



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2016 – 11:17 AM EDT

PDB ID : 4ZX8  
Title : X-ray crystal structure of PfA-M17 in complex with hydroxamic acid-based inhibitor 9b  
Authors : Drinkwater, N.; McGowan, S.  
Deposited on : 2015-05-20  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

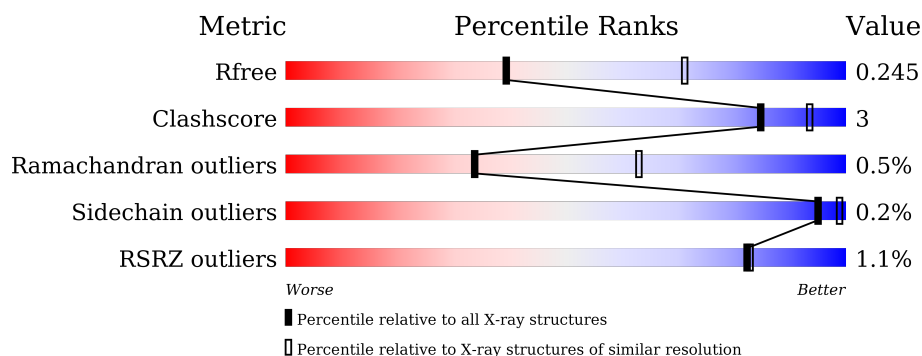
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	522	<div> <div>%</div> <div>92% 8% .</div> </div>
1	B	522	<div> <div>2%</div> <div>90% 9% ..</div> </div>
1	C	522	<div> <div>%</div> <div>92% 7% .</div> </div>
1	D	522	<div> <div>%</div> <div>90% 8% .</div> </div>
1	E	522	<div> <div></div> <div>91% 7% .</div> </div>
1	F	522	<div> <div>2%</div> <div>92% 6% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	522	
1	H	522	
1	I	522	
1	J	522	
1	K	522	
1	L	522	

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
2	4TY	B	1001	-	-	-	X
2	4TY	K	1001	-	-	-	X
2	4TY	L	1001	-	-	-	X
4	CO3	J	1004	-	-	-	X
5	GOL	A	1005	-	-	-	X
5	GOL	C	1005	-	-	-	X
5	GOL	I	1005	-	-	-	X
6	DMS	A	1007	-	-	-	X
7	1PE	A	1009	-	-	-	X
7	1PE	D	1006	-	-	-	X
7	1PE	F	1006	-	-	-	X
7	1PE	F	1007	-	-	-	X
7	1PE	G	1005	-	-	-	X
7	1PE	K	1006	-	-	-	X
8	SO4	D	1007	-	-	-	X
8	SO4	E	1008	-	-	-	X
8	SO4	J	1007	-	-	-	X
8	SO4	J	1009	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 49322 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3960	2540	637	764	19			
1	B	516	Total	C	N	O	S	0	0	0
			3906	2509	636	742	19			
1	C	517	Total	C	N	O	S	0	0	0
			3910	2516	628	747	19			
1	D	512	Total	C	N	O	S	0	0	0
			3888	2507	630	731	20			
1	E	510	Total	C	N	O	S	0	0	0
			3895	2509	626	741	19			
1	F	513	Total	C	N	O	S	0	0	0
			3833	2468	620	726	19			
1	G	519	Total	C	N	O	S	0	0	0
			3972	2548	638	767	19			
1	H	517	Total	C	N	O	S	0	0	0
			3894	2499	633	743	19			
1	I	517	Total	C	N	O	S	0	0	0
			3938	2529	637	753	19			
1	J	513	Total	C	N	O	S	0	0	0
			3894	2508	631	735	20			
1	K	509	Total	C	N	O	S	0	0	0
			3896	2506	627	744	19			
1	L	512	Total	C	N	O	S	0	0	0
			3840	2468	621	732	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	546	GLN	ASN	engineered mutation	UNP A0A024V0B1

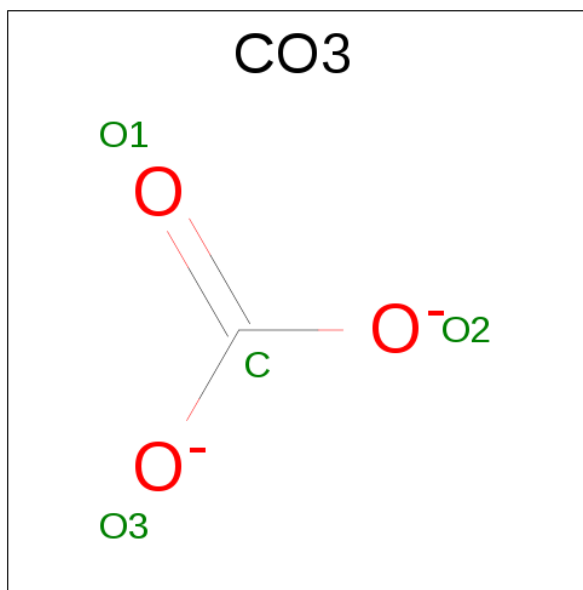
- Molecule 2 is tert-butyl [(1R)-1-(4-bromophenyl)-2-(hydroxyamino)-2-oxoethyl]carbamate (three-letter code: 4TY) (formula: C<sub>13</sub>H<sub>17</sub>BrN<sub>2</sub>O<sub>4</sub>).



- Molecule 3 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

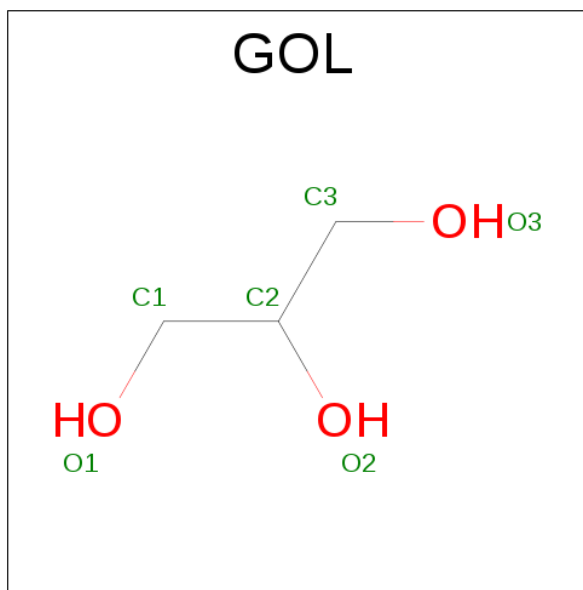
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total 2	Zn 2	0	0
3	J	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	K	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0
3	L	2	Total 2	Zn 2	0	0
3	F	2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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

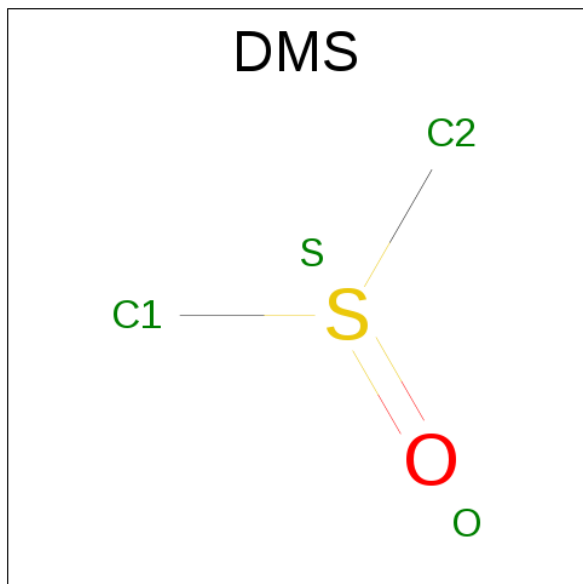
- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





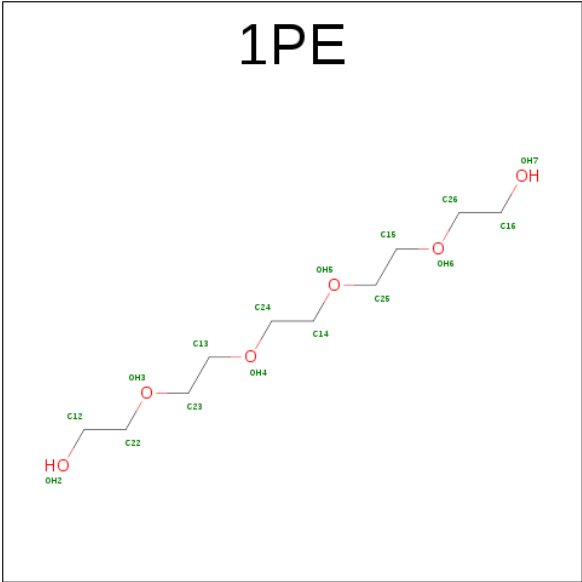
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



