



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:34 AM UTC

PDB ID : 6WVV / pdb_00006wvv
Title : Plasmodium vivax M17 leucyl aminopeptidase
Authors : Malcolm, T.R.; Drinkwater, N.; McGowan, S.
Deposited on : 2020-05-07
Resolution : 2.33 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

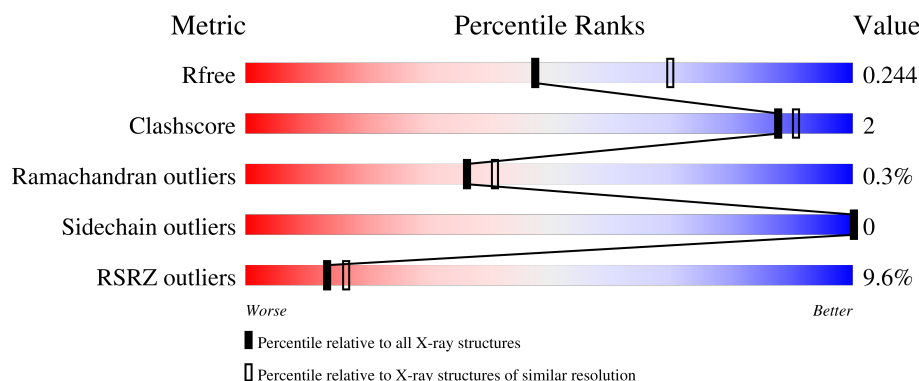
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

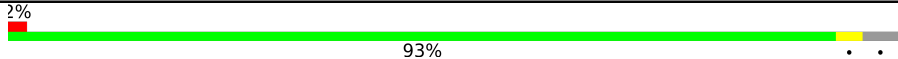
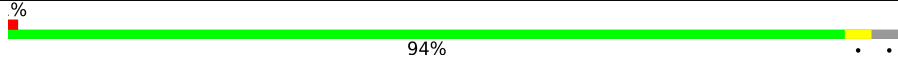
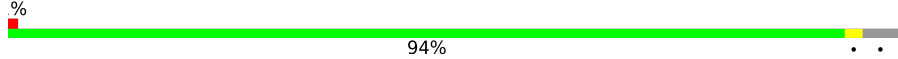
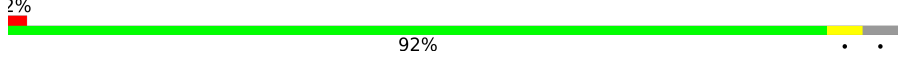
The reported resolution of this entry is 2.33 Å.

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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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 $\leq 5\%$. 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	 2% 93% . .
1	B	528	 % 94% . .
1	C	528	 % 94% . .
1	D	528	 2% 92% . .
1	E	528	 12% 87% 7% . 5%

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Mol	Chain	Length	Quality of chain
1	F	528	9% 91% 6%
1	G	528	11% 85% 12%
1	H	528	9% 86% 9%
1	I	528	12% 85% 12%
1	J	528	15% 80% 7% 13%
1	K	528	13% 78% 5% 17%
1	L	528	20% 79% 7% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 86464 atoms, of which 41597 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	509	Total	C	H	N	O	S	0	0	0
			7847	2523	3920	637	751	16			
1	B	508	Total	C	H	N	O	S	0	0	0
			7839	2519	3919	634	751	16			
1	C	507	Total	C	H	N	O	S	0	0	0
			7837	2518	3918	633	752	16			
1	D	507	Total	C	H	N	O	S	0	1	0
			7806	2512	3896	632	750	16			
1	E	503	Total	C	H	N	O	S	0	0	0
			7240	2377	3523	611	715	14			
1	F	497	Total	C	H	N	O	S	0	0	0
			7259	2366	3565	608	706	14			
1	G	466	Total	C	H	N	O	S	0	0	0
			6543	2159	3161	561	648	14			
1	H	478	Total	C	H	N	O	S	0	0	0
			6772	2228	3280	579	671	14			
1	I	467	Total	C	H	N	O	S	0	0	0
			6564	2164	3163	568	656	13			
1	J	458	Total	C	H	N	O	S	0	0	0
			6328	2095	3027	549	643	14			
1	K	440	Total	C	H	N	O	S	0	0	0
			6076	2003	2920	531	609	13			
1	L	453	Total	C	H	N	O	S	0	0	0
			6175	2053	2946	543	619	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	622	HIS	-	expression tag	UNP A0A1G4HHP8
A	623	HIS	-	expression tag	UNP A0A1G4HHP8
A	624	HIS	-	expression tag	UNP A0A1G4HHP8
A	625	HIS	-	expression tag	UNP A0A1G4HHP8
A	626	HIS	-	expression tag	UNP A0A1G4HHP8

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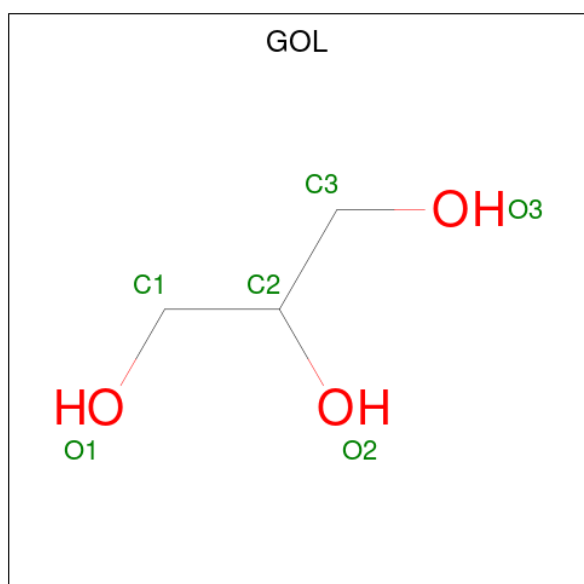
Chain	Residue	Modelled	Actual	Comment	Reference
A	627	HIS	-	expression tag	UNP A0A1G4HHP8
B	622	HIS	-	expression tag	UNP A0A1G4HHP8
B	623	HIS	-	expression tag	UNP A0A1G4HHP8
B	624	HIS	-	expression tag	UNP A0A1G4HHP8
B	625	HIS	-	expression tag	UNP A0A1G4HHP8
B	626	HIS	-	expression tag	UNP A0A1G4HHP8
B	627	HIS	-	expression tag	UNP A0A1G4HHP8
C	622	HIS	-	expression tag	UNP A0A1G4HHP8
C	623	HIS	-	expression tag	UNP A0A1G4HHP8
C	624	HIS	-	expression tag	UNP A0A1G4HHP8
C	625	HIS	-	expression tag	UNP A0A1G4HHP8
C	626	HIS	-	expression tag	UNP A0A1G4HHP8
C	627	HIS	-	expression tag	UNP A0A1G4HHP8
D	622	HIS	-	expression tag	UNP A0A1G4HHP8
D	623	HIS	-	expression tag	UNP A0A1G4HHP8
D	624	HIS	-	expression tag	UNP A0A1G4HHP8
D	625	HIS	-	expression tag	UNP A0A1G4HHP8
D	626	HIS	-	expression tag	UNP A0A1G4HHP8
D	627	HIS	-	expression tag	UNP A0A1G4HHP8
E	622	HIS	-	expression tag	UNP A0A1G4HHP8
E	623	HIS	-	expression tag	UNP A0A1G4HHP8
E	624	HIS	-	expression tag	UNP A0A1G4HHP8
E	625	HIS	-	expression tag	UNP A0A1G4HHP8
E	626	HIS	-	expression tag	UNP A0A1G4HHP8
E	627	HIS	-	expression tag	UNP A0A1G4HHP8
F	622	HIS	-	expression tag	UNP A0A1G4HHP8
F	623	HIS	-	expression tag	UNP A0A1G4HHP8
F	624	HIS	-	expression tag	UNP A0A1G4HHP8
F	625	HIS	-	expression tag	UNP A0A1G4HHP8
F	626	HIS	-	expression tag	UNP A0A1G4HHP8
F	627	HIS	-	expression tag	UNP A0A1G4HHP8
G	622	HIS	-	expression tag	UNP A0A1G4HHP8
G	623	HIS	-	expression tag	UNP A0A1G4HHP8
G	624	HIS	-	expression tag	UNP A0A1G4HHP8
G	625	HIS	-	expression tag	UNP A0A1G4HHP8
G	626	HIS	-	expression tag	UNP A0A1G4HHP8
G	627	HIS	-	expression tag	UNP A0A1G4HHP8
H	622	HIS	-	expression tag	UNP A0A1G4HHP8
H	623	HIS	-	expression tag	UNP A0A1G4HHP8
H	624	HIS	-	expression tag	UNP A0A1G4HHP8
H	625	HIS	-	expression tag	UNP A0A1G4HHP8
H	626	HIS	-	expression tag	UNP A0A1G4HHP8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	627	HIS	-	expression tag	UNP A0A1G4HHP8
I	622	HIS	-	expression tag	UNP A0A1G4HHP8
I	623	HIS	-	expression tag	UNP A0A1G4HHP8
I	624	HIS	-	expression tag	UNP A0A1G4HHP8
I	625	HIS	-	expression tag	UNP A0A1G4HHP8
I	626	HIS	-	expression tag	UNP A0A1G4HHP8
I	627	HIS	-	expression tag	UNP A0A1G4HHP8
J	622	HIS	-	expression tag	UNP A0A1G4HHP8
J	623	HIS	-	expression tag	UNP A0A1G4HHP8
J	624	HIS	-	expression tag	UNP A0A1G4HHP8
J	625	HIS	-	expression tag	UNP A0A1G4HHP8
J	626	HIS	-	expression tag	UNP A0A1G4HHP8
J	627	HIS	-	expression tag	UNP A0A1G4HHP8
K	622	HIS	-	expression tag	UNP A0A1G4HHP8
K	623	HIS	-	expression tag	UNP A0A1G4HHP8
K	624	HIS	-	expression tag	UNP A0A1G4HHP8
K	625	HIS	-	expression tag	UNP A0A1G4HHP8
K	626	HIS	-	expression tag	UNP A0A1G4HHP8
K	627	HIS	-	expression tag	UNP A0A1G4HHP8
L	622	HIS	-	expression tag	UNP A0A1G4HHP8
L	623	HIS	-	expression tag	UNP A0A1G4HHP8
L	624	HIS	-	expression tag	UNP A0A1G4HHP8
L	625	HIS	-	expression tag	UNP A0A1G4HHP8
L	626	HIS	-	expression tag	UNP A0A1G4HHP8
L	627	HIS	-	expression tag	UNP A0A1G4HHP8

