20	0
7	1PE	K	4	-	11,11,15	1.66	1 (9%)	9,10,14	0.69	0
7	1PE	K	42	-	9,10,15	0.84	0	8,9,14	0.42	0
7	1PE	K	5	-	11,11,15	2.03	1 (9%)	9,10,14	0.85	0
7	1PE	K	50	-	3,5,15	0.64	0	2,4,14	0.16	0
7	1PE	L	1	-	9,9,15	0.49	0	8,8,14	0.91	1 (12%)
2	CO3	L	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	BES	L	1003	3,5	22,22,22	0.69	0	29,29,29	1.32	4 (13%)
6	SO4	L	25	-	4,4,4	0.46	0	6,6,6	0.23	0
7	1PE	L	56	-	9,10,15	0.57	0	8,9,14	0.24	0
7	1PE	L	612	-	11,11,15	2.92	1 (9%)	9,10,14	0.58	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
6	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	CO3	A	1002	-	-	0/0/0/0	0/0/0/0
4	BES	A	1003	3,5	-	0/24/24/24	0/1/1/1
7	1PE	A	19	-	-	0/6/6/13	0/0/0/0
6	SO4	A	2	-	-	0/0/0/0	0/0/0/0
7	1PE	A	20	-	-	0/9/9/13	0/0/0/0
6	SO4	A	24	-	-	0/0/0/0	0/0/0/0
2	CO3	B	1002	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BES	B	1003	3,5	-	0/24/24/24	0/1/1/1
6	SO4	B	3	-	-	0/0/0/0	0/0/0/0
7	1PE	B	60	-	-	0/7/7/13	0/0/0/0
7	1PE	B	61	-	-	0/7/7/13	0/0/0/0
7	1PE	B	62	-	-	0/7/7/13	0/0/0/0
2	CO3	C	1002	-	-	0/0/0/0	0/0/0/0
4	BES	C	1003	3,5	-	0/24/24/24	0/1/1/1
7	1PE	C	17	-	-	0/10/10/13	0/0/0/0
7	1PE	C	18	-	-	0/6/6/13	0/0/0/0
2	CO3	D	1002	-	-	0/0/0/0	0/0/0/0
4	BES	D	1003	3,5	-	0/24/24/24	0/1/1/1
7	1PE	D	44	-	-	0/8/8/13	0/0/0/0
6	SO4	D	5	-	-	0/0/0/0	0/0/0/0
7	1PE	D	63	-	-	0/7/7/13	0/0/0/0
7	1PE	D	67	-	-	1/4/4/13	0/0/0/0
6	SO4	D	7	-	-	0/0/0/0	0/0/0/0
7	1PE	D	9	-	-	0/7/7/13	0/0/0/0
2	CO3	E	1002	-	-	0/0/0/0	0/0/0/0
4	BES	E	1003	3,5	-	0/24/24/24	0/1/1/1
6	SO4	E	22	-	-	0/0/0/0	0/0/0/0
7	1PE	E	43	-	-	0/5/5/13	0/0/0/0
7	1PE	E	7	-	-	0/9/9/13	0/0/0/0
7	1PE	E	8	-	-	0/9/9/13	0/0/0/0
2	CO3	F	1002	-	-	0/0/0/0	0/0/0/0
4	BES	F	1003	3,5	-	0/24/24/24	0/1/1/1
6	SO4	F	21	-	-	0/0/0/0	0/0/0/0
7	1PE	F	31	-	-	0/7/7/13	0/0/0/0
7	1PE	F	32	-	-	0/7/7/13	0/0/0/0
7	1PE	F	33	-	-	0/7/7/13	0/0/0/0
2	CO3	G	1002	-	-	0/0/0/0	0/0/0/0
4	BES	G	1003	3,5	-	0/24/24/24	0/1/1/1
7	1PE	G	12	-	-	0/6/6/13	0/0/0/0
6	SO4	G	17	-	-	0/0/0/0	0/0/0/0
6	SO4	G	23	-	-	0/0/0/0	0/0/0/0
7	1PE	G	30	-	-	0/4/4/13	0/0/0/0
7	1PE	G	47	-	-	0/3/3/13	0/0/0/0
7	1PE	G	48	-	-	0/3/3/13	0/0/0/0
7	1PE	G	58	-	-	0/12/12/13	0/0/0/0
2	CO3	H	1002	-	-	0/0/0/0	0/0/0/0
4	BES	H	1003	3,5	-	0/24/24/24	0/1/1/1
7	1PE	H	64	-	-	0/7/7/13	0/0/0/0