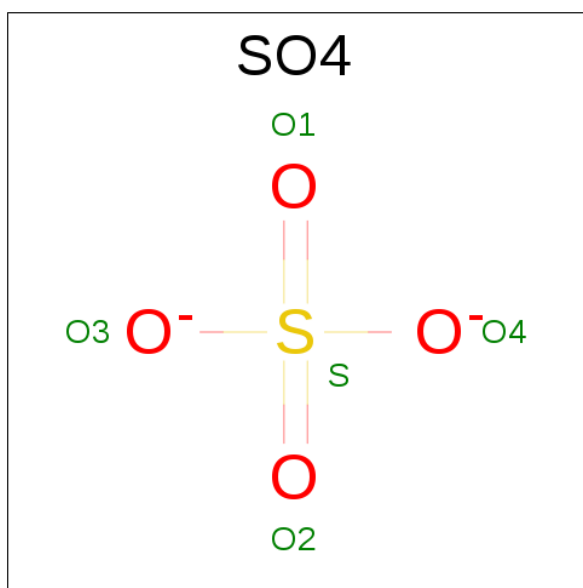
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	4	2		
7	A	1	Total	C	O	0	0
			9	6	3		
7	A	1	Total	C	O	0	0
			6	4	2		
7	A	1	Total	C	O	0	0
			6	4	2		
7	B	1	Total	C	O	0	0
			10	7	3		
7	C	1	Total	C	O	0	0
			12	8	4		
7	C	1	Total	C	O	0	0
			11	8	3		
7	D	1	Total	C	O	0	0
			11	7	4		
7	D	1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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			9	6	3		
7	G	1	Total	C	O	0	0
			12	8	4		
7	H	1	Total	C	O	0	0
			10	7	3		
7	H	1	Total	C	O	0	0
			10	7	3		
7	I	1	Total	C	O	0	0
			13	9	4		
7	I	1	Total	C	O	0	0
			9	6	3		
7	J	1	Total	C	O	0	0
			10	7	3		
7	J	1	Total	C	O	0	0
			10	7	3		
7	K	1	Total	C	O	0	0
			12	8	4		
7	K	1	Total	C	O	0	0
			12	8	4		
7	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	163	Total O 163 163	0	0
9	B	138	Total O 138 138	0	0
9	C	155	Total O 155 155	0	0
9	D	166	Total O 166 166	0	0
9	E	155	Total O 155 155	0	0
9	F	138	Total O 138 138	0	0
9	G	148	Total O 148 148	0	0

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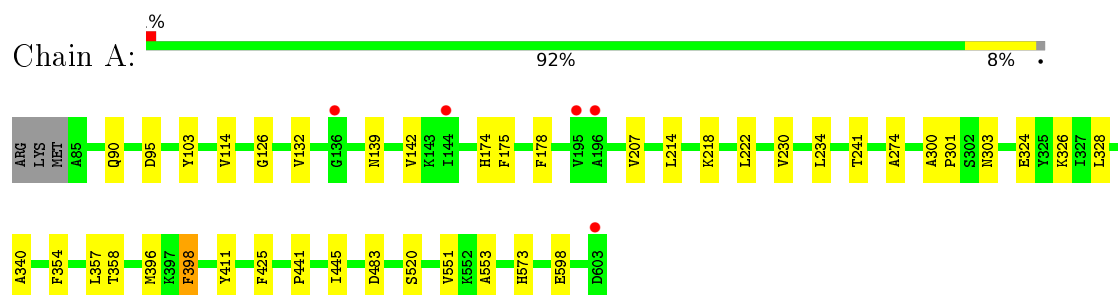
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	127	Total 127	O 127	0	0
9	I	160	Total 160	O 160	0	0
9	J	152	Total 152	O 152	0	0
9	K	196	Total 196	O 196	0	0
9	L	121	Total 121	O 121	0	0

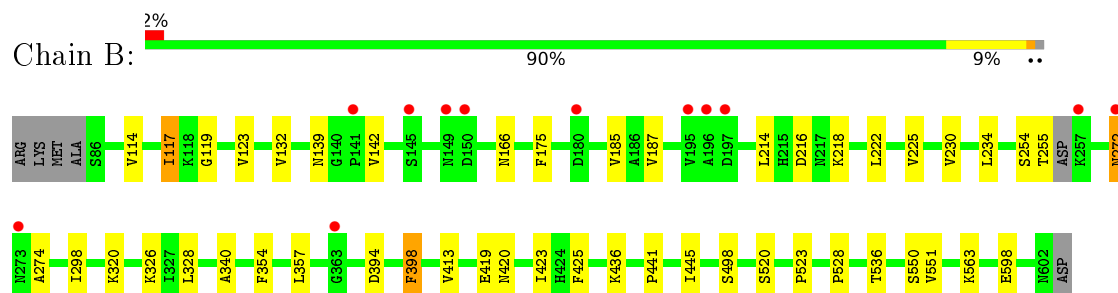
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

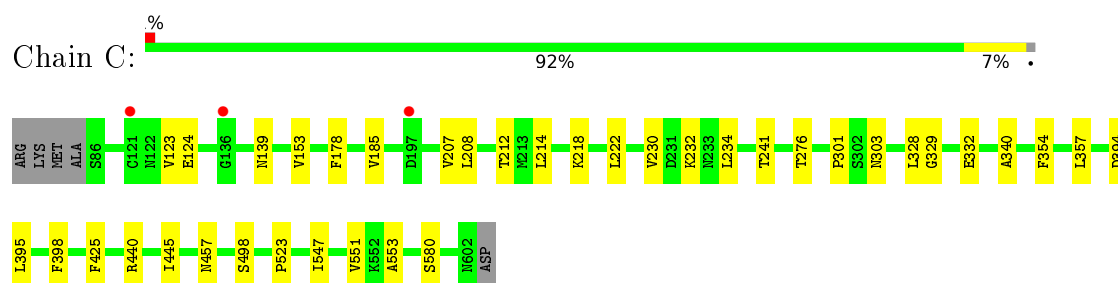
- Molecule 1: Probable M17 family aminopeptidase



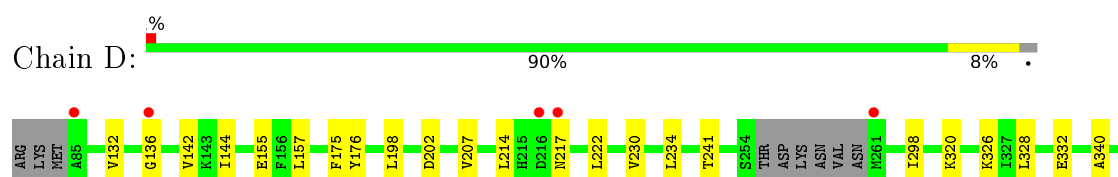
- Molecule 1: Probable M17 family aminopeptidase



- Molecule 1: Probable M17 family aminopeptidase



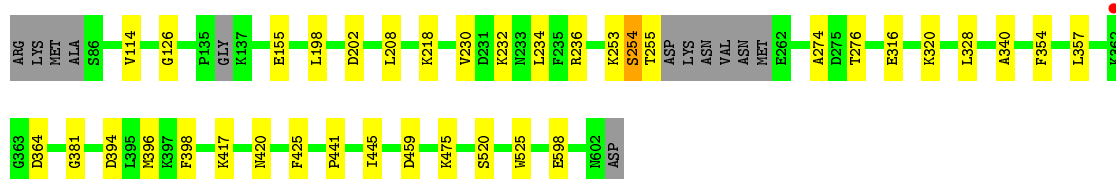
- Molecule 1: Probable M17 family aminopeptidase





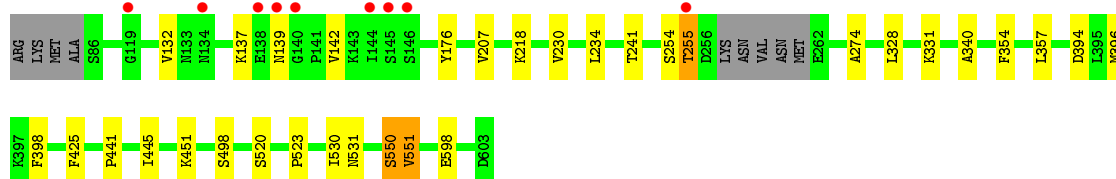
- Molecule 1: Probable M17 family aminopeptidase

Chain E: 91% 7% .



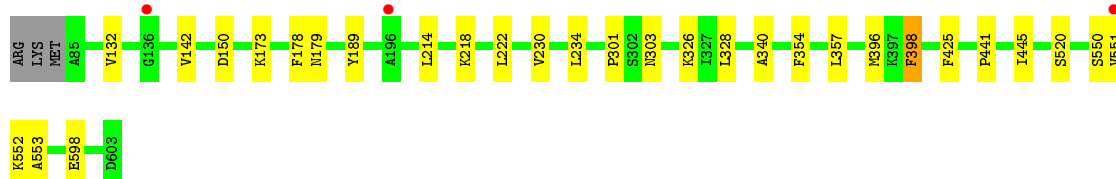
- Molecule 1: Probable M17 family aminopeptidase

Chain F: 92% 6% 2% .



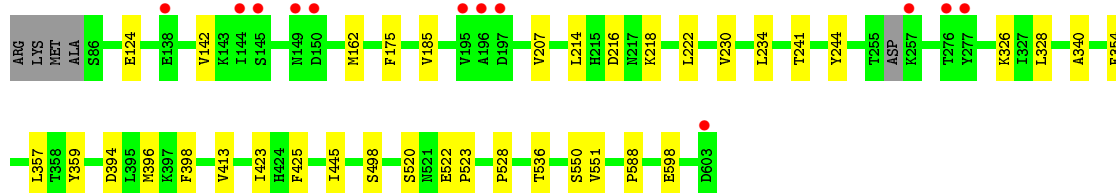
- Molecule 1: Probable M17 family aminopeptidase

Chain G: 94% 6% .



- Molecule 1: Probable M17 family aminopeptidase

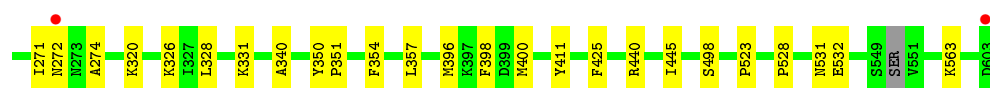
Chain H: 92% 7% 2% .