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



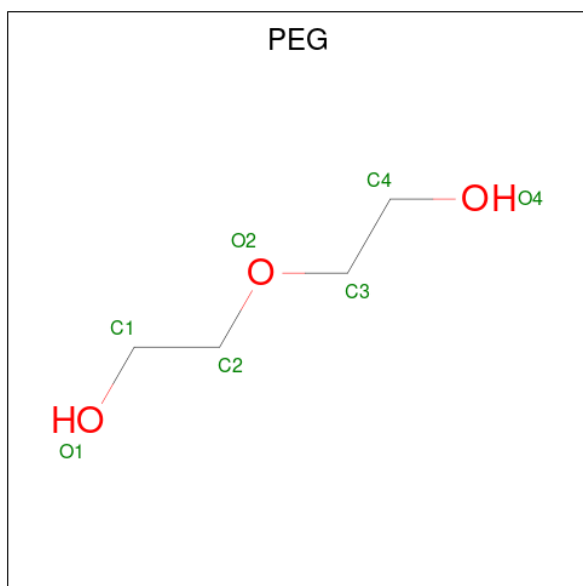
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	H	O	0	0
			14	3	8	3		
2	G	1	Total	C	H	O	0	0
			14	3	8	3		
2	H	1	Total	C	H	O	0	0
			14	3	8	3		
2	I	1	Total	C	H	O	0	0
			14	3	8	3		
2	I	1	Total	C	H	O	0	0
			14	3	8	3		
2	J	1	Total	C	H	O	0	0
			14	3	8	3		
2	J	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		
3	E	1	Total	C	H	O	0	0
			17	4	10	3		
3	E	1	Total	C	H	O	0	0
			17	4	10	3		
3	E	1	Total	C	H	O	0	0
			17	4	10	3		
3	F	1	Total	C	H	O	0	0
			17	4	10	3		
3	F	1	Total	C	H	O	0	0
			17	4	10	3		
3	G	1	Total	C	H	O	0	0
			17	4	10	3		
3	H	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

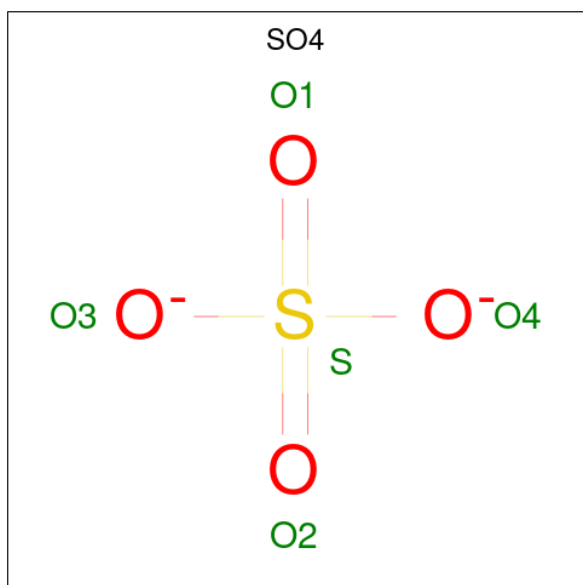
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	E	2	Total	Zn	0	0
			2	2		
4	F	2	Total	Zn	0	0
			2	2		
4	G	2	Total	Zn	0	0
			2	2		
4	H	2	Total	Zn	0	0
			2	2		
4	I	2	Total	Zn	0	0
			2	2		
4	J	2	Total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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	2	Total	Zn	0	0
			2	2		
4	L	2	Total	Zn	0	0
			2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	206	Total O 206 206	0	0
6	B	182	Total O 182 182	0	0
6	C	201	Total O 201 201	0	0
6	D	179	Total O 179 179	0	0
6	E	154	Total O 154 154	0	0
6	F	128	Total O 128 128	0	0
6	G	108	Total O 108 108	0	0
6	H	83	Total O 83 83	0	0
6	I	56	Total O 56 56	0	0
6	J	47	Total O 47 47	0	0

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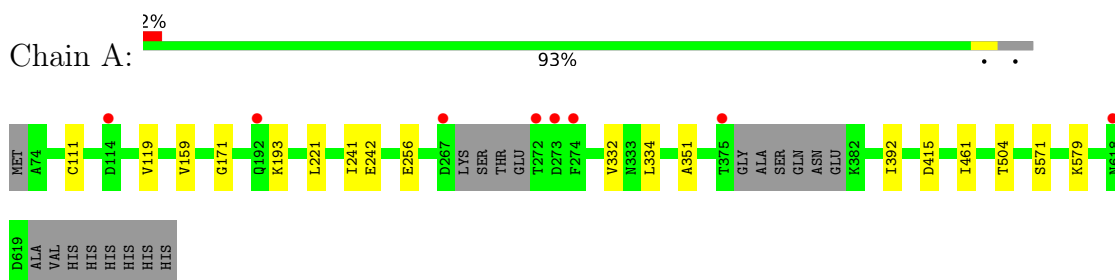
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	53	Total	O	0	0
			53	53		
6	L	44	Total	O	0	0
			44	44		

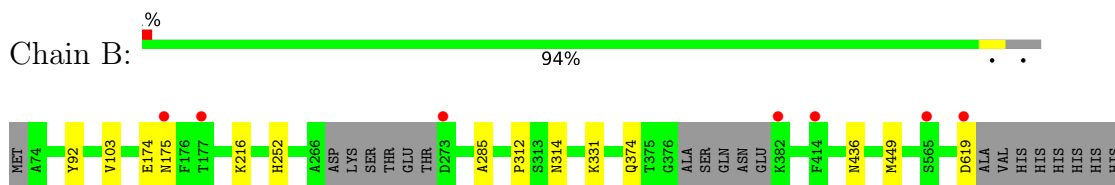
3 Residue-property plots

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.

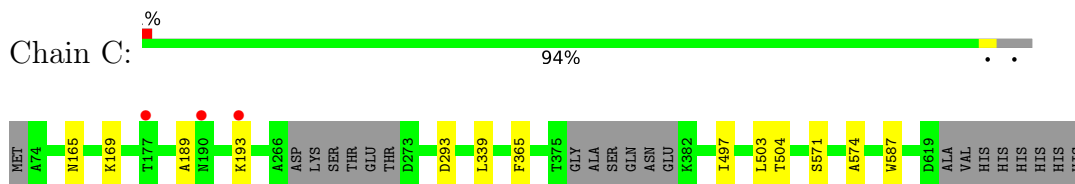
- Molecule 1: M17 leucyl aminopeptidase



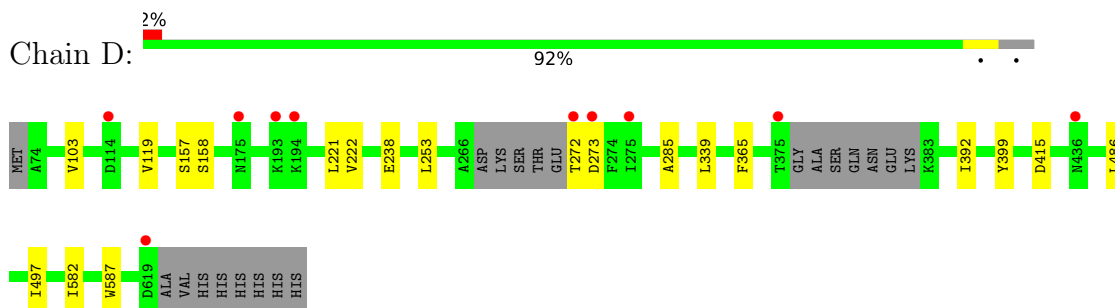
- Molecule 1: M17 leucyl aminopeptidase



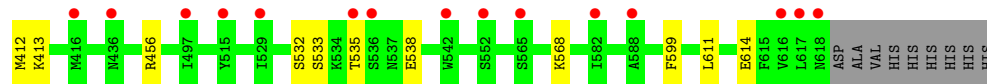
- Molecule 1: M17 leucyl aminopeptidase



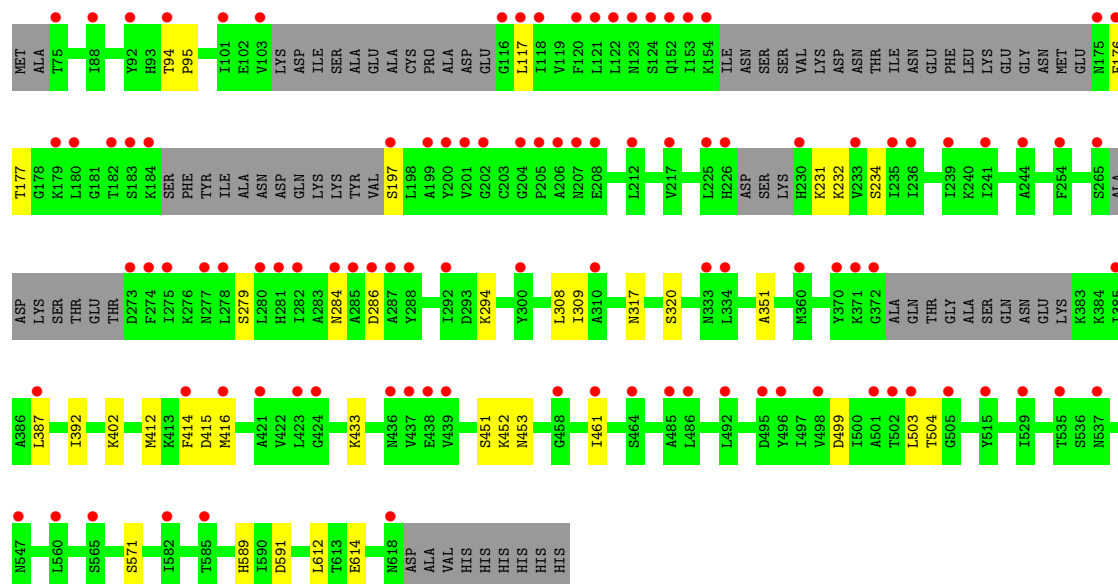
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



