



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 04:56 PM EDT

PDB ID : 6WVV
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

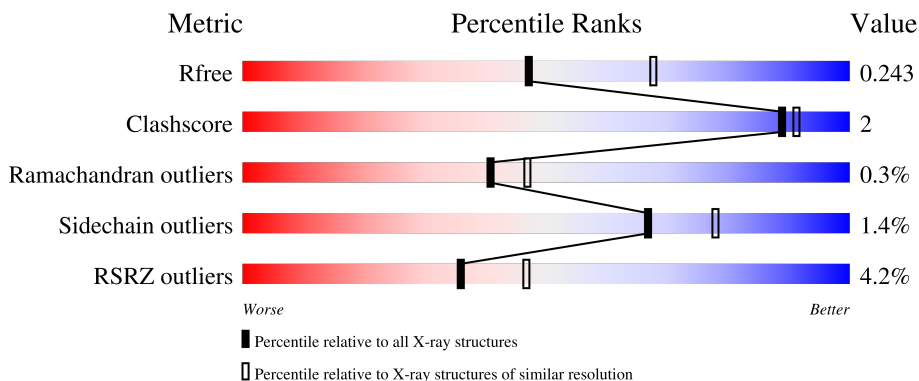
1 Overall quality at a glance

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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	 92% . .
1	B	528	 93% . .
1	C	528	 92% . .
1	D	528	 92% . .
1	E	528	 87% 8% . 5%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	F	704	-	-	-	X

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

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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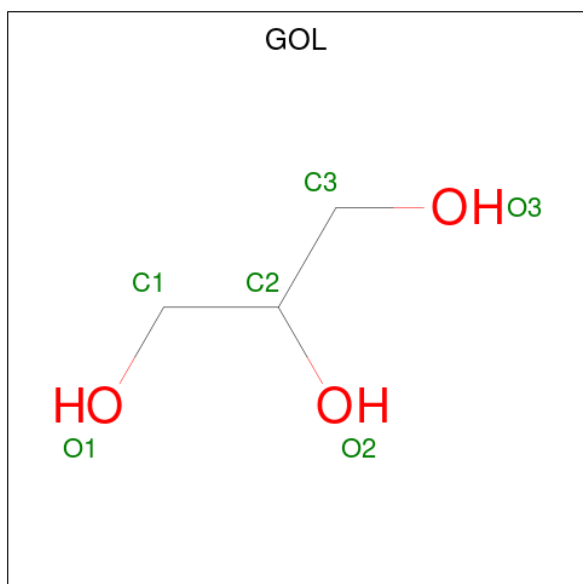
Chain	Residue	Modelled	Actual	Comment	Reference
A	627	HIS	-	expression tag	UNP A0A1G4HHP8
B	622	HIS	-	expression tag	UNP A0A1G4HHP8
B	623	HIS	-	expression tag	UNP A0A1G4HHP8
B	624	HIS	-	expression tag	UNP A0A1G4HHP8
B	625	HIS	-	expression tag	UNP A0A1G4HHP8
B	626	HIS	-	expression tag	UNP A0A1G4HHP8
B	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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



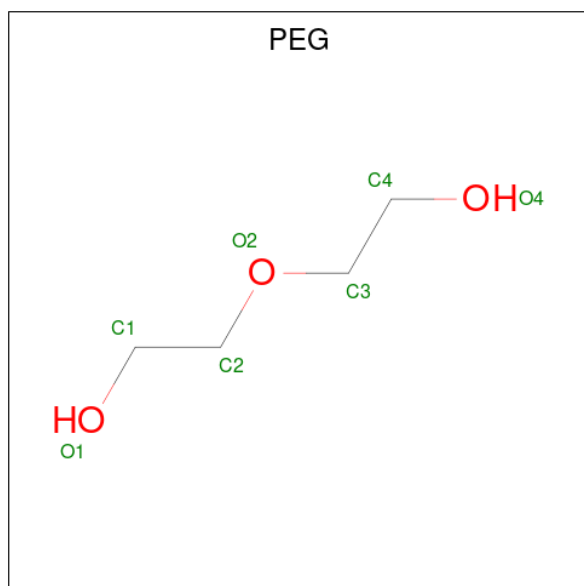
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	A	1	Total 13	C 3	H 7	O 3	0	0
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total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

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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 (three-letter code: PEG) (formula: C₄H₁₀O₃).



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 (three-letter code: ZN) (formula: Zn).

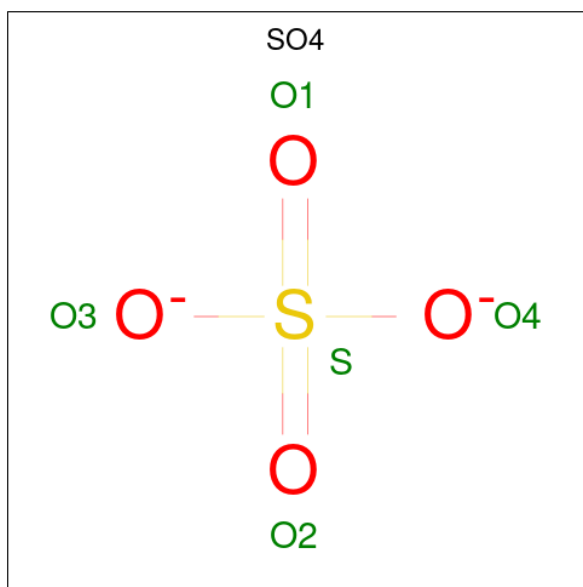
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	E	2	Total	Zn	0	0
			2	2		
4	F	2	Total	Zn	0	0
			2	2		
4	G	2	Total	Zn	0	0
			2	2		
4	H	2	Total	Zn	0	0
			2	2		
4	I	2	Total	Zn	0	0
			2	2		
4	J	2	Total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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 6 is water.

