



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 8SW9 / pdb_00008sw9
Title : Plasmodium falciparum M17 (A460S) mutant
Authors : McGowan, S.; Suraweera, C.; Drinkwater, N.
Deposited on : 2023-05-17
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

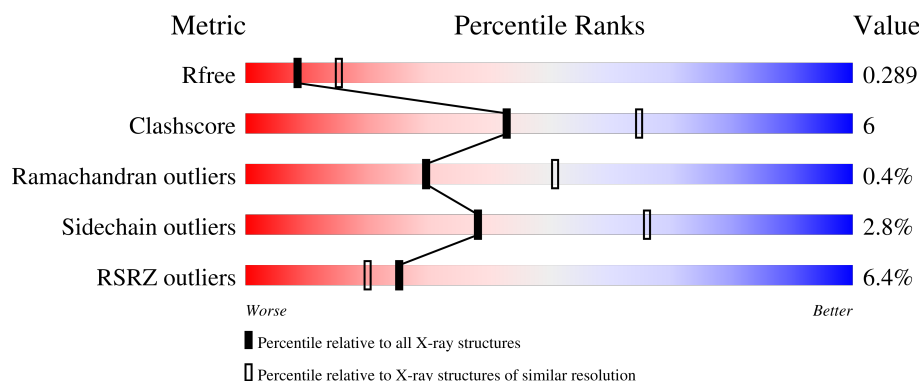
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	4% 83% 15% .
1	B	528	9% 79% 17% ..
1	C	528	4% 84% 13% ..
1	D	528	3% 82% 15% ..
1	E	528	2% 82% 14% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CO3	H	703	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 93534 atoms, of which 45524 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 Leucine aminopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	517	Total	C	H	N	O	S	0	1	0
			7782	2533	3841	632	757	19			
1	B	511	Total	C	H	N	O	S	0	0	0
			7528	2470	3698	618	723	19			
1	C	518	Total	C	H	N	O	S	0	0	0
			7820	2540	3871	637	753	19			
1	D	513	Total	C	H	N	O	S	0	0	0
			7748	2520	3832	631	745	20			
1	E	509	Total	C	H	N	O	S	0	0	0
			7674	2499	3789	623	744	19			
1	F	510	Total	C	H	N	O	S	0	0	0
			7365	2428	3589	609	720	19			
1	G	514	Total	C	H	N	O	S	0	0	0
			7798	2530	3862	633	754	19			
1	H	511	Total	C	H	N	O	S	0	0	0
			7605	2485	3742	622	737	19			
1	I	515	Total	C	H	N	O	S	0	0	0
			7736	2518	3827	631	741	19			
1	J	514	Total	C	H	N	O	S	0	0	0
			7753	2521	3840	632	741	19			
1	K	509	Total	C	H	N	O	S	3	0	0
			7624	2489	3757	620	739	19			
1	L	508	Total	C	H	N	O	S	1	0	0
			7424	2442	3623	611	729	19			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	460	SER	ALA	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	607	HIS	-	expression tag	UNP Q8IL11
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	460	SER	ALA	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	460	SER	ALA	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	460	SER	ALA	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	460	SER	ALA	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	460	SER	ALA	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	460	SER	ALA	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	460	SER	ALA	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	460	SER	ALA	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	460	SER	ALA	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	460	SER	ALA	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	460	SER	ALA	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

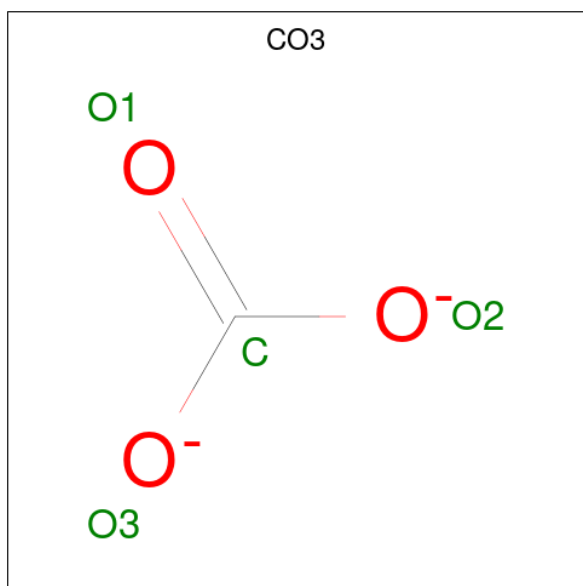
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		
2	G	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		
2	I	2	Total	Zn	0	0
			2	2		
2	J	2	Total	Zn	0	0
			2	2		
2	K	2	Total	Zn	0	0
			2	2		
2	L	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



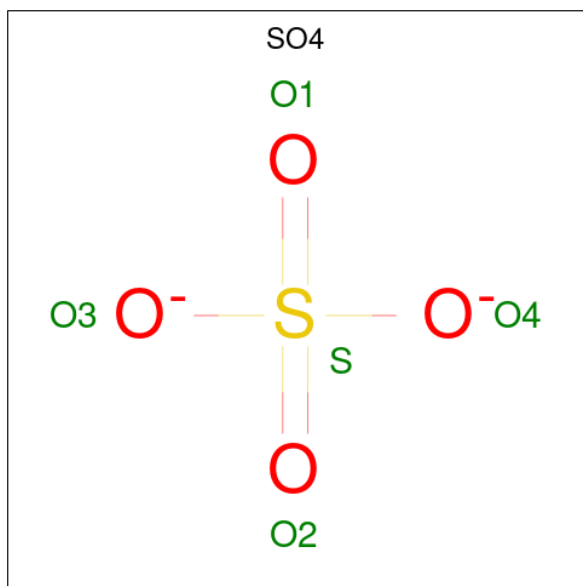
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



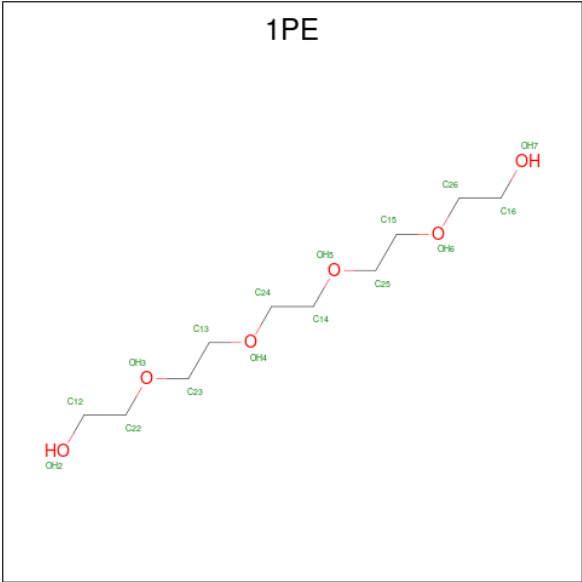
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