Chain L: 20% 79% 7% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.03Å 201.55Å 166.22Å 90.00° 106.01° 90.00°	Depositor
Resolution (Å)	44.32 – 2.33 44.32 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.32-2.33) 99.9 (44.32-2.33)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.205 , 0.243 0.207 , 0.244	Depositor DCC
R_{free} test set	15703 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	86464	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.12	0/4003	0.28	0/5421
1	B	0.12	0/3996	0.28	0/5412
1	C	0.12	0/3995	0.28	0/5411
1	D	0.11	0/3989	0.28	0/5406
1	E	0.16	0/3783	0.39	2/5137 (0.0%)
1	F	0.13	0/3759	0.29	0/5101
1	G	0.14	0/3440	0.30	0/4673
1	H	0.11	0/3554	0.28	0/4830
1	I	0.12	0/3460	0.29	0/4697
1	J	0.13	0/3355	0.28	0/4560
1	K	0.13	0/3207	0.31	0/4356
1	L	0.12	0/3284	0.29	0/4458
All	All	0.13	0/43825	0.30	2/59462 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	196	VAL	N-CA-C	5.61	121.01	109.34
1	E	195	TYR	N-CA-C	5.17	121.81	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	195	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3927	3920	3924	11	0
1	B	3920	3919	3919	10	0
1	C	3919	3918	3918	7	0
1	D	3910	3896	3896	13	0
1	E	3717	3523	3540	28	0
1	F	3694	3565	3561	10	0
1	G	3382	3161	3162	10	0
1	H	3492	3280	3281	15	0
1	I	3401	3163	3160	9	0
1	J	3301	3027	3039	20	0
1	K	3156	2920	2918	19	0
1	L	3229	2946	2948	24	0
2	A	36	47	48	0	0
2	B	18	24	24	1	0
2	C	12	16	16	0	0
2	D	18	24	24	0	0
2	E	30	40	40	1	0
2	F	18	24	24	0	0
2	G	12	16	16	0	0
2	H	6	8	8	0	0
2	I	12	16	16	2	0
2	J	18	24	24	0	0
3	A	7	10	10	0	0
3	B	14	20	20	1	0
3	C	7	10	10	0	0
3	D	7	10	10	0	0
3	E	21	30	30	1	0
3	F	14	20	20	0	0
3	G	7	10	10	1	0
3	H	7	10	10	0	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	15	0	0	0	0
5	B	15	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	G	10	0	0	0	0
5	H	5	0	0	0	0
5	I	5	0	0	0	0
5	J	5	0	0	0	0
5	K	5	0	0	0	0
5	L	10	0	0	0	0
6	A	206	0	0	2	0
6	B	182	0	0	3	0
6	C	201	0	0	1	0
6	D	179	0	0	1	0
6	E	154	0	0	3	0
6	F	128	0	0	1	0
6	G	108	0	0	3	0
6	H	83	0	0	2	0
6	I	56	0	0	2	0
6	J	47	0	0	2	0
6	K	53	0	0	2	0
6	L	44	0	0	0	0
All	All	44867	41597	41626	172	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 2.

