Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 07:01 AM EDT

PDB ID	:	4JIW
Title	:	c1882 PAAR-repeat protein from Escherichia coli in complex with a VgrG-like beta-helix that is based on a fragment of T4 gp5
Authors	:	Buth, S.A.; Leiman, P.G.; Shneider, M.M.
Deposited on	:	2013-03-07
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

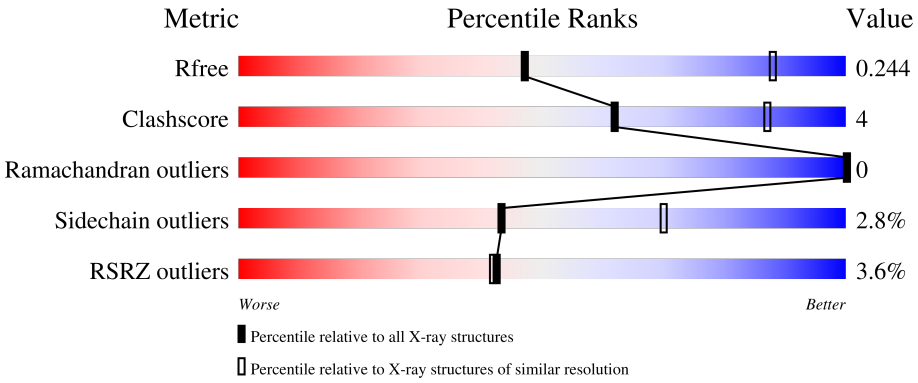
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	96	2% 83% 14%
1	B	96	2% 95%
1	C	96	80% 17%
1	E	96	2% 81% 14%
1	F	96	82% 15%

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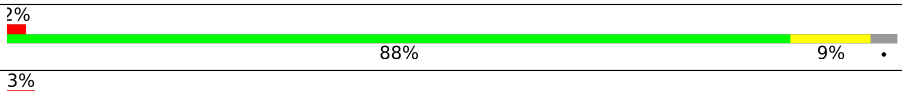
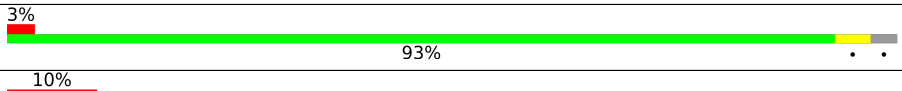
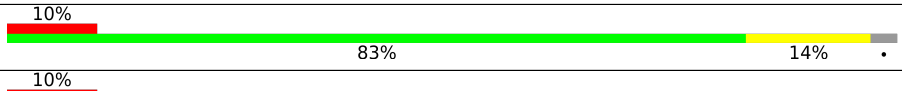
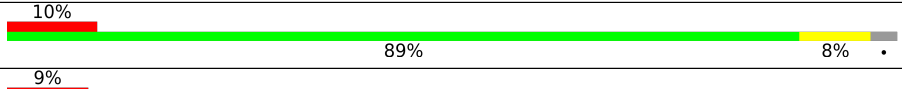
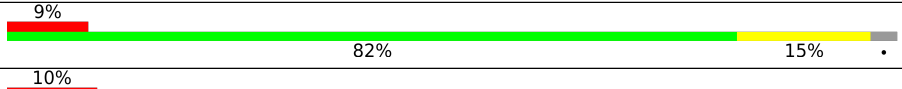
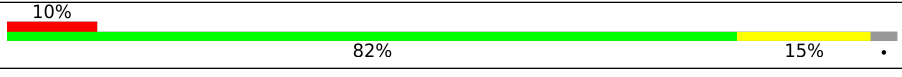
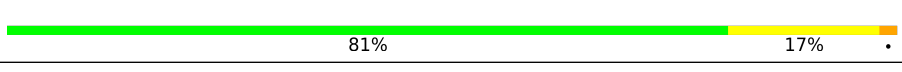
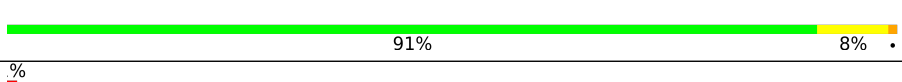
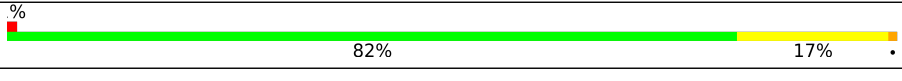
Mol	Chain	Length	Quality of chain
1	G	96	
1	I	96	
1	J	96	
1	K	96	
1	M	96	
1	N	96	
1	O	96	
2	D	93	
2	H	93	
2	L	93	
2	P	93	

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
5	CL	D	102	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10908 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 Tail-associated lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	B	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	C	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	E	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	F	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	G	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	I	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	J	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	K	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	M	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	N	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			
1	O	93	Total	C	N	O	S	0	0	0
			679	415	114	148	2			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	480	GLY	-	expression tag	UNP P16009
A	481	SER	-	expression tag	UNP P16009
A	482	GLY	-	expression tag	UNP P16009
A	483	SER	-	expression tag	UNP P16009
A	566	ASP	THR	engineered mutation	UNP P16009