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

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			19	6	10	3		
5	A	1	Total	C	H	O	0	0
			23	6	13	4		
5	B	1	Total	C	H	O	0	0
			13	5	6	2		
5	C	1	Total	C	H	O	0	0
			27	9	14	4		
5	C	1	Total	C	H	O	0	0
			19	6	10	3		
5	C	1	Total	C	H	O	0	0
			23	6	13	4		
5	D	1	Total	C	H	O	0	0
			20	7	10	3		
5	D	1	Total	C	H	O	0	0
			20	7	10	3		
5	D	1	Total	C	H	O	0	0
			20	6	11	3		
5	E	1	Total	C	H	O	0	0
			26	8	14	4		
5	E	1	Total	C	H	O	0	0
			20	6	11	3		
5	F	1	Total	C	H	O	0	0
			23	6	13	4		
5	G	1	Total	C	H	O	0	0
			19	6	10	3		
5	G	1	Total	C	H	O	0	0
			23	6	13	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	H	O	0	0
			30	8	17	5		
5	H	1	Total	C	H	O	0	0
			20	7	10	3		
5	J	1	Total	C	H	O	0	0
			23	6	13	4		
5	K	1	Total	C	H	O	0	0
			20	6	11	3		
5	K	1	Total	C	H	O	0	0
			38	10	22	6		
5	L	1	Total	C	H	O	0	0
			38	10	22	6		

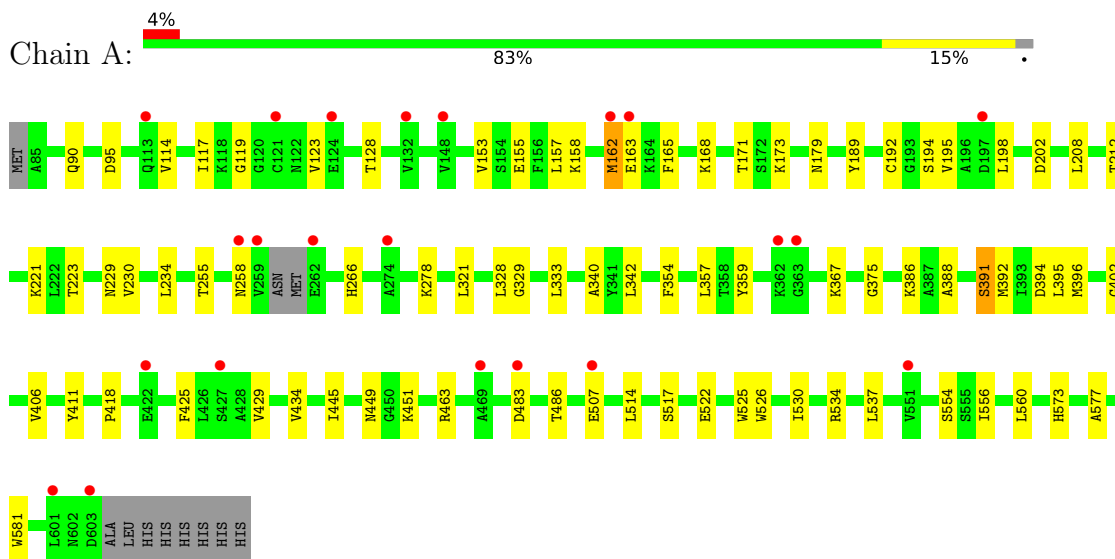
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total	O	0	0
			97	97		
6	B	78	Total	O	0	0
			78	78		
6	C	79	Total	O	0	0
			79	79		
6	D	87	Total	O	0	0
			87	87		
6	E	119	Total	O	0	0
			119	119		
6	F	94	Total	O	0	0
			94	94		
6	G	85	Total	O	0	0
			85	85		
6	H	79	Total	O	0	0
			79	79		
6	I	98	Total	O	0	0
			98	98		
6	J	86	Total	O	0	0
			86	86		
6	K	88	Total	O	0	0
			88	88		
6	L	66	Total	O	0	0
			66	66		

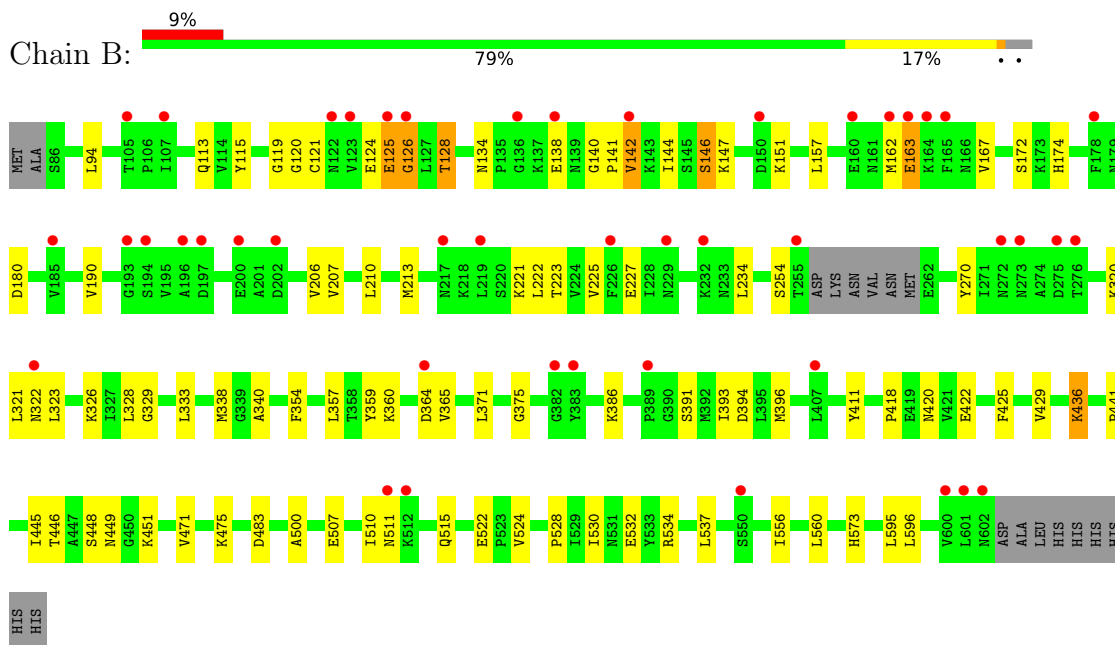
3 Residue-property plots [i](#)

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.