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

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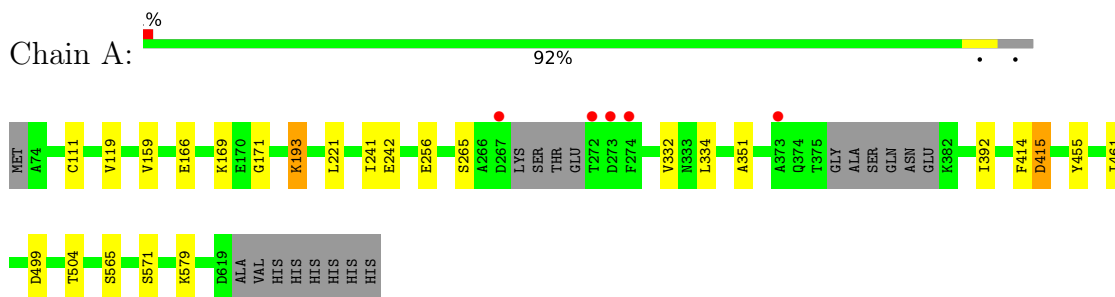
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	53	Total O 53 53	0	0
6	L	44	Total O 44 44	0	0

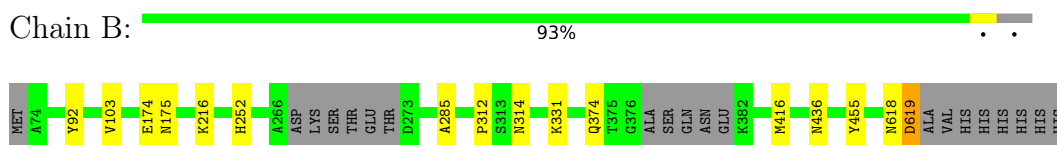
3 Residue-property plots [i](#)

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.

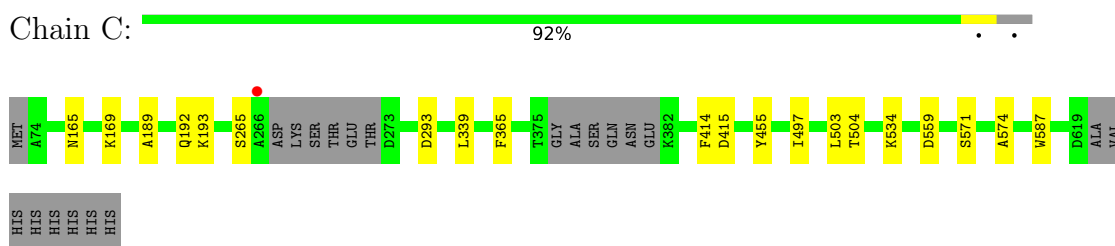
- Molecule 1: M17 leucyl aminopeptidase



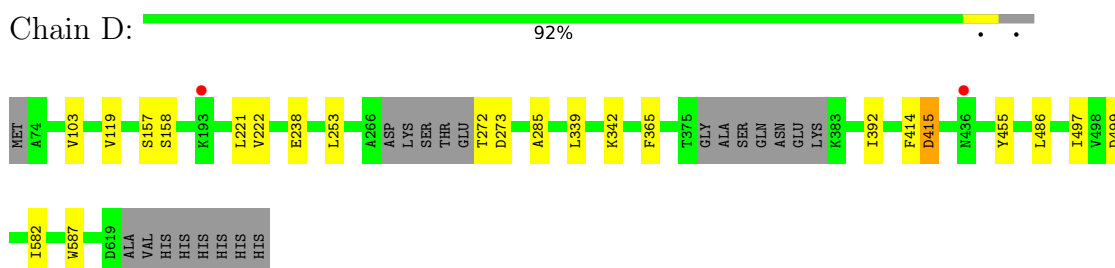
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