All (172) 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)
3:G:702:PEG:O4	6:G:801:HOH:O	1.98	0.82
1:L:433:LYS:HA	1:L:433:LYS:HE2	1.62	0.79
1:E:534:LYS:NZ	6:E:802:HOH:O	2.17	0.77
1:E:165:ASN:O	1:E:168:LEU:CB	2.36	0.73
1:B:216:LYS:NZ	6:B:803:HOH:O	2.22	0.73
1:J:513:THR:OG1	6:J:801:HOH:O	2.06	0.72
1:E:346:GLU:OE2	6:E:801:HOH:O	2.09	0.69
1:B:619:ASP:O	6:B:801:HOH:O	2.11	0.69
1:I:416:MET:CE	1:I:420:ALA:HB2	2.23	0.69
1:A:256:GLU:OE1	6:A:801:HOH:O	2.11	0.68
1:L:503:LEU:HD22	1:L:504:THR:HG23	1.76	0.68
1:K:407:SER:O	6:K:801:HOH:O	2.11	0.67
1:C:293:ASP:OD2	6:C:801:HOH:O	2.15	0.63
1:L:504:THR:HG21	1:L:571:SER:HA	1.80	0.63
1:A:579:LYS:NZ	6:A:802:HOH:O	2.31	0.63
1:E:162:ASN:O	1:E:164:ILE:N	2.32	0.62
1:H:308:LEU:HB3	1:H:416:MET:HE1	1.82	0.61
1:G:524:GLN:NE2	6:G:805:HOH:O	2.33	0.61
1:G:384:LYS:NZ	6:G:802:HOH:O	2.29	0.60
1:E:189:ALA:O	1:E:193:LYS:HA	2.03	0.59
1:J:210:THR:OG1	1:J:213:GLU:OE2	2.19	0.59
1:A:119:VAL:HG11	1:A:221:LEU:HD12	1.85	0.58
1:F:187:TYR:OH	6:F:801:HOH:O	2.02	0.57
1:E:164:ILE:CB	1:E:167:PHE:HB3	2.35	0.57
1:L:504:THR:OG1	1:L:591:ASP:OD2	2.22	0.57
1:D:238:GLU:OE1	6:D:801:HOH:O	2.18	0.54
1:H:324:ALA:O	6:H:801:HOH:O	2.18	0.54
1:F:99:LEU:HD13	1:F:275:ILE:HG13	1.90	0.54
1:E:214:ILE:HD12	1:E:245:LEU:HG	1.90	0.53
1:J:537:ASN:ND2	6:J:802:HOH:O	2.34	0.53
1:E:174:GLU:O	1:E:175:ASN:CB	2.57	0.52
1:D:272:THR:OG1	1:D:273:ASP:N	2.42	0.52
1:L:308:LEU:HB3	1:L:416:MET:HE1	1.91	0.52
1:J:499:ASP:OD1	1:J:589:HIS:ND1	2.42	0.52
1:J:241:ILE:O	1:J:242:GLU:CB	2.56	0.52
1:G:105:ASP:O	1:G:109:GLU:CB	2.58	0.51
1:I:499:ASP:OD1	1:I:589:HIS:ND1	2.42	0.51
1:B:252:HIS:ND1	2:B:701:GOL:H11	2.26	0.51
1:E:162:ASN:CB	1:E:191:ASP:H	2.24	0.50
1:C:189:ALA:HB1	1:C:193:LYS:HE3	1.94	0.50
1:B:174:GLU:O	1:B:175:ASN:HB2	2.11	0.50
1:E:456:ARG:NH1	6:E:813:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:ASN:OD1	1:J:239:ILE:HG22	2.12	0.49
1:J:396:SER:OG	1:J:448:ASN:O	2.25	0.49
1:K:535:THR:CB	1:K:614:GLU:HG2	2.42	0.49
1:B:449:MET:HE3	1:D:399:TYR:CZ	2.48	0.49
1:K:409:ILE:HA	1:K:412:MET:HG2	1.95	0.48
3:B:703:PEG:O2	6:B:802:HOH:O	2.20	0.48
1:A:332:VAL:HG13	1:A:334:LEU:HG	1.95	0.48
1:E:164:ILE:O	1:E:167:PHE:HB3	2.14	0.48
1:E:164:ILE:CB	1:E:167:PHE:CB	2.92	0.48
1:G:339:LEU:HD12	1:G:339:LEU:N	2.29	0.48
1:L:499:ASP:OD1	1:L:589:HIS:ND1	2.45	0.47
1:I:183:SER:O	1:I:183:SER:OG	2.28	0.47
1:E:326:VAL:HG13	2:E:705:GOL:H2	1.96	0.47
1:C:339:LEU:HB2	1:C:365:PHE:HB3	1.96	0.47
1:F:99:LEU:O	1:F:296:ARG:NH2	2.47	0.47
1:H:80:VAL:HG22	1:H:84:ASP:OD2	2.15	0.47
1:G:470:GLU:OE1	1:G:555:SER:OG	2.33	0.47
1:J:92:TYR:HA	1:J:300:TYR:OH	2.15	0.47
1:L:176:PHE:O	1:L:177:THR:CB	2.63	0.47
1:E:191:ASP:O	1:E:192:GLN:CB	2.63	0.46
1:E:395:ASP:O	1:E:412:MET:HG3	2.15	0.46
1:I:246:PHE:O	1:I:250:LEU:HD23	2.15	0.46
1:E:332:VAL:HG23	1:E:334:LEU:HG	1.96	0.46
1:J:326:VAL:HG23	1:J:338:ILE:HD11	1.97	0.46
1:K:532:SER:OG	1:K:611:LEU:HD22	2.16	0.46
1:E:501:ALA:HB3	1:E:503:LEU:HD13	1.98	0.46
1:G:185:SER:O	1:G:186:PHE:C	2.58	0.46
1:K:568:LYS:HE2	1:K:568:LYS:HA	1.97	0.46
1:L:117:LEU:HA	1:L:197:SER:CB	2.46	0.46
1:D:103:VAL:HG12	1:D:285:ALA:HB1	1.97	0.46
1:J:284:ASN:O	1:J:286:ASP:N	2.47	0.46
1:K:360:MET:HE2	1:L:453:ASN:HA	1.97	0.46
1:L:317:ASN:H	1:L:320:SER:HG	1.64	0.46
1:E:340:ASP:OD1	1:E:364:LYS:NZ	2.47	0.46
1:H:568:LYS:NZ	6:H:815:HOH:O	2.49	0.46
1:E:339:LEU:HB2	1:E:365:PHE:HB3	1.97	0.45
1:J:590:ILE:HD13	1:J:611:LEU:HD21	1.97	0.45
1:L:284:ASN:O	1:L:286:ASP:N	2.42	0.45
1:A:504:THR:HG21	1:A:571:SER:HA	1.99	0.45
1:H:80:VAL:HG21	1:K:357:LYS:HE3	1.98	0.45
1:L:387:LEU:HD22	1:L:612:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:309:ILE:HA	1:G:416:MET:SD	2.56	0.45
1:G:234:SER:HA	1:G:279:SER:O	2.16	0.45
1:F:328:LEU:O	1:F:332:VAL:HG22	2.17	0.45
1:C:504:THR:HG21	1:C:571:SER:HA	1.99	0.45
1:D:339:LEU:HB2	1:D:365:PHE:HB3	1.98	0.45
1:F:504:THR:HG21	1:F:571:SER:HA	1.99	0.44
1:E:164:ILE:HA	1:E:167:PHE:H	1.81	0.44
1:L:231:LYS:HD2	1:L:231:LYS:H	1.82	0.44
1:A:119:VAL:HG11	1:A:221:LEU:CD1	2.46	0.44
1:F:103:VAL:HG12	1:F:285:ALA:HB1	1.99	0.44
1:K:532:SER:HB3	1:K:611:LEU:HD21	1.99	0.44
1:E:568:LYS:O	1:E:570:SER:N	2.51	0.44
1:G:503:LEU:HD22	1:G:589:HIS:CE1	2.52	0.44
1:A:111:CYS:HB3	1:A:159:VAL:HG23	1.99	0.44
1:F:161:ASP:O	1:F:162:ASN:CB	2.66	0.44
1:K:413:LYS:NZ	6:K:808:HOH:O	2.51	0.44
1:B:374:GLN:HA	1:B:436:ASN:OD1	2.18	0.43
1:B:449:MET:HE3	1:D:399:TYR:OH	2.18	0.43
1:K:408:MET:HE3	1:K:599:PHE:HE1	1.83	0.43
1:G:117:LEU:O	1:G:234:SER:N	2.50	0.43
1:L:412:MET:SD	1:L:414:PHE:HE1	2.41	0.43
1:L:309:ILE:HA	1:L:416:MET:SD	2.59	0.43
1:C:503:LEU:HD21	1:C:574:ALA:HB1	2.00	0.43
1:E:164:ILE:O	1:E:168:LEU:N	2.50	0.43
1:H:214:ILE:CG1	1:H:245:LEU:HD11	2.49	0.43
1:H:106:ILE:O	1:H:110:ALA:HB2	2.19	0.43
2:I:702:GOL:H12	1:J:461:ILE:HG22	2.01	0.43
1:A:241:ILE:HG22	1:A:242:GLU:O	2.19	0.43
1:H:80:VAL:CG1	1:H:360:MET:HE1	2.49	0.43
1:E:467:LYS:NZ	1:E:580:GLU:O	2.49	0.43
1:I:505:GLY:H	2:I:701:GOL:HO3	1.65	0.43
1:J:451:SER:OG	1:J:452:LYS:N	2.52	0.42
1:F:391:GLY:O	1:F:445:VAL:HA	2.20	0.42
1:H:80:VAL:HG21	1:K:357:LYS:HG2	2.00	0.42
1:H:449:MET:HE1	1:K:456:ARG:HG2	2.00	0.42
1:I:510:SER:OG	1:I:511:LEU:N	2.42	0.42
1:J:236:ILE:HA	1:J:281:HIS:N	2.34	0.42
1:K:532:SER:C	1:K:611:LEU:CD2	2.92	0.42
1:H:510:SER:OG	1:H:511:LEU:N	2.43	0.42
1:L:94:THR:HG22	1:L:95:PRO:HD2	2.02	0.42
1:L:234:SER:HA	1:L:279:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:LEU:HD22	1:E:370:TYR:HB2	2.01	0.42
1:K:354:SER:HA	1:K:357:LYS:HG3	2.01	0.42
1:D:157:SER:OG	1:D:158:SER:N	2.53	0.42
1:D:392:ILE:HB	1:D:415:ASP:HB3	2.01	0.42
1:D:486:LEU:HD22	1:D:582:ILE:HD11	2.02	0.42
1:D:497:ILE:O	1:D:587:TRP:HA	2.20	0.42
1:F:80:VAL:HG23	1:F:360:MET:HE1	2.01	0.42
1:I:92:TYR:N	6:I:806:HOH:O	2.43	0.42
1:J:455:TYR:CE2	1:J:471:VAL:HG11	2.55	0.42
1:L:402:LYS:HE3	1:L:412:MET:SD	2.59	0.42
1:H:309:ILE:HA	1:H:416:MET:SD	2.60	0.42
1:B:103:VAL:HG12	1:B:285:ALA:HB1	2.02	0.42
1:E:570:SER:HB2	3:E:707:PEG:H12	2.01	0.42
1:A:392:ILE:HB	1:A:415:ASP:HB3	2.00	0.41
1:B:92:TYR:CZ	1:B:331:LYS:HE3	2.54	0.41
1:H:451:SER:OG	1:H:452:LYS:N	2.53	0.41
1:E:392:ILE:HB	1:E:415:ASP:HB3	2.01	0.41
1:K:211:GLU:OE1	1:K:215:ARG:NH2	2.51	0.41
1:K:533:SER:OG	1:K:538:GLU:O	2.37	0.41
1:L:451:SER:OG	1:L:452:LYS:N	2.54	0.41
1:K:317:ASN:HB2	1:K:318:PRO:HD2	2.02	0.41
1:H:213:GLU:O	1:H:217:VAL:HG23	2.20	0.41
1:J:531:SER:O	1:J:535:THR:HG23	2.20	0.41
1:D:119:VAL:HG21	1:D:221:LEU:HD13	2.02	0.41
1:L:309:ILE:HG12	1:L:416:MET:SD	2.61	0.41
1:L:392:ILE:HB	1:L:415:ASP:HB3	2.02	0.41
1:H:105:ASP:HA	1:H:285:ALA:HB2	2.02	0.41
1:L:231:LYS:HG2	1:L:232:LYS:N	2.35	0.41
1:C:497:ILE:O	1:C:587:TRP:HA	2.21	0.41
1:D:582:ILE:HD13	1:D:582:ILE:HA	1.95	0.41
1:E:477:GLU:OE1	1:E:477:GLU:N	2.45	0.41
1:J:500:ILE:HD11	1:J:592:ILE:HG21	2.02	0.41
1:E:96:ILE:O	1:E:296:ARG:NH2	2.54	0.41
1:J:317:ASN:HB2	1:J:318:PRO:HD2	2.03	0.41
1:J:388:ILE:HD12	1:J:486:LEU:HD23	2.02	0.41
1:J:500:ILE:HD11	1:J:592:ILE:HD13	2.03	0.41
1:L:294:LYS:NZ	1:L:614:GLU:OE2	2.53	0.41
1:L:351:ALA:HA	1:L:461:ILE:HD12	2.03	0.41
1:A:351:ALA:HA	1:A:461:ILE:HD12	2.02	0.41
1:B:312:PRO:HB2	1:B:314:ASN:OD1	2.21	0.40
1:F:339:LEU:HB2	1:F:365:PHE:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:456:ARG:NH1	6:I:811:HOH:O	2.51	0.40
1:C:165:ASN:OD1	1:C:169:LYS:HE2	2.22	0.40
1:D:222:VAL:HG23	1:D:253:LEU:HD12	2.04	0.40
1:A:193:LYS:N	1:A:193:LYS:HD2	2.37	0.40
1:I:351:ALA:HA	1:I:461:ILE:HD12	2.03	0.40
1:K:233:VAL:O	1:K:278:LEU:HA	2.22	0.40
1:K:303:TYR:O	1:K:307:GLN:HG3	2.22	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	503/528 (95%)	490 (97%)	12 (2%)	1 (0%)	43	50
1	B	502/528 (95%)	490 (98%)	12 (2%)	0	100	100
1	C	501/528 (95%)	488 (97%)	13 (3%)	0	100	100
1	D	502/528 (95%)	490 (98%)	12 (2%)	0	100	100
1	E	491/528 (93%)	464 (94%)	19 (4%)	8 (2%)	7	5
1	F	484/528 (92%)	466 (96%)	17 (4%)	1 (0%)	43	50
1	G	452/528 (86%)	435 (96%)	15 (3%)	2 (0%)	30	32
1	H	468/528 (89%)	443 (95%)	23 (5%)	2 (0%)	30	32
1	I	453/528 (86%)	433 (96%)	18 (4%)	2 (0%)	30	32
1	J	442/528 (84%)	420 (95%)	20 (4%)	2 (0%)	24	26
1	K	426/528 (81%)	410 (96%)	15 (4%)	1 (0%)	43	50
1	L	439/528 (83%)	415 (94%)	24 (6%)	0	100	100
All	All	5663/6336 (89%)	5444 (96%)	200 (4%)	19 (0%)	36	41

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	163	THR
1	E	192	GLN
1	F	273	ASP
1	I	112	PRO
1	I	205	PRO
1	J	242	GLU
1	E	175	ASN
1	E	194	LYS
1	E	108	ALA
1	E	569	ALA
1	G	185	SER
1	H	113	ALA
1	E	193	LYS
1	E	195	TYR
1	G	231	LYS
1	K	182	THR
1	J	230	HIS
1	A	171	GLY
1	H	111	CYS