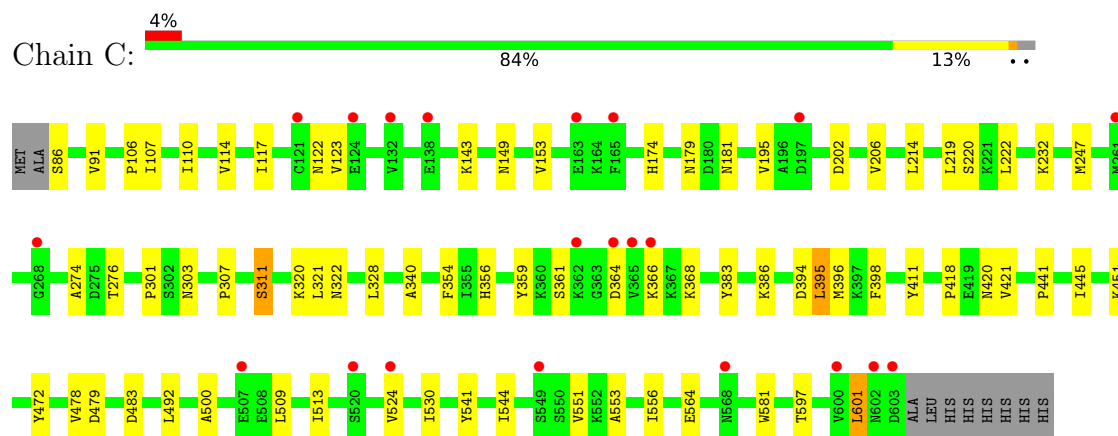
• Molecule 1: Leucine aminopeptidase



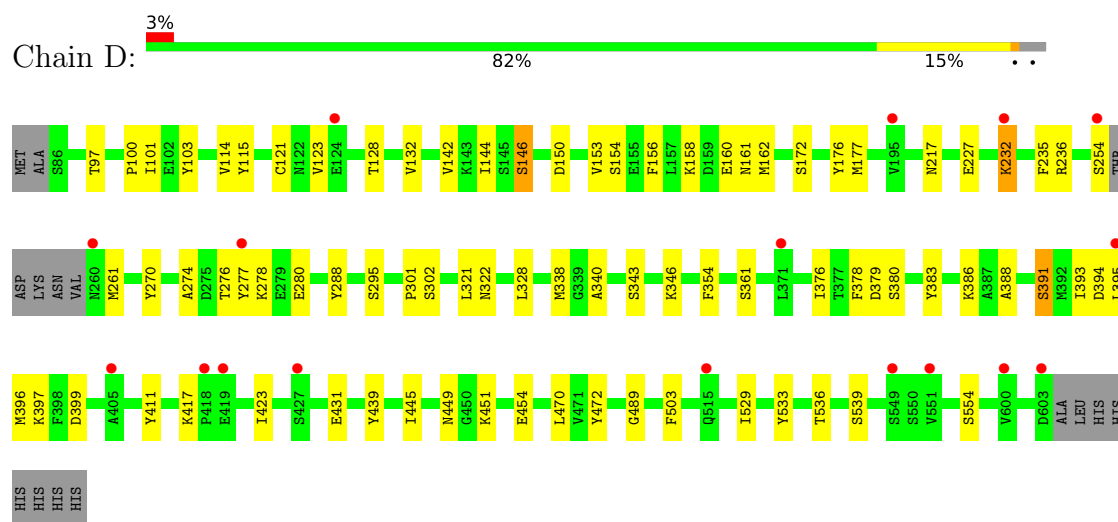
• Molecule 1: Leucine aminopeptidase



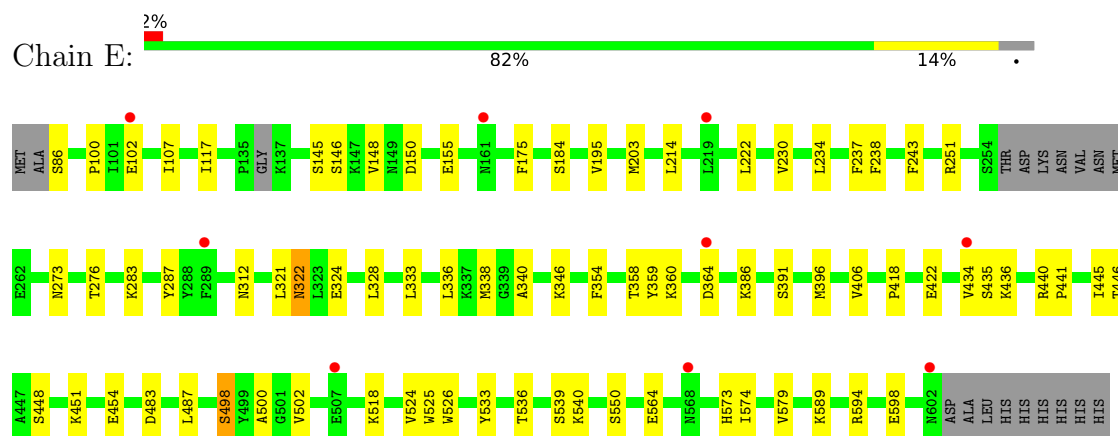
- Molecule 1: Leucine aminopeptidase



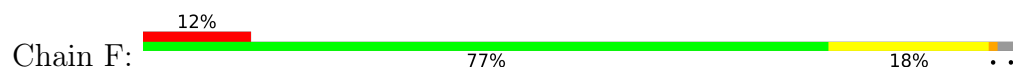
- Molecule 1: Leucine aminopeptidase