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Chain	Residue	Modelled	Actual	Comment	Reference
A	568	LYS	ASP	engineered mutation	UNP P16009
A	570	ALA	SER	engineered mutation	UNP P16009
A	571	LYS	ARG	engineered mutation	UNP P16009
A	573	ASN	ASP	engineered mutation	UNP P16009
A	574	LEU	ILE	engineered mutation	UNP P16009
A	575	ASN	GLY	engineered mutation	UNP P16009
B	480	GLY	-	expression tag	UNP P16009
B	481	SER	-	expression tag	UNP P16009
B	482	GLY	-	expression tag	UNP P16009
B	483	SER	-	expression tag	UNP P16009
B	566	ASP	THR	engineered mutation	UNP P16009
B	568	LYS	ASP	engineered mutation	UNP P16009
B	570	ALA	SER	engineered mutation	UNP P16009
B	571	LYS	ARG	engineered mutation	UNP P16009
B	573	ASN	ASP	engineered mutation	UNP P16009
B	574	LEU	ILE	engineered mutation	UNP P16009
B	575	ASN	GLY	engineered mutation	UNP P16009
C	480	GLY	-	expression tag	UNP P16009
C	481	SER	-	expression tag	UNP P16009
C	482	GLY	-	expression tag	UNP P16009
C	483	SER	-	expression tag	UNP P16009
C	566	ASP	THR	engineered mutation	UNP P16009
C	568	LYS	ASP	engineered mutation	UNP P16009
C	570	ALA	SER	engineered mutation	UNP P16009
C	571	LYS	ARG	engineered mutation	UNP P16009
C	573	ASN	ASP	engineered mutation	UNP P16009
C	574	LEU	ILE	engineered mutation	UNP P16009
C	575	ASN	GLY	engineered mutation	UNP P16009
E	480	GLY	-	expression tag	UNP P16009
E	481	SER	-	expression tag	UNP P16009
E	482	GLY	-	expression tag	UNP P16009
E	483	SER	-	expression tag	UNP P16009
E	566	ASP	THR	engineered mutation	UNP P16009
E	568	LYS	ASP	engineered mutation	UNP P16009
E	570	ALA	SER	engineered mutation	UNP P16009
E	571	LYS	ARG	engineered mutation	UNP P16009
E	573	ASN	ASP	engineered mutation	UNP P16009
E	574	LEU	ILE	engineered mutation	UNP P16009
E	575	ASN	GLY	engineered mutation	UNP P16009
F	480	GLY	-	expression tag	UNP P16009
F	481	SER	-	expression tag	UNP P16009
F	482	GLY	-	expression tag	UNP P16009

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Chain	Residue	Modelled	Actual	Comment	Reference
F	483	SER	-	expression tag	UNP P16009
F	566	ASP	THR	engineered mutation	UNP P16009
F	568	LYS	ASP	engineered mutation	UNP P16009
F	570	ALA	SER	engineered mutation	UNP P16009
F	571	LYS	ARG	engineered mutation	UNP P16009
F	573	ASN	ASP	engineered mutation	UNP P16009
F	574	LEU	ILE	engineered mutation	UNP P16009
F	575	ASN	GLY	engineered mutation	UNP P16009
G	480	GLY	-	expression tag	UNP P16009
G	481	SER	-	expression tag	UNP P16009
G	482	GLY	-	expression tag	UNP P16009
G	483	SER	-	expression tag	UNP P16009
G	566	ASP	THR	engineered mutation	UNP P16009
G	568	LYS	ASP	engineered mutation	UNP P16009
G	570	ALA	SER	engineered mutation	UNP P16009
G	571	LYS	ARG	engineered mutation	UNP P16009
G	573	ASN	ASP	engineered mutation	UNP P16009
G	574	LEU	ILE	engineered mutation	UNP P16009
G	575	ASN	GLY	engineered mutation	UNP P16009
I	480	GLY	-	expression tag	UNP P16009
I	481	SER	-	expression tag	UNP P16009
I	482	GLY	-	expression tag	UNP P16009
I	483	SER	-	expression tag	UNP P16009
I	566	ASP	THR	engineered mutation	UNP P16009
I	568	LYS	ASP	engineered mutation	UNP P16009
I	570	ALA	SER	engineered mutation	UNP P16009
I	571	LYS	ARG	engineered mutation	UNP P16009
I	573	ASN	ASP	engineered mutation	UNP P16009
I	574	LEU	ILE	engineered mutation	UNP P16009
I	575	ASN	GLY	engineered mutation	UNP P16009
J	480	GLY	-	expression tag	UNP P16009
J	481	SER	-	expression tag	UNP P16009
J	482	GLY	-	expression tag	UNP P16009
J	483	SER	-	expression tag	UNP P16009
J	566	ASP	THR	engineered mutation	UNP P16009
J	568	LYS	ASP	engineered mutation	UNP P16009
J	570	ALA	SER	engineered mutation	UNP P16009
J	571	LYS	ARG	engineered mutation	UNP P16009
J	573	ASN	ASP	engineered mutation	UNP P16009
J	574	LEU	ILE	engineered mutation	UNP P16009
J	575	ASN	GLY	engineered mutation	UNP P16009
K	480	GLY	-	expression tag	UNP P16009