- Molecule 1: Probable M17 family aminopeptidase

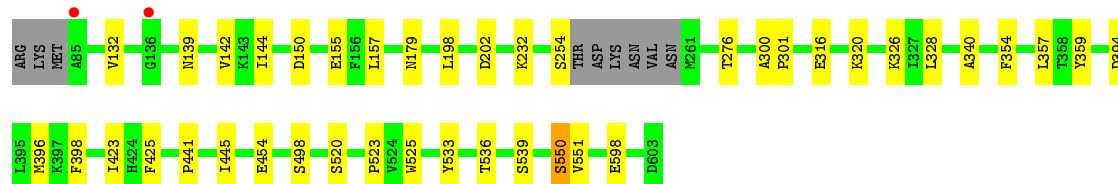
Chain I: 89% 10% .





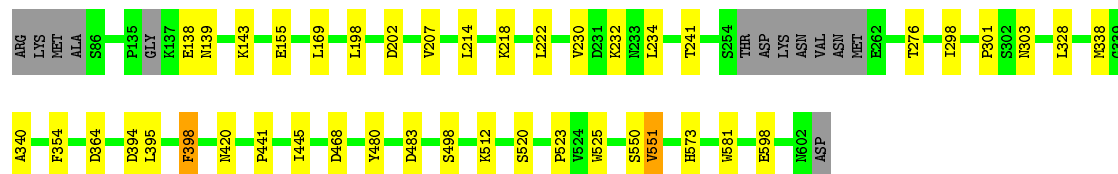
- Molecule 1: Probable M17 family aminopeptidase

Chain J: 90% 8% .



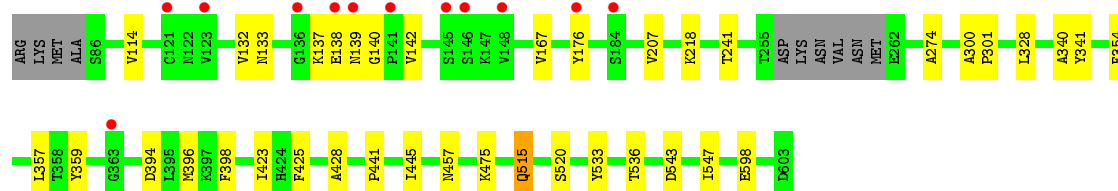
- Molecule 1: Probable M17 family aminopeptidase

Chain K: 89% 8% .



- Molecule 1: Probable M17 family aminopeptidase

Chain L: 2% 91% 7% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.39Å 177.47Å 231.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 2.70 48.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.95-2.70) 92.6 (48.95-2.70)	Depositor EDS
$R_{merge}$	0.47	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, $R_{free}$	0.197 , 0.245 0.203 , 0.245	Depositor DCC
$R_{free}$ test set	9911 reflections (5.74%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 17.7	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	52 of 196269 reflections (0.026%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	49322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.45 % 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 9.9050e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 4TY, ZN, 1PE, DMS, SO4, 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	0.24	0/4038	0.42	0/5485
1	B	0.24	0/3983	0.42	0/5411
1	C	0.24	0/3988	0.41	0/5422
1	D	0.24	0/3965	0.43	0/5381
1	E	0.24	0/3971	0.41	0/5387
1	F	0.23	0/3910	0.42	0/5321
1	G	0.24	0/4050	0.41	0/5499
1	H	0.24	0/3971	0.41	0/5399
1	I	0.25	0/4015	0.41	0/5450
1	J	0.24	0/3971	0.43	0/5389
1	K	0.24	0/3972	0.42	0/5388
1	L	0.23	0/3917	0.42	0/5329
All	All	0.24	0/47751	0.42	0/64861

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	K	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	K	138	GLU	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	3960	0	3853	25	0
1	B	3906	0	3799	31	0
1	C	3910	0	3778	21	0
1	D	3888	0	3813	25	0
1	E	3895	0	3815	24	0
1	F	3833	0	3677	21	0
1	G	3972	0	3871	17	0
1	H	3894	0	3752	21	0
1	I	3938	0	3839	31	0
1	J	3894	0	3811	25	0
1	K	3896	0	3819	22	0
1	L	3840	0	3685	25	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
2	E	20	0	0	0	0
2	F	20	0	0	0	0
2	G	20	0	0	0	0
2	H	20	0	0	0	0
2	I	20	0	0	0	0
2	J	20	0	0	0	0
2	K	20	0	0	0	0
2	L	20	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	12	0	16	1	0
5	C	6	0	8	0	0
5	E	6	0	8	1	0
5	F	6	0	8	1	0
5	I	6	0	8	2	0
6	A	4	0	6	0	0
7	A	27	0	26	1	0
7	B	10	0	10	2	0
7	C	23	0	26	0	0
7	D	21	0	26	1	0
7	E	24	0	28	4	0
7	F	38	0	47	3	0
7	G	21	0	22	1	0
7	H	20	0	20	0	0
7	I	22	0	24	4	0
7	J	20	0	20	3	0
7	K	24	0	28	0	0
7	L	10	0	13	0	0
8	A	5	0	0	1	0
8	B	5	0	0	1	0
8	D	5	0	0	0	0
8	E	10	0	0	0	0
8	F	10	0	0	0	0
8	H	5	0	0	0	0
8	J	15	0	0	0	0
8	K	10	0	0	0	0
9	A	163	0	0	1	0
9	B	138	0	0	1	0
9	C	155	0	0	1	0
9	D	166	0	0	1	0
9	E	155	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	138	0	0	1	0
9	G	148	0	0	1	0
9	H	127	0	0	1	0
9	I	160	0	0	4	0
9	J	152	0	0	0	0
9	K	196	0	0	0	0
9	L	121	0	0	1	0
All	All	49322	0	45856	269	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 3.