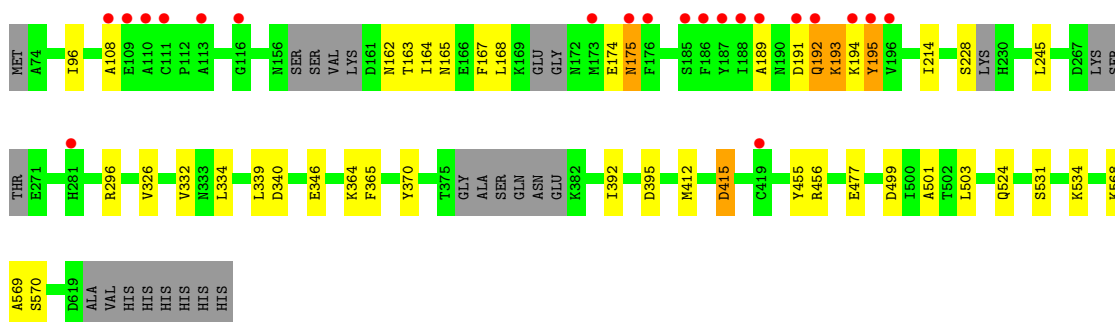


- Molecule 1: M17 leucyl aminopeptidase



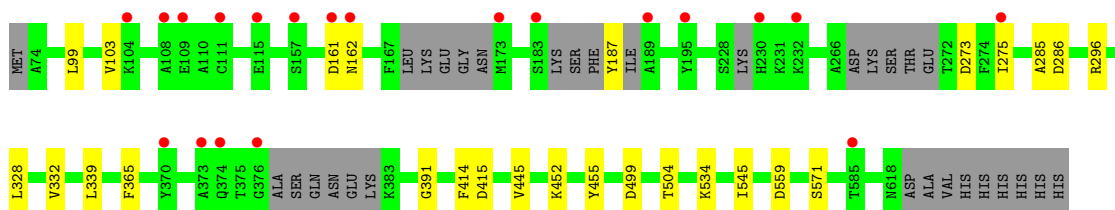
- Molecule 1: M17 leucyl aminopeptidase

Chain E: 4% 87% 8% 5%



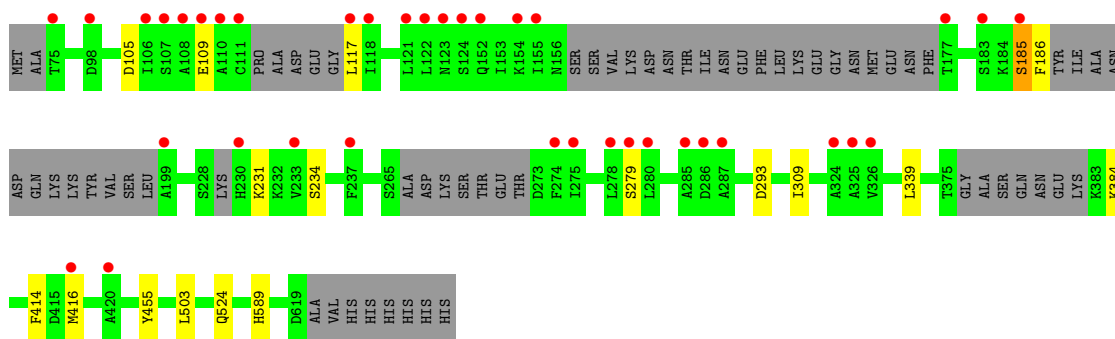
- Molecule 1: M17 leucyl aminopeptidase

Chain F: 4% 89% 5% 6%



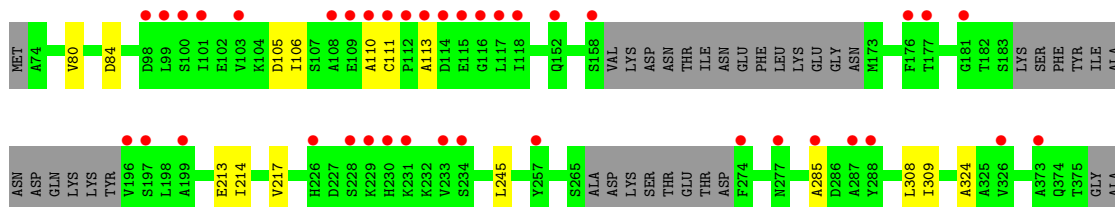
- Molecule 1: M17 leucyl aminopeptidase

Chain G: 7% 85% 12%



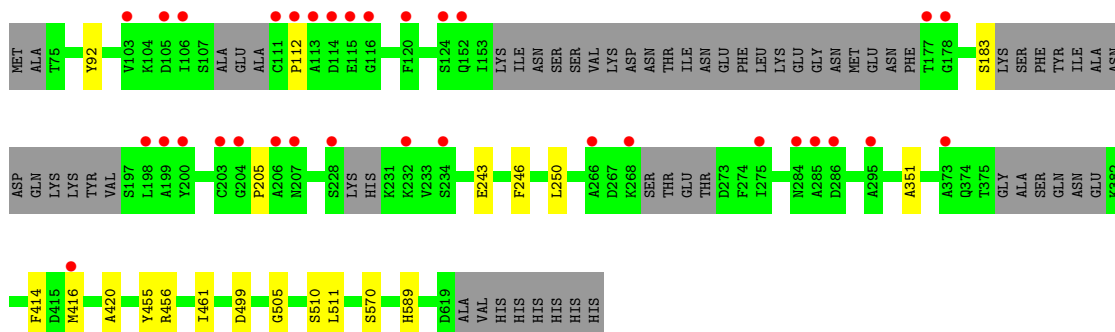
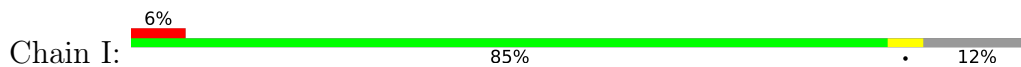
- Molecule 1: M17 leucyl aminopeptidase

Chain H: 7% 86% 9%

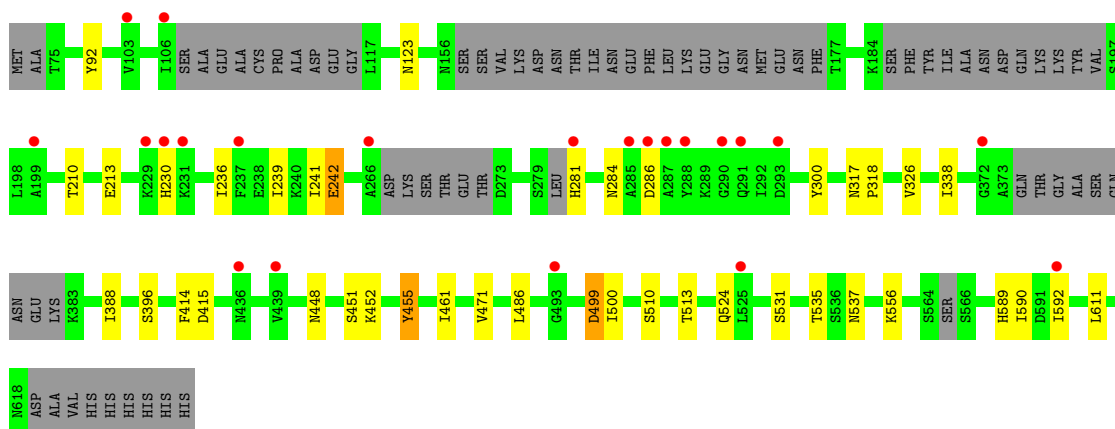
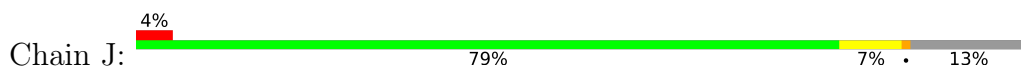




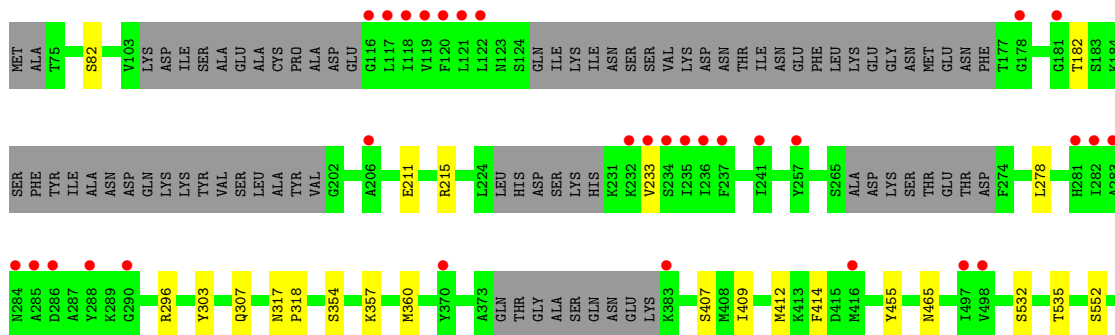
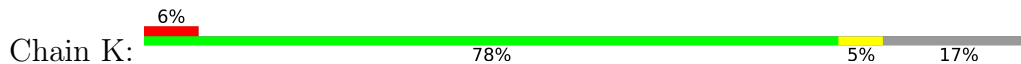
● Molecule 1: M17 leucyl aminopeptidase