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Chain	Residue	Modelled	Actual	Comment	Reference
K	481	SER	-	expression tag	UNP P16009
K	482	GLY	-	expression tag	UNP P16009
K	483	SER	-	expression tag	UNP P16009
K	566	ASP	THR	engineered mutation	UNP P16009
K	568	LYS	ASP	engineered mutation	UNP P16009
K	570	ALA	SER	engineered mutation	UNP P16009
K	571	LYS	ARG	engineered mutation	UNP P16009
K	573	ASN	ASP	engineered mutation	UNP P16009
K	574	LEU	ILE	engineered mutation	UNP P16009
K	575	ASN	GLY	engineered mutation	UNP P16009
M	480	GLY	-	expression tag	UNP P16009
M	481	SER	-	expression tag	UNP P16009
M	482	GLY	-	expression tag	UNP P16009
M	483	SER	-	expression tag	UNP P16009
M	566	ASP	THR	engineered mutation	UNP P16009
M	568	LYS	ASP	engineered mutation	UNP P16009
M	570	ALA	SER	engineered mutation	UNP P16009
M	571	LYS	ARG	engineered mutation	UNP P16009
M	573	ASN	ASP	engineered mutation	UNP P16009
M	574	LEU	ILE	engineered mutation	UNP P16009
M	575	ASN	GLY	engineered mutation	UNP P16009
N	480	GLY	-	expression tag	UNP P16009
N	481	SER	-	expression tag	UNP P16009
N	482	GLY	-	expression tag	UNP P16009
N	483	SER	-	expression tag	UNP P16009
N	566	ASP	THR	engineered mutation	UNP P16009
N	568	LYS	ASP	engineered mutation	UNP P16009
N	570	ALA	SER	engineered mutation	UNP P16009
N	571	LYS	ARG	engineered mutation	UNP P16009
N	573	ASN	ASP	engineered mutation	UNP P16009
N	574	LEU	ILE	engineered mutation	UNP P16009
N	575	ASN	GLY	engineered mutation	UNP P16009
O	480	GLY	-	expression tag	UNP P16009
O	481	SER	-	expression tag	UNP P16009
O	482	GLY	-	expression tag	UNP P16009
O	483	SER	-	expression tag	UNP P16009
O	566	ASP	THR	engineered mutation	UNP P16009
O	568	LYS	ASP	engineered mutation	UNP P16009
O	570	ALA	SER	engineered mutation	UNP P16009
O	571	LYS	ARG	engineered mutation	UNP P16009
O	573	ASN	ASP	engineered mutation	UNP P16009
O	574	LEU	ILE	engineered mutation	UNP P16009

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Chain	Residue	Modelled	Actual	Comment	Reference
O	575	ASN	GLY	engineered mutation	UNP P16009

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	93	Total	C	N	O	S	0	0	0
			675	421	121	132	1			
2	H	93	Total	C	N	O	S	0	0	0
			675	421	121	132	1			
2	L	93	Total	C	N	O	S	0	0	0
			675	421	121	132	1			
2	P	93	Total	C	N	O	S	0	0	0
			675	421	121	132	1			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	P	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	M	1	Total Cl 1 1	0	0

- Molecule 6 is water.

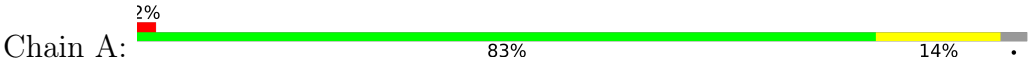
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total O 3 3	0	0
6	B	10	Total O 10 10	0	0
6	C	4	Total O 4 4	0	0
6	D	1	Total O 1 1	0	0
6	E	3	Total O 3 3	0	0
6	F	2	Total O 2 2	0	0
6	G	4	Total O 4 4	0	0
6	I	4	Total O 4 4	0	0
6	J	5	Total O 5 5	0	0
6	K	4	Total O 4 4	0	0
6	L	3	Total O 3 3	0	0
6	M	1	Total O 1 1	0	0
6	N	2	Total O 2 2	0	0
6	O	3	Total O 3 3	0	0

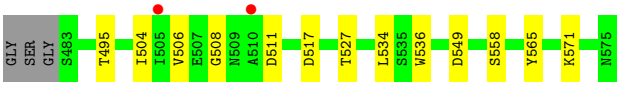
3 Residue-property plots (i)

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

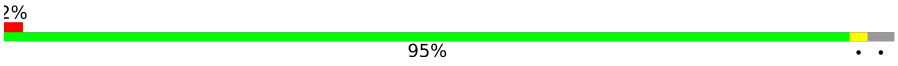
Chain A:

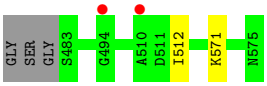




• Molecule 1: Tail-associated lysozyme

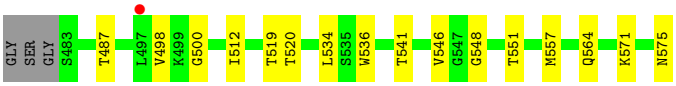
Chain B:





• Molecule 1: Tail-associated lysozyme

Chain C:

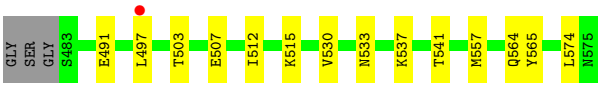


• Molecule 1: Tail-associated lysozyme

Chain E:

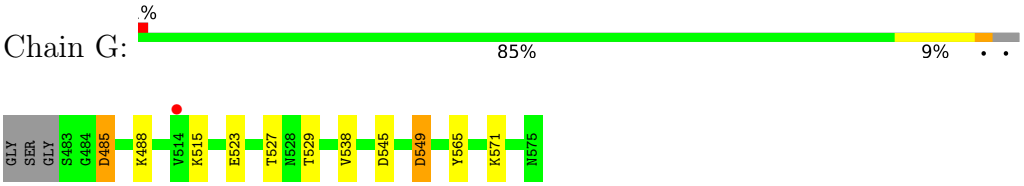
• Molecule 1: Tail-associated lysozyme

Chain F:



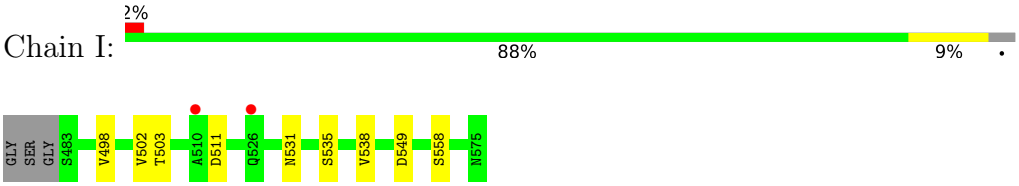
• Molecule 1: Tail-associated lysozyme

Chain G:



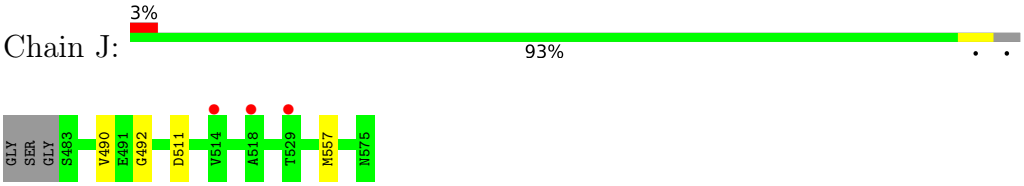
• Molecule 1: Tail-associated lysozyme

Chain I:



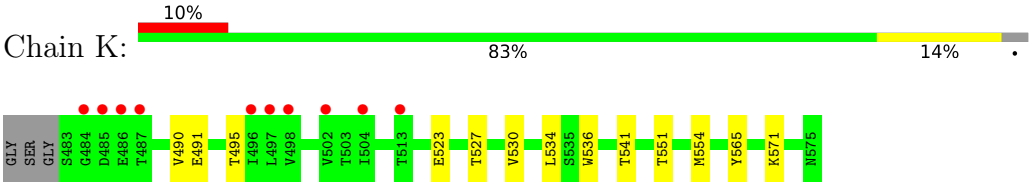
• Molecule 1: Tail-associated lysozyme

Chain J:



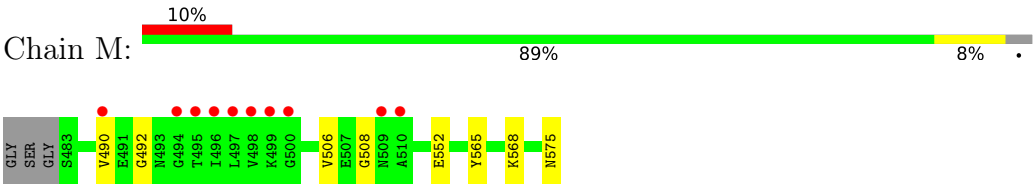
• Molecule 1: Tail-associated lysozyme

Chain K:



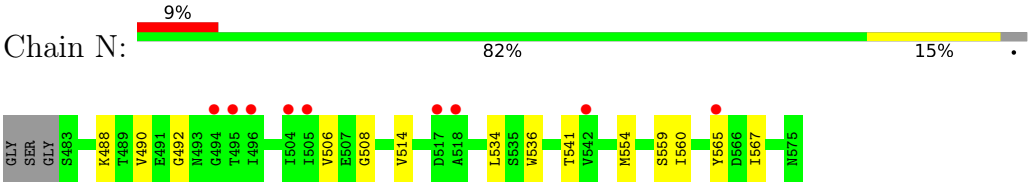
• Molecule 1: Tail-associated lysozyme

Chain M:



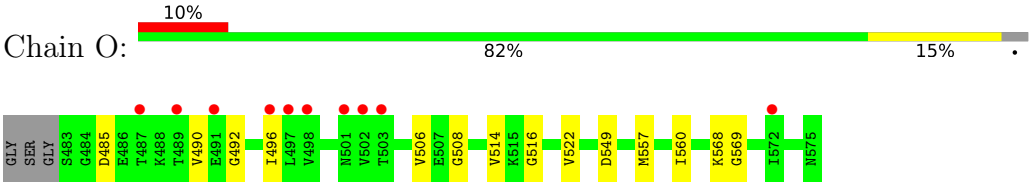
• Molecule 1: Tail-associated lysozyme

Chain N:



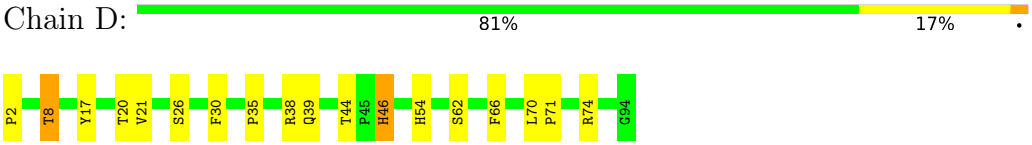
• Molecule 1: Tail-associated lysozyme

Chain O:



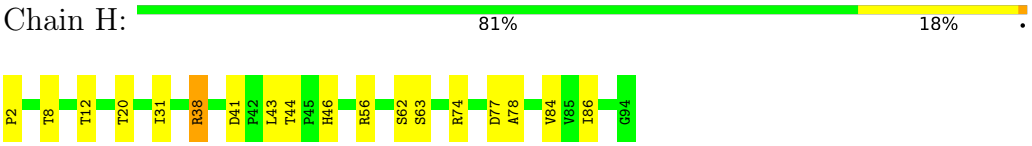
• Molecule 2: Putative uncharacterized protein

Chain D:



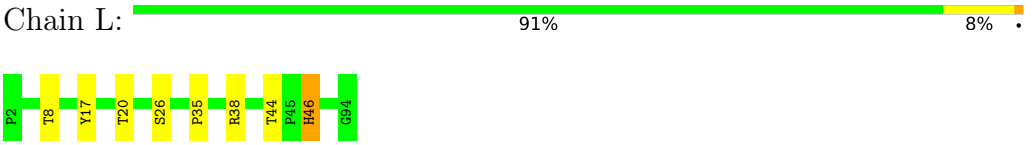
• Molecule 2: Putative uncharacterized protein

Chain H:



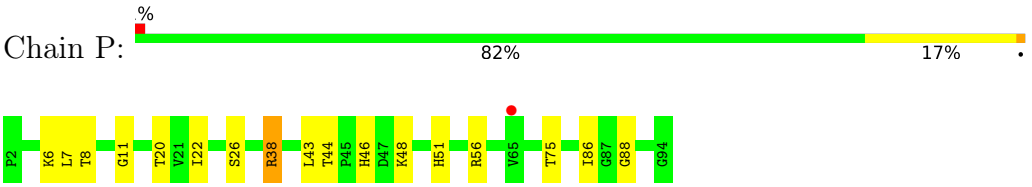
• Molecule 2: Putative uncharacterized protein

Chain L:



• Molecule 2: Putative uncharacterized protein

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	184.16Å 184.16Å 238.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.57 – 3.40 48.57 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.57-3.40) 99.8 (48.57-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.184 , 0.243 0.185 , 0.244	Depositor DCC
R_{free} test set	1692 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	90.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 116.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10908	wwPDB-VP
Average B, all atoms (Å^2)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, ZN

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	0.20	0/685	0.38	0/928
1	B	0.20	0/685	0.38	0/928
1	C	0.20	0/685	0.38	0/928
1	E	0.20	0/685	0.38	0/928
1	F	0.20	0/685	0.36	0/928
1	G	0.20	0/685	0.38	0/928
1	I	0.20	0/685	0.38	0/928
1	J	0.20	0/685	0.37	0/928
1	K	0.20	0/685	0.37	0/928
1	M	0.20	0/685	0.37	0/928
1	N	0.20	0/685	0.37	0/928
1	O	0.19	0/685	0.36	0/928
2	D	0.21	0/691	0.43	0/940
2	H	0.21	0/691	0.43	0/940
2	L	0.21	0/691	0.43	0/940
2	P	0.20	0/691	0.41	0/940
All	All	0.20	0/10984	0.39	0/14896

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

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	679	0	662	9	0
1	B	679	0	662	3	0
1	C	679	0	662	12	0
1	E	679	0	662	10	0
1	F	679	0	662	14	0
1	G	679	0	662	11	0
1	I	679	0	662	8	0
1	J	679	0	662	2	0
1	K	679	0	662	9	0
1	M	679	0	662	6	0
1	N	679	0	662	11	0
1	O	679	0	662	10	0
2	D	675	0	667	12	0
2	H	675	0	667	9	0
2	L	675	0	667	4	0
2	P	675	0	667	8	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	O	1	0	0	0	0
4	D	1	0	0	0	0
4	H	1	0	0	0	0
4	L	1	0	0	0	0
4	P	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	1	0
5	M	1	0	0	1	0
6	A	3	0	0	0	0
6	B	10	0	0	0	0
6	C	4	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	2	0	0	0	0
6	G	4	0	0	0	0
6	I	4	0	0	0	0
6	J	5	0	0	0	0
6	K	4	0	0	0	0
6	L	3	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
6	O	3	0	0	0	0
All	All	10908	0	10612	95	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 4.