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	425/448 (95%)	425 (100%)	0	100	100
1	B	425/448 (95%)	425 (100%)	0	100	100
1	C	426/448 (95%)	426 (100%)	0	100	100
1	D	423/448 (94%)	423 (100%)	0	100	100
1	E	372/448 (83%)	372 (100%)	0	100	100
1	F	373/448 (83%)	373 (100%)	0	100	100
1	G	325/448 (72%)	325 (100%)	0	100	100
1	H	337/448 (75%)	337 (100%)	0	100	100
1	I	325/448 (72%)	325 (100%)	0	100	100
1	J	315/448 (70%)	315 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	298/448 (66%)	298 (100%)	0	100	100
1	L	296/448 (66%)	296 (100%)	0	100	100
All	All	4340/5376 (81%)	4340 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	GLN
1	B	207	ASN
1	C	230	HIS
1	C	277	ASN
1	D	230	HIS
1	E	207	ASN
1	E	281	HIS
1	F	152	GLN
1	F	207	ASN
1	G	207	ASN
1	G	330	GLN
1	I	252	HIS
1	I	537	ASN
1	J	226	HIS
1	J	252	HIS
1	K	79	GLN
1	L	537	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 84 ligands modelled in this entry, 24 are monoatomic - leaving 60 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	E	703	-	5,5,5	0.75	0	5,5,5	1.02	0
2	GOL	G	701	-	5,5,5	0.84	0	5,5,5	1.02	0
3	PEG	E	707	-	6,6,6	0.49	0	5,5,5	0.26	0
5	SO4	F	708	-	4,4,4	0.23	0	6,6,6	0.21	0
5	SO4	J	706	-	4,4,4	0.23	0	6,6,6	0.14	0
5	SO4	B	708	-	4,4,4	0.25	0	6,6,6	0.33	0
3	PEG	F	703	4	6,6,6	0.52	0	5,5,5	0.41	0
3	PEG	B	704	-	6,6,6	0.50	0	5,5,5	0.44	0
2	GOL	F	705	-	5,5,5	0.95	0	5,5,5	0.94	0
3	PEG	D	702	-	6,6,6	0.50	0	5,5,5	0.26	0
5	SO4	L	704	-	4,4,4	0.23	0	6,6,6	0.16	0
2	GOL	C	701	-	5,5,5	0.84	0	5,5,5	1.10	0
5	SO4	K	703	-	4,4,4	0.23	0	6,6,6	0.15	0
2	GOL	I	702	-	5,5,5	0.89	0	5,5,5	1.07	0
5	SO4	L	703	-	4,4,4	0.24	0	6,6,6	0.16	0
3	PEG	C	702	-	6,6,6	0.50	0	5,5,5	0.37	0
2	GOL	C	703	-	5,5,5	0.88	0	5,5,5	1.05	0
3	PEG	G	702	-	6,6,6	0.50	0	5,5,5	0.27	0
2	GOL	E	702	-	5,5,5	0.86	0	5,5,5	1.10	0
2	GOL	A	702	-	5,5,5	0.90	0	5,5,5	1.16	1 (20%)
3	PEG	B	703	-	6,6,6	0.50	0	5,5,5	0.22	0
5	SO4	I	705	-	4,4,4	0.26	0	6,6,6	0.21	0
2	GOL	E	705	-	5,5,5	0.82	0	5,5,5	1.04	0
5	SO4	D	707	-	4,4,4	0.26	0	6,6,6	0.11	0
2	GOL	E	701	-	5,5,5	0.87	0	5,5,5	1.05	0
5	SO4	A	711	-	4,4,4	0.22	0	6,6,6	0.20	0
5	SO4	H	705	-	4,4,4	0.22	0	6,6,6	0.06	0
3	PEG	A	703	-	6,6,6	0.49	0	5,5,5	0.42	0
3	PEG	E	706	-	6,6,6	0.49	0	5,5,5	0.38	0
2	GOL	A	706	-	5,5,5	0.86	0	5,5,5	1.03	0
2	GOL	D	701	-	5,5,5	0.90	0	5,5,5	1.08	0
2	GOL	E	704	-	5,5,5	0.88	0	5,5,5	1.14	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	705	-	5,5,5	0.89	0	5,5,5	1.12	0
5	SO4	C	706	-	4,4,4	0.22	0	6,6,6	0.11	0
2	GOL	J	701	-	5,5,5	0.91	0	5,5,5	1.06	0
2	GOL	G	703	-	5,5,5	0.82	0	5,5,5	1.09	0
2	GOL	D	704	-	5,5,5	0.92	0	5,5,5	1.07	0
3	PEG	H	702	-	6,6,6	0.50	0	5,5,5	0.30	0
2	GOL	J	703	-	5,5,5	0.93	0	5,5,5	1.10	1 (20%)
2	GOL	F	701	-	5,5,5	0.91	0	5,5,5	1.06	0
5	SO4	G	706	-	4,4,4	0.26	0	6,6,6	0.14	0
2	GOL	A	705	-	5,5,5	0.86	0	5,5,5	1.07	0
5	SO4	E	711	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	G	707	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	A	710	-	4,4,4	0.26	0	6,6,6	0.09	0
2	GOL	D	703	-	5,5,5	0.83	0	5,5,5	1.00	0
2	GOL	A	707	-	5,5,5	0.89	0	5,5,5	1.10	0
2	GOL	A	704	-	5,5,5	0.84	0	5,5,5	1.18	1 (20%)
2	GOL	I	701	-	5,5,5	0.95	0	5,5,5	1.15	1 (20%)
2	GOL	J	702	-	5,5,5	0.84	0	5,5,5	1.15	1 (20%)
2	GOL	B	702	-	5,5,5	0.89	0	5,5,5	1.14	0
2	GOL	F	702	-	5,5,5	1.05	0	5,5,5	1.13	1 (20%)
5	SO4	A	712	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	B	709	-	4,4,4	0.26	0	6,6,6	0.18	0
2	GOL	A	701	-	5,5,5	0.91	0	5,5,5	1.06	0
2	GOL	H	701	-	5,5,5	0.88	0	5,5,5	1.13	1 (20%)
3	PEG	E	708	-	6,6,6	0.49	0	5,5,5	0.25	0
3	PEG	F	704	-	6,6,6	0.50	0	5,5,5	0.43	0
5	SO4	B	710	-	4,4,4	0.24	0	6,6,6	0.13	0
2	GOL	B	701	-	5,5,5	1.01	0	5,5,5	1.20	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	703	-	-	2/4/4/4	-
2	GOL	G	701	-	-	2/4/4/4	-
3	PEG	E	707	-	-	2/4/4/4	-
3	PEG	F	703	4	-	3/4/4/4	-
3	PEG	B	704	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	F	705	-	-	2/4/4/4	-
3	PEG	D	702	-	-	2/4/4/4	-
2	GOL	C	701	-	-	2/4/4/4	-
2	GOL	I	702	-	-	2/4/4/4	-
3	PEG	C	702	-	-	3/4/4/4	-
2	GOL	C	703	-	-	0/4/4/4	-
3	PEG	G	702	-	-	2/4/4/4	-
2	GOL	E	702	-	-	0/4/4/4	-
2	GOL	A	702	-	-	2/4/4/4	-
3	PEG	B	703	-	-	1/4/4/4	-
2	GOL	E	705	-	-	2/4/4/4	-
2	GOL	E	701	-	-	0/4/4/4	-
3	PEG	A	703	-	-	2/4/4/4	-
3	PEG	E	706	-	-	1/4/4/4	-
2	GOL	A	706	-	-	0/4/4/4	-
2	GOL	D	701	-	-	2/4/4/4	-
2	GOL	E	704	-	-	0/4/4/4	-
2	GOL	B	705	-	-	2/4/4/4	-
2	GOL	J	701	-	-	1/4/4/4	-
2	GOL	G	703	-	-	0/4/4/4	-
2	GOL	D	704	-	-	1/4/4/4	-
3	PEG	H	702	-	-	1/4/4/4	-
2	GOL	J	703	-	-	0/4/4/4	-
2	GOL	F	701	-	-	0/4/4/4	-
2	GOL	A	705	-	-	2/4/4/4	-
2	GOL	D	703	-	-	3/4/4/4	-
2	GOL	A	707	-	-	2/4/4/4	-
2	GOL	A	704	-	-	0/4/4/4	-
2	GOL	I	701	-	-	0/4/4/4	-
2	GOL	J	702	-	-	2/4/4/4	-
2	GOL	B	702	-	-	0/4/4/4	-
2	GOL	F	702	-	-	0/4/4/4	-
2	GOL	A	701	-	-	0/4/4/4	-
2	GOL	H	701	-	-	0/4/4/4	-
3	PEG	E	708	-	-	0/4/4/4	-
3	PEG	F	704	-	-	3/4/4/4	-
2	GOL	B	701	-	-	2/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	GOL	C3-C2-C1	-2.19	103.78	111.80
2	I	701	GOL	C3-C2-C1	-2.10	104.08	111.80
2	A	704	GOL	C3-C2-C1	-2.07	104.20	111.80
2	H	701	GOL	C3-C2-C1	-2.07	104.20	111.80
2	A	702	GOL	C3-C2-C1	-2.07	104.22	111.80
2	F	702	GOL	C3-C2-C1	-2.06	104.23	111.80
2	E	704	GOL	C3-C2-C1	-2.06	104.26	111.80
2	J	702	GOL	C3-C2-C1	-2.02	104.37	111.80
2	J	703	GOL	C3-C2-C1	-2.02	104.39	111.80