All (269) 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:L:515:GLN:HA	1:L:515:GLN:HE21	1.20	1.06
1:I:531:ASN:H	5:I:1005:GOL:H12	1.42	0.84
1:J:320:LYS:HZ1	7:J:1005:1PE:H142	1.46	0.81
1:L:515:GLN:HA	1:L:515:GLN:NE2	1.97	0.76
1:B:123:VAL:HG12	1:B:185:VAL:HG11	1.67	0.75
1:L:515:GLN:HE21	1:L:515:GLN:CA	1.99	0.73
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.71	0.72
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.58	0.69
1:A:551:VAL:O	9:A:1101:HOH:O	2.10	0.69
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.75	0.68
1:G:551:VAL:HG12	1:G:553:ALA:H	1.59	0.68
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.76	0.68
1:E:232:LYS:NZ	1:E:276:THR:O	2.27	0.67
1:B:214:LEU:HD21	1:B:222:LEU:HD22	1.74	0.67
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.77	0.67
1:F:531:ASN:H	7:F:1007:1PE:H141	1.60	0.67
1:A:126:GLY:H	5:A:1005:GOL:H11	1.61	0.66
1:K:232:LYS:NZ	1:K:276:THR:O	2.27	0.66
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.77	0.66
1:B:132:VAL:HG21	1:B:142:VAL:HG13	1.77	0.66
1:I:320:LYS:HZ1	7:I:1006:1PE:H142	1.61	0.66
1:C:357:LEU:HB2	1:C:425:PHE:HB2	1.77	0.66
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.79	0.65
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.79	0.65
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.79	0.65
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.63	0.62
1:F:451:LYS:HE2	7:F:1006:1PE:H161	1.82	0.62
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.82	0.61
1:G:326:LYS:HE3	1:G:328:LEU:HD11	1.82	0.60
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.82	0.60
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.67	0.60
1:B:436:LYS:NZ	8:B:1006:SO4:O2	2.33	0.60
1:I:440:ARG:NH2	9:I:1106:HOH:O	2.34	0.60
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.83	0.60
1:I:123:VAL:HG12	1:I:185:VAL:HG11	1.83	0.60
1:K:395:LEU:HD11	1:K:581:TRP:CE2	2.36	0.60
1:H:214:LEU:HD21	1:H:222:LEU:HD22	1.83	0.60
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.83	0.60
1:A:326:LYS:HE3	1:A:328:LEU:HD11	1.84	0.59
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.82	0.59
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.84	0.59
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.85	0.59
1:J:396:MET:SD	1:J:398:PHE:HE2	2.25	0.58
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.85	0.58
1:J:326:LYS:HE3	1:J:328:LEU:HD11	1.84	0.58
1:B:139:ASN:HB3	1:B:166:ASN:ND2	2.19	0.58
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.87	0.57
1:A:396:MET:SD	1:A:398:PHE:HE2	2.26	0.57
1:C:398:PHE:CE1	1:C:580:SER:HB3	2.39	0.57
1:E:396:MET:SD	1:E:398:PHE:HE2	2.27	0.57
1:H:396:MET:SD	1:H:398:PHE:HE2	2.28	0.57
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.86	0.57
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.86	0.57
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.70	0.57
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.86	0.56
1:I:143:LYS:NZ	9:I:1108:HOH:O	2.37	0.56
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.86	0.56
1:A:520:SER:HB3	1:A:598:GLU:HG3	1.88	0.56
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.86	0.56
1:A:483:ASP:OD1	1:A:573:HIS:ND1	2.35	0.56
1:F:331:LYS:H	5:F:1005:GOL:H11	1.71	0.56
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.88	0.56
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.88	0.56
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.88	0.56
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.87	0.55
1:D:357:LEU:HB2	1:D:425:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:MET:SD	1:G:398:PHE:HE2	2.30	0.55
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.89	0.55
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.89	0.55
1:J:316:GLU:HG3	7:J:1005:1PE:H221	1.87	0.55
1:B:563:LYS:NZ	9:B:1104:HOH:O	2.37	0.54
1:H:142:VAL:HG23	1:H:162:MET:HB3	1.88	0.54
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.89	0.54
1:K:198:LEU:HD22	1:K:202:ASP:HB3	1.90	0.54
1:G:173:LYS:NZ	9:G:1114:HOH:O	2.41	0.54
1:I:396:MET:SD	1:I:398:PHE:HE2	2.31	0.54
1:C:440:ARG:NH2	9:C:1110:HOH:O	2.40	0.54
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.72	0.54
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.89	0.54
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.90	0.53
1:A:90:GLN:NE2	1:A:95:ASP:O	2.40	0.53
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.90	0.53
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.91	0.53
1:K:230:VAL:HG12	1:K:234:LEU:HD23	1.90	0.53
1:B:175:PHE:HD1	1:F:176:TYR:HB2	1.74	0.52
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.91	0.52
1:B:326:LYS:HE3	1:B:328:LEU:HD11	1.92	0.52
1:C:395:LEU:O	1:C:398:PHE:HB3	2.09	0.52
1:A:551:VAL:HG12	1:A:553:ALA:H	1.75	0.52
1:I:116:ASP:HA	1:I:271:ILE:O	2.09	0.52
1:A:411:TYR:HE1	7:A:1009:1PE:H132	1.75	0.52
1:F:530:ILE:HG23	7:F:1007:1PE:H242	1.92	0.52
1:D:326:LYS:HE3	1:D:328:LEU:HD11	1.91	0.52
1:L:207:VAL:HG11	1:L:241:THR:HG22	1.91	0.52
1:B:320:LYS:NZ	7:B:1005:1PE:H141	2.25	0.51
1:F:254:SER:OG	1:F:255:THR:N	2.44	0.51
1:F:357:LEU:HB2	1:F:425:PHE:HB2	1.92	0.51
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.91	0.51
1:J:520:SER:HB3	1:J:598:GLU:HG3	1.92	0.51
1:E:316:GLU:HG3	7:E:1006:1PE:H251	1.91	0.51
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.93	0.51
1:H:326:LYS:HE3	1:H:328:LEU:HD11	1.92	0.51
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.92	0.51
1:C:123:VAL:HG21	1:C:153:VAL:HG21	1.93	0.51
1:C:230:VAL:HG12	1:C:234:LEU:HD23	1.92	0.51
1:D:207:VAL:HG11	1:D:241:THR:HG22	1.93	0.50
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.93	0.50
1:H:498:SER:O	1:H:523:PRO:HG2	2.12	0.50
1:E:417:LYS:NZ	9:E:1115:HOH:O	2.45	0.49
1:I:326:LYS:HE3	1:I:328:LEU:HD11	1.94	0.49
1:F:396:MET:SD	1:F:398:PHE:HE2	2.35	0.49
1:L:396:MET:SD	1:L:398:PHE:HE2	2.35	0.49
1:B:139:ASN:HB3	1:B:166:ASN:HD21	1.76	0.49
1:D:533:TYR:O	1:D:536:THR:HG22	2.12	0.49
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.94	0.49
1:I:320:LYS:NZ	7:I:1006:1PE:H142	2.27	0.49
1:L:357:LEU:HB2	1:L:425:PHE:HB2	1.95	0.49
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.94	0.48
1:C:398:PHE:HE1	1:C:580:SER:HB3	1.78	0.48
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.94	0.48
1:J:533:TYR:O	1:J:536:THR:HG22	2.12	0.48
1:H:522:GLU:OE2	9:H:1101:HOH:O	2.19	0.48
1:B:254:SER:OG	1:B:255:THR:N	2.47	0.48
1:J:254:SER:HB3	1:L:543:ASP:OD2	2.14	0.47
1:G:301:PRO:HB2	1:G:303:ASN:OD1	2.14	0.47
1:J:320:LYS:NZ	7:J:1005:1PE:H142	2.22	0.47
1:J:550:SER:HA	1:J:551:VAL:C	2.35	0.47
1:L:475:LYS:NZ	9:L:1106:HOH:O	2.47	0.47
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.95	0.47
1:K:550:SER:OG	1:K:551:VAL:N	2.46	0.47
1:F:137:LYS:C	1:F:139:ASN:HA	2.34	0.47
1:J:198:LEU:HD12	1:J:202:ASP:HB3	1.97	0.47