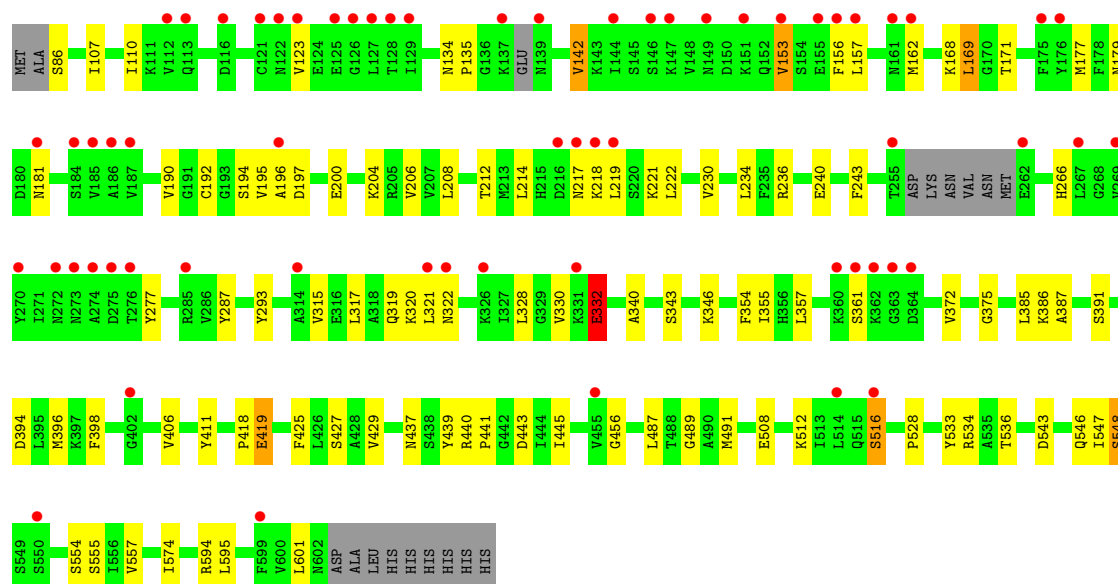


- Molecule 1: Leucine aminopeptidase

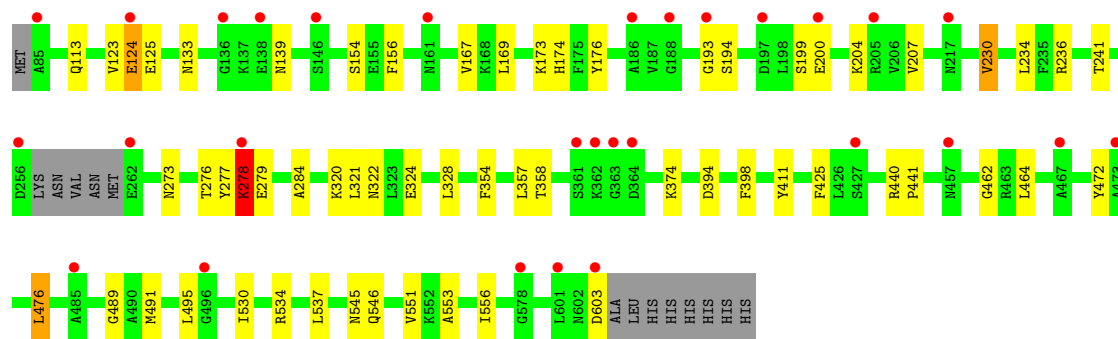
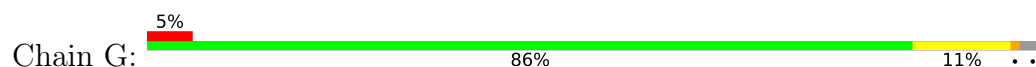


- Molecule 1: Leucine aminopeptidase

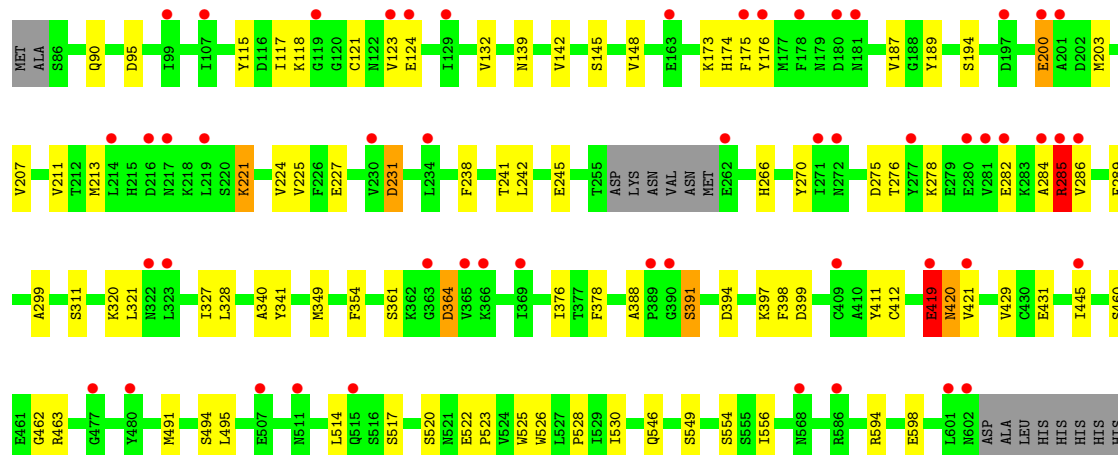
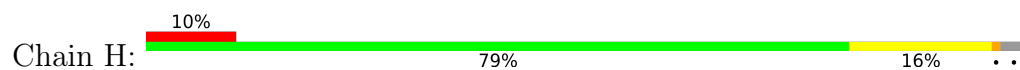