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	GOL	C1-C2-C3-O3
2	B	701	GOL	C1-C2-C3-O3
2	B	705	GOL	C1-C2-C3-O3
2	E	703	GOL	O1-C1-C2-C3
2	F	705	GOL	C1-C2-C3-O3
2	G	701	GOL	C1-C2-C3-O3
2	G	701	GOL	O2-C2-C3-O3
2	I	702	GOL	C1-C2-C3-O3
2	J	702	GOL	C1-C2-C3-O3
3	C	702	PEG	O2-C3-C4-O4
3	H	702	PEG	O1-C1-C2-O2
2	A	705	GOL	O1-C1-C2-C3
2	C	701	GOL	O1-C1-C2-C3
2	D	703	GOL	O1-C1-C2-C3
2	E	705	GOL	O1-C1-C2-C3
2	A	702	GOL	O2-C2-C3-O3
2	B	701	GOL	O2-C2-C3-O3
2	E	703	GOL	O1-C1-C2-O2
2	E	705	GOL	O1-C1-C2-O2
2	F	705	GOL	O2-C2-C3-O3
2	I	702	GOL	O2-C2-C3-O3
2	J	702	GOL	O2-C2-C3-O3
3	E	707	PEG	O1-C1-C2-O2
2	B	705	GOL	O2-C2-C3-O3
3	G	702	PEG	O1-C1-C2-O2
2	C	701	GOL	O1-C1-C2-O2
2	J	701	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	702	PEG	O1-C1-C2-O2
2	D	703	GOL	O2-C2-C3-O3
3	C	702	PEG	C1-C2-O2-C3
3	B	704	PEG	C1-C2-O2-C3
3	B	704	PEG	O2-C3-C4-O4
3	B	704	PEG	C4-C3-O2-C2
3	F	704	PEG	C4-C3-O2-C2
3	F	704	PEG	C1-C2-O2-C3
3	F	704	PEG	O2-C3-C4-O4
3	D	702	PEG	C1-C2-O2-C3
3	G	702	PEG	O2-C3-C4-O4
2	A	707	GOL	O1-C1-C2-C3
2	D	701	GOL	C1-C2-C3-O3
2	D	701	GOL	O2-C2-C3-O3
3	E	707	PEG	C1-C2-O2-C3
2	A	705	GOL	O1-C1-C2-O2
2	D	703	GOL	O1-C1-C2-O2
2	D	704	GOL	O2-C2-C3-O3
2	A	707	GOL	O1-C1-C2-O2
3	E	706	PEG	O2-C3-C4-O4
3	B	703	PEG	O1-C1-C2-O2
3	F	703	PEG	O2-C3-C4-O4
3	F	703	PEG	C1-C2-O2-C3
3	D	702	PEG	O1-C1-C2-O2
3	F	703	PEG	C4-C3-O2-C2
3	A	703	PEG	O1-C1-C2-O2
3	A	703	PEG	C4-C3-O2-C2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	707	PEG	1	0
2	I	702	GOL	1	0
3	G	702	PEG	1	0
3	B	703	PEG	1	0
2	E	705	GOL	1	0
2	I	701	GOL	1	0
2	B	701	GOL	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, 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	509/528 (96%)	-0.07	8 (1%) 70 75	24, 34, 57, 72	0
1	B	508/528 (96%)	-0.08	7 (1%) 73 77	24, 34, 54, 73	0
1	C	507/528 (96%)	-0.14	3 (0%) 85 88	23, 33, 50, 73	0
1	D	507/528 (96%)	0.00	10 (1%) 65 70	24, 36, 54, 74	1 (0%)
1	E	503/528 (95%)	0.40	61 (12%) 8 10	25, 37, 76, 90	0
1	F	497/528 (94%)	0.40	48 (9%) 13 16	25, 39, 75, 85	0
1	G	466/528 (88%)	0.51	57 (12%) 8 10	30, 42, 78, 93	0
1	H	478/528 (90%)	0.58	48 (10%) 12 15	34, 46, 78, 94	0
1	I	467/528 (88%)	0.96	65 (13%) 6 7	36, 54, 80, 98	0
1	J	458/528 (86%)	1.04	79 (17%) 4 4	38, 58, 83, 97	0
1	K	440/528 (83%)	1.12	69 (15%) 5 5	38, 57, 79, 90	0
1	L	453/528 (85%)	1.29	103 (22%) 2 2	42, 59, 84, 100	0
All	All	5793/6336 (91%)	0.48	558 (9%) 13 16	23, 44, 77, 100	1 (0%)