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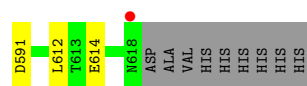
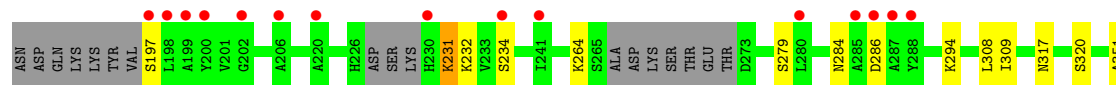
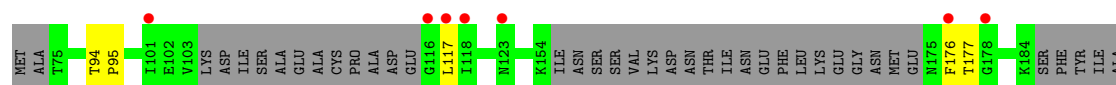
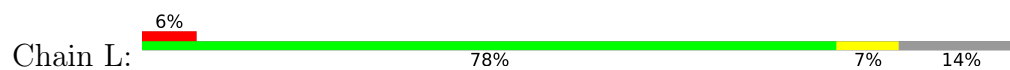


● Molecule 1: M17 leucyl aminopeptidase





• Molecule 1: M17 leucyl aminopeptidase



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)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.205 , 0.243 0.205 , 0.243	Depositor DCC
R_{free} test set	15702 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtrriage
Anisotropy	0.323	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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, PEG, SO4

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	0.26	0/4003	0.43	0/5421
1	B	0.26	0/3996	0.43	0/5412
1	C	0.26	0/3995	0.43	0/5411
1	D	0.26	0/3989	0.43	0/5406
1	E	0.26	0/3783	0.46	0/5137
1	F	0.26	0/3759	0.43	0/5101
1	G	0.26	0/3440	0.43	0/4673
1	H	0.26	0/3554	0.43	0/4830
1	I	0.25	0/3460	0.43	0/4697
1	J	0.25	0/3355	0.42	0/4560
1	K	0.26	0/3207	0.44	0/4356
1	L	0.25	0/3284	0.42	0/4458
All	All	0.26	0/43825	0.43	0/59462

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.

There are no bond angle outliers.

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	13	0
1	B	3920	3919	3919	8	0
1	C	3919	3918	3918	9	0
1	D	3910	3896	3896	11	0
1	E	3717	3523	3540	27	0
1	F	3694	3565	3561	11	0
1	G	3382	3161	3162	9	0
1	H	3492	3280	3281	12	0
1	I	3401	3163	3160	10	0
1	J	3301	3027	3039	20	0
1	K	3156	2920	2918	13	0
1	L	3229	2946	2948	23	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	1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
6	I	56	0	0	2	0
6	J	47	0	0	2	0
6	K	53	0	0	1	0
6	L	44	0	0	0	0
All	All	44867	41597	41626	164	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 (164) 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:F:187:TYR:OH	6:F:801:HOH:O	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:I:510:SER:OG	1:I:511:LEU:N	2.42	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
1:J:396:SER:OG	1:J:448:ASN:O	2.25	0.50
1:J:123:ASN:OD1	1:J:239:ILE:HG22	2.12	0.49
1:K:535:THR:CB	1:K:614:GLU:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:510:SER:OG	1:H:511:LEU:N	2.43	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: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: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:E:340:ASP:OD1	1:E:364:LYS:NZ	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:265:SER:OG	1:C:559:ASP:OD2	2.26	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:F:545:ILE:H	2:F:705:GOL:HO2	1.61	0.43
1:B:374:GLN:HA	1:B:436:ASN:OD1	2.18	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:J:451:SER:OG	1:J:452:LYS:N	2.52	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:I:505:GLY:H	2:I:701:GOL:HO3	1.65	0.43
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:J:236:ILE:HA	1:J:281:HIS:N	2.34	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
1:D:157:SER:OG	1:D:158:SER:N	2.53	0.42
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:L:317:ASN:H	1:L:320:SER:HG	1.66	0.42
1:C:265:SER:OG	1:F:559:ASP:OD2	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:416:MET:HE1	1:I:420:ALA:HB2	1.99	0.41
1:E:392:ILE:HB	1:E:415:ASP:HB3	2.01	0.41
1:G:185:SER:O	1:G:186:PHE:C	2.58	0.41
1:K:211:GLU:OE1	1:K:215:ARG:NH2	2.51	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:A:166:GLU:OE1	1:A:169:LYS:NZ	2.47	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:H:308:LEU:O	1:H:416:MET:HE3	2.21	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
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%)	47	55
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%)	9	7
1	F	484/528 (92%)	466 (96%)	17 (4%)	1 (0%)	47	55
1	G	452/528 (86%)	435 (96%)	15 (3%)	2 (0%)	34	38
1	H	468/528 (89%)	443 (95%)	23 (5%)	2 (0%)	34	38
1	I	453/528 (86%)	433 (96%)	18 (4%)	2 (0%)	34	38
1	J	442/528 (84%)	420 (95%)	20 (4%)	2 (0%)	29	31
1	K	426/528 (81%)	410 (96%)	15 (4%)	1 (0%)	47	55
1	L	439/528 (83%)	415 (94%)	24 (6%)	0	100	100
All	All	5663/6336 (89%)	5444 (96%)	200 (4%)	19 (0%)	41	47