1:D:396:MET:SD	1:D:398:PHE:HE2	2.38	0.47
1:J:359:TYR:HD2	1:J:423:ILE:HD12	1.79	0.47
1:A:103:TYR:N	8:A:1012:SO4:O4	2.47	0.47
1:B:298:ILE:HG23	1:B:398:PHE:HA	1.96	0.47
1:I:532:GLU:H	5:I:1005:GOL:H31	1.80	0.47
1:I:411:TYR:HE1	7:I:1007:1PE:H232	1.80	0.47
1:A:207:VAL:HG11	1:A:241:THR:HG22	1.96	0.47
1:K:338:MET:HE2	1:K:468:ASP:HB3	1.97	0.47
1:L:359:TYR:HD2	1:L:423:ILE:HD12	1.80	0.47
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.97	0.46
1:H:413:VAL:HG11	1:H:423:ILE:HD13	1.96	0.46
1:H:207:VAL:HG11	1:H:241:THR:HG22	1.97	0.46
1:E:198:LEU:HD22	1:E:202:ASP:HB3	1.97	0.46
1:B:175:PHE:N	1:B:187:VAL:O	2.36	0.46
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:LYS:HZ3	7:D:1005:1PE:H161	1.81	0.46
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.97	0.46
1:I:90:GLN:NE2	1:I:95:ASP:O	2.46	0.46
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.96	0.46
1:C:208:LEU:O	1:C:212:THR:HG23	2.16	0.46
1:G:132:VAL:HG21	1:G:142:VAL:HG13	1.97	0.46
1:H:244:TYR:OH	1:H:588:PRO:O	2.34	0.46
1:B:520:SER:HB3	1:B:598:GLU:HG3	1.97	0.46
1:B:419:GLU:HG3	1:B:420:ASN:N	2.31	0.45
1:D:230:VAL:HG12	1:D:234:LEU:HD23	1.98	0.45
1:F:230:VAL:HG12	1:F:234:LEU:HD23	1.98	0.45
1:F:498:SER:O	1:F:523:PRO:HG2	2.16	0.45
1:H:359:TYR:HD2	1:H:423:ILE:HD12	1.81	0.45
1:J:498:SER:O	1:J:523:PRO:HG2	2.16	0.45
1:L:114:VAL:HG12	1:L:274:ALA:HB1	1.98	0.45
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.98	0.45
1:I:175:PHE:N	1:I:187:VAL:O	2.41	0.45
1:A:214:LEU:HD21	1:A:222:LEU:HD22	1.98	0.45
1:E:126:GLY:H	5:E:1005:GOL:H11	1.81	0.45
1:G:550:SER:O	1:G:552:LYS:N	2.47	0.45
1:K:207:VAL:HG11	1:K:241:THR:HG22	1.99	0.45
1:L:533:TYR:O	1:L:536:THR:HG22	2.17	0.45
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.97	0.45
1:F:207:VAL:HG11	1:F:241:THR:HG22	1.99	0.45
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.98	0.45
1:B:498:SER:O	1:B:523:PRO:HG2	2.17	0.45
1:I:207:VAL:HG11	1:I:241:THR:HG22	1.99	0.45
1:J:454:GLU:OE1	1:J:539:SER:OG	2.30	0.45
1:B:320:LYS:HZ1	7:B:1005:1PE:H141	1.82	0.45
1:K:520:SER:HB3	1:K:598:GLU:HG3	1.98	0.45
1:E:230:VAL:HG12	1:E:234:LEU:HD23	1.99	0.44
1:G:230:VAL:HG12	1:G:234:LEU:HD23	1.99	0.44
1:E:254:SER:HA	1:E:255:THR:HA	1.51	0.44
1:B:117:ILE:HD11	1:B:225:VAL:HG13	2.00	0.44
1:J:150:ASP:OD1	1:J:179:ASN:HB2	2.17	0.44
1:H:528:PRO:HB3	1:K:525:TRP:CZ3	2.53	0.44
1:I:230:VAL:HG12	1:I:234:LEU:HD23	1.99	0.44
1:H:520:SER:HB3	1:H:598:GLU:HG3	1.99	0.44
7:I:1007:1PE:H242	7:I:1007:1PE:H231	1.80	0.44
1:K:301:PRO:HB2	1:K:303:ASN:OD1	2.18	0.44
1:H:175:PHE:CD1	1:L:176:TYR:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:ASP:OD1	1:D:573:HIS:ND1	2.39	0.44
1:E:236:ARG:NH2	9:E:1108:HOH:O	2.36	0.44
1:L:137:LYS:CB	1:L:140:GLY:H	2.31	0.44
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.99	0.44
1:I:198:LEU:HD22	1:I:202:ASP:HB3	2.00	0.44
1:C:498:SER:O	1:C:523:PRO:HG2	2.19	0.43
1:K:298:ILE:HG23	1:K:398:PHE:HA	2.00	0.43
1:C:551:VAL:HG12	1:C:553:ALA:H	1.83	0.43
1:D:198:LEU:HD22	1:D:202:ASP:HB3	2.00	0.43
1:E:441:PRO:HB2	1:F:394:ASP:HA	2.00	0.43
1:I:246:TYR:HE2	1:I:264:ILE:HG12	1.83	0.43
1:C:207:VAL:HG11	1:C:241:THR:HG22	2.01	0.43
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.87	0.43
1:I:563:LYS:NZ	9:I:1107:HOH:O	2.35	0.43
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.54	0.42
1:D:132:VAL:HG11	1:D:144:ILE:HD13	2.02	0.42
1:I:208:LEU:O	1:I:212:THR:HG23	2.19	0.42
1:B:413:VAL:HG11	1:B:423:ILE:HD13	2.02	0.42
1:B:550:SER:OG	1:B:551:VAL:N	2.53	0.42
1:C:232:LYS:NZ	1:C:276:THR:O	2.51	0.42
1:C:301:PRO:HB2	1:C:303:ASN:OD1	2.19	0.42
1:B:175:PHE:CD1	1:F:176:TYR:HB2	2.54	0.42
1:I:350:TYR:HA	1:I:351:PRO:HD3	1.95	0.42
1:D:298:ILE:HG23	1:D:398:PHE:HA	2.01	0.42
7:G:1006:1PE:H142	7:G:1006:1PE:H152	1.74	0.42
1:K:480:TYR:OH	1:K:512:LYS:NZ	2.41	0.42
1:F:274:ALA:N	9:F:1101:HOH:O	2.52	0.42
1:J:300:ALA:HA	1:J:301:PRO:HD3	1.89	0.42
1:A:324:GLU:HB2	1:A:358:THR:HB	2.01	0.42
1:A:441:PRO:HB2	1:B:394:ASP:HA	2.00	0.42
7:E:1007:1PE:H141	7:E:1007:1PE:H152	1.83	0.42
1:L:138:GLU:N	1:L:139:ASN:HA	2.35	0.42
1:B:114:VAL:HG12	1:B:274:ALA:HB1	2.01	0.42
1:E:520:SER:HB3	1:E:598:GLU:HG3	2.01	0.42
1:K:143:LYS:HE2	1:K:143:LYS:HB3	1.89	0.42
1:L:300:ALA:HA	1:L:301:PRO:HD3	1.86	0.42
1:C:124:GLU:O	1:C:185:VAL:HG12	2.20	0.41
1:I:114:VAL:HG12	1:I:274:ALA:HB1	2.01	0.41
1:I:498:SER:O	1:I:523:PRO:HG2	2.20	0.41
1:L:341:TYR:CE1	1:L:428:ALA:HB1	2.55	0.41
1:D:328:LEU:HA	1:D:332:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:GLU:O	1:H:185:VAL:HG12	2.20	0.41
1:E:320:LYS:HZ3	7:E:1006:1PE:H252	1.84	0.41
1:A:175:PHE:HD1	1:D:176:TYR:HB2	1.86	0.41
1:C:329:GLY:N	1:C:332:GLU:OE1	2.49	0.41
1:B:117:ILE:HG22	1:B:272:ASN:ND2	2.35	0.41
1:C:214:LEU:HD21	1:C:222:LEU:HD22	2.02	0.41
1:K:214:LEU:HD11	1:K:222:LEU:HD22	2.02	0.41
1:L:457:ASN:HB2	1:L:547:ILE:HD13	2.03	0.41
1:A:230:VAL:HG12	1:A:234:LEU:HD23	2.02	0.41
1:E:208:LEU:HD23	1:E:208:LEU:HA	1.93	0.41
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.55	0.41
1:G:441:PRO:HB2	1:H:394:ASP:HA	2.01	0.41
1:D:498:SER:O	1:D:523:PRO:HG2	2.21	0.41
1:F:550:SER:O	1:F:551:VAL:C	2.59	0.41
1:I:172:SER:C	1:I:173:LYS:HD2	2.41	0.41
1:K:364:ASP:O	1:K:420:ASN:HA	2.20	0.41
1:K:483:ASP:OD2	1:K:573:HIS:ND1	2.42	0.41
1:K:498:SER:O	1:K:523:PRO:HG2	2.21	0.41
1:L:133:ASN:HA	1:L:167:VAL:HG21	2.01	0.41
1:E:114:VAL:HG12	1:E:274:ALA:HB1	2.02	0.41
1:G:173:LYS:HB2	1:G:189:TYR:CE1	2.56	0.41
1:G:214:LEU:HD21	1:G:222:LEU:HD22	2.02	0.41
1:K:340:ALA:HA	1:K:445:ILE:HD12	2.02	0.41
1:A:301:PRO:HB2	1:A:303:ASN:OD1	2.21	0.40
1:B:528:PRO:HB3	1:E:525:TRP:CZ3	2.56	0.40
1:G:150:ASP:OD1	1:G:179:ASN:HB2	2.20	0.40
1:E:381:GLY:HA2	1:E:459:ASP:OD1	2.21	0.40
1:I:173:LYS:NZ	9:I:1124:HOH:O	2.52	0.40
1:J:232:LYS:NZ	1:J:276:THR:O	2.54	0.40
1:D:568:ASN:ND2	9:D:1118:HOH:O	2.54	0.40
1:E:253:LYS:O	1:E:254:SER:HB3	2.22	0.40
1:E:475:LYS:NZ	9:E:1106:HOH:O	2.35	0.40
1:J:144:ILE:HG13	1:J:157:LEU:HD22	2.02	0.40
1:C:457:ASN:HB2	1:C:547:ILE:HD13	2.04	0.40
7:E:1007:1PE:H132	7:E:1007:1PE:H221	1.87	0.40
1:E:364:ASP:O	1:E:420:ASN:HA	2.22	0.40
1:G:520:SER:HB3	1:G:598:GLU:HG3	2.04	0.40
1:I:331:LYS:HB3	1:I:331:LYS:HE2	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/522 (99%)	497 (96%)	18 (4%)	2 (0%)	39	69
1	B	512/522 (98%)	492 (96%)	17 (3%)	3 (1%)	30	59
1	C	515/522 (99%)	495 (96%)	18 (4%)	2 (0%)	39	69
1	D	508/522 (97%)	489 (96%)	16 (3%)	3 (1%)	30	59
1	E	504/522 (97%)	488 (97%)	14 (3%)	2 (0%)	39	69
1	F	509/522 (98%)	489 (96%)	16 (3%)	4 (1%)	24	51
1	G	517/522 (99%)	496 (96%)	20 (4%)	1 (0%)	52	80
1	H	513/522 (98%)	492 (96%)	18 (4%)	3 (1%)	30	59
1	I	513/522 (98%)	494 (96%)	17 (3%)	2 (0%)	39	69
1	J	509/522 (98%)	491 (96%)	16 (3%)	2 (0%)	39	69
1	K	503/522 (96%)	485 (96%)	15 (3%)	3 (1%)	30	59
1	L	508/522 (97%)	492 (97%)	15 (3%)	1 (0%)	52	80
All	All	6128/6264 (98%)	5900 (96%)	200 (3%)	28 (0%)	34	63