All (558) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	186	PHE	5.9
1	K	124	SER	5.8
1	E	185	SER	5.7
1	H	112	PRO	5.3
1	E	161	ASP	5.3
1	F	167	PHE	5.2
1	G	186	PHE	5.1
1	E	165	ASN	5.0
1	E	187	TYR	5.0
1	E	163	THR	4.9
1	F	273	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	195	TYR	4.9
1	F	164	ILE	4.9
1	E	194	LYS	4.8
1	E	188	ILE	4.8
1	I	284	ASN	4.8
1	G	111	CYS	4.7
1	K	103	VAL	4.7
1	J	230	HIS	4.6
1	K	274	PHE	4.6
1	I	228	SER	4.5
1	L	275	ILE	4.5
1	E	189	ALA	4.5
1	G	156	ASN	4.5
1	I	103	VAL	4.4
1	E	230	HIS	4.3
1	G	375	THR	4.3
1	E	114	ASP	4.3
1	G	619	ASP	4.3
1	I	111	CYS	4.3
1	H	173	MET	4.3
1	E	172	ASN	4.3
1	K	373	ALA	4.2
1	G	75	THR	4.2
1	J	153	ILE	4.2
1	L	101	ILE	4.2
1	J	284	ASN	4.2
1	E	169	LYS	4.2
1	L	385	ILE	4.2
1	J	618	ASN	4.2
1	J	237	PHE	4.2
1	H	200	TYR	4.2
1	G	185	SER	4.1
1	L	103	VAL	4.1
1	L	284	ASN	4.1
1	E	113	ALA	4.1
1	F	195	TYR	4.1
1	L	274	PHE	4.1
1	G	241	ILE	4.1
1	F	111	CYS	4.1
1	K	123	ASN	4.1
1	L	235	ILE	4.1
1	K	120	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	173	MET	4.0
1	J	180	LEU	4.0
1	L	123	ASN	4.0
1	G	177	THR	4.0
1	L	153	ILE	4.0
1	E	111	CYS	4.0
1	E	619	ASP	4.0
1	E	196	VAL	3.9
1	H	176	PHE	3.9
1	C	190	ASN	3.9
1	F	175	ASN	3.9
1	H	175	ASN	3.9
1	E	164	ILE	3.9
1	E	198	LEU	3.9
1	F	189	ALA	3.9
1	L	286	ASP	3.9
1	I	107	SER	3.9
1	E	192	GLN	3.9
1	K	436	ASN	3.9
1	F	228	SER	3.8
1	I	197	SER	3.8
1	I	241	ILE	3.8
1	I	105	ASP	3.8
1	J	281	HIS	3.8
1	H	375	THR	3.8
1	I	205	PRO	3.8
1	J	106	ILE	3.8
1	F	230	HIS	3.8
1	I	273	ASP	3.7
1	L	285	ALA	3.7
1	F	161	ASP	3.7
1	F	162	ASN	3.7
1	K	618	ASN	3.7
1	G	237	PHE	3.7
1	E	116	GLY	3.7
1	I	225	LEU	3.7
1	E	191	ASP	3.7
1	K	177	THR	3.7
1	F	159	VAL	3.7
1	G	275	ILE	3.6
1	L	414	PHE	3.6
1	J	121	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	122	LEU	3.6
1	L	117	LEU	3.6
1	F	165	ASN	3.6
1	D	619	ASP	3.6
1	K	284	ASN	3.6
1	J	184	LYS	3.6
1	K	219	TYR	3.6
1	K	416	MET	3.6
1	K	497	ILE	3.6
1	I	153	ILE	3.5
1	B	273	ASP	3.5
1	H	114	ASP	3.5
1	H	183	SER	3.5
1	L	154	LYS	3.5
1	I	180	LEU	3.5
1	L	498	VAL	3.5
1	K	565	SER	3.5
1	K	288	TYR	3.5
1	F	272	THR	3.4
1	J	103	VAL	3.4
1	K	292	ILE	3.4
1	D	273	ASP	3.4
1	I	114	ASP	3.4
1	G	274	PHE	3.4
1	I	118	ILE	3.4
1	K	224	LEU	3.4
1	L	201	VAL	3.4
1	H	196	VAL	3.4
1	K	203	CYS	3.4
1	F	191	ASP	3.4
1	H	227	ASP	3.4
1	J	241	ILE	3.3
1	F	174	GLU	3.3
1	L	208	GLU	3.3
1	J	227	ASP	3.3
1	G	118	ILE	3.3
1	I	106	ILE	3.3
1	I	115	GLU	3.3
1	K	257	TYR	3.3
1	F	157	SER	3.3
1	J	102	GLU	3.3
1	K	233	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	501	ALA	3.3
1	G	273	ASP	3.3
1	G	106	ILE	3.3
1	H	274	PHE	3.3
1	G	228	SER	3.3
1	K	536	SER	3.3
1	J	437	VAL	3.3
1	F	114	ASP	3.2
1	I	227	ASP	3.2
1	I	224	LEU	3.2
1	L	230	HIS	3.2
1	K	183	SER	3.2
1	L	124	SER	3.2
1	L	288	TYR	3.2
1	A	114	ASP	3.2
1	F	109	GLU	3.2
1	J	104	LYS	3.2
1	I	121	LEU	3.2
1	K	121	LEU	3.2
1	L	225	LEU	3.2
1	L	280	LEU	3.2
1	J	277	ASN	3.2
1	I	235	ILE	3.2
1	J	275	ILE	3.2
1	J	291	GLN	3.2
1	I	177	THR	3.2
1	G	279	SER	3.2
1	J	566	SER	3.2
1	J	199	ALA	3.2
1	J	219	TYR	3.2
1	J	436	ASN	3.2
1	K	207	ASN	3.2
1	L	205	PRO	3.2
1	L	585	THR	3.2
1	E	166	GLU	3.1
1	L	310	ALA	3.1
1	L	485	ALA	3.1
1	K	616	VAL	3.1
1	G	282	ILE	3.1
1	E	108	ALA	3.1
1	G	284	ASN	3.1
1	J	105	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	200	TYR	3.1
1	H	107	SER	3.1
1	F	156	ASN	3.1
1	L	277	ASN	3.1
1	L	152	GLN	3.1
1	E	109	GLU	3.1
1	A	272	THR	3.1
1	I	375	THR	3.1
1	J	182	THR	3.1
1	K	286	ASP	3.1
1	H	110	ALA	3.1
1	H	113	ALA	3.1
1	J	386	ALA	3.1
1	K	117	LEU	3.1
1	F	101	ILE	3.0
1	J	292	ILE	3.0
1	K	239	ILE	3.0
1	H	197	SER	3.0
1	A	273	ASP	3.0
1	L	437	VAL	3.0
1	A	375	THR	3.0
1	E	103	VAL	3.0
1	G	280	LEU	3.0
1	L	438	GLU	3.0
1	L	560	LEU	3.0
1	G	101	ILE	3.0
1	J	200	TYR	3.0
1	K	182	THR	3.0
1	L	182	THR	3.0
1	K	231	LYS	3.0
1	J	197	SER	3.0
1	J	332	VAL	3.0
1	G	155	ILE	3.0
1	H	118	ILE	3.0
1	I	239	ILE	3.0
1	K	282	ILE	3.0
1	F	187	TYR	3.0
1	L	370	TYR	3.0
1	L	496	TYR	3.0
1	G	124	SER	3.0
1	L	204	GLY	3.0
1	J	120	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	274	PHE	2.9
1	F	108	ALA	2.9
1	L	278	LEU	2.9
1	K	582	ILE	2.9
1	I	223	THR	2.9
1	G	107	SER	2.9
1	L	207	ASN	2.9
1	I	120	PHE	2.9
1	G	121	LEU	2.9
1	K	588	ALA	2.9
1	L	486	LEU	2.9
1	G	153	ILE	2.9
1	K	529	ILE	2.9
1	E	173	MET	2.9
1	H	158	SER	2.9
1	I	204	GLY	2.9
1	J	229	LYS	2.9
1	L	120	PHE	2.9
1	L	121	LEU	2.9
1	L	122	LEU	2.9
1	G	103	VAL	2.9
1	H	106	ILE	2.9
1	J	282	ILE	2.9
1	K	118	ILE	2.9
1	F	166	GLU	2.9
1	D	114	ASP	2.9
1	E	107	SER	2.9
1	L	179	LYS	2.9
1	H	233	VAL	2.9
1	H	326	VAL	2.9
1	E	106	ILE	2.9
1	E	272	THR	2.9
1	D	175	ASN	2.9
1	L	116	GLY	2.8
1	F	176	PHE	2.8
1	L	254	PHE	2.8
1	L	233	VAL	2.8
1	C	177	THR	2.8
1	G	223	THR	2.8
1	I	203	CYS	2.8
1	J	385	ILE	2.8
1	K	235	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	227	ASP	2.8
1	L	618	ASN	2.8
1	G	230	HIS	2.8
1	G	278	LEU	2.8
1	I	122	LEU	2.8
1	L	423	LEU	2.8
1	H	108	ALA	2.8
1	E	267	ASP	2.8
1	K	116	GLY	2.8
1	E	168	LEU	2.8
1	H	109	GLU	2.8
1	K	237	PHE	2.8
1	K	249	PHE	2.8
1	E	184	LYS	2.8
1	J	439	VAL	2.8
1	F	155	ILE	2.8
1	E	190	ASN	2.8
1	I	207	ASN	2.8
1	J	152	GLN	2.8
1	E	115	GLU	2.8
1	D	375	THR	2.7
1	F	153	ILE	2.7
1	F	618	ASN	2.7
1	D	193	LYS	2.7
1	I	257	TYR	2.7
1	H	226	HIS	2.7
1	I	286	ASP	2.7
1	L	241	ILE	2.7
1	G	184	LYS	2.7
1	K	122	LEU	2.7
1	G	287	ALA	2.7
1	J	370	TYR	2.7
1	E	167	PHE	2.7
1	F	193	LYS	2.7
1	L	197	SER	2.7
1	I	117	LEU	2.7
1	L	287	ALA	2.7
1	B	619	ASP	2.7
1	L	175	ASN	2.7
1	L	292	ILE	2.7
1	J	198	LEU	2.7
1	G	200	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	515	TYR	2.6
1	F	106	ILE	2.6
1	H	153	ILE	2.6
1	F	192	GLN	2.6
1	H	600	LYS	2.6
1	J	285	ALA	2.6
1	E	271	GLU	2.6
1	E	162	ASN	2.6
1	L	273	ASP	2.6
1	B	177	THR	2.6
1	I	116	GLY	2.6
1	L	94	THR	2.6
1	I	416	MET	2.6
1	L	529	ILE	2.6
1	G	104	LYS	2.6
1	E	175	ASN	2.6
1	J	293	ASP	2.6
1	I	254	PHE	2.6
1	F	375	THR	2.6
1	L	424	GLY	2.6
1	I	236	ILE	2.6
1	L	183	SER	2.6
1	L	582	ILE	2.6
1	H	230	HIS	2.6
1	L	184	LYS	2.6
1	E	227	ASP	2.6
1	J	205	PRO	2.6
1	K	241	ILE	2.6
1	L	565	SER	2.6
1	H	229	LYS	2.6
1	G	224	LEU	2.5
1	H	111	CYS	2.5
1	K	285	ALA	2.5
1	I	619	ASP	2.5
1	H	504	THR	2.5
1	K	76	THR	2.5
1	L	505	GLY	2.5
1	E	119	VAL	2.5
1	D	275	ILE	2.5
1	E	565	SER	2.5
1	F	158	SER	2.5
1	F	196	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	207	ASN	2.5
1	C	193	LYS	2.5
1	K	290	GLY	2.5
1	I	182	THR	2.5
1	J	222	VAL	2.5
1	J	529	ILE	2.5
1	G	109	GLU	2.5
1	H	117	LEU	2.5
1	H	122	LEU	2.5
1	L	212	LEU	2.5
1	L	371	LYS	2.5
1	J	434	PRO	2.5
1	J	535	THR	2.5
1	K	535	THR	2.5
1	I	101	ILE	2.5
1	J	494	VAL	2.5
1	G	154	LYS	2.5
1	F	190	ASN	2.5
1	G	105	ASP	2.5
1	J	283	ALA	2.5
1	F	183	SER	2.4
1	G	183	SER	2.4
1	G	236	ILE	2.4
1	I	275	ILE	2.4
1	K	236	ILE	2.4
1	G	117	LEU	2.4
1	L	334	LEU	2.4
1	E	156	ASN	2.4
1	J	273	ASP	2.4
1	J	286	ASP	2.4
1	H	374	GLN	2.4
1	E	112	PRO	2.4
1	K	205	PRO	2.4
1	L	176	PHE	2.4
1	K	180	LEU	2.4