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

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Mol	Chain	Res	Type
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 [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	425/448 (95%)	419 (99%)	6 (1%)	67 78
1	B	425/448 (95%)	421 (99%)	4 (1%)	78 87
1	C	426/448 (95%)	421 (99%)	5 (1%)	71 82
1	D	423/448 (94%)	418 (99%)	5 (1%)	71 82
1	E	372/448 (83%)	366 (98%)	6 (2%)	62 74
1	F	373/448 (83%)	366 (98%)	7 (2%)	57 68
1	G	325/448 (72%)	322 (99%)	3 (1%)	78 87
1	H	337/448 (75%)	334 (99%)	3 (1%)	78 87
1	I	325/448 (72%)	321 (99%)	4 (1%)	71 82
1	J	315/448 (70%)	308 (98%)	7 (2%)	52 63
1	K	298/448 (66%)	291 (98%)	7 (2%)	50 61
1	L	296/448 (66%)	291 (98%)	5 (2%)	60 72
All	All	4340/5376 (81%)	4278 (99%)	62 (1%)	67 78

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LYS
1	A	414	PHE
1	A	415	ASP

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Mol	Chain	Res	Type
1	A	455	TYR
1	A	499	ASP
1	A	565	SER
1	B	416	MET
1	B	455	TYR
1	B	618	ASN
1	B	619	ASP
1	C	192	GLN
1	C	414	PHE
1	C	415	ASP
1	C	455	TYR
1	C	534	LYS
1	D	342	LYS
1	D	414	PHE
1	D	415	ASP
1	D	455	TYR
1	D	499	ASP
1	E	228	SER
1	E	415	ASP
1	E	455	TYR
1	E	499	ASP
1	E	524	GLN
1	E	531	SER
1	F	286	ASP
1	F	414	PHE
1	F	415	ASP
1	F	452	LYS
1	F	455	TYR
1	F	499	ASP
1	F	534	LYS
1	G	293	ASP
1	G	414	PHE
1	G	455	TYR
1	H	414	PHE
1	H	455	TYR
1	H	568	LYS
1	I	243	GLU
1	I	414	PHE
1	I	455	TYR
1	I	570	SER
1	J	414	PHE
1	J	415	ASP

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Mol	Chain	Res	Type
1	J	455	TYR
1	J	499	ASP
1	J	510	SER
1	J	524	GLN
1	J	556	LYS
1	K	82	SER
1	K	296	ARG
1	K	360	MET
1	K	414	PHE
1	K	455	TYR
1	K	465	ASN
1	K	552	SER
1	L	231	LYS
1	L	264	LYS
1	L	414	PHE
1	L	455	TYR
1	L	551	SER

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

Mol	Chain	Res	Type
1	G	207	ASN
1	L	537	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	SO4	B	710	-	4,4,4	0.14	0	6,6,6	0.10	0
2	GOL	J	702	-	5,5,5	0.82	0	5,5,5	1.07	0
2	GOL	F	702	-	5,5,5	1.01	0	5,5,5	1.05	0
3	PEG	F	703	4	6,6,6	0.51	0	5,5,5	0.41	0
2	GOL	A	704	-	5,5,5	0.83	0	5,5,5	1.09	0
2	GOL	E	704	-	5,5,5	0.85	0	5,5,5	1.06	0
5	SO4	K	703	-	4,4,4	0.13	0	6,6,6	0.15	0
2	GOL	B	705	-	5,5,5	0.87	0	5,5,5	1.05	0
2	GOL	I	701	-	5,5,5	0.91	0	5,5,5	1.07	0
5	SO4	A	710	-	4,4,4	0.16	0	6,6,6	0.07	0
2	GOL	E	705	-	5,5,5	0.80	0	5,5,5	0.97	0
2	GOL	E	703	-	5,5,5	0.73	0	5,5,5	0.95	0
3	PEG	E	706	-	6,6,6	0.48	0	5,5,5	0.38	0
2	GOL	G	701	-	5,5,5	0.81	0	5,5,5	0.95	0
2	GOL	A	706	-	5,5,5	0.83	0	5,5,5	0.96	0
5	SO4	G	707	-	4,4,4	0.13	0	6,6,6	0.12	0
3	PEG	C	702	-	6,6,6	0.48	0	5,5,5	0.37	0
5	SO4	A	711	-	4,4,4	0.13	0	6,6,6	0.17	0
5	SO4	I	705	-	4,4,4	0.17	0	6,6,6	0.18	0
2	GOL	E	702	-	5,5,5	0.84	0	5,5,5	1.02	0
3	PEG	H	702	-	6,6,6	0.49	0	5,5,5	0.30	0
3	PEG	A	703	-	6,6,6	0.48	0	5,5,5	0.42	0
2	GOL	J	701	-	5,5,5	0.88	0	5,5,5	0.98	0
2	GOL	J	703	-	5,5,5	0.90	0	5,5,5	1.02	0
3	PEG	G	702	-	6,6,6	0.49	0	5,5,5	0.27	0
5	SO4	B	709	-	4,4,4	0.17	0	6,6,6	0.14	0
2	GOL	C	703	-	5,5,5	0.85	0	5,5,5	0.98	0
5	SO4	A	712	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	H	705	-	4,4,4	0.13	0	6,6,6	0.08	0
2	GOL	H	701	-	5,5,5	0.85	0	5,5,5	1.05	0
2	GOL	B	702	-	5,5,5	0.87	0	5,5,5	1.06	0
5	SO4	G	706	-	4,4,4	0.17	0	6,6,6	0.19	0
5	SO4	E	711	-	4,4,4	0.15	0	6,6,6	0.13	0
5	SO4	F	708	-	4,4,4	0.15	0	6,6,6	0.19	0
2	GOL	E	701	-	5,5,5	0.84	0	5,5,5	0.97	0
5	SO4	D	707	-	4,4,4	0.16	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	707	-	5,5,5	0.85	0	5,5,5	1.03	0
3	PEG	E	707	-	6,6,6	0.48	0	5,5,5	0.26	0
2	GOL	A	702	-	5,5,5	0.88	0	5,5,5	1.07	0
2	GOL	D	704	-	5,5,5	0.89	0	5,5,5	1.00	0
2	GOL	F	701	-	5,5,5	0.88	0	5,5,5	0.99	0
2	GOL	I	702	-	5,5,5	0.86	0	5,5,5	0.99	0
2	GOL	C	701	-	5,5,5	0.82	0	5,5,5	1.02	0
2	GOL	A	701	-	5,5,5	0.87	0	5,5,5	0.98	0
3	PEG	B	704	-	6,6,6	0.49	0	5,5,5	0.44	0
2	GOL	D	703	-	5,5,5	0.81	0	5,5,5	0.93	0
5	SO4	L	704	-	4,4,4	0.14	0	6,6,6	0.13	0
5	SO4	B	708	-	4,4,4	0.15	0	6,6,6	0.32	0
2	GOL	D	701	-	5,5,5	0.87	0	5,5,5	1.00	0
2	GOL	B	701	-	5,5,5	0.97	0	5,5,5	1.12	1 (20%)
2	GOL	F	705	-	5,5,5	0.92	0	5,5,5	0.87	0
3	PEG	F	704	-	6,6,6	0.48	0	5,5,5	0.43	0
3	PEG	D	702	-	6,6,6	0.49	0	5,5,5	0.26	0
2	GOL	G	703	-	5,5,5	0.79	0	5,5,5	1.01	0
3	PEG	E	708	-	6,6,6	0.48	0	5,5,5	0.25	0
5	SO4	J	706	-	4,4,4	0.13	0	6,6,6	0.10	0
3	PEG	B	703	-	6,6,6	0.49	0	5,5,5	0.22	0
2	GOL	A	705	-	5,5,5	0.83	0	5,5,5	0.99	0
5	SO4	L	703	-	4,4,4	0.15	0	6,6,6	0.15	0
5	SO4	C	706	-	4,4,4	0.12	0	6,6,6	0.11	0