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	255	THR
1	F	550	SER
1	F	551	VAL
1	A	139	ASN
1	C	139	ASN
1	D	136	GLY
1	E	218	LYS
1	F	218	LYS
1	G	218	LYS
1	H	218	LYS
1	H	550	SER
1	I	139	ASN

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Mol	Chain	Res	Type
1	K	139	ASN
1	K	218	LYS
1	K	551	VAL
1	L	218	LYS
1	A	218	LYS
1	B	218	LYS
1	C	218	LYS
1	D	217	ASN
1	H	216	ASP
1	I	218	LYS
1	B	216	ASP
1	D	551	VAL
1	E	254	SER
1	J	139	ASN
1	B	119	GLY
1	J	550	SER

### 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	420/450 (93%)	419 (100%)	1 (0%)	95	99
1	B	410/450 (91%)	407 (99%)	3 (1%)	88	96
1	C	406/450 (90%)	406 (100%)	0	100	100
1	D	407/450 (90%)	406 (100%)	1 (0%)	95	99
1	E	412/450 (92%)	412 (100%)	0	100	100
1	F	392/450 (87%)	392 (100%)	0	100	100
1	G	422/450 (94%)	421 (100%)	1 (0%)	95	99
1	H	405/450 (90%)	405 (100%)	0	100	100
1	I	416/450 (92%)	413 (99%)	3 (1%)	88	96
1	J	408/450 (91%)	408 (100%)	0	100	100
1	K	415/450 (92%)	413 (100%)	2 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	396/450 (88%)	395 (100%)	1 (0%)	94	99
All	All	4909/5400 (91%)	4897 (100%)	12 (0%)	95	99

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	398	PHE
1	B	117	ILE
1	B	272	ASN
1	B	398	PHE
1	D	398	PHE
1	G	398	PHE
1	I	200	GLU
1	I	272	ASN
1	I	400	MET
1	K	169	LEU
1	K	398	PHE
1	L	515	GLN