All (95) 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)
2:D:46:HIS:CD2	2:D:54:HIS:CE1	2.58	0.83
1:F:530:VAL:HB	1:G:538:VAL:HG12	1.74	0.69
1:I:535:SER:HB3	1:K:527:THR:HG22	1.80	0.62
1:E:525:ASN:HB3	1:F:533:ASN:H	1.66	0.60
1:M:490:VAL:HG22	1:M:492:GLY:H	1.67	0.60
1:O:490:VAL:HG12	1:O:492:GLY:H	1.66	0.59
2:H:20:THR:HB	2:H:44:THR:HB	1.85	0.59
2:D:39:GLN:HB3	2:D:70:LEU:HD22	1.85	0.58
1:M:506:VAL:HG12	1:M:508:GLY:H	1.69	0.57
1:F:564:GLN:HG2	1:G:571:LYS:HB3	1.87	0.56
1:N:506:VAL:HG12	1:N:508:GLY:H	1.70	0.56
5:E:601:CL:CL	1:G:488:LYS:NZ	2.76	0.55
2:H:43:LEU:HB2	2:H:56:ARG:HB2	1.90	0.54
2:P:20:THR:HB	2:P:44:THR:HB	1.90	0.53
2:P:48:LYS:HB2	2:P:51:HIS:HB2	1.91	0.53
1:I:549:ASP:H	1:K:541:THR:HG22	1.75	0.52
1:E:499:LYS:HG2	1:F:507:GLU:HG3	1.90	0.52
2:H:78:ALA:HA	2:H:84:VAL:HG12	1.92	0.52
1:A:549:ASP:H	1:C:541:THR:HG22	1.74	0.52
2:P:6:LYS:NZ	2:P:88:GLY:O	2.34	0.52
1:F:541:THR:HG22	1:G:549:ASP:H	1.75	0.52
2:D:2:PRO:HB2	2:D:74:ARG:HB3	1.91	0.51
1:I:558:SER:HB3	1:K:551:THR:HG22	1.91	0.51
1:I:531:ASN:ND2	1:K:523:GLU:OE2	2.39	0.51
1:F:537:LYS:HD2	1:G:545:ASP:HB3	1.92	0.51
1:N:490:VAL:HG12	1:N:492:GLY:H	1.76	0.51
1:C:571:LYS:HD2	2:D:66:PHE:HE1	1.76	0.50
1:E:489:THR:HG22	1:F:497:LEU:HB3	1.93	0.50
1:I:503:THR:HB	1:K:495:THR:HG22	1.93	0.49
2:D:20:THR:HB	2:D:44:THR:HB	1.92	0.49
1:M:575:ASN:ND2	1:O:569:GLY:O	2.44	0.49
2:L:20:THR:HB	2:L:44:THR:HB	1.95	0.49
1:J:557:MET:HG2	1:K:565:TYR:CZ	2.48	0.49
2:P:75:THR:HG23	2:P:86:ILE:HA	1.94	0.49
2:D:70:LEU:HD23	2:D:71:PRO:HD2	1.95	0.49
1:E:557:MET:HB3	1:F:565:TYR:HA	1.95	0.49
2:P:26:SER:HB2	2:P:38:ARG:HD2	1.95	0.48
2:P:7:LEU:HD12	2:P:22:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:THR:HG22	2:H:86:ILE:HD11	1.96	0.48
1:K:534:LEU:HD21	1:K:536:TRP:HE1	1.79	0.48
1:E:537:LYS:HB2	1:G:529:THR:HG22	1.96	0.47
1:I:498:VAL:HG11	1:I:502:VAL:HG22	1.97	0.47
1:A:527:THR:HB	1:C:519:THR:HG22	1.97	0.46
1:C:571:LYS:HD2	2:D:66:PHE:CE1	2.50	0.46
2:D:8:THR:HA	2:D:21:VAL:HB	1.98	0.46
1:N:560:ILE:HG23	1:O:568:LYS:HB2	1.97	0.46
1:J:490:VAL:HG12	1:J:492:GLY:H	1.81	0.46
1:N:514:VAL:HB	1:O:522:VAL:HG22	1.97	0.46
1:A:495:THR:HB	1:C:487:THR:HG23	1.98	0.46
1:E:535:SER:HB2	1:G:527:THR:HG23	1.97	0.46
1:I:538:VAL:HG22	1:K:530:VAL:HB	1.98	0.46
1:M:552:GLU:HB2	1:N:559:SER:HA	1.98	0.46
1:O:506:VAL:HG12	1:O:508:GLY:H	1.80	0.45
2:P:43:LEU:HB2	2:P:56:ARG:HB2	1.98	0.45
1:N:554:MET:SD	1:N:554:MET:N	2.90	0.45
1:E:495:THR:HG23	1:F:503:THR:HB	1.99	0.45
1:A:565:TYR:CZ	1:C:557:MET:HG2	2.51	0.45
5:M:601:CL:CL	1:N:488:LYS:NZ	2.84	0.45
1:A:504:ILE:HG23	1:B:512:ILE:HG23	1.99	0.44
1:O:514:VAL:HG12	1:O:516:GLY:H	1.82	0.44
2:L:46:HIS:H	2:L:46:HIS:CD2	2.36	0.44
2:P:11:GLY:N	2:P:20:THR:O	2.45	0.44
2:D:26:SER:O	2:D:35:PRO:HB3	2.18	0.44
1:M:565:TYR:CZ	1:O:557:MET:HG2	2.53	0.44
2:H:38:ARG:NH1	2:H:41:ASP:OD1	2.50	0.44
1:E:507:GLU:HA	1:F:515:LYS:HB3	2.00	0.43
1:C:498:VAL:HG12	1:C:500:GLY:H	1.84	0.43
1:A:571:LYS:HB2	1:C:564:GLN:HG2	2.00	0.43
1:F:564:GLN:NE2	1:G:571:LYS:HD3	2.33	0.43
2:D:17:TYR:HB3	2:D:46:HIS:CG	2.54	0.43
1:G:485:ASP:OD1	1:G:485:ASP:N	2.52	0.43
1:C:534:LEU:HD21	1:C:536:TRP:HE1	1.83	0.43
1:N:541:THR:HG22	1:O:549:ASP:H	1.83	0.43
1:F:507:GLU:HA	1:G:515:LYS:HD3	2.01	0.42
1:N:534:LEU:HD21	1:N:536:TRP:HE1	1.84	0.42
1:I:498:VAL:HG13	1:K:490:VAL:HG13	2.01	0.42
1:M:568:LYS:HD2	1:O:560:ILE:HD12	2.01	0.42
2:H:74:ARG:N	2:H:77:ASP:OD2	2.40	0.42
2:D:62:SER:O	2:D:71:PRO:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:SER:OG	2:H:63:SER:N	2.53	0.41
1:A:534:LEU:HD21	1:A:536:TRP:HE1	1.86	0.41
1:B:571:LYS:HE2	2:D:30:PHE:CD1	2.55	0.41
1:A:558:SER:HB3	1:C:551:THR:HG22	2.01	0.41
1:B:512:ILE:HB	1:C:520:THR:HG22	2.02	0.41
2:L:17:TYR:HB3	2:L:46:HIS:CG	2.55	0.41
1:N:488:LYS:HB2	1:O:496:ILE:HD13	2.02	0.41
2:H:2:PRO:HB2	2:H:74:ARG:HB3	2.03	0.41
2:L:26:SER:O	2:L:35:PRO:HB3	2.21	0.41
1:E:485:ASP:N	1:E:485:ASP:OD1	2.53	0.41
1:N:565:TYR:HE1	1:N:567:ILE:HD11	1.86	0.41
1:A:506:VAL:HG12	1:A:508:GLY:H	1.86	0.41
1:E:534:LEU:HD21	1:E:536:TRP:HE1	1.86	0.41
1:F:574:LEU:HD12	2:H:31:ILE:HG12	2.02	0.41
1:C:546:VAL:HG12	1:C:548:GLY:H	1.85	0.41
1:F:557:MET:HG2	1:G:565:TYR:CZ	2.57	0.40