7	1PE	H	65	-	-	0/7/7/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO3	I	1002	-	-	0/0/0/0	0/0/0/0
4	BES	I	1003	3,5	-	0/24/24/24	0/1/1/1
7	1PE	I	21	-	-	1/12/12/13	0/0/0/0
7	1PE	I	22	-	-	0/8/8/13	0/0/0/0
7	1PE	I	66	-	-	0/4/4/13	0/0/0/0
2	CO3	J	1002	-	-	0/0/0/0	0/0/0/0
4	BES	J	1003	3,5	-	0/24/24/24	0/1/1/1
6	SO4	J	18	-	-	0/0/0/0	0/0/0/0
7	1PE	J	2	-	-	0/8/8/13	0/0/0/0
6	SO4	J	20	-	-	0/0/0/0	0/0/0/0
7	1PE	J	3	-	-	0/7/7/13	0/0/0/0
7	1PE	J	45	-	-	0/7/7/13	0/0/0/0
2	CO3	K	1002	-	-	0/0/0/0	0/0/0/0
4	BES	K	1003	3,5	-	0/24/24/24	0/1/1/1
6	SO4	K	19	-	-	0/0/0/0	0/0/0/0
7	1PE	K	4	-	-	0/9/9/13	0/0/0/0
7	1PE	K	42	-	-	0/8/8/13	0/0/0/0
7	1PE	K	5	-	-	0/9/9/13	0/0/0/0
7	1PE	K	50	-	-	0/3/3/13	0/0/0/0
7	1PE	L	1	-	-	0/7/7/13	0/0/0/0
2	CO3	L	1002	-	-	0/0/0/0	0/0/0/0
4	BES	L	1003	3,5	-	0/24/24/24	0/1/1/1
6	SO4	L	25	-	-	0/0/0/0	0/0/0/0
7	1PE	L	56	-	-	0/8/8/13	0/0/0/0
7	1PE	L	612	-	-	0/9/9/13	0/0/0/0

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	612	1PE	C12-C22	-9.49	1.51	1.55
7	B	61	1PE	C12-C22	-9.31	1.51	1.55
7	H	65	1PE	C12-C22	-9.09	1.51	1.55
7	D	63	1PE	C12-C22	-8.19	1.51	1.55
7	B	60	1PE	C12-C22	-7.91	1.52	1.55

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1003	BES	O2-C2-C1	4.47	121.01	110.19
4	G	1003	BES	O2-C2-C3	-4.24	100.69	110.51
4	G	1003	BES	O2-C2-C1	4.22	120.41	110.19
4	K	1003	BES	O2-C2-C3	-4.07	101.08	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1003	BES	O2-C2-C3	-4.06	101.11	110.51

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	21	1PE	C23-OH3-C22-C12
7	D	67	1PE	C13-OH4-C24-C14

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	518/528 (98%)	-0.40	3 (0%) 86 88	7, 14, 29, 39	1 (0%)
1	B	518/528 (98%)	-0.24	14 (2%) 52 52	7, 16, 42, 51	0
1	C	518/528 (98%)	-0.35	3 (0%) 86 88	7, 15, 31, 42	0
1	D	516/528 (97%)	-0.36	6 (1%) 75 76	8, 15, 29, 39	0
1	E	510/528 (96%)	-0.46	4 (0%) 83 84	8, 14, 25, 37	0
1	F	510/528 (96%)	-0.26	5 (0%) 79 80	8, 17, 37, 46	0
1	G	516/528 (97%)	-0.36	4 (0%) 83 84	7, 14, 28, 40	0
1	H	509/528 (96%)	-0.23	9 (1%) 65 66	7, 16, 42, 52	0
1	I	518/528 (98%)	-0.33	1 (0%) 93 94	7, 14, 31, 41	0
1	J	513/528 (97%)	-0.34	3 (0%) 86 88	8, 15, 29, 40	0
1	K	509/528 (96%)	-0.46	3 (0%) 86 88	9, 14, 25, 38	0
1	L	513/528 (97%)	-0.26	6 (1%) 75 76	8, 16, 40, 46	0