• Molecule 1: Leucine aminopeptidase



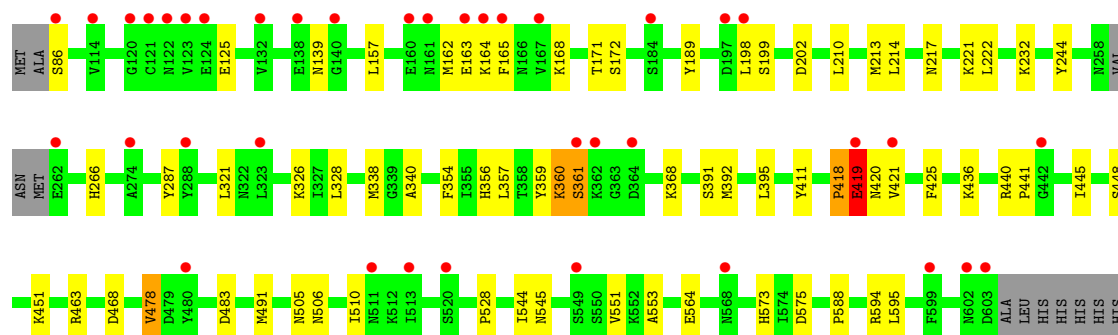
• Molecule 1: Leucine aminopeptidase



HIS

- Molecule 1: Leucine aminopeptidase

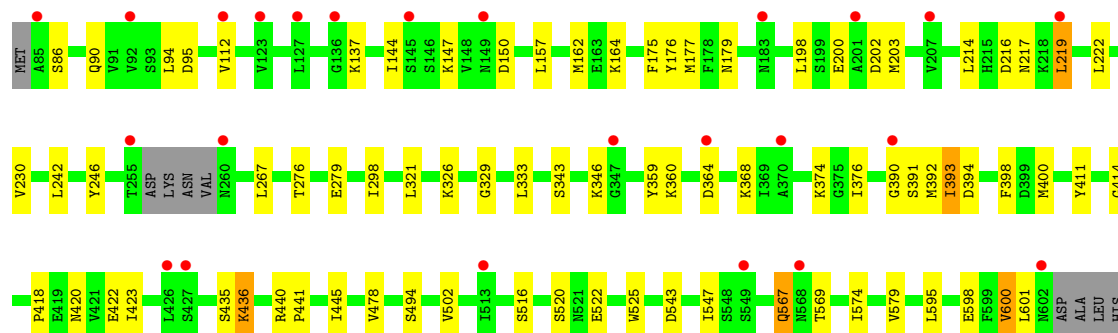
Chain I: 7% 84% 12% ..



HIS

- Molecule 1: Leucine aminopeptidase

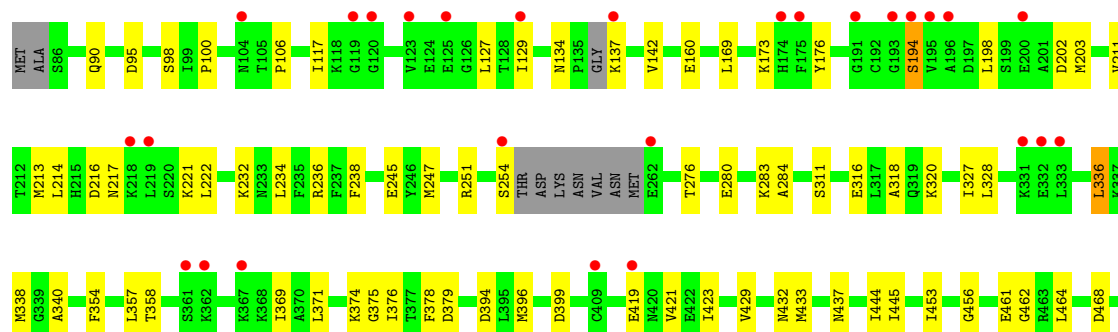
Chain J: 5% 82% 14% ..



HIS

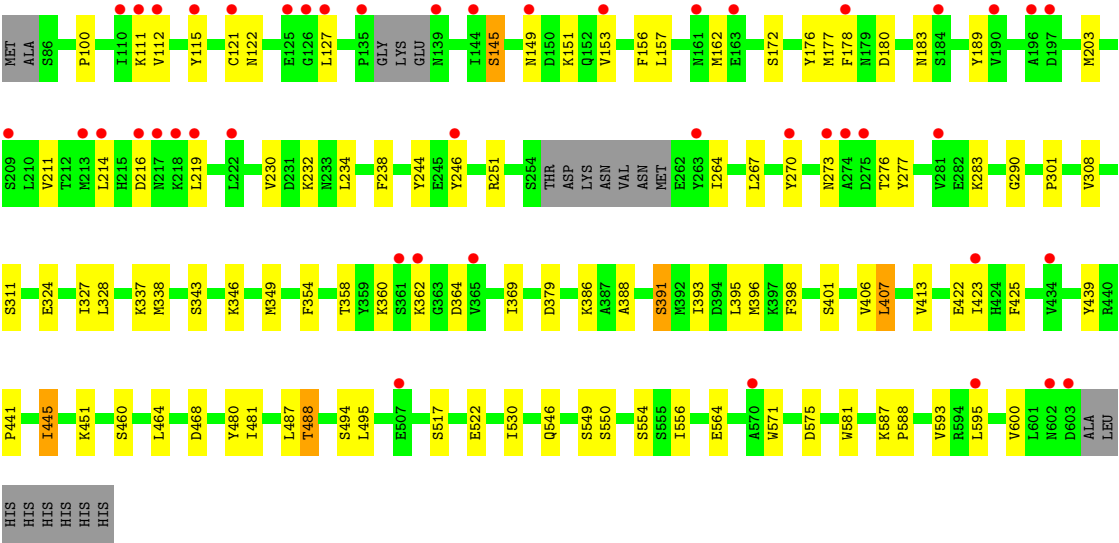
- Molecule 1: Leucine aminopeptidase

Chain K: 6% 79% 17% .





● Molecule 1: Leucine aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.34Å 176.72Å 225.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 2.60 49.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.57-2.60) 100.0 (49.57-2.60)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.235 , 0.281 (Not available) , 0.289	Depositor DCC
R_{free} test set	10861 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.882	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	93534	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1391e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, SO4, ZN, CO3

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	0.16	1/4021 (0.0%)	0.32	0/5459
1	B	0.16	0/3907	0.54	3/5312 (0.1%)
1	C	0.10	0/4027	0.29	0/5465
1	D	0.18	0/3993	0.30	0/5417
1	E	0.09	0/3961	0.27	0/5375
1	F	0.10	0/3850	0.27	0/5241
1	G	0.09	0/4012	0.28	0/5442
1	H	0.11	0/3940	0.32	0/5354
1	I	0.15	1/3986 (0.0%)	0.30	0/5410
1	J	0.09	0/3990	0.28	0/5414
1	K	0.13	0/3943	0.28	0/5354
1	L	0.09	0/3876	0.28	0/5277
All	All	0.13	2/47506 (0.0%)	0.32	3/64520 (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	A	0	1
1	D	0	1
1	F	0	1
1	G	0	1
1	H	0	2
1	I	0	4
1	K	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	ASN	CG-OD1	5.40	1.33	1.23
1	I	545	ASN	CG-OD1	5.02	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLU	CG-CD-OE2	-18.07	76.84	118.40
1	B	125	GLU	OE1-CD-OE2	-17.93	79.88	122.90
1	B	125	GLU	CG-CD-OE1	16.57	156.51	118.40