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	91/96 (95%)	90 (99%)	1 (1%)	0	100	100
1	B	91/96 (95%)	89 (98%)	2 (2%)	0	100	100
1	C	91/96 (95%)	89 (98%)	2 (2%)	0	100	100
1	E	91/96 (95%)	91 (100%)	0	0	100	100
1	F	91/96 (95%)	90 (99%)	1 (1%)	0	100	100
1	G	91/96 (95%)	91 (100%)	0	0	100	100
1	I	91/96 (95%)	88 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	91/96 (95%)	90 (99%)	1 (1%)	0	100	100
1	K	91/96 (95%)	88 (97%)	3 (3%)	0	100	100
1	M	91/96 (95%)	89 (98%)	2 (2%)	0	100	100
1	N	91/96 (95%)	87 (96%)	4 (4%)	0	100	100
1	O	91/96 (95%)	90 (99%)	1 (1%)	0	100	100
2	D	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
2	H	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
2	L	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
2	P	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
All	All	1456/1524 (96%)	1422 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	75/76 (99%)	73 (97%)	2 (3%)	44	70
1	B	75/76 (99%)	75 (100%)	0	100	100
1	C	75/76 (99%)	73 (97%)	2 (3%)	44	70
1	E	75/76 (99%)	69 (92%)	6 (8%)	12	38
1	F	75/76 (99%)	73 (97%)	2 (3%)	44	70
1	G	75/76 (99%)	72 (96%)	3 (4%)	31	60
1	I	75/76 (99%)	74 (99%)	1 (1%)	69	84
1	J	75/76 (99%)	74 (99%)	1 (1%)	69	84
1	K	75/76 (99%)	72 (96%)	3 (4%)	31	60
1	M	75/76 (99%)	75 (100%)	0	100	100
1	N	75/76 (99%)	75 (100%)	0	100	100
1	O	75/76 (99%)	74 (99%)	1 (1%)	69	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	71/71 (100%)	68 (96%)	3 (4%)	30 59
2	H	71/71 (100%)	68 (96%)	3 (4%)	30 59
2	L	71/71 (100%)	68 (96%)	3 (4%)	30 59
2	P	71/71 (100%)	68 (96%)	3 (4%)	30 59
All	All	1184/1196 (99%)	1151 (97%)	33 (3%)	43 70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	511	ASP
1	A	517	ASP
1	C	512	ILE
1	C	575	ASN
2	D	8	THR
2	D	38	ARG
2	D	46	HIS
1	E	485	ASP
1	E	505	ILE
1	E	525	ASN
1	E	529	THR
1	E	546	VAL
1	E	554	MET
1	F	491	GLU
1	F	512	ILE
1	G	485	ASP
1	G	523	GLU
1	G	549	ASP
2	H	8	THR
2	H	38	ARG
2	H	46	HIS
1	I	511	ASP
1	J	511	ASP
1	K	491	GLU
1	K	554	MET
1	K	571	LYS
2	L	8	THR
2	L	38	ARG
2	L	46	HIS
1	O	485	ASP
2	P	8	THR
2	P	38	ARG