All	All	6168/6336 (97%)	-0.34	61 (0%) 75 80	7, 15, 34, 52	1 (0%)

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	GLY	6.1
1	J	136	GLY	6.0
1	B	136	GLY	5.3
1	H	181	ASN	4.1
1	B	256	ASP	3.9

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MG	A	1004	1/1	0.58	58.85	24,24,24,24	0
5	MG	L	1004	1/1	0.54	39.65	33,33,33,33	0
5	MG	G	1004	1/1	0.39	35.10	23,23,23,23	0
5	MG	F	1004	1/1	0.51	32.73	37,37,37,37	0
5	MG	I	1004	1/1	0.52	29.70	15,15,15,15	0
7	1PE	B	62	10/16	0.68	26.89	91,95,97,98	0
5	MG	D	1004	1/1	0.45	24.22	28,28,28,28	0
5	MG	C	1004	1/1	0.48	23.58	27,27,27,27	0
5	MG	K	1004	1/1	0.34	22.68	23,23,23,23	0
5	MG	H	1004	1/1	0.52	21.14	40,40,40,40	0
5	MG	J	1004	1/1	0.55	20.37	22,22,22,22	0
5	MG	B	1004	1/1	0.42	19.73	16,16,16,16	0
5	MG	E	1004	1/1	0.36	18.46	26,26,26,26	0
7	1PE	F	33	10/16	0.18	10.04	21,29,31,34	0
7	1PE	K	50	6/16	0.20	9.78	37,40,45,46	0
7	1PE	G	30	7/16	0.17	8.14	35,38,42,43	0
4	BES	F	1003	22/22	0.20	5.66	13,27,36,40	0
4	BES	G	1003	22/22	0.17	5.47	13,28,34,39	0
4	BES	H	1003	22/22	0.18	5.11	15,25,34,37	0
6	SO4	L	25	5/5	0.26	5.07	56,59,59,60	0
2	CO3	A	1002	4/4	0.13	4.98	13,14,14,17	0
4	BES	B	1003	22/22	0.18	4.77	17,30,39,45	0
4	BES	A	1003	22/22	0.15	4.63	20,29,35,40	0
4	BES	K	1003	22/22	0.16	4.44	16,26,32,39	0
6	SO4	A	24	5/5	0.13	3.85	52,55,56,57	0
6	SO4	E	22	5/5	0.26	3.72	44,45,47,48	0
6	SO4	J	20	5/5	0.25	3.67	60,62,62,62	0
7	1PE	J	45	10/16	0.28	3.58	44,48,51,51	0
7	1PE	E	43	8/16	0.17	3.55	33,35,35,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	1PE	D	44	11/16	0.29	3.55	36,38,43,44	0
7	1PE	A	19	9/16	0.16	3.52	20,24,28,31	0
7	1PE	G	58	15/16	0.21	3.48	37,42,52,53	0
4	BES	L	1003	22/22	0.17	3.41	12,26,33,34	0
6	SO4	G	23	5/5	0.22	3.22	46,49,50,50	0
4	BES	E	1003	22/22	0.14	2.78	19,29,35,39	0
7	1PE	B	61	10/16	0.19	2.76	38,40,42,43	0
7	1PE	L	56	11/16	0.17	2.66	43,45,48,50	0
7	1PE	A	20	12/16	0.18	2.58	40,43,46,47	0
7	1PE	G	12	9/16	0.16	2.54	27,28,32,32	0
7	1PE	K	42	11/16	0.17	2.43	33,42,47,47	0
7	1PE	H	65	10/16	0.16	2.26	32,40,41,41	0
7	1PE	L	612	12/16	0.17	2.17	22,36,39,40	0
7	1PE	D	67	7/16	0.21	2.09	29,33,41,41	0
4	BES	D	1003	22/22	0.14	2.09	13,28,32,33	0
4	BES	J	1003	22/22	0.15	2.02	11,28,37,40	0
7	1PE	G	48	6/16	0.13	2.01	25,31,33,36	0
6	SO4	F	21	5/5	0.20	2.00	56,59,59,59	0