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	MET	Peptide
1	D	232	LYS	Peptide
1	F	332	GLU	Peptide
1	G	277	TYR	Peptide
1	H	284	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3941	3841	3841	47	1
1	B	3830	3698	3698	52	0
1	C	3949	3871	3871	39	0
1	D	3916	3832	3832	51	0
1	E	3885	3789	3789	47	0
1	F	3776	3589	3588	61	0
1	G	3936	3862	3862	37	1
1	H	3863	3742	3742	63	0
1	I	3909	3827	3827	41	0
1	J	3913	3840	3836	49	0
1	K	3867	3757	3757	60	0
1	L	3801	3623	3623	61	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	2	0
3	I	4	0	0	1	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	10	0	0	1	0
4	B	5	0	0	1	0
4	C	10	0	0	1	0
4	D	5	0	0	1	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
4	I	10	0	0	1	0
4	J	5	0	0	1	0
4	K	5	0	0	0	0
4	L	10	0	0	0	0
5	A	19	23	23	3	0
5	B	7	6	6	0	0
5	C	32	37	37	1	0
5	D	29	31	31	2	0
5	E	21	25	25	1	0
5	F	10	13	13	4	0
5	G	32	40	40	4	0
5	H	10	10	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	10	13	13	0	0
5	K	25	33	33	2	0
5	L	16	22	22	2	0
6	A	97	0	0	1	0
6	B	78	0	0	1	0
6	C	79	0	0	0	0
6	D	87	0	0	2	0
6	E	119	0	0	4	0
6	F	94	0	0	7	0
6	G	85	0	0	4	0
6	H	79	0	0	1	0
6	I	98	0	0	2	0
6	J	86	0	0	5	0
6	K	88	0	0	3	0
6	L	66	0	0	0	0
All	All	48010	45524	45519	573	1

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 6.

The worst 5 of 573 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:400:MET:HE2	6:J:805:HOH:O	1.44	1.17
1:J:400:MET:CE	6:J:805:HOH:O	2.04	1.00
1:J:298:ILE:HA	1:J:400:MET:HE1	1.45	0.96
1:H:286:VAL:HG11	1:H:412:CYS:HA	1.60	0.81
1:E:273:ASN:OD1	1:E:276:THR:OG1	1.99	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:HD21	1:G:113:GLN:HE22[2_564]	1.19	0.41

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	514/528 (97%)	493 (96%)	17 (3%)	4 (1%)	16	34
1	B	507/528 (96%)	483 (95%)	19 (4%)	5 (1%)	12	28
1	C	516/528 (98%)	500 (97%)	16 (3%)	0	100	100
1	D	509/528 (96%)	495 (97%)	14 (3%)	0	100	100
1	E	503/528 (95%)	489 (97%)	13 (3%)	1 (0%)	43	66
1	F	504/528 (96%)	486 (96%)	15 (3%)	3 (1%)	21	42
1	G	510/528 (97%)	494 (97%)	14 (3%)	2 (0%)	30	51
1	H	507/528 (96%)	482 (95%)	21 (4%)	4 (1%)	16	34
1	I	511/528 (97%)	489 (96%)	20 (4%)	2 (0%)	30	51
1	J	510/528 (97%)	496 (97%)	12 (2%)	2 (0%)	30	51
1	K	503/528 (95%)	493 (98%)	10 (2%)	0	100	100
1	L	502/528 (95%)	484 (96%)	18 (4%)	0	100	100
All	All	6096/6336 (96%)	5884 (96%)	189 (3%)	23 (0%)	30	51

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
1	H	285	ARG
1	H	419	GLU
1	H	420	ASN
1	I	419	GLU

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	380/456 (83%)	377 (99%)	3 (1%)	73	88
1	B	394/456 (86%)	384 (98%)	10 (2%)	42	69
1	C	419/456 (92%)	407 (97%)	12 (3%)	37	65
1	D	414/456 (91%)	400 (97%)	14 (3%)	32	60
1	E	412/456 (90%)	402 (98%)	10 (2%)	43	70
1	F	382/456 (84%)	365 (96%)	17 (4%)	24	50
1	G	420/456 (92%)	410 (98%)	10 (2%)	43	70
1	H	404/456 (89%)	390 (96%)	14 (4%)	32	59
1	I	412/456 (90%)	403 (98%)	9 (2%)	45	72
1	J	412/456 (90%)	398 (97%)	14 (3%)	32	60
1	K	407/456 (89%)	398 (98%)	9 (2%)	45	72
1	L	391/456 (86%)	376 (96%)	15 (4%)	29	56
All	All	4847/5472 (89%)	4710 (97%)	137 (3%)	38	66