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Mol	Chain	Res	Type
2	P	46	HIS

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

Mol	Chain	Res	Type
1	E	526	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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^{th} 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	93/96 (96%)	0.15	2 (2%) 62 60	112, 155, 211, 231	0
1	B	93/96 (96%)	0.13	2 (2%) 62 60	111, 149, 224, 256	0
1	C	93/96 (96%)	0.03	1 (1%) 80 79	99, 158, 199, 232	0
1	E	93/96 (96%)	0.10	2 (2%) 62 60	102, 162, 224, 239	0
1	F	93/96 (96%)	0.14	1 (1%) 80 79	106, 163, 230, 247	0
1	G	93/96 (96%)	0.12	1 (1%) 80 79	112, 167, 220, 254	0
1	I	93/96 (96%)	0.33	2 (2%) 62 60	113, 163, 222, 270	0
1	J	93/96 (96%)	0.30	3 (3%) 47 46	112, 162, 237, 277	0
1	K	93/96 (96%)	0.44	10 (10%) 5 7	112, 163, 244, 331	0
1	M	93/96 (96%)	0.40	10 (10%) 5 7	129, 207, 271, 305	0
1	N	93/96 (96%)	0.44	9 (9%) 7 9	129, 204, 259, 268	0
1	O	93/96 (96%)	0.52	10 (10%) 5 7	146, 207, 275, 293	1 (1%)
2	D	93/93 (100%)	-0.06	0 100 100	95, 117, 164, 177	0
2	H	93/93 (100%)	-0.18	0 100 100	101, 129, 175, 195	0
2	L	93/93 (100%)	-0.06	0 100 100	92, 119, 162, 175	0
2	P	93/93 (100%)	0.09	1 (1%) 80 79	107, 131, 159, 196	0
All	All	1488/1524 (97%)	0.18	54 (3%) 42 42	92, 158, 244, 331	1 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	487	THR	6.5
1	N	495	THR	4.7
1	O	497	LEU	4.5
1	B	494	GLY	4.1
1	O	498	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	M	496	ILE	4.0
1	N	505	ILE	3.8
1	N	494	GLY	3.6
1	M	497	LEU	3.5
1	M	499	LYS	3.4
1	I	510	ALA	3.4
1	B	510	ALA	3.2
1	O	487	THR	3.2
1	O	503	THR	3.1
1	O	491	GLU	3.0
1	F	497	LEU	3.0
1	M	510	ALA	2.9
1	E	497	LEU	2.8
1	M	509	ASN	2.8
1	A	510	ALA	2.8
1	K	496	ILE	2.8
1	I	526	GLN	2.6
1	M	494	GLY	2.6
1	K	484	GLY	2.6
1	O	501	ASN	2.6
1	K	504	ILE	2.6
1	N	496	ILE	2.5
1	M	498	VAL	2.5
1	N	504	ILE	2.5
1	K	513	THR	2.5
1	K	485	ASP	2.5
1	N	565	TYR	2.4
1	O	496	ILE	2.4
1	K	497	LEU	2.4
1	N	518	ALA	2.4
1	J	518	ALA	2.3
1	C	497	LEU	2.3
1	J	529	THR	2.3
1	O	502	VAL	2.3
1	K	502	VAL	2.3
1	N	517	ASP	2.3
1	J	514	VAL	2.3
1	E	498	VAL	2.3
1	O	572	ILE	2.3
1	O	489	THR	2.2
1	M	500	GLY	2.2
1	M	495	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	542	VAL	2.2
1	K	498	VAL	2.1
2	P	65	VAL	2.1
1	M	490	VAL	2.1
1	K	486	GLU	2.1
1	G	514	VAL	2.0
1	A	505	ILE	2.0

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
5	CL	E	601	1/1	0.43	0.10	225,225,225,225	0
5	CL	M	601	1/1	0.43	0.10	221,221,221,221	0
5	CL	D	102	1/1	0.79	0.86	150,150,150,150	1
4	ZN	D	101	1/1	0.98	0.23	123,123,123,123	0
3	MG	F	601	1/1	0.98	0.11	150,150,150,150	0
3	MG	I	601	1/1	0.98	0.11	188,188,188,188	0
3	MG	O	601	1/1	0.98	0.14	315,315,315,315	0
4	ZN	P	101	1/1	0.99	0.14	113,113,113,113	0
3	MG	B	601	1/1	0.99	0.11	160,160,160,160	0
4	ZN	H	101	1/1	0.99	0.12	133,133,133,133	0
4	ZN	L	101	1/1	0.99	0.21	127,127,127,127	0

6.5 Other polymers (i)

There are no such residues in this entry.