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

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	GOL	C3-C2-C1	-2.04	103.78	111.70

There are no chirality outliers.

All (55) 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
3	G	702	PEG	O1-C1-C2-O2
2	B	705	GOL	O2-C2-C3-O3
3	C	702	PEG	O1-C1-C2-O2
2	C	701	GOL	O1-C1-C2-O2
2	J	701	GOL	O2-C2-C3-O3
3	B	704	PEG	O2-C3-C4-O4
3	C	702	PEG	C1-C2-O2-C3
3	B	704	PEG	C1-C2-O2-C3
3	B	704	PEG	C4-C3-O2-C2
2	D	703	GOL	O2-C2-C3-O3
3	F	704	PEG	C4-C3-O2-C2
2	A	707	GOL	O1-C1-C2-C3
2	D	701	GOL	C1-C2-C3-O3
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

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

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	701	GOL	1	0
2	E	705	GOL	1	0
3	G	702	PEG	1	0
3	E	707	PEG	1	0
2	I	702	GOL	1	0
2	B	701	GOL	1	0
2	F	705	GOL	1	0
3	B	703	PEG	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%)	0.01	5 (0%) 82 88	22, 30, 52, 64	0
1	B	508/528 (96%)	-0.02	0 100 100	22, 31, 50, 65	0
1	C	507/528 (96%)	-0.08	1 (0%) 95 97	21, 30, 46, 64	0
1	D	507/528 (96%)	-0.01	2 (0%) 92 96	22, 33, 49, 69	0
1	E	503/528 (95%)	0.32	21 (4%) 36 47	23, 34, 72, 85	0
1	F	497/528 (94%)	0.38	20 (4%) 38 49	23, 36, 70, 82	0
1	G	466/528 (88%)	0.53	37 (7%) 12 19	28, 39, 73, 88	0
1	H	478/528 (90%)	0.55	39 (8%) 11 17	31, 42, 73, 89	0
1	I	467/528 (88%)	0.51	33 (7%) 16 23	34, 49, 75, 93	0
1	J	458/528 (86%)	0.46	22 (4%) 30 41	36, 53, 77, 87	0
1	K	440/528 (83%)	0.60	32 (7%) 15 22	35, 52, 74, 83	0
1	L	453/528 (85%)	0.64	32 (7%) 16 23	38, 54, 79, 89	0
All	All	5793/6336 (91%)	0.31	244 (4%) 36 47	21, 40, 72, 93	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	107	SER	6.6
1	K	178	GLY	6.4
1	G	110	ALA	5.7
1	H	110	ALA	5.7
1	E	195	TYR	5.6
1	H	112	PRO	5.4
1	I	200	TYR	5.1
1	E	194	LYS	4.6
1	G	287	ALA	4.6
1	L	101	ILE	4.6
1	J	230	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	326	VAL	4.6
1	G	121	LEU	4.6
1	K	285	ALA	4.5
1	F	108	ALA	4.5
1	F	173	MET	4.4
1	H	111	CYS	4.4
1	E	186	PHE	4.4
1	I	275	ILE	4.4
1	G	108	ALA	4.4
1	G	155	ILE	4.3
1	I	152	GLN	4.3
1	H	108	ALA	4.3
1	H	113	ALA	4.3
1	L	285	ALA	4.3
1	H	231	LYS	4.2
1	G	280	LEU	4.2
1	G	75	THR	4.1
1	E	176	PHE	4.1
1	I	206	ALA	4.1
1	H	199	ALA	4.0
1	K	121	LEU	4.0
1	J	199	ALA	4.0
1	H	233	VAL	4.0
1	A	274	PHE	3.9
1	E	188	ILE	3.9
1	I	178	GLY	3.9
1	K	237	PHE	3.9
1	J	286	ASP	3.8
1	H	114	ASP	3.8
1	G	326	VAL	3.8
1	J	287	ALA	3.7
1	E	187	TYR	3.7
1	G	233	VAL	3.7
1	L	198	LEU	3.6
1	H	116	GLY	3.6
1	I	285	ALA	3.6
1	H	109	GLU	3.6
1	H	285	ALA	3.6
1	H	229	LYS	3.5
1	K	120	PHE	3.5
1	I	124	SER	3.5
1	I	284	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	376	GLY	3.5
1	G	279	SER	3.5
1	E	109	GLU	3.5
1	J	103	VAL	3.4
1	L	178	GLY	3.3
1	L	493	GLY	3.3
1	J	290	GLY	3.3
1	K	257	TYR	3.3
1	I	111	CYS	3.3
1	L	199	ALA	3.3
1	J	229	LYS	3.2
1	H	230	HIS	3.2
1	I	199	ALA	3.2
1	I	115	GLU	3.2
1	J	372	GLY	3.2
1	E	192	GLN	3.2
1	I	116	GLY	3.2
1	J	285	ALA	3.2
1	K	117	LEU	3.2
1	I	228	SER	3.1
1	H	176	PHE	3.1
1	K	234	SER	3.1
1	I	204	GLY	3.1
1	E	196	VAL	3.1
1	F	370	TYR	3.1
1	E	191	ASP	3.1
1	L	234	SER	3.1
1	K	122	LEU	3.1
1	L	176	PHE	3.1
1	G	278	LEU	3.0
1	F	373	ALA	3.0
1	G	324	ALA	3.0
1	J	493	GLY	3.0
1	K	416	MET	3.0
1	I	207	ASN	3.0
1	G	185	SER	3.0