4	BES	C	1003	22/22	0.15	1.98	22,27,36,36	0
6	SO4	K	19	5/5	0.19	1.94	52,53,54,54	0
6	SO4	A	1	5/5	0.15	1.93	50,51,53,53	0
7	1PE	D	63	10/16	0.18	1.93	22,30,33,36	0
6	SO4	A	2	5/5	0.14	1.78	45,46,50,51	0
6	SO4	D	5	5/5	0.20	1.77	53,53,56,56	0
4	BES	I	1003	22/22	0.14	1.74	11,27,30,32	0
7	1PE	C	17	13/16	0.19	1.68	22,36,38,38	0
7	1PE	I	22	11/16	0.13	1.67	18,23,36,38	0
7	1PE	D	9	10/16	0.15	1.51	21,25,35,37	0
7	1PE	I	66	7/16	0.13	1.42	30,32,34,34	0
7	1PE	E	8	12/16	0.13	1.36	20,23,35,35	0
7	1PE	K	4	12/16	0.14	1.25	31,32,34,35	0
7	1PE	F	32	10/16	0.16	1.21	37,39,39,39	0
2	CO3	E	1002	4/4	0.11	1.19	16,17,18,19	0
2	CO3	B	1002	4/4	0.12	1.08	11,12,12,16	0
7	1PE	B	60	10/16	0.13	1.05	23,28,33,35	0
7	1PE	I	21	15/16	0.18	1.04	26,33,46,47	0
7	1PE	J	3	10/16	0.15	1.02	36,37,40,41	0
7	1PE	E	7	12/16	0.14	1.01	32,34,36,36	0
7	1PE	K	5	12/16	0.12	0.89	25,27,38,38	0
3	ZN	G	1001	1/1	0.09	0.83	38,38,38,38	0
7	1PE	H	64	10/16	0.12	0.67	19,26,34,35	0
2	CO3	L	1002	4/4	0.09	0.66	14,15,15,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	1PE	G	47	6/16	0.12	0.53	30,31,32,35	0
7	1PE	J	2	11/16	0.12	0.45	23,26,37,42	0
2	CO3	D	1002	4/4	0.10	0.40	11,12,12,16	0
7	1PE	C	18	9/16	0.10	0.31	20,21,26,29	0
3	ZN	C	1001	1/1	0.10	0.28	39,39,39,39	0
7	1PE	L	1	10/16	0.11	0.20	25,27,32,38	0
3	ZN	F	1001	1/1	0.09	0.15	40,40,40,40	0
2	CO3	F	1002	4/4	0.08	0.15	12,12,13,15	0
2	CO3	K	1002	4/4	0.09	-0.01	13,14,14,18	0
2	CO3	C	1002	4/4	0.09	-0.17	12,13,13,16	0
3	ZN	A	1001	1/1	0.08	-0.26	39,39,39,39	0
2	CO3	J	1002	4/4	0.10	-0.27	12,14,15,16	0
7	1PE	F	31	10/16	0.09	-0.38	26,27,29,29	0
3	ZN	L	1001	1/1	0.08	-0.56	37,37,37,37	0
6	SO4	D	7	5/5	0.09	-0.82	8,11,11,12	0
2	CO3	I	1002	4/4	0.09	-0.88	14,15,15,18	0
3	ZN	B	1001	1/1	0.07	-1.01	37,37,37,37	0
3	ZN	H	1001	1/1	0.08	-1.05	34,34,34,34	0
2	CO3	G	1002	4/4	0.07	-1.09	11,12,12,15	0
6	SO4	J	18	5/5	0.09	-1.19	11,11,12,14	0
6	SO4	G	17	5/5	0.07	-1.23	10,11,13,14	0
2	CO3	H	1002	4/4	0.09	-1.29	10,10,11,14	0
3	ZN	I	1001	1/1	0.08	-1.42	36,36,36,36	0
6	SO4	B	3	5/5	0.06	-1.51	8,9,10,10	0
3	ZN	K	1001	1/1	0.07	-2.21	37,37,37,37	0
3	ZN	E	1001	1/1	0.04	-2.57	38,38,38,38	0
3	ZN	D	1001	1/1	0.04	-3.00	34,34,34,34	0
3	ZN	J	1001	1/1	0.04	-3.60	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.