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

Mol	Chain	Res	Type
1	B	272	ASN
1	L	515	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 94 ligands modelled in this entry, 24 are monoatomic - leaving 70 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	4TY	A	1001	3	20,20,20	1.45	3 (15%)	28,28,28	1.57	4 (14%)
4	CO3	A	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	A	1005	-	5,5,5	0.33	0	5,5,5	0.32	0
5	GOL	A	1006	-	5,5,5	0.34	0	5,5,5	0.28	0
6	DMS	A	1007	-	3,3,3	0.65	0	3,3,3	0.48	0
7	1PE	A	1008	-	5,5,15	0.69	0	4,4,14	0.48	0
7	1PE	A	1009	-	8,8,15	0.57	0	7,7,14	0.27	0
7	1PE	A	1010	-	5,5,15	0.67	0	4,4,14	0.50	0
7	1PE	A	1011	-	5,5,15	0.68	0	4,4,14	0.45	0
8	SO4	A	1012	-	4,4,4	0.24	0	6,6,6	0.11	0
2	4TY	B	1001	3	20,20,20	1.45	3 (15%)	28,28,28	1.68	5 (17%)
4	CO3	B	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
7	1PE	B	1005	-	9,9,15	0.56	0	8,8,14	0.34	0
8	SO4	B	1006	-	4,4,4	0.29	0	6,6,6	0.08	0
2	4TY	C	1001	3	20,20,20	1.47	3 (15%)	28,28,28	1.63	3 (10%)
4	CO3	C	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	C	1005	-	5,5,5	0.35	0	5,5,5	0.25	0
7	1PE	C	1006	-	11,11,15	0.61	0	10,10,14	0.41	0
7	1PE	C	1007	-	10,10,15	0.58	0	9,9,14	0.34	0
2	4TY	D	1001	3	20,20,20	1.46	3 (15%)	28,28,28	1.64	4 (14%)
4	CO3	D	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
7	1PE	D	1005	-	10,10,15	0.90	0	9,9,14	0.35	0
7	1PE	D	1006	-	9,9,15	0.92	0	8,8,14	0.42	0
8	SO4	D	1007	-	4,4,4	0.22	0	6,6,6	0.08	0
2	4TY	E	1001	3	20,20,20	1.47	3 (15%)	28,28,28	1.59	4 (14%)
4	CO3	E	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	E	1005	-	5,5,5	0.37	0	5,5,5	0.43	0
7	1PE	E	1006	-	11,11,15	0.60	0	10,10,14	0.44	0
7	1PE	E	1007	-	11,11,15	0.62	0	10,10,14	0.35	0
8	SO4	E	1008	-	4,4,4	0.22	0	6,6,6	0.05	0
8	SO4	E	1009	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	4TY	F	1001	3	20,20,20	1.45	3 (15%)	28,28,28	1.68	5 (17%)
4	CO3	F	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	F	1005	-	5,5,5	0.35	0	5,5,5	0.35	0
7	1PE	F	1006	-	10,10,15	0.91	0	9,9,14	0.34	0
7	1PE	F	1007	-	6,6,15	0.63	0	5,5,14	0.54	0
7	1PE	F	1008	-	9,9,15	0.90	0	8,8,14	0.45	0
7	1PE	F	1009	-	9,9,15	0.88	0	8,8,14	0.49	0
8	SO4	F	1010	-	4,4,4	0.27	0	6,6,6	0.09	0
8	SO4	F	1011	-	4,4,4	0.23	0	6,6,6	0.09	0
2	4TY	G	1001	3	20,20,20	1.45	3 (15%)	28,28,28	1.68	5 (17%)
4	CO3	G	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
7	1PE	G	1005	-	8,8,15	0.55	0	7,7,14	0.41	0
7	1PE	G	1006	-	11,11,15	0.65	0	10,10,14	0.35	0
2	4TY	H	1001	3	20,20,20	1.44	3 (15%)	28,28,28	1.57	4 (14%)
4	CO3	H	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
7	1PE	H	1005	-	9,9,15	0.55	0	8,8,14	0.33	0
7	1PE	H	1006	-	9,9,15	0.57	0	8,8,14	0.32	0
8	SO4	H	1007	-	4,4,4	0.28	0	6,6,6	0.10	0
2	4TY	I	1001	3	20,20,20	1.45	3 (15%)	28,28,28	1.61	3 (10%)
4	CO3	I	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	I	1005	-	5,5,5	0.29	0	5,5,5	0.27	0
7	1PE	I	1006	-	12,12,15	0.66	0	11,11,14	0.32	0
7	1PE	I	1007	-	8,8,15	0.55	0	7,7,14	0.41	0
2	4TY	J	1001	3	20,20,20	1.48	4 (20%)	28,28,28	1.51	3 (10%)
4	CO3	J	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
7	1PE	J	1005	-	9,9,15	0.57	0	8,8,14	0.32	0
7	1PE	J	1006	-	9,9,15	0.56	0	8,8,14	0.33	0
8	SO4	J	1007	-	4,4,4	0.23	0	6,6,6	0.07	0
8	SO4	J	1008	-	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	J	1009	-	4,4,4	0.23	0	6,6,6	0.07	0
2	4TY	K	1001	3	20,20,20	1.47	3 (15%)	28,28,28	1.46	2 (7%)
4	CO3	K	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
7	1PE	K	1005	-	11,11,15	0.61	0	10,10,14	0.35	0
7	1PE	K	1006	-	11,11,15	0.60	0	10,10,14	0.39	0
8	SO4	K	1007	-	4,4,4	0.27	0	6,6,6	0.11	0
8	SO4	K	1008	-	4,4,4	0.22	0	6,6,6	0.08	0
2	4TY	L	1001	3	20,20,20	1.45	3 (15%)	28,28,28	1.61	3 (10%)
4	CO3	L	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
7	1PE	L	1005	-	9,9,15	0.94	0	8,8,14	0.39	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	4TY	A	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	A	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1006	-	-	0/4/4/4	0/0/0/0
6	DMS	A	1007	-	-	0/0/0/0	0/0/0/0
7	1PE	A	1008	-	-	0/3/3/13	0/0/0/0
7	1PE	A	1009	-	-	0/6/6/13	0/0/0/0
7	1PE	A	1010	-	-	0/3/3/13	0/0/0/0
7	1PE	A	1011	-	-	0/3/3/13	0/0/0/0
8	SO4	A	1012	-	-	0/0/0/0	0/0/0/0
2	4TY	B	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	B	1004	-	-	0/0/0/0	0/0/0/0
7	1PE	B	1005	-	-	0/7/7/13	0/0/0/0
8	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
2	4TY	C	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	C	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	C	1005	-	-	0/4/4/4	0/0/0/0
7	1PE	C	1006	-	-	0/9/9/13	0/0/0/0
7	1PE	C	1007	-	-	0/8/8/13	0/0/0/0
2	4TY	D	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	D	1004	-	-	0/0/0/0	0/0/0/0
7	1PE	D	1005	-	-	0/8/8/13	0/0/0/0
7	1PE	D	1006	-	-	0/7/7/13	0/0/0/0
8	SO4	D	1007	-	-	0/0/0/0	0/0/0/0
2	4TY	E	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	E	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	E	1005	-	-	0/4/4/4	0/0/0/0
7	1PE	E	1006	-	-	0/9/9/13	0/0/0/0
7	1PE	E	1007	-	-	0/9/9/13	0/0/0/0
8	SO4	E	1008	-	-	0/0/0/0	0/0/0/0
8	SO4	E	1009	-	-	0/0/0/0	0/0/0/0
2	4TY	F	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	F	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	F	1005	-	-	0/4/4/4	0/0/0/0
7	1PE	F	1006	-	-	0/8/8/13	0/0/0/0
7	1PE	F	1007	-	-	0/4/4/13	0/0/0/0
7	1PE	F	1008	-	-	0/7/7/13	0/0/0/0
7	1PE	F	1009	-	-	0/7/7/13	0/0/0/0
8	SO4	F	1010	-	-	0/0/0/0	0/0/0/0
8	SO4	F	1011	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4TY	G	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	G	1004	-	-	0/0/0/0	0/0/0/0
7	1PE	G	1005	-	-	0/6/6/13	0/0/0/0
7	1PE	G	1006	-	-	0/9/9/13	0/0/0/0
2	4TY	H	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	H	1004	-	-	0/0/0/0	0/0/0/0
7	1PE	H	1005	-	-	0/7/7/13	0/0/0/0
7	1PE	H	1006	-	-	0/7/7/13	0/0/0/0
8	SO4	H	1007	-	-	0/0/0/0	0/0/0/0
2	4TY	I	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	I	1004	-	-	0/0/0/0	0/0/0/0
5	GOL	I	1005	-	-	0/4/4/4	0/0/0/0
7	1PE	I	1006	-	-	0/10/10/13	0/0/0/0
7	1PE	I	1007	-	-	0/6/6/13	0/0/0/0
2	4TY	J	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	J	1004	-	-	0/0/0/0	0/0/0/0
7	1PE	J	1005	-	-	0/7/7/13	0/0/0/0
7	1PE	J	1006	-	-	0/7/7/13	0/0/0/0
8	SO4	J	1007	-	-	0/0/0/0	0/0/0/0
8	SO4	J	1008	-	-	0/0/0/0	0/0/0/0
8	SO4	J	1009	-	-	0/0/0/0	0/0/0/0
2	4TY	K	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	K	1004	-	-	0/0/0/0	0/0/0/0
7	1PE	K	1005	-	-	0/9/9/13	0/0/0/0
7	1PE	K	1006	-	-	0/9/9/13	0/0/0/0
8	SO4	K	1007	-	-	0/0/0/0	0/0/0/0
8	SO4	K	1008	-	-	0/0/0/0	0/0/0/0
2	4TY	L	1001	3	-	0/19/19/19	0/1/1/1
4	CO3	L	1004	-	-	0/0/0/0	0/0/0/0
7	1PE	L	1005	-	-	0/7/7/13	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1001	4TY	O1-C7	-3.71	1.41	1.48
2	G	1001	4TY	O1-C7	-3.61	1.41	1.48
2	A	1001	4TY	O1-C7	-3.58	1.41	1.48
2	F	1001	4TY	O1-C7	-3.52	1.41	1.48
2	E	1001	4TY	O1-C7	-3.50	1.41	1.48
2	D	1001	4TY	O1-C7	-3.48	1.41	1.48
2	C	1001	4TY	O1-C7	-3.43	1.41	1.48
2	I	1001	4TY	O1-C7	-3.43	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1001	4TY	O1-C7	-3.35	1.41	1.48
2	K	1001	4TY	O1-C7	-3.35	1.41	1.48
2	B	1001	4TY	O1-C7	-3.28	1.42	1.48
2	H	1001	4TY	O1-C7	-3.27	1.42	1.48
2	J	1001	4TY	C5-N1	-2.05	1.42	1.46
2	J	1001	4TY	O1-C6	2.86	1.41	1.34
2	G	1001	4TY	O1-C6	3.07	1.41	1.34
2	E	1001	4TY	O1-C6	3.09	1.41	1.34
2	A	1001	4TY	O1-C6	3.09	1.41	1.34
2	F	1001	4TY	O1-C6	3.13	1.41	1.34
2	B	1001	4TY	O1-C6	3.19	1.41	1.34
2	I	1001	4TY	O1-C6	3.21	1.41	1.34
2	D	1001	4TY	O1-C6	3.23	1.41	1.34
2	C	1001	4TY	O1-C6	3.25	1.41	1.34
2	K	1001	4TY	O1-C6	3.26	1.41	1.34
2	L	1001	4TY	O1-C6	3.29	1.41	1.34
2	H	1001	4TY	O1-C6	3.31	1.41	1.34
2	L	1001	4TY	O4-N2	3.49	1.46	1.39
2	F	1001	4TY	O4-N2	3.50	1.46	1.39
2	A	1001	4TY	O4-N2	3.50	1.46	1.39
2	I	1001	4TY	O4-N2	3.51	1.46	1.39
2	C	1001	4TY	O4-N2	3.51	1.46	1.39
2	D	1001	4TY	O4-N2	3.52	1.46	1.39
2	E	1001	4TY	O4-N2	3.52	1.46	1.39
2	H	1001	4TY	O4-N2	3.53	1.46	1.39
2	G	1001	4TY	O4-N2	3.54	1.46	1.39
2	K	1001	4TY	O4-N2	3.56	1.46	1.39
2	B	1001	4TY	O4-N2	3.60	1.46	1.39
2	J	1001	4TY	O4-N2	3.63	1.46	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1001	4TY	O2-C6-N1	-4.65	116.82	124.89
2	L	1001	4TY	O2-C6-N1	-4.57	116.95	124.89
2	B	1001	4TY	O2-C6-N1	-4.47	117.12	124.89
2	G	1001	4TY	O2-C6-N1	-4.42	117.22	124.89
2	K	1001	4TY	O2-C6-N1	-4.40	117.26	124.89
2	I	1001	4TY	O2-C6-N1	-4.35	117.33	124.89
2	D	1001	4TY	O2-C6-N1	-4.20	117.60	124.89
2	C	1001	4TY	O2-C6-N1	-4.15	117.69	124.89
2	A	1001	4TY	O2-C6-N1	-4.08	117.81	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1001	4TY	O2-C6-N1	-4.01	117.92	124.89
2	F	1001	4TY	O2-C6-N1	-3.64	118.57	124.89