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	142	VAL
1	K	358	THR
1	L	445	ILE
1	E	550	SER
1	E	498	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	602	ASN
1	J	217	ASN
1	H	90	GLN
1	I	161	ASN
1	J	531	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 24 are monoatomic - leaving 49 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CO3	B	1001	-	3,3,3	0.82	0	2,3,3	0.11	0
5	1PE	A	706	-	8,8,15	0.17	0	7,7,14	0.16	0
4	SO4	K	706	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	D	704	-	4,4,4	0.24	0	6,6,6	0.12	0
5	1PE	E	705	-	11,11,15	0.15	0	10,10,14	0.14	0
5	1PE	E	706	-	8,8,15	0.15	0	7,7,14	0.10	0
4	SO4	A	705	-	4,4,4	0.23	0	6,6,6	0.07	0
5	1PE	B	1005	-	6,6,15	0.20	0	5,5,14	0.10	0
4	SO4	A	704	-	4,4,4	0.24	0	6,6,6	0.12	0
3	CO3	J	703	-	3,3,3	0.82	0	2,3,3	0.14	0
4	SO4	G	704	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	G	708	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	E	704	-	4,4,4	0.23	0	6,6,6	0.09	0
5	1PE	G	707	-	12,12,15	0.10	0	11,11,14	0.12	0
3	CO3	K	703	-	3,3,3	0.83	0	2,3,3	0.10	0
3	CO3	F	704	-	3,3,3	0.84	0	2,3,3	0.13	0
5	1PE	K	705	-	15,15,15	0.11	0	14,14,14	0.12	0
4	SO4	L	705	-	4,4,4	0.23	0	6,6,6	0.07	0
3	CO3	A	703	-	3,3,3	0.83	0	2,3,3	0.19	0
3	CO3	C	703	-	3,3,3	0.84	0	2,3,3	0.14	0
4	SO4	I	705	-	4,4,4	0.24	0	6,6,6	0.07	0
5	1PE	J	704	-	9,9,15	0.10	0	8,8,14	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1PE	A	707	-	9,9,15	0.10	0	8,8,14	0.14	0
3	CO3	L	704	-	3,3,3	0.83	0	2,3,3	0.12	0
4	SO4	C	704	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	F	701	-	4,4,4	0.23	0	6,6,6	0.09	0
5	1PE	F	705	-	9,9,15	0.08	0	8,8,14	0.15	0
5	1PE	L	706	-	15,15,15	0.13	0	14,14,14	0.16	0
5	1PE	H	704	-	9,9,15	0.19	0	8,8,14	0.12	0
4	SO4	C	708	-	4,4,4	0.24	0	6,6,6	0.07	0
3	CO3	G	701	-	3,3,3	0.83	0	2,3,3	0.16	0
5	1PE	D	705	-	9,9,15	0.19	0	8,8,14	0.12	0
5	1PE	D	706	-	9,9,15	0.20	0	8,8,14	0.11	0
3	CO3	E	703	-	3,3,3	0.85	0	2,3,3	0.15	0
3	CO3	H	703	-	3,3,3	0.82	0	2,3,3	0.26	0
5	1PE	C	706	-	8,8,15	0.17	0	7,7,14	0.15	0
4	SO4	J	705	-	4,4,4	0.22	0	6,6,6	0.09	0
3	CO3	I	703	-	3,3,3	0.83	0	2,3,3	0.14	0
4	SO4	B	1004	-	4,4,4	0.23	0	6,6,6	0.13	0
5	1PE	K	704	-	8,8,15	0.16	0	7,7,14	0.09	0
4	SO4	H	705	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	L	701	-	4,4,4	0.23	0	6,6,6	0.07	0
5	1PE	C	705	-	12,12,15	0.18	0	11,11,14	0.12	0
5	1PE	D	707	-	8,8,15	0.16	0	7,7,14	0.09	0
4	SO4	I	704	-	4,4,4	0.23	0	6,6,6	0.09	0
5	1PE	G	706	-	9,9,15	0.11	0	8,8,14	0.13	0
3	CO3	D	703	-	3,3,3	0.82	0	2,3,3	0.12	0
5	1PE	C	707	-	9,9,15	0.11	0	8,8,14	0.13	0
5	1PE	G	705	-	8,8,15	0.17	0	7,7,14	0.14	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
5	1PE	A	706	-	-	3/6/6/13	-
5	1PE	E	705	-	-	5/9/9/13	-
5	1PE	B	1005	-	-	2/4/4/13	-
5	1PE	C	707	-	-	4/7/7/13	-
5	1PE	G	707	-	-	4/10/10/13	-
5	1PE	K	705	-	-	4/13/13/13	-
5	1PE	J	704	-	-	5/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	A	707	-	-	6/7/7/13	-
5	1PE	F	705	-	-	4/7/7/13	-
5	1PE	L	706	-	-	6/13/13/13	-
5	1PE	H	704	-	-	6/7/7/13	-
5	1PE	D	705	-	-	5/7/7/13	-
5	1PE	D	706	-	-	2/7/7/13	-
5	1PE	C	706	-	-	2/6/6/13	-
5	1PE	K	704	-	-	1/6/6/13	-
5	1PE	C	705	-	-	2/10/10/13	-
5	1PE	D	707	-	-	5/6/6/13	-
5	1PE	G	706	-	-	2/7/7/13	-
5	1PE	E	706	-	-	2/6/6/13	-
5	1PE	G	705	-	-	4/6/6/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	706	1PE	C14-C24-OH4-C13
5	L	706	1PE	C12-C22-OH3-C23
5	D	705	1PE	OH4-C13-C23-OH3
5	G	707	1PE	OH5-C14-C24-OH4
5	A	707	1PE	OH5-C14-C24-OH4

There are no ring outliers.

23 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	706	1PE	2	0
4	D	704	SO4	1	0
5	E	706	1PE	1	0
4	A	704	SO4	1	0
4	E	704	SO4	1	0
5	G	707	1PE	2	0
5	K	705	1PE	2	0
3	A	703	CO3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	707	1PE	1	0
4	C	704	SO4	1	0
5	F	705	1PE	4	0
5	L	706	1PE	2	0
5	H	704	1PE	1	0
5	D	705	1PE	1	0
3	H	703	CO3	2	0
4	J	705	SO4	1	0
3	I	703	CO3	1	0
4	B	1004	SO4	1	0
5	C	705	1PE	1	0
5	D	707	1PE	1	0
4	I	704	SO4	1	0
5	G	706	1PE	1	0
5	G	705	1PE	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	517/528 (97%)	0.72	22 (4%)	40	34	26, 37, 59, 88	1 (0%)
1	B	511/528 (96%)	0.81	45 (8%)	15	12	28, 39, 69, 108	0
1	C	518/528 (98%)	0.66	21 (4%)	41	36	27, 36, 59, 87	0
1	D	513/528 (97%)	0.56	17 (3%)	49	43	23, 31, 52, 81	0
1	E	509/528 (96%)	0.48	9 (1%)	67	63	24, 32, 46, 69	0
1	F	510/528 (96%)	0.96	63 (12%)	8	6	24, 38, 70, 92	0
1	G	514/528 (97%)	0.81	29 (5%)	30	24	32, 40, 57, 79	0
1	H	511/528 (96%)	0.95	52 (10%)	12	9	26, 40, 73, 116	1 (0%)
1	I	515/528 (97%)	0.83	38 (7%)	20	16	28, 37, 60, 105	0
1	J	514/528 (97%)	0.65	24 (4%)	36	30	24, 34, 51, 70	0
1	K	509/528 (96%)	0.66	30 (5%)	28	23	26, 33, 49, 77	3 (0%)
1	L	508/528 (96%)	0.92	45 (8%)	15	12	28, 39, 65, 95	1 (0%)
All	All	6149/6336 (97%)	0.75	395 (6%)	25	20	23, 37, 63, 116	6 (0%)