1	G	177	THR	3.0
1	H	277	ASN	3.0
1	E	116	GLY	2.9
1	H	257	TYR	2.9
1	E	111	CYS	2.9
1	H	234	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	485	ALA	2.9
1	K	181	GLY	2.9
1	L	117	LEU	2.9
1	I	112	PRO	2.9
1	K	497	ILE	2.8
1	L	230	HIS	2.8
1	G	183	SER	2.8
1	I	177	THR	2.8
1	L	495	ASP	2.8
1	G	109	GLU	2.8
1	I	106	ILE	2.8
1	J	592	ILE	2.8
1	E	108	ALA	2.8
1	K	588	ALA	2.8
1	G	124	SER	2.8
1	E	189	ALA	2.8
1	K	282	ILE	2.8
1	I	113	ALA	2.7
1	G	117	LEU	2.7
1	H	115	GLU	2.7
1	F	230	HIS	2.7
1	J	266	ALA	2.7
1	I	373	ALA	2.7
1	K	283	ALA	2.7
1	J	288	TYR	2.7
1	J	237	PHE	2.7
1	J	106	ILE	2.6
1	G	152	GLN	2.6
1	I	232	LYS	2.6
1	F	374	GLN	2.6
1	K	206	ALA	2.6
1	F	109	GLU	2.6
1	L	414	PHE	2.6
1	G	275	ILE	2.6
1	G	122	LEU	2.6
1	K	288	TYR	2.6
1	K	118	ILE	2.6
1	L	118	ILE	2.6
1	H	181	GLY	2.6
1	G	230	HIS	2.6
1	G	325	ALA	2.6
1	F	111	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	233	VAL	2.6
1	G	199	ALA	2.6
1	K	290	GLY	2.6
1	H	228	SER	2.5
1	E	110	ALA	2.5
1	D	436	ASN	2.5
1	H	274	PHE	2.5
1	F	115	GLU	2.5
1	F	157	SER	2.5
1	L	200	TYR	2.5
1	L	385	ILE	2.5
1	H	197	SER	2.5
1	G	285	ALA	2.5
1	K	241	ILE	2.5
1	L	116	GLY	2.5
1	G	286	ASP	2.5
1	H	103	VAL	2.4
1	H	287	ALA	2.4
1	K	284	ASN	2.4
1	H	101	ILE	2.4
1	G	420	ALA	2.4
1	I	120	PHE	2.4
1	I	105	ASP	2.4
1	K	235	ILE	2.4
1	J	231	LYS	2.4
1	H	100	SER	2.4
1	I	234	SER	2.4
1	I	114	ASP	2.4
1	H	117	LEU	2.4
1	K	281	HIS	2.4
1	F	189	ALA	2.4
1	G	123	ASN	2.4
1	I	203	CYS	2.4
1	G	154	LYS	2.3
1	J	281	HIS	2.3
1	L	202	GLY	2.3
1	E	113	ALA	2.3
1	E	173	MET	2.3
1	L	286	ASP	2.3
1	L	123	ASN	2.3
1	L	288	TYR	2.3
1	K	498	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	287	ALA	2.3
1	F	195	TYR	2.3
1	G	416	MET	2.3
1	L	491	LYS	2.3
1	K	232	LYS	2.3
1	K	236	ILE	2.3
1	K	116	GLY	2.3
1	E	175	ASN	2.3
1	E	185	SER	2.3
1	G	106	ILE	2.3
1	L	386	ALA	2.3
1	E	281	HIS	2.2
1	D	193	LYS	2.2
1	F	275	ILE	2.2
1	L	438	GLU	2.2
1	C	266	ALA	2.2
1	L	206	ALA	2.2
1	K	370	TYR	2.2
1	G	274	PHE	2.2
1	J	525	LEU	2.2
1	L	280	LEU	2.2
1	H	196	VAL	2.2
1	A	272	THR	2.2
1	A	273	ASP	2.2
1	J	293	ASP	2.2
1	H	226	HIS	2.2
1	H	98	ASP	2.2
1	K	286	ASP	2.2
1	L	197	SER	2.2
1	J	436	ASN	2.1
1	A	373	ALA	2.1
1	I	286	ASP	2.1
1	H	152	GLN	2.1
1	K	119	VAL	2.1
1	H	373	ALA	2.1
1	I	295	ALA	2.1
1	G	98	ASP	2.1
1	G	118	ILE	2.1
1	H	118	ILE	2.1
1	G	111	CYS	2.1
1	H	177	THR	2.1
1	I	268	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	267	ASP	2.1
1	H	288	TYR	2.1
1	F	162	ASN	2.1
1	L	241	ILE	2.1
1	I	266	ALA	2.1
1	I	103	VAL	2.1
1	G	237	PHE	2.1
1	L	370	TYR	2.1
1	H	99	LEU	2.1
1	L	220	ALA	2.1
1	E	419	CYS	2.1
1	J	439	VAL	2.1
1	I	198	LEU	2.0
1	F	232	LYS	2.0
1	I	416	MET	2.0
1	K	383	LYS	2.0
1	F	585	THR	2.0
1	H	158	SER	2.0
1	J	291	GLN	2.0
1	L	618	ASN	2.0
1	F	183	SER	2.0
1	F	161	ASP	2.0
1	F	104	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 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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	F	704	7/7	0.62	0.43	46,63,76,81	0
2	GOL	J	702	6/6	0.65	0.26	65,83,91,102	0
2	GOL	I	701	6/6	0.68	0.40	62,78,94,94	0
2	GOL	A	701	6/6	0.72	0.35	51,62,71,71	0
3	PEG	E	708	7/7	0.73	0.32	52,63,76,76	0
3	PEG	B	704	7/7	0.74	0.27	46,62,74,77	0
3	PEG	H	702	7/7	0.75	0.19	53,64,74,79	0
3	PEG	B	703	7/7	0.76	0.24	47,57,62,62	0