2	F	1001	4TY	C7-O1-C6	-3.23	115.91	121.03
2	G	1001	4TY	O1-C6-O2	-3.19	119.17	125.55
2	J	1001	4TY	O2-C6-N1	-3.11	119.49	124.89
2	J	1001	4TY	C7-O1-C6	-2.86	116.50	121.03
2	A	1001	4TY	O1-C6-O2	-2.75	120.05	125.55
2	I	1001	4TY	O1-C6-O2	-2.73	120.10	125.55
2	D	1001	4TY	O1-C6-O2	-2.64	120.27	125.55
2	G	1001	4TY	C7-O1-C6	-2.63	116.86	121.03
2	L	1001	4TY	O1-C6-O2	-2.58	120.40	125.55
2	C	1001	4TY	O1-C6-O2	-2.50	120.55	125.55
2	E	1001	4TY	O1-C6-O2	-2.44	120.67	125.55
2	B	1001	4TY	O1-C6-O2	-2.42	120.71	125.55
2	F	1001	4TY	O1-C6-O2	-2.40	120.77	125.55
2	D	1001	4TY	C7-O1-C6	-2.25	117.46	121.03
2	B	1001	4TY	C3-C4-C5	-2.18	117.15	120.80
2	A	1001	4TY	C7-O1-C6	-2.15	117.62	121.03
2	H	1001	4TY	O1-C6-O2	-2.13	121.29	125.55
2	B	1001	4TY	C5-N1-C6	-2.09	117.67	121.14
2	E	1001	4TY	C7-O1-C6	-2.09	117.72	121.03
2	F	1001	4TY	O3-C11-N2	-2.05	120.15	122.97
2	G	1001	4TY	C5-N1-C6	-2.05	117.75	121.14
2	H	1001	4TY	C5-N1-C6	-2.02	117.79	121.14
2	K	1001	4TY	O1-C6-N1	4.16	117.63	110.07
2	L	1001	4TY	O1-C6-N1	4.37	118.01	110.07
2	H	1001	4TY	O1-C6-N1	4.44	118.14	110.07
2	A	1001	4TY	O1-C6-N1	4.49	118.23	110.07
2	I	1001	4TY	O1-C6-N1	4.60	118.43	110.07
2	C	1001	4TY	O1-C6-N1	4.61	118.44	110.07
2	J	1001	4TY	O1-C6-N1	4.72	118.64	110.07
2	B	1001	4TY	O1-C6-N1	4.74	118.68	110.07
2	G	1001	4TY	O1-C6-N1	4.79	118.77	110.07
2	E	1001	4TY	O1-C6-N1	4.88	118.94	110.07
2	D	1001	4TY	O1-C6-N1	5.09	119.31	110.07
2	F	1001	4TY	O1-C6-N1	5.40	119.88	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	GOL	1	0
7	A	1009	1PE	1	0
8	A	1012	SO4	1	0
7	B	1005	1PE	2	0
8	B	1006	SO4	1	0
7	D	1005	1PE	1	0
5	E	1005	GOL	1	0
7	E	1006	1PE	2	0
7	E	1007	1PE	2	0
5	F	1005	GOL	1	0
7	F	1006	1PE	1	0
7	F	1007	1PE	2	0
7	G	1006	1PE	1	0
5	I	1005	GOL	2	0
7	I	1006	1PE	2	0
7	I	1007	1PE	2	0
7	J	1005	1PE	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	519/522 (99%)	-0.43	5 (0%) 84 85	7, 16, 41, 61	4 (0%)
1	B	516/522 (98%)	-0.17	12 (2%) 64 64	8, 20, 54, 76	5 (0%)
1	C	517/522 (99%)	-0.36	3 (0%) 90 91	7, 17, 45, 60	1 (0%)
1	D	512/522 (98%)	-0.46	5 (0%) 84 85	7, 16, 37, 73	2 (0%)
1	E	510/522 (97%)	-0.49	1 (0%) 95 96	8, 17, 34, 55	3 (0%)
1	F	513/522 (98%)	-0.33	9 (1%) 71 72	9, 20, 47, 79	0
1	G	519/522 (99%)	-0.37	3 (0%) 90 91	8, 17, 41, 58	3 (0%)
1	H	517/522 (99%)	-0.14	12 (2%) 64 64	7, 19, 57, 71	5 (0%)
1	I	517/522 (99%)	-0.35	5 (0%) 84 85	6, 17, 45, 61	3 (0%)
1	J	513/522 (98%)	-0.45	2 (0%) 93 94	8, 17, 38, 62	0
1	K	509/522 (97%)	-0.49	0 100 100	8, 16, 32, 55	5 (0%)
1	L	512/522 (98%)	-0.23	12 (2%) 64 64	10, 23, 52, 72	3 (0%)
All	All	6174/6264 (98%)	-0.36	69 (1%) 82 83	6, 18, 46, 79	34 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	MET	5.9
1	F	138	GLU	5.4
1	D	85	ALA	3.8
1	G	136	GLY	3.8
1	H	603	ASP	3.7
1	A	136	GLY	3.6
1	L	138	GLU	3.5
1	H	144	ILE	3.4
1	F	139	ASN	3.3
1	B	257	LYS	3.2
1	H	138	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	255	THR	3.1
1	G	551	VAL	3.1
1	L	121	CYS	3.0
1	L	145	SER	3.0
1	J	85	ALA	3.0
1	B	195	VAL	2.9
1	B	196	ALA	2.9
1	C	121	CYS	2.9
1	L	123	VAL	2.9
1	F	134	ASN	2.9
1	B	197	ASP	2.8
1	H	195	VAL	2.7
1	D	216	ASP	2.7
1	L	148	VAL	2.7
1	I	136	GLY	2.7
1	G	196	ALA	2.6
1	H	196	ALA	2.6
1	L	141	PRO	2.6
1	D	217	ASN	2.6
1	C	136	GLY	2.6
1	L	139	ASN	2.6
1	H	276	THR	2.5
1	B	149	ASN	2.5
1	B	150	ASP	2.5
1	L	136	GLY	2.5
1	J	136	GLY	2.5
1	F	145	SER	2.4
1	H	277	TYR	2.4
1	L	363	GLY	2.4
1	A	603	ASP	2.4
1	I	117	ILE	2.4
1	H	149	ASN	2.3
1	A	196	ALA	2.3
1	D	136	GLY	2.3
1	E	362	LYS	2.3
1	H	150	ASP	2.3
1	H	145	SER	2.3
1	B	141	PRO	2.3
1	I	272	ASN	2.3
1	L	146	SER	2.2
1	H	197	ASP	2.2
1	A	144	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	202	ASP	2.2
1	H	257	LYS	2.2
1	B	272	ASN	2.1
1	B	273	ASN	2.1
1	C	197	ASP	2.1
1	I	603	ASP	2.1
1	A	195	VAL	2.1
1	F	144	ILE	2.1
1	L	184	SER	2.1
1	B	363	GLY	2.1
1	B	180	ASP	2.1
1	F	140	GLY	2.1
1	L	176	TYR	2.1
1	B	145	SER	2.1
1	F	119	GLY	2.1
1	F	146	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	I	1005	6/6	0.75	0.34	7.40	23,28,37,47	0
7	1PE	D	1006	10/16	0.89	0.21	7.10	23,30,71,75	0
5	GOL	C	1005	6/6	0.65	0.44	6.89	54,72,76,87	0
8	SO4	J	1009	5/5	0.93	0.29	5.99	44,56,73,82	0
8	SO4	J	1007	5/5	0.96	0.34	5.77	39,40,50,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	D	1007	5/5	0.95	0.33	5.63	28,34,49,57	0
8	SO4	E	1008	5/5	0.95	0.28	5.24	25,36,49,61	0
7	1PE	F	1006	11/16	0.80	0.29	4.96	34,49,69,74	0
5	GOL	A	1005	6/6	0.80	0.30	4.93	23,30,36,50	0
7	1PE	A	1009	9/16	0.87	0.21	4.91	25,32,43,46	0
7	1PE	K	1006	12/16	0.92	0.20	4.61	14,28,54,57	0
4	CO3	J	1004	4/4	0.96	0.20	3.51	10,12,12,16	0
2	4TY	K	1001	20/20	0.90	0.20	2.73	8,16,29,70	20
7	1PE	F	1007	7/16	0.84	0.24	2.67	20,27,37,38	0
2	4TY	L	1001	20/20	0.92	0.17	2.51	7,16,32,52	20
6	DMS	A	1007	4/4	0.90	0.22	2.29	38,39,42,57	0
7	1PE	G	1005	9/16	0.91	0.17	2.23	20,24,30,31	0
2	4TY	B	1001	20/20	0.93	0.19	2.10	11,15,39,62	20
2	4TY	E	1001	20/20	0.92	0.19	1.89	10,18,38,61	20
2	4TY	C	1001	20/20	0.94	0.18	1.72	11,16,35,57	20
7	1PE	E	1007	12/16	0.95	0.15	1.30	20,30,44,45	0
4	CO3	F	1004	4/4	0.97	0.17	1.29	12,14,15,18	0
7	1PE	C	1007	11/16	0.88	0.19	1.27	24,33,42,44	0
2	4TY	F	1001	20/20	0.93	0.17	1.21	9,16,33,57	20
7	1PE	F	1008	10/16	0.93	0.16	1.19	22,32,46,46	0
7	1PE	H	1005	10/16	0.86	0.20	1.13	33,38,54,56	0
7	1PE	J	1006	10/16	0.93	0.15	1.02	24,27,35,41	0
2	4TY	I	1001	20/20	0.94	0.16	0.99	8,17,29,63	20
2	4TY	D	1001	20/20	0.95	0.16	0.94	11,15,26,70	20
4	CO3	H	1004	4/4	0.96	0.14	0.77	9,9,10,14	0
7	1PE	A	1010	6/16	0.94	0.21	0.72	15,23,26,27	0
2	4TY	A	1001	20/20	0.94	0.16	0.71	9,15,27,60	20
7	1PE	L	1005	10/16	0.89	0.18	0.66	21,33,36,49	0
4	CO3	E	1004	4/4	0.96	0.15	0.66	11,15,18,21	0
7	1PE	I	1007	9/16	0.91	0.15	0.57	11,27,35,45	0
7	1PE	A	1011	6/16	0.91	0.18	0.53	17,26,29,35	0
5	GOL	A	1006	6/6	0.89	0.21	0.47	33,38,42,43	0
4	CO3	K	1004	4/4	0.96	0.14	0.45	10,15,17,19	0
2	4TY	J	1001	20/20	0.94	0.15	0.35	9,18,30,70	20
5	GOL	E	1005	6/6	0.86	0.19	0.18	31,36,45,47	0
4	CO3	D	1004	4/4	0.98	0.12	0.16	9,12,13,17	0
2	4TY	H	1001	20/20	0.95	0.15	0.09	7,12,23,73	20
2	4TY	G	1001	20/20	0.95	0.15	0.06	10,16,28,71	20
4	CO3	B	1004	4/4	0.95	0.12	-0.29	9,10,11,18	0
4	CO3	I	1004	4/4	0.98	0.12	-0.31	9,12,12,14	0
4	CO3	L	1004	4/4	0.98	0.11	-0.49	11,15,15,19	0
4	CO3	C	1004	4/4	0.97	0.12	-0.78	9,11,12,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	F	1010	5/5	0.99	0.10	-1.70	15,19,20,22	0
8	SO4	H	1007	5/5	0.99	0.10	-1.83	10,11,16,18	0
8	SO4	K	1007	5/5	0.98	0.11	-2.25	12,13,18,20	0
8	SO4	B	1006	5/5	0.99	0.10	-2.49	11,14,14,17	0
4	CO3	A	1004	4/4	0.98	0.11	-2.72	8,9,10,10	0
4	CO3	G	1004	4/4	0.98	0.09	-2.86	11,13,13,14	0
3	ZN	G	1002	1/1	0.94	0.07	-3.11	31,31,31,31	0
3	ZN	D	1002	1/1	0.96	0.04	-3.25	29,29,29,29	0
3	ZN	J	1003	1/1	0.99	0.06	-3.51	21,21,21,21	0
3	ZN	L	1002	1/1	0.99	0.06	-3.52	25,25,25,25	0
3	ZN	A	1002	1/1	0.98	0.05	-3.76	22,22,22,22	0
3	ZN	E	1003	1/1	0.98	0.06	-4.16	25,25,25,25	0
3	ZN	J	1002	1/1	0.98	0.04	-4.28	22,22,22,22	0
3	ZN	I	1002	1/1	0.98	0.03	-4.43	18,18,18,18	0
3	ZN	I	1003	1/1	0.99	0.05	-4.50	24,24,24,24	0
3	ZN	F	1003	1/1	0.99	0.03	-4.64	21,21,21,21	0
3	ZN	D	1003	1/1	0.99	0.04	-4.68	26,26,26,26	0
3	ZN	A	1003	1/1	0.98	0.05	-4.69	19,19,19,19	0
3	ZN	F	1002	1/1	0.98	0.05	-4.71	24,24,24,24	0
3	ZN	C	1003	1/1	0.97	0.06	-4.90	25,25,25,25	0
3	ZN	E	1002	1/1	0.98	0.05	-5.18	23,23,23,23	0
3	ZN	G	1003	1/1	0.99	0.04	-5.33	17,17,17,17	0
3	ZN	B	1003	1/1	0.99	0.04	-5.37	17,17,17,17	0
3	ZN	H	1003	1/1	1.00	0.03	-5.88	21,21,21,21	0
3	ZN	K	1002	1/1	0.97	0.04	-6.18	27,27,27,27	0
3	ZN	B	1002	1/1	0.99	0.04	-6.55	23,23,23,23	0
3	ZN	H	1002	1/1	0.99	0.05	-6.71	23,23,23,23	0
3	ZN	K	1003	1/1	0.99	0.05	-7.25	22,22,22,22	0
3	ZN	L	1003	1/1	0.99	0.04	-7.42	24,24,24,24	0
3	ZN	C	1002	1/1	0.95	0.03	-10.06	24,24,24,24	0
8	SO4	J	1008	5/5	0.97	0.27	-	43,45,60,63	0
7	1PE	A	1008	6/16	0.92	0.18	-	22,28,36,42	0
7	1PE	B	1005	10/16	0.92	0.17	-	21,31,47,51	0
7	1PE	K	1005	12/16	0.85	0.20	-	28,39,48,65	0
7	1PE	I	1006	13/16	0.86	0.24	-	19,33,47,47	0
8	SO4	K	1008	5/5	0.97	0.21	-	32,49,57,59	0
5	GOL	F	1005	6/6	0.87	0.25	-	26,41,54,73	0
8	SO4	E	1009	5/5	0.97	0.20	-	33,52,56,67	0
7	1PE	D	1005	11/16	0.84	0.20	-	29,36,50,55	0
7	1PE	E	1006	12/16	0.87	0.20	-	32,42,47,56	0
7	1PE	G	1006	12/16	0.88	0.21	-	32,44,52,59	0
7	1PE	C	1006	12/16	0.89	0.20	-	27,34,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	1PE	J	1005	10/16	0.86	0.21	-	20,36,41,69	0
8	SO4	A	1012	5/5	0.96	0.25	-	36,38,48,56	0
7	1PE	F	1009	10/16	0.79	0.41	-	35,45,57,74	0
8	SO4	F	1011	5/5	0.95	0.22	-	32,49,53,56	0
7	1PE	H	1006	10/16	0.84	0.24	-	30,41,53,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.