The worst 5 of 395 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	419	GLU	6.1
1	L	603	ASP	6.0
1	I	603	ASP	5.4
1	H	285	ARG	5.3
1	I	361	SER	5.2

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	Q<0.9
4	SO4	L	701	5/5	0.27	0.12	123,127,143,154	0
4	SO4	L	705	5/5	0.38	0.14	123,128,135,152	0
4	SO4	E	704	5/5	0.58	0.34	122,123,124,148	0
4	SO4	D	704	5/5	0.62	0.27	112,113,119,125	0
4	SO4	A	705	5/5	0.65	0.20	92,92,106,117	0
5	1PE	B	1005	7/16	0.68	0.23	37,47,51,53	0
3	CO3	J	703	4/4	0.72	0.21	26,26,27,44	0
5	1PE	C	705	13/16	0.72	0.17	37,49,62,64	0
5	1PE	D	706	10/16	0.72	0.17	36,55,59,62	0
5	1PE	K	704	9/16	0.73	0.16	31,34,42,42	0
5	1PE	D	707	9/16	0.75	0.18	28,38,51,51	0
5	1PE	K	705	16/16	0.75	0.16	45,59,72,75	0
4	SO4	G	708	5/5	0.76	0.20	75,77,92,95	0
4	SO4	I	705	5/5	0.77	0.16	64,68,75,77	0
5	1PE	G	707	13/16	0.79	0.16	41,50,64,67	0
4	SO4	A	704	5/5	0.79	0.36	84,85,101,116	0
5	1PE	G	705	9/16	0.79	0.18	40,50,58,58	0
5	1PE	L	706	16/16	0.79	0.17	48,64,75,78	0
5	1PE	A	706	9/16	0.80	0.16	37,37,46,49	0
5	1PE	G	706	10/16	0.80	0.16	35,44,54,56	0
5	1PE	A	707	10/16	0.80	0.18	39,43,52,55	0
4	SO4	H	705	5/5	0.81	0.13	52,55,81,85	0
3	CO3	A	703	4/4	0.82	0.18	35,38,38,43	0
5	1PE	C	707	10/16	0.82	0.17	28,35,50,51	0
3	CO3	G	701	4/4	0.83	0.17	39,39,46,50	0
5	1PE	H	704	10/16	0.83	0.17	44,51,59,61	0
5	1PE	C	706	9/16	0.83	0.13	33,38,46,48	0
4	SO4	C	704	5/5	0.83	0.15	66,72,75,94	0
5	1PE	D	705	10/16	0.83	0.17	33,39,41,45	0
3	CO3	D	703	4/4	0.84	0.15	23,23,25,31	0
5	1PE	F	705	10/16	0.84	0.13	33,38,44,48	0
3	CO3	L	704	4/4	0.84	0.13	37,43,44,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	K	706	5/5	0.85	0.18	46,53,74,74	0
5	1PE	J	704	10/16	0.86	0.14	33,37,46,51	0
5	1PE	E	705	12/16	0.86	0.14	28,33,64,64	0
4	SO4	G	704	5/5	0.87	0.12	45,54,65,69	0
3	CO3	E	703	4/4	0.87	0.12	37,38,39,42	0
5	1PE	E	706	9/16	0.88	0.14	23,33,41,41	0
3	CO3	H	703	4/4	0.89	0.11	37,37,39,39	0
3	CO3	F	704	4/4	0.91	0.11	25,29,32,36	0
3	CO3	I	703	4/4	0.91	0.10	29,31,32,33	0
4	SO4	C	708	5/5	0.92	0.12	49,52,54,65	0
3	CO3	C	703	4/4	0.92	0.09	33,34,35,43	0
4	SO4	B	1004	5/5	0.93	0.11	33,33,33,37	0
3	CO3	K	703	4/4	0.94	0.09	26,29,34,42	0
3	CO3	B	1001	4/4	0.94	0.09	29,30,32,33	0
2	ZN	F	702	1/1	0.95	0.09	31,31,31,31	0
2	ZN	L	702	1/1	0.95	0.07	32,32,32,32	0
4	SO4	J	705	5/5	0.96	0.08	24,31,34,41	0
4	SO4	I	704	5/5	0.96	0.08	34,34,34,40	0
2	ZN	B	1003	1/1	0.97	0.08	35,35,35,35	0
2	ZN	F	703	1/1	0.97	0.05	24,24,24,24	0
2	ZN	C	701	1/1	0.97	0.10	29,29,29,29	0
2	ZN	J	701	1/1	0.98	0.10	30,30,30,30	0
2	ZN	A	701	1/1	0.98	0.04	32,32,32,32	0
2	ZN	L	703	1/1	0.98	0.05	28,28,28,28	0
2	ZN	D	701	1/1	0.98	0.06	25,25,25,25	0
2	ZN	G	703	1/1	0.98	0.07	34,34,34,34	0
2	ZN	H	702	1/1	0.98	0.04	30,30,30,30	0
4	SO4	F	701	5/5	0.98	0.05	20,24,29,33	0
2	ZN	I	701	1/1	0.98	0.09	29,29,29,29	0
2	ZN	I	702	1/1	0.98	0.09	29,29,29,29	0
2	ZN	B	1002	1/1	0.99	0.06	29,29,29,29	0
2	ZN	J	702	1/1	0.99	0.06	24,24,24,24	0
2	ZN	K	701	1/1	0.99	0.06	25,25,25,25	0
2	ZN	K	702	1/1	0.99	0.06	32,32,32,32	0
2	ZN	C	702	1/1	0.99	0.08	29,29,29,29	0
2	ZN	G	702	1/1	0.99	0.05	34,34,34,34	0
2	ZN	A	702	1/1	0.99	0.04	32,32,32,32	0
2	ZN	H	701	1/1	0.99	0.04	31,31,31,31	0
2	ZN	D	702	1/1	0.99	0.05	30,30,30,30	0
2	ZN	E	701	1/1	0.99	0.04	23,23,23,23	0
2	ZN	E	702	1/1	0.99	0.09	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.