2	GOL	A	707	6/6	0.77	0.26	58,69,74,74	0
2	GOL	G	701	6/6	0.77	0.32	46,55,68,82	0
3	PEG	E	707	7/7	0.77	0.36	37,47,63,63	0
3	PEG	G	702	7/7	0.78	0.34	56,67,76,76	0
3	PEG	A	703	7/7	0.80	0.22	50,64,76,82	0
2	GOL	E	703	6/6	0.81	0.32	44,55,63,66	0
3	PEG	C	702	7/7	0.82	0.18	40,54,66,66	0
2	GOL	A	705	6/6	0.82	0.28	44,55,67,71	0
2	GOL	F	705	6/6	0.83	0.30	40,52,73,73	0
2	GOL	B	701	6/6	0.83	0.20	37,44,53,57	0
3	PEG	E	706	7/7	0.83	0.19	52,62,72,72	0
2	GOL	A	706	6/6	0.83	0.24	46,63,72,76	0
2	GOL	D	703	6/6	0.84	0.31	59,75,79,93	0
2	GOL	J	703	6/6	0.84	0.20	58,69,80,81	0
4	ZN	L	701	1/1	0.84	0.16	53,53,53,53	1
2	GOL	E	704	6/6	0.85	0.46	44,53,60,62	0
3	PEG	F	703	7/7	0.85	0.20	44,53,61,74	0
2	GOL	I	702	6/6	0.86	0.33	44,57,64,69	0
3	PEG	D	702	7/7	0.88	0.25	47,57,68,68	0
2	GOL	B	702	6/6	0.88	0.21	44,53,64,64	0
2	GOL	F	702	6/6	0.88	0.30	39,53,64,64	0
2	GOL	E	705	6/6	0.89	0.28	30,48,59,67	0
2	GOL	H	701	6/6	0.90	0.23	47,56,64,67	0
2	GOL	C	701	6/6	0.90	0.17	42,51,61,71	0
2	GOL	G	703	6/6	0.90	0.16	37,53,57,65	0
4	ZN	I	703	1/1	0.91	0.12	46,46,46,46	1
2	GOL	E	702	6/6	0.91	0.30	39,53,63,63	0
2	GOL	D	701	6/6	0.92	0.36	44,57,64,68	0
2	GOL	J	701	6/6	0.92	0.25	43,52,59,60	0
2	GOL	F	701	6/6	0.92	0.17	33,45,51,55	0
2	GOL	A	702	6/6	0.94	0.16	40,51,57,61	0
2	GOL	B	705	6/6	0.94	0.19	34,41,48,56	0
4	ZN	A	708	1/1	0.94	0.12	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	D	706	1/1	0.94	0.12	30,30,30,30	1
4	ZN	E	709	1/1	0.94	0.13	32,32,32,32	1
4	ZN	H	704	1/1	0.94	0.19	44,44,44,44	1
2	GOL	E	701	6/6	0.94	0.26	35,44,51,54	0
4	ZN	K	702	1/1	0.94	0.10	52,52,52,52	1
2	GOL	A	704	6/6	0.94	0.16	34,42,50,60	0
5	SO4	L	703	5/5	0.94	0.16	45,46,49,50	5
4	ZN	F	707	1/1	0.95	0.10	31,31,31,31	1
2	GOL	D	704	6/6	0.95	0.16	35,42,47,47	0
2	GOL	C	703	6/6	0.95	0.33	38,46,50,57	0
4	ZN	K	701	1/1	0.96	0.09	48,48,48,48	1
4	ZN	G	704	1/1	0.96	0.19	38,38,38,38	1
4	ZN	D	705	1/1	0.97	0.12	44,44,44,44	1
4	ZN	I	704	1/1	0.97	0.10	46,46,46,46	1
4	ZN	J	705	1/1	0.97	0.10	42,42,42,42	1
4	ZN	A	709	1/1	0.97	0.12	37,37,37,37	1
4	ZN	G	705	1/1	0.97	0.15	52,52,52,52	1
4	ZN	H	703	1/1	0.97	0.12	41,41,41,41	1
5	SO4	A	712	5/5	0.97	0.37	57,62,72,75	0
5	SO4	B	710	5/5	0.97	0.21	56,58,65,67	0
4	ZN	B	707	1/1	0.97	0.07	33,33,33,33	1
4	ZN	J	704	1/1	0.98	0.13	46,46,46,46	1
4	ZN	L	702	1/1	0.98	0.13	56,56,56,56	1
4	ZN	E	710	1/1	0.98	0.09	43,43,43,43	1
5	SO4	B	708	5/5	0.98	0.15	28,31,32,34	0
4	ZN	F	706	1/1	0.98	0.13	36,36,36,36	1
5	SO4	F	708	5/5	0.98	0.16	35,35,36,38	0
5	SO4	G	706	5/5	0.98	0.22	30,33,36,42	5
5	SO4	K	703	5/5	0.98	0.12	48,50,52,56	0
4	ZN	B	706	1/1	0.98	0.10	38,38,38,38	1
5	SO4	L	704	5/5	0.98	0.15	37,41,42,46	0
5	SO4	C	706	5/5	0.99	0.08	28,30,38,38	0
5	SO4	D	707	5/5	0.99	0.12	31,34,37,37	0
5	SO4	E	711	5/5	0.99	0.16	32,33,38,39	0
5	SO4	A	711	5/5	0.99	0.13	23,27,29,31	0
4	ZN	C	704	1/1	0.99	0.09	28,28,28,28	1
5	SO4	G	707	5/5	0.99	0.12	31,32,35,35	0
5	SO4	H	705	5/5	0.99	0.20	36,37,39,43	5
5	SO4	I	705	5/5	0.99	0.16	34,39,42,49	5
5	SO4	J	706	5/5	0.99	0.17	39,45,46,49	5
4	ZN	C	705	1/1	0.99	0.08	47,47,47,47	1
5	SO4	B	709	5/5	0.99	0.15	25,28,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	710	5/5	0.99	0.14	32,32,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.