1	J	92	TYR	2.4
1	G	286	ASP	2.4
1	A	274	PHE	2.4
1	J	432	ILE	2.4
1	K	307	GLN	2.4
1	F	376	GLY	2.4
1	G	505	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	206	ALA	2.4
1	L	244	ALA	2.4
1	J	504	THR	2.4
1	K	184	LYS	2.4
1	F	107	SER	2.4
1	J	279	SER	2.4
1	K	234	SER	2.4
1	I	258	VAL	2.4
1	L	236	ILE	2.4
1	L	282	ILE	2.4
1	I	102	GLU	2.4
1	L	515	TYR	2.3
1	L	537	ASN	2.3
1	F	116	GLY	2.3
1	I	231	LYS	2.3
1	E	275	ILE	2.3
1	H	437	VAL	2.3
1	L	281	HIS	2.3
1	H	280	LEU	2.3
1	L	503	LEU	2.3
1	H	115	GLU	2.3
1	H	277	ASN	2.3
1	L	436	ASN	2.3
1	E	382	LYS	2.3
1	I	255	TYR	2.3
1	L	199	ALA	2.3
1	D	272	THR	2.3
1	G	510	SER	2.3
1	L	265	SER	2.3
1	I	292	ILE	2.3
1	G	233	VAL	2.3
1	I	119	VAL	2.3
1	H	198	LEU	2.3
1	D	436	ASN	2.3
1	I	232	LYS	2.3
1	L	333	ASN	2.3
1	K	181	GLY	2.3
1	L	202	GLY	2.3
1	I	285	ALA	2.3
1	L	75	THR	2.3
1	K	617	LEU	2.3
1	A	618	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	175	ASN	2.3
1	I	200	TYR	2.3
1	F	113	ALA	2.3
1	L	421	ALA	2.3
1	H	265	SER	2.3
1	H	565	SER	2.3
1	J	564	SER	2.3
1	H	152	GLN	2.3
1	E	118	ILE	2.3
1	J	600	LYS	2.3
1	K	88	ILE	2.3
1	G	414	PHE	2.2
1	J	339	LEU	2.2
1	K	222	VAL	2.3
1	K	332	VAL	2.3
1	L	495	ASP	2.2
1	J	373	ALA	2.2
1	J	177	THR	2.2
1	L	226	HIS	2.2
1	F	265	SER	2.2
1	H	101	ILE	2.2
1	L	88	ILE	2.2
1	L	118	ILE	2.2
1	J	99	LEU	2.2
1	L	439	VAL	2.2
1	I	112	PRO	2.2
1	F	194	LYS	2.2
1	K	82	SER	2.2
1	L	300	TYR	2.2
1	K	542	TRP	2.2
1	J	224	LEU	2.2
1	L	492	LEU	2.2
1	B	414	PHE	2.2
1	E	176	PHE	2.2
1	E	226	HIS	2.2
1	J	238	GLU	2.2
1	I	506	ALA	2.2
1	J	94	THR	2.2
1	L	535	THR	2.2
1	L	92	TYR	2.2
1	F	122	LEU	2.2
1	F	224	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	560	LEU	2.2
1	L	239	ILE	2.2
1	L	387	LEU	2.2
1	A	267	ASP	2.2
1	H	222	VAL	2.2
1	J	616	VAL	2.2
1	G	204	GLY	2.2
1	I	608	GLY	2.2
1	G	182	THR	2.2
1	G	199	ALA	2.2
1	H	206	ALA	2.2
1	I	266	ALA	2.2
1	G	122	LEU	2.1
1	J	118	ILE	2.1
1	G	227	ASP	2.1
1	G	326	VAL	2.1
1	I	222	VAL	2.1
1	I	567	VAL	2.1
1	J	201	VAL	2.1
1	K	258	VAL	2.1
1	L	217	VAL	2.1
1	H	174	GLU	2.1
1	K	208	GLU	2.1
1	K	232	LYS	2.1
1	K	240	LYS	2.1
1	B	565	SER	2.1
1	I	113	ALA	2.1
1	I	421	ALA	2.1
1	J	588	ALA	2.1
1	J	289	LYS	2.1
1	K	383	LYS	2.1
1	L	180	LEU	2.1
1	G	93	HIS	2.1
1	K	89	PRO	2.1
1	E	223	THR	2.1
1	E	199	ALA	2.1
1	F	266	ALA	2.1
1	I	100	SER	2.1
1	H	534	LYS	2.1
1	E	174	GLU	2.1
1	I	208	GLU	2.1
1	E	214	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	117	LEU	2.1
1	G	277	ASN	2.1
1	I	370	TYR	2.1
1	J	101	ILE	2.1
1	K	255	TYR	2.1
1	J	119	VAL	2.1
1	G	178	GLY	2.1
1	E	182	THR	2.1
1	F	565	SER	2.1
1	D	194	LYS	2.1
1	H	287	ALA	2.1
1	L	360	MET	2.1
1	G	238	GLU	2.1
1	I	278	LEU	2.1
1	E	153	ILE	2.1
1	L	461	ILE	2.1
1	L	547	ASN	2.1
1	I	92	TYR	2.1
1	J	288	TYR	2.1
1	J	181	GLY	2.1
1	E	240	LYS	2.0
1	J	183	SER	2.0
1	K	552	SER	2.0
1	L	502	THR	2.0
1	J	206	ALA	2.0
1	A	192	GLN	2.0
1	I	226	HIS	2.0
1	K	278	LEU	2.0
1	E	241	ILE	2.0
1	J	236	ILE	2.0
1	L	372	GLY	2.0
1	L	458	GLY	2.0
1	I	599	PHE	2.0
1	E	104	LYS	2.0
1	E	193	LYS	2.0
1	L	416	MET	2.0
1	E	228	SER	2.0
1	H	234	SER	2.0
1	L	464	SER	2.0
1	G	108	ALA	2.0
1	K	218	ALA	2.0
1	B	382	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	154	LYS	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	I	701	6/6	0.55	0.25	62,78,94,94	0
2	GOL	J	702	6/6	0.57	0.21	65,83,91,102	0
3	PEG	B	704	7/7	0.63	0.24	46,62,74,77	0
3	PEG	F	704	7/7	0.64	0.26	46,63,76,81	0
3	PEG	G	702	7/7	0.69	0.23	56,67,76,76	0
2	GOL	D	703	6/6	0.71	0.14	59,75,79,93	0
3	PEG	H	702	7/7	0.71	0.19	53,64,74,79	0
3	PEG	E	707	7/7	0.74	0.27	37,47,63,63	0
3	PEG	A	703	7/7	0.74	0.18	50,64,76,82	0
2	GOL	A	701	6/6	0.74	0.23	51,62,71,71	0
3	PEG	C	702	7/7	0.74	0.17	40,54,66,66	0
3	PEG	E	708	7/7	0.75	0.17	52,63,76,76	0
2	GOL	G	701	6/6	0.76	0.23	46,55,68,82	0
2	GOL	J	703	6/6	0.76	0.15	58,69,80,81	0
3	PEG	E	706	7/7	0.77	0.17	52,62,72,72	0
2	GOL	A	706	6/6	0.77	0.20	46,63,72,76	0
3	PEG	F	703	7/7	0.78	0.16	44,53,61,74	0
3	PEG	B	703	7/7	0.80	0.19	47,57,62,62	0
2	GOL	A	707	6/6	0.82	0.17	58,69,74,74	0
2	GOL	B	701	6/6	0.82	0.19	37,44,53,57	0
2	GOL	H	701	6/6	0.83	0.20	47,56,64,67	0
2	GOL	E	704	6/6	0.83	0.29	44,53,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	705	6/6	0.83	0.19	44,55,67,71	0
2	GOL	F	705	6/6	0.84	0.19	40,52,73,73	0
4	ZN	L	701	1/1	0.84	0.12	53,53,53,53	1
3	PEG	D	702	7/7	0.85	0.19	47,57,68,68	0
2	GOL	B	702	6/6	0.86	0.13	44,53,64,64	0
2	GOL	E	703	6/6	0.86	0.20	44,55,63,66	0
2	GOL	G	703	6/6	0.86	0.16	37,53,57,65	0
4	ZN	K	701	1/1	0.86	0.08	48,48,48,48	1
2	GOL	D	701	6/6	0.86	0.18	44,57,64,68	0
2	GOL	E	702	6/6	0.87	0.12	39,53,63,63	0
2	GOL	E	705	6/6	0.87	0.19	30,48,59,67	0
2	GOL	F	702	6/6	0.87	0.18	39,53,64,64	0
2	GOL	C	701	6/6	0.88	0.11	42,51,61,71	0
2	GOL	I	702	6/6	0.88	0.18	44,57,64,69	0
2	GOL	A	702	6/6	0.89	0.11	40,51,57,61	0
5	SO4	A	712	5/5	0.89	0.18	57,62,72,75	0
4	ZN	E	709	1/1	0.90	0.07	32,32,32,32	1
2	GOL	J	701	6/6	0.90	0.17	43,52,59,60	0
2	GOL	F	701	6/6	0.90	0.16	33,45,51,55	0
2	GOL	E	701	6/6	0.90	0.18	35,44,51,54	0
4	ZN	I	703	1/1	0.92	0.11	46,46,46,46	1
2	GOL	C	703	6/6	0.92	0.18	38,46,50,57	0
5	SO4	K	703	5/5	0.92	0.12	48,50,52,56	0
4	ZN	A	708	1/1	0.93	0.08	34,34,34,34	1
2	GOL	A	704	6/6	0.93	0.13	34,42,50,60	0
4	ZN	G	704	1/1	0.93	0.09	38,38,38,38	1
5	SO4	B	710	5/5	0.93	0.16	56,58,65,67	0
2	GOL	B	705	6/6	0.93	0.12	34,41,48,56	0
5	SO4	L	703	5/5	0.93	0.10	45,46,49,50	5
4	ZN	H	704	1/1	0.94	0.09	44,44,44,44	1
2	GOL	D	704	6/6	0.94	0.13	35,42,47,47	0
4	ZN	K	702	1/1	0.95	0.08	52,52,52,52	1
5	SO4	G	706	5/5	0.95	0.11	30,33,36,42	5
5	SO4	I	705	5/5	0.96	0.09	34,39,42,49	5
4	ZN	C	705	1/1	0.97	0.04	47,47,47,47	1
5	SO4	B	708	5/5	0.97	0.07	28,31,32,34	0
4	ZN	D	706	1/1	0.97	0.03	30,30,30,30	1
5	SO4	D	707	5/5	0.97	0.11	31,34,37,37	0
5	SO4	F	708	5/5	0.97	0.07	35,35,36,38	0
4	ZN	J	704	1/1	0.97	0.05	46,46,46,46	1
5	SO4	H	705	5/5	0.97	0.09	36,37,39,43	5
4	ZN	A	709	1/1	0.97	0.04	37,37,37,37	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	J	706	5/5	0.97	0.07	39,45,46,49	5
4	ZN	F	707	1/1	0.97	0.04	31,31,31,31	1
4	ZN	B	707	1/1	0.97	0.05	33,33,33,33	1
5	SO4	E	711	5/5	0.98	0.05	32,33,38,39	0
4	ZN	E	710	1/1	0.98	0.03	43,43,43,43	1
5	SO4	A	710	5/5	0.98	0.06	32,32,33,35	0
4	ZN	F	706	1/1	0.98	0.04	36,36,36,36	1
4	ZN	C	704	1/1	0.98	0.04	28,28,28,28	1
4	ZN	D	705	1/1	0.98	0.03	44,44,44,44	1
5	SO4	C	706	5/5	0.98	0.08	28,30,38,38	0
4	ZN	G	705	1/1	0.98	0.06	52,52,52,52	1
5	SO4	L	704	5/5	0.98	0.06	37,41,42,46	0
4	ZN	I	704	1/1	0.99	0.04	46,46,46,46	1
5	SO4	G	707	5/5	0.99	0.05	31,32,35,35	0
5	SO4	B	709	5/5	0.99	0.04	25,28,28,29	0
4	ZN	B	706	1/1	0.99	0.03	38,38,38,38	1
4	ZN	L	702	1/1	0.99	0.05	56,56,56,56	1
4	ZN	J	705	1/1	0.99	0.03	42,42,42,42	1
5	SO4	A	711	5/5	0.99	0.04	23,27,29,31	0
4	ZN	H	703	1/1	0.99	0.04	41,41,41,41	1

6.5 Other polymers

There are no such residues